

# Human-Like Biomechanics

A Unified Mathematical Approach to Human  
Biomechanics and Humanoid Robotics

by

VLADIMIR G. IVANCEVIC

AND TIJANA T. IVANCEVIC

**MICROPROCESSOR-BASED AND  
INTELLIGENT SYSTEMS ENGINEERING**

## Human-Like Biomechanics

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*A Unified Mathematical Approach  
to Human Biomechanics  
and Humanoid Robotics*

by

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Dedicated to Nitya, Atma and Kali

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# Contents

<b>Preface</b> .....	xi
<b>Acknowledgments</b> .....	xiv
0.1 Glossary of Frequently Used Symbols .....	1
<b>1 Introduction</b> .....	5
1.1 Local Tensorial Language of Human–Like Biomechanics .....	6
1.1.1 Classical Translational Biomechanics .....	6
1.1.2 Calculus of Geometric Objects .....	8
1.1.3 Lagrangian Action and Feynman Path Integral .....	18
1.1.4 Noether Theorem .....	22
1.1.5 Symplectic Mechanics .....	24
1.1.6 Modern Rotational Biomechanics .....	25
1.1.7 Muscular Dynamics and Control .....	28
1.2 Global Functorial Language of Human–Like Biomechanics ....	30
1.2.1 Preliminaries from Calculus, Algebra and Topology ....	31
1.2.2 Categories .....	42
1.2.3 Functors .....	46
1.2.4 Natural Transformations .....	48
1.2.5 Limits and Colimits .....	51
1.2.6 The Adjunction .....	52
1.2.7 $n$ –Categories .....	53
1.2.8 Abelian Functorial Algebra .....	60
<b>2 Geometric Basis of Human–Like Biomechanics</b> .....	63
2.1 Biomechanical Manifold $M$ .....	63
2.1.1 Definition of the Manifold $M$ .....	64
2.1.2 Smooth Maps Between Manifolds .....	65
2.2 Biomechanical Bundles .....	66
2.2.1 The Tangent Bundle of the Manifold $M$ .....	66
2.2.2 The Cotangent Bundle of the Manifold $M$ .....	68
2.2.3 Fibre Bundles .....	69
2.2.4 Jet Bundles .....	77
2.3 Sections of Biomechanical Bundles .....	79

2.3.1	Biomechanical Evolution and Flow	79
2.3.2	Vector-Fields and Their Flows	80
2.3.3	Differential Forms on $M$	87
2.4	Lie Categories in Human-Like Biomechanics	102
2.4.1	Lie Derivative in Biomechanics	102
2.4.2	Lie Groups in Human-Like Biomechanics	110
2.4.3	Dynamical Games on Lie Groups	126
2.4.4	Group Structure of the Biomechanical Manifold $M$	134
2.4.5	Lie Symmetries in Biomechanics	138
2.5	Riemannian Geometry in Human-Like Biomechanics	156
2.5.1	Local Riemannian Geometry on $M$	157
2.5.2	Global Riemannian Geometry on $M$	165
2.5.3	Complex and Kähler Manifolds	176
2.5.4	Conformal Killing-Riemannian Geometry	181
2.6	Symplectic Geometry in Human-Like Biomechanics	184
2.6.1	Symplectic Algebra	185
2.6.2	Symplectic Geometry on $M$	185
2.6.3	Momentum Map and Symplectic Reduction of $M$	187
2.7	The Covariant Force Functor	188
<b>3</b>	<b>Mechanical Basis of Human-Like Biomechanics</b>	<b>191</b>
3.1	Lagrangian Formalism in Human-Like Biomechanics	191
3.1.1	Basis of Lagrangian Mechanics	193
3.1.2	Basics of Poincaré Dynamics	195
3.2	Hamiltonian Formalism in Human-Like Biomechanics	196
3.2.1	Nonlinear Dynamics in Hamiltonian Form	198
3.2.2	Hamiltonian Geometry in Human-Like Biomechanics	217
3.2.3	Hamilton-Poisson Geometry in Biomechanics	219
3.2.4	Completely Integrable Hamiltonian Systems	224
3.2.5	Killing Vector and Tensor Fields in Biomechanics	231
3.3	Variational Formalism in Human-Like Biomechanics	234
3.3.1	Biomechanical Action Functional	235
3.3.2	Lagrangian Action	235
3.3.3	Hamiltonian Action	237
3.3.4	Hamiltonian-Action Formulation of Biomechanics	238
3.3.5	Maupertuis Stationary Action in Biomechanics	240
3.3.6	Geometric Action	242
3.3.7	Feynman Quantum-Mechanical Action	247
3.4	Nonholonomic Problems in Human-Like Biomechanics	251
3.4.1	Lagrangian Approach	251
3.4.2	Hamiltonian Approach	253
3.4.3	Biomechanical Example: Bicycle Dynamics	254
3.4.4	Constraint Dirac-Hamiltonian Dynamics	256
3.5	Lie Functors in Human-Like Biomechanics	272
3.5.1	Lie-Lagrangian Biomechanical Functor	272

3.5.2	Lie–Hamiltonian Biomechanical Functor . . . . .	278
3.5.3	Stochastic–Lie–Hamiltonian Biomechanical Functor . . . . .	282
3.5.4	Fuzzy–Stochastic–Lie–Hamiltonian Functor . . . . .	283
3.6	Biomechanics of Spinal Injuries . . . . .	286
<b>4</b>	<b>Topology of Human–Like Biomechanics . . . . .</b>	<b>289</b>
4.1	Category of (Co)Chain Complexes in Human–Like Biomechanics . . . . .	289
4.1.1	(Co)Homologies in Abelian Categories Related to $M$ . . . . .	290
4.1.2	$M$ –Reduction and its Euler Characteristic . . . . .	291
4.2	Morse Theory in Human–Like Biomechanics . . . . .	292
4.2.1	Morse Geometry of $M$ . . . . .	292
4.2.2	Morse Topology of $M$ . . . . .	297
4.3	Hodge–De Rham Theory in Human–Like Biomechanics . . . . .	301
4.3.1	Hodge Laplacian on $M$ . . . . .	301
4.3.2	Heat Kernel and Thermodynamics on $M$ . . . . .	303
4.4	Topological Duality in Human–Like Biomechanics . . . . .	304
4.4.1	Geometric Duality Theorem for $M$ . . . . .	305
4.4.2	Topological Duality Theorem for $M$ . . . . .	309
4.4.3	Lagrangian Versus Hamiltonian Duality . . . . .	311
4.4.4	Globally Dual Structure of Rotational Biomechanics . . . . .	312
<b>5</b>	<b>Nonlinear Control in Human–Like Biomechanics . . . . .</b>	<b>313</b>
5.1	The Basics of Classical Control and Stability . . . . .	313
5.1.1	Brief Introduction into Feedback Control . . . . .	313
5.1.2	Linear Stationary Systems and Operators . . . . .	318
5.1.3	Stability and Boundedness . . . . .	322
5.1.4	Lyapunov’s Stability Method . . . . .	324
5.2	The Basis of Modern Geometric Control . . . . .	325
5.2.1	Feedback Linearization . . . . .	325
5.2.2	Controllability . . . . .	333
5.3	Modern Control Techniques for Mechanical Systems . . . . .	338
5.3.1	Abstract Control System . . . . .	338
5.3.2	Controllability of a Linear Control System . . . . .	339
5.3.3	Affine Control System and Local Controllability . . . . .	340
5.3.4	Lagrangian Control Systems . . . . .	340
5.3.5	Lie–Adaptive Control in Human–Like Biomechanics . . . . .	348
5.3.6	Intelligent Robot Control: Interaction with Environment . . . . .	350
5.4	Neural Path Integral Motion Controller . . . . .	352
5.4.1	Spinal Autogenetic Reflex Control . . . . .	353
5.4.2	Cerebellum – the Comparator . . . . .	354
5.4.3	Hamiltonian Action and Neural Path Integral . . . . .	356
5.5	Brain–Like Control Functor in Human–Like Biomechanics . . . . .	357

<b>6</b>	<b>Covariant Biophysics of Electro–Muscular Stimulation</b> . . . . .	371
6.1	Basics of Electrical Muscular Stimulation . . . . .	371
6.2	EMS Functor . . . . .	375
6.2.1	Global macro–level of $EMS_{total}$ . . . . .	375
6.2.2	Local Micro–Level of $EMS_{total}$ . . . . .	377
6.2.3	Micro–Level Adaptation and Muscular Training . . . . .	378
6.3	Electrical Stimulation Fields: $EMS_{fields}$ . . . . .	379
6.3.1	External Smooth Maxwell Electrodynamics . . . . .	379
6.3.2	Internal Cellular Bio–Quantum Electrodynamics . . . . .	381
6.4	Stimulated Muscular Contraction Paths: $EMS_{paths}$ . . . . .	382
6.4.1	External Anatomical Muscular Mechanics . . . . .	382
6.4.2	Internal Myofibrillar Bio–Quantum Mechanics . . . . .	382
6.5	Anatomical Geometry of the Face & Body Shape: $EMS_{geom}$ . . . . .	384
6.5.1	External Face & Body Geometry . . . . .	384
6.5.2	Cellular Muscle–Fat Geometry . . . . .	389
<b>A</b>	<b>Appendix</b> . . . . .	391
A.1	Basic Formulas from Tensor Analysis . . . . .	391
A.1.1	Transformation of Coordinates and Elementary Tensors . . . . .	391
A.1.2	Euclidean Tensors . . . . .	397
A.1.3	Tensor Derivatives on Riemannian Manifolds . . . . .	398
A.1.4	The Covariant Force Law in Human–Like Biomechanics . . . . .	405
A.1.5	The Essence of Hamiltonian Biomechanics . . . . .	407
A.2	Muscular System . . . . .	408
A.2.1	Muscular Histology . . . . .	408
A.2.2	Classical Theories of Muscular Contraction . . . . .	410
A.2.3	The Equivalent Muscular Actuator . . . . .	417
A.2.4	Biochemistry of Muscular Contraction . . . . .	418
A.3	Path Integral Methods . . . . .	419
A.3.1	Historical Remarks . . . . .	419
A.3.2	Standard Path Integral Quantization . . . . .	427
A.3.3	Modern String Actions and Transition Amplitudes . . . . .	435
	<b>References</b> . . . . .	439
	<b>Index</b> . . . . .	455

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## Preface

This monographic textbook is a comprehensive introduction into modern geometric methods to be used as a unified research approach in two apparently separate and rapidly growing fields: *mathematical biomechanics & humanoid robotics*. The term *human-like biomechanics* is used to denote this unified modelling and control approach based on: theoretical mechanics, differential geometry and topology, nonlinear dynamics and control as well as modern path-integral methods. This approach has been realized in the form of the world-leading human-motion simulator called *Human Biodynamics Engine* (developed in the Land Operations Division, Defence Science & Technology Organisation, Australia).

This book is designed for a rigorous, one-semester course at the graduate level. The intended audience includes mechanical, control and biomedical engineers (with stronger mathematical background), mathematicians, physicists, computer scientists and mathematical biologists, as well as all researchers and technical professionals interested in modelling and control of humanoid robots and biomechanical systems.

From this *geometry-mechanics-control* modelling perspective, ‘human’ and ‘humanoid’ means the *same*. This unified approach, locally tensorial and globally functorial, enables both design of humanoid systems of immense complexity and prediction/prevention of subtle neuro-musculo-skeletal injuries. Consider, for example, human spine. Even if we ignore the highly irregular multi-vertebral geometry, a popular ‘spinal column’ is not columnar at all; it is a chain of 26 flexibly-coupled rigid bodies, including 25 movable spinal joints, each with three rotations (restricted to about 6–7 angular degrees in average) as well as three translations (each restricted to about 5 millimeters), which gives a total number of 150 constraint degrees of freedom (DOF). To perform a predictive analysis of the mechanism of a very common ‘back pain’ syndrome, in which there is no evidence at all for any tissue damage (measured by X-ray, CT, PET or functional MRI scans), and yet the patient suffers from spastic pain and drastically reduced motion capability — we need to take into account *all* 150 DOF. Dynamically speaking, we have a chain of 25 constrained

Euclidean  $SE(3)$  groups acting in all movable spinal joints, and we need to develop a rigorous kinematics and dynamics, as well as a hierarchical control model for this chain — to be able to accurately predict/control all possible motions (between any initial and final body configurations) and prevent spinal injuries, and thus efficiently cope with the back pain syndrome.

Spine is just one of many examples in which current biomechanics (or biomedical engineering) tries to *predict* and *control* the behavior of highly complex physiological systems using trivial models, like a very popular 1 DOF *inverted pendulum model* for the whole human body that has more than 300 DOF driven by more than 600 muscles, or similarly popular ‘Hybrid III’ crash-test dummy, that has one cylinder for the spine and one for the neck.<sup>1</sup>

In all monograph we try to follow the path-showing words of Paul Dirac [Dir30]: “...The main object of physical science is not the provision of pictures, but is the formulation of *laws* governing phenomena and the application of these *laws* to the discovery of new phenomena...” Modern scientific way of implementing this idea is to follow the slogan of Ralph Abraham [AS92]: “...*dynamics* is *geometry* of *behavior*...” Therefore, the whole text is dominated by tensorial geometry and topology, as a set of variations to the central theme of the book – our *covariant force law*, that states:

**Force 1–form–field = Mass distribution  $\times$  Acceleration vector–field**

This *law* is the *core* of human-like biomechanics. It is essentially mechanical, but at the same time it makes necessary three other related mathematical fields: differential geometry and topology, as well as nonlinear control theory.

---

<sup>1</sup> *Human Biodynamics Engine* (HBE) is a generalized Hamiltonian system with 264 DOF, including 132 rotational DOF (considered active) and 132 translational DOF (considered passive). Passive joint dynamics models visco-elastic properties of intervertebral discs, joint tendons and muscle ligaments as a nonlinear spring-damper system. Active joint dynamics is driven by 264 *nonlinear muscular actuators*, each with its own excitation-contraction dynamics (following traditional biomechanical models) and two-level neural-like control. The lower control level resembles spinal-reflex positive and negative force feedbacks (stretch and Golgi reflexes). The higher control level resembles cerebellum’s postural stabilization and velocity control (modelled as a high-dimensional Lie-derivative controller). The HBE includes over 2000 body parameters, all derived from individual user data, using standard biomechanical tables. It models stabilizing and reaching body movements at a spot, walking and running with any speed and a generic crash simulator. The HBE incorporates a new theory of soft neuro-musculo-skeletal injuries, much more sensitive than the traditional Principal Loading Hypothesis (of tension, compression, bending and shear) for spinal and other neuro-musculo-skeletal injuries. It is based on the concept of the local Jolts and Torque-Jolts, which are the time derivatives of the total forces and torques localized in each joint at a particular time instant.

The book contains six Chapters and Appendix. The first Chapter is Introduction, giving the brief review of mathematical techniques to be used in the text. The second Chapter develops geometric basis of human-like biomechanics, while the third Chapter develops its mechanical basis, mainly from generalized Lagrangian and Hamiltonian perspective. The fourth Chapter develops topology of human-like biomechanics, while the fifth Chapter reviews related nonlinear control techniques. The sixth Chapter develops covariant biophysics of electro-muscular stimulation. The Appendix includes three parts: (i) basic formulas from tensor calculus, including the derivation of our *covariant force law*, (ii) classical muscular mechanics, and (iii) modern path integral methods, which are all used frequently in the main text. The whole book is based on authors' own research papers in human-like biomechanics.

Adelaide,  
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## 0.1 Glossary of Frequently Used Symbols

### General

- ‘iff’ means ‘if and only if’;
- ‘r.h.s’ means ‘right hand side’; ‘l.h.s’ means ‘left hand side’;
- *Einstein’s summation convention over repeated indices* (not necessarily one up and one down) *is assumed in the whole text*, unless explicitly stated otherwise.

### Sets

- $\mathbb{N}$  – natural numbers;
- $\mathbb{Z}$  – integers;
- $\mathbb{R}$  – real numbers;
- $\mathbb{C}$  – complex numbers;
- $\mathbb{H}$  – quaternions;
- $\mathbb{K}$  – number field of real numbers, complex numbers, or quaternions.

### Maps

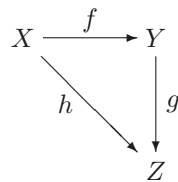
$f : A \rightarrow B$  – a function, (or map) between sets  $A \equiv \text{Dom } f$  and  $B \equiv \text{Cod } f$ ;

$\text{Ker } f = f^{-1}(e_B)$  – a kernel of  $f$ ;

$\text{Im } f = f(A)$  – an image of  $f$ ;

$\text{Coker } f = \text{Cod } f / \text{Im } f$  – a cokernel of  $f$ ;

$\text{Coim } f = \text{Dom } f / \text{Ker } f$  – a coimage of  $f$ ;



– a commutative diagram, requiring  $h = g \circ f$ .

### Derivatives

$C^k(A, B)$  – set of  $k$ -times differentiable functions between sets  $A$  to  $B$ ;

$C^\infty(A, B)$  – set of *smooth* functions between sets  $A$  to  $B$ ;

$C^0(A, B)$  – set of *continuous* functions between sets  $A$  to  $B$ ;

$f'(x) = \frac{df(x)}{dx}$  – derivative of  $f$  with respect to  $x$ ;

$\dot{x}$  – total time derivative of  $x$ ;

$\partial_t \equiv \frac{\partial}{\partial t}$  – partial time derivative;

$\partial_{x^i} \equiv \partial_i \equiv \frac{\partial}{\partial x^i}$  – partial coordinate derivative;

$\dot{f} = \partial_t f + \partial_{x^i} f \dot{x}^i$  – total time derivative of the scalar field  $f = f(t, x^i)$ ;  
 $u_t \equiv \partial_t u$ ,  $u_x \equiv \partial_x u$ ,  $u_{xx} \equiv \partial_{x^2} u$  – only in partial differential equations;  
 $L_{x^i} \equiv \partial_{x^i} L$ ,  $L_{\dot{x}^i} \equiv \partial_{\dot{x}^i} L$  – coordinate and velocity partial derivatives of the Lagrangian function;  
 $d$  – exterior derivative;  
 $d^n$  – coboundary operator;  
 $\partial_n$  – boundary operator;  
 $\nabla = \nabla(g)$  – Levi-Civita affine connection on a smooth manifold  $M$  with Riemannian metric tensor  $g = g_{ij}$ ;  
 $\Gamma_{jk}^i$  – Christoffel symbols of the connection  $\nabla$ ;  
 $\nabla_X T$  – covariant derivative of the tensor-field  $T$  with respect to the vector-field  $X$ , defined by means of  $\Gamma_{jk}^i$ ;  
 $T_{;x^i}$  – covariant derivative of the tensor-field  $T$  with respect to the coordinate basis  $\{x^i\}$ ;  
 $\bar{T} \equiv \frac{DT}{dt}$  – absolute (intrinsic, or Bianchi) derivative of the tensor-field  $T$  upon the parameter  $t$ ; e.g., acceleration vector is the *absolute time derivative* of the velocity vector,  $a^i = \dot{v}^i \equiv \frac{Dv^i}{dt}$ ; note that in general,  $a^i \neq \dot{v}^i$  – this is crucial for *proper definition of Newtonian force* (see Appendix);  
 $\mathcal{L}_X T$  – Lie derivative of the tensor-field  $T$  in direction of the vector-field  $X$ ;  
 $[X, Y]$  – Lie bracket (commutator) of two vector-fields  $X$  and  $Y$ ;  
 $[F, G]$  – Poisson bracket of two functions  $F$  and  $G$ ;  
 $\{F, G\}$  – Lie-Poisson bracket of two functions  $F$  and  $G$ .

## Manifolds and Fibre Bundles

$M$  – manifold, usually the biomechanical configuration manifold;  
 $TM$  – tangent bundle of the manifold  $M$ ;  
 $\pi_M : TM \rightarrow M$  – natural projection;  
 $T^*M$  – cotangent bundle of the manifold  $M$ ;  
 $(E, \pi, M)$  – a vector bundle with total space  $E$ , base  $M$  and projection  $\pi$ ;  
 $(E, p, M, F)$  – a fibre bundle with total space  $E$ , base  $M$ , projection  $p$  and standard fibre  $F$ ;  
 $J^k(M, N)$  – bundle of  $k$ -jets of smooth functions between manifolds  $M, N$ .

## Groups

$G$  – usually a general Lie group;  
 $GL(n)$  – general linear group with real coefficients in dimension  $n$ ;  
 $SO(n)$  – group of rotations in dimension  $n$ ;  
 $T^n$  – toral (Abelian) group in dimension  $n$ ;  
 $Sp(n)$  – symplectic group in dimension  $n$ ;  
 $T(n)$  – group of translations in dimension  $n$ ;  
 $SE(n)$  – Euclidean group in dimension  $n$ ;  
 $H_n(M) = \text{Ker } \partial_n / \text{Im } \partial_{n-1}$  –  $n$ th homology group of the manifold  $M$ ;  
 $H^n(M) = \text{Ker } d^n / \text{Im } d^{n+1}$  –  $n$ th cohomology group of the manifold  $M$ .

## Other Spaces and Operators

$C^k(M)$  – space of  $k$ -differentiable functions on the manifold  $M$ ;

$\Omega^k(M)$  – space of  $k$ -forms on the manifold  $M$ ;

$\mathfrak{g}$  – Lie algebra of a Lie group  $G$ , i.e., the tangent space of  $G$  at its identity element;

$Ad(g)$  – adjoint endomorphism; recall that *adjoint representation* of a Lie group  $G$  is the linearized version of the action of  $G$  on itself by conjugation, i.e., for each  $g \in G$ , the inner automorphism  $x \mapsto gxg^{-1}$  gives a linear transformation  $Ad(g) : \mathfrak{g} \rightarrow \mathfrak{g}$ , from the Lie algebra  $\mathfrak{g}$  of  $G$  to itself;

$nD$  space (group, system) means  $n$ -dimensional space (group, system), for  $n \in \mathbb{N}$ ;

$\lrcorner$  – interior product, or contraction, of a vector-field and a 1-form;

$\triangleright$  – semidirect (noncommutative) product; e.g.,  $SE(3) = SO(3) \triangleright \mathbb{R}^3$ ;

$\int$  – Feynman path integral symbol, denoting integration over continuous spectrum of smooth paths and summation over discrete spectrum of Markov chains; e.g.,  $\int \mathcal{D}[x] e^{iS[x]}$  denotes the path integral (i.e., sum-over-histories) over all possible paths  $x^i = x^i(t)$  defined by the Hamilton action,  $S[x] = \frac{1}{2} \int_{t_0}^{t_1} g_{ij} \dot{x}^i \dot{x}^j dt$ , while  $\int \mathcal{D}[\Phi] e^{iS[\Phi]}$  denotes the path integral over all possible fields  $\Phi^i = \Phi^i(x)$  defined by some field action  $S[\Phi]$ .

## Categories

$\mathcal{S}$  – all sets as objects and all functions between them as morphisms;

$\mathcal{PS}$  – all pointed sets as objects and all functions between them preserving base point as morphisms;

$\mathcal{V}$  – all vector spaces as objects and all linear maps between them as morphisms;

$\mathcal{B}$  – Banach spaces over  $\mathbb{R}$  as objects and bounded linear maps between them as morphisms;

$\mathcal{G}$  – all groups as objects, all homomorphisms between them as morphisms;

$\mathcal{A}$  – Abelian groups as objects, homomorphisms between them as morphisms;

$\mathcal{AL}$  – all algebras (over a given number field  $\mathbb{K}$ ) as objects, all their homomorphisms between them as morphisms;

$\mathcal{T}$  – all topological spaces as objects, all continuous functions between them as morphisms;

$\mathcal{PT}$  – pointed topological spaces as objects, continuous functions between them preserving base point as morphisms;

$\mathcal{TG}$  – all topological groups as objects, their continuous homomorphisms as morphisms;

$\mathcal{M}$  – all smooth manifolds as objects, all smooth maps between them as morphisms;

$\mathcal{M}_n$  –  $nD$  manifolds as objects, their local diffeomorphisms as morphisms;

$\mathcal{LG}$  – all Lie groups as objects, all smooth homomorphisms between them as morphisms;

$\mathcal{LAL}$  – all Lie algebras (over a given field  $\mathbb{K}$ ) as objects, all smooth homomorphisms between them as morphisms;

$\mathcal{TB}$  – all tangent bundles as objects, all smooth tangent maps between them as morphisms;

$\mathcal{T}^*\mathcal{B}$  – all cotangent bundles as objects, all smooth cotangent maps between them as morphisms;

$\mathcal{VB}$  – all smooth vector bundles as objects, all smooth homomorphisms between them as morphisms;

$\mathcal{FB}$  – all smooth fibre bundles as objects, all smooth homomorphisms between them as morphisms;

**Symplec** – all symplectic manifolds (i.e., physical phase-spaces), all symplectic maps (i.e., canonical transformations) between them as morphisms;

**Hilbert** – all Hilbert spaces and all unitary operators as morphisms.

## Introduction

*Human-like biomechanics* is a modern scientific approach to *human-like motion dynamics and control*. Its *human perspective* has been developed in the work of the present authors (see [Iva91, ILI95, IS01, IP01b, IP01a, Iva02, Iva04, Iva05, IB05, PI03, PI04]). The dynamics of human motion is extremely complex, multi-dimensional, highly nonlinear and hierarchical. Human skeleton has more than two hundred rigid bones, connected by rotational joints, which have up to three axes of rotation. Nevertheless, in classical biomechanics the main analytical tool was *translational vector geometry* (see Figure 1.1). The skeleton is driven by a synergistic action of its 640 skeletal muscles. Each of these muscles has its own *excitation* and *contraction* dynamics, in which neural action potentials are transformed into muscular force vectors (see [Hat77a, Hat77b, Hat78]).

On the other hand, *robotic approach* to human-like motion dynamics and control has been developed in the last three decades in the work of M. Vukobratovic (and his collaborators). He started in the early 1970s with pioneering papers on synthesis, control and stability of biped gait [VJ69, VJF70, VFJ70], followed by mathematical models of locomotion robots and anthropomorphic mechanisms [VS72, VS73, Vuk75, Vuk78]. later, in 1980s, he developed the scientific fundamentals of robotics in seven volumes of the Springer-Verlag book series [VP82, VS82, VK85a, VK85b, VSK85, VP85, VBS89]. In recent years, within the realm of mature robotic science, Vukobratovic has been revising the study of anthropomorphism and intelligence of humanoid robots [VPM03, KV03a, KV03b, VB04, VPR, VPT04, VAB04, VBB05, PV05, RV05].

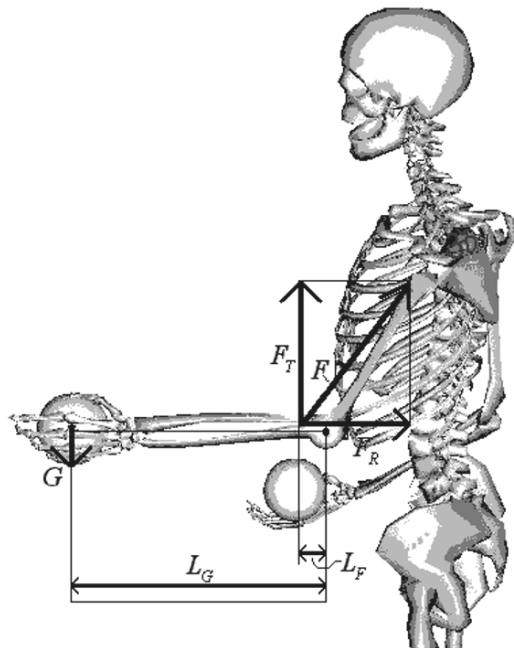
In this introductory Chapter we introduce the reader to the subject of modern human-like biomechanics, presenting its local (tensorial) language as well as its global (functorial) one. The objective here is to introduce our *covariant force law* (see subsection A.1.4 in Appendix),

$$F_i = mg_{ij}a^j, \quad \text{that 'in plain English' reads :}$$

**Force 1-form-field = Mass distribution  $\times$  Acceleration vector-field**

## 1.1 Local Tensorial Language of Human-Like Biomechanics

The local tensorial language of human-like biomechanics can be introduced in the following way. As it is pointed out in Appendix, the acceleration vector *is not* an ordinary time derivative of the velocity vector; ‘even worse’, the force, which is a paradigm of a vector in statics and engineering vector mechanics, *is not* a vector at all. The acceleration vector is the absolute time derivative of the velocity vector, while the force is a differential one-form. Proper description of these ideas is called *geometrodynamic*s.<sup>1</sup>



**Fig. 1.1.** Force vectors and their corresponding lever arms in classical translational biomechanics.

### 1.1.1 Classical Translational Biomechanics

Classical biomechanics consists of inverse and forward dynamics. *Inverse dynamics* is the commonly used technique used to gain insight into the net summation of all muscle activity at each joint. In this method, the joint forces

<sup>1</sup> Term *geometrodynamic*s was coined by John A. Wheeler from Princeton.

and torques are calculated from a prescribed movement. Since the segmental movements, in contrast to the internal forces, can be measured, this method is commonly applied for the analysis of measured movements. A full kinematic description obtained from *motion capture* of marker positions is sufficient to get an inverse solution; however, motion capture is often combined with output from other sensors, including *force plates*, in order to improve the precision of the estimated joint loads [Dar]. On the other hand, the rarely used *forward dynamics* takes joint forces and torques as input to simulate translational and rotational motion. This paper focuses on the basic principles of rotational forward dynamics.

Most of the classical biomechanics is based on the *Newton's second law*, which states that a *conservative particle* of mass  $m > 0$  immersed in a *potential*  $V(q)$  moves along a *curve*  $q^i(t)$  in *Euclidean 3D space*  $\mathbb{R}^3$ , in such a way that the *Newtonian equation of motion* is satisfied

$$m\ddot{q}^i = -\text{grad } V(q), \quad (1.1)$$

for  $q^i = \{q^1 \equiv x, q^2 \equiv y, q^3 \equiv z\} \in \mathbb{R}^3$ .

Now, if we introduce the translational (or, the so-called 'linear') momenta  $p_i = m\dot{q}^i$  and the total energy  $H(q, p) = \frac{1}{2m}\|p\|^2 + V(q)$ , (where  $\|\cdot\|$  denotes the Euclidean norm in  $\mathbb{R}^3$ ), then the second Newton's law of motion is equivalent to *translational Hamiltonian equations of motion* (see [AMR88, Arn89, MR99]):

$$\dot{q}^i = \frac{\partial H}{\partial p_i} \equiv \partial_{p_i} H, \quad \dot{p}_i = -\frac{\partial H}{\partial q^i} \equiv \partial_{q^i} H, \quad (i = 1, \dots, n). \quad (1.2)$$

One proceeds to study this system of first-order equations for a general  $H(q, p)$ . To do this, we introduce the matrix  $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$ , where  $I$  is the  $3 \times 3$  identity, and note that the equations become  $\dot{\xi} = J \cdot \text{grad } H(\xi)$ , where  $\xi = (q, p)$ .

Set  $X_H = J \cdot \text{grad } H$ . Then  $\xi(t)$  satisfies Hamilton's equations iff  $\xi(t)$  is an integral curve of  $X_H$ , that is,  $\dot{\xi}(t) = X_H(\xi(t))$  [AMR88].

The space  $\mathbb{R}^3 \times \mathbb{R}^3$  of the  $\xi$ 's is called the *phase space*. For a system of  $n$  particles we would use  $\mathbb{R}^{3n} \times \mathbb{R}^{3n}$ .

The conservative Hamiltonian system (1.2) is characterized by conservation of energy, and consequently momentum; the classical example of the later is reactive recoil of a gun after shooting.

The left,  $\dot{q}$ -equation in (1.2) is called the 'Velocity equation', while the right,  $\dot{p}$ -equation is called the 'Force equation'. Combined, they give the biomechanical sense of the celebrated Hill's 'Force-Velocity relation' ([Hil38]). All biologically essential non-conservative forces, like neuro-muscular servo-drives, tendon elasticities and joint dampings, are to be added to the force equation. This is probably the most plausible way of presenting the *translational biomechanics*.

### 1.1.2 Calculus of Geometric Objects

Following the trend that has prevailed in physical sciences for several decades (see, e.g., [MTW73]), we state here the leading idea of this book: *every biomechanical quantity can be described by a geometric object; all biomechanical laws can be expressed as geometric relationships between these geometric objects.* This trend has its mathematical beginnings in the Erlanger Program of Felix Klein and entered the physical sciences in the form of the ‘principle of general covariance’ of Albert Einstein: *physical laws must be independent of any particular coordinate systems if they are to be valid.* A study of the consequences of this requirement leded, at first, to classical tensor calculus, and subsequently, to its modern development, *calculus of coordinate-free geometric objects*, the most natural machinery for analysis of biomechanical systems. We assume that our reader is familiar with classical tensor calculus, while the modern calculus of coordinate-free geometric objects will be developed as we proceed in our study of human-like biomechanics.

In biomechanics, the most important geometric objects are Riemannian metric and curvature tensors (see Appendix), as well as several exterior differential forms.

#### Metric Tensor – the Core of Geometrodynamics

The act of measurement in curved spaces is performed by the use of Riemannian metrics. The general result is this: at each point of any smooth *Riemannian manifold* there exists a geometric object called the *metric tensor*  $g$ , usually given by its *covariant components*  $g_{ij}$ . However, it is easier to start with our familiar ordinary Euclidean three-dimensional space with rectilinear Cartesian axes defined on it.

In any case, the metric tensor  $g = (g_{ij})$  defines a linear symmetrical machine  $g(\cdot, \cdot)$  with two input slots for the insertion of two vectors, producing a real number as an output. It can be used for calculating the *scalar product*

$$v \cdot w = g(v, w) = g_{ij}v^i w^j$$

of two different vectors  $v = (v^i)$  and  $w = (w^i)$ , or the square length

$$g(v, v) = v^2$$

of a single vector  $v$ .

In particular, in *Euclidean 3D space*  $\mathbb{R}^3$ , with the coordinate basis

$$\{e_1 = dx, e_2 = dy, e_3 = dz\}$$

along the standard *Cartesian axes*  $\{x, y, z\}$ , the metric tensor  $g = (g_{ij})$  is defined by

$$g = g(e_i, e_j) = e_i \cdot e_j,$$

while the vector  $v = (v^i)$  is expressed in components as

$$v = v^1 e_1 + v^2 e_2 + v^3 e_3 = v^i e_i$$

(Einstein’s summation convention is always in place).

At this point we need to emphasize that more fundamental than the components of a tensor (or a vector) is the tensor (respectively vector) itself, a geometric object with a physical or biomechanical meaning independent of all coordinates. For example, velocity of a particle moving in  $\mathbb{R}^3$  is a *tangent vector* to the trajectory of the particle, defined locally as a derivative of the trajectory at a certain point. However, coordinates necessarily enter the scene when numerical analysis is required.

### Classical Tensor Dynamics in Brief

Now we switch from geometry to dynamics, intending to show that they are actually the same thing, sometimes called *geotrodynamics*. Recall that a material system is regarded from the dynamical standpoint as a collection of particles which are subject to interconnections and constraints of various kinds (e.g., a rigid body is regarded as a number of particles rigidly connected together so as to remain at invariable distances from each other). The *number of independent coordinates which determine the configuration of a dynamical system completely* is called the *number of degrees of freedom* (DOF) of the system. In other words, this number,  $n$ , is the *dimension of the system’s configuration manifold*. This viewpoint is the core of our geometric biomechanics.

For simplicity, let us suppose that we have a dynamical system with three DOF (e.g., a particle of mass  $M$ , or a rigid body of mass  $M$  with one point fixed); generalization to  $n$  DOF, with  $N$  included masses  $M_\alpha$ , is straightforward. The configuration of our system at any time is then given by three coordinates  $\{q^1, q^2, q^3\}$ . As the coordinates change in value the dynamical system changes its configuration. Obviously, there is an infinite number of sets of independent coordinates which will determine the configuration of a dynamical system, but since the position of the system is completely given by any one set, these sets of coordinates must be functionally related. Hence, if  $\bar{q}^i$  is any other set of coordinates, these quantities must be connected with  $q^i$  by formulae of the type

$$\bar{q}^i = \bar{q}^i(q^i), \quad (i = 1, \dots, n(= 3)). \quad (1.3)$$

Relations (1.3) are the equations of transformation from one set of dynamical coordinates to another and, in a standard tensorial way (see Appendix, as well as e.g., [McC60, SS78, BL81, LR89, LC03], although we recommend [MTW73]), we can define tensors relative to this coordinate transformation. The generalized coordinates  $q^i$ , ( $i = 1, \dots, n$ ) constitute the system’s *configuration manifold*.

In particular, in our ordinary Euclidean 3–dimensional (3D) space  $\mathbb{R}^3$ , the ordinary Cartesian axes are  $x^i = \{x, y, z\}$ , and the *system's center of mass* (COM) is given by

$$C^i = \frac{M_\alpha x_\alpha^i}{\sum_{\alpha=1}^N M_\alpha},$$

where Greek subscript  $\alpha$  labels the masses included in the system. If we have a continuous distribution of matter  $V = V(M)$  rather than the discrete system of masses  $M_\alpha$ , all the  $\alpha$ –sums should be replaced by volume integrals, the element of mass  $dM$  taking the place of  $M_\alpha$ ,

$$\sum_{\alpha=1}^N M_\alpha \Rightarrow \iiint_V dM.$$

An important quantity related to the system's COM is the double symmetric contravariant tensor

$$I^{ij} = M_\alpha x_\alpha^i x_\alpha^j, \quad (1.4)$$

called the *inertia tensor*, calculated relative to the origin  $O$  of the Cartesian axes  $x_\alpha^i = \{x_\alpha, y_\alpha, z_\alpha\}$ . If we are given a straight line through  $O$ , defined by its unit vector  $\lambda^i$ , and perpendiculars  $p_\alpha$  are drawn from the different particles on the line  $\lambda^i$ , the quantity

$$I(\lambda^i) = M_\alpha p_\alpha^2$$

is called the *moment of inertia* around  $\lambda^i$ . The moment of inertia  $I(\lambda^i)$  can be expressed through inertia tensor (1.4) as

$$I(\lambda^i) = (I g_{ij} - I_{ij}) \lambda^i \lambda^j,$$

where  $g_{ij}$  is the system's *Euclidean 3D metric tensor* (as defined above),  $I = g_{ij} I^{ij}$ , and  $I_{ij} = g_{rm} g_{sn} I^{mn}$  is the *covariant inertia tensor*. If we now consider the quadric  $Q$  whose equation is

$$(I g_{ij} - I_{ij}) x^i x^j = 1, \quad (1.5)$$

we find that the moment of inertia around  $\lambda^i$  is  $1/R$ , where  $R$  is the radius vector of  $Q$  in the direction of  $\lambda^i$ . The quadric  $Q$  defined by relation (1.5) is called the *ellipsoid of inertia* at the origin  $O$ . It has always three principal axes, which are called the *principal axes of inertia* at  $O$ , and the planes containing them in pairs are called the *principal planes of inertia* at  $O$ . The principal axes of inertia are given by the equations

$$(I g_{ij} - I_{ij}) \lambda^j = \theta \lambda^i,$$

where  $\theta$  is a root of the determinant equation

$$|(I - \theta) g_{ij} - I_{ij}| = 0.$$

More generally, if we suppose that the points of our dynamical system are referred to rectilinear Cartesian axes  $x^i$  in a Euclidean  $n$ -dimensional ( $nD$ ) space  $\mathbb{R}^n$ , then when we are given the time and a set of *generalized coordinates*  $q^i$  we are also given all the points  $x^i$  of the dynamical system, as the system is determined uniquely. Consequently, the  $x^i$  are functions of  $q^i$  and possibly also of the time, that is,

$$x^i = x^i(q^i, t).$$

If we restrict ourselves to the *autonomous dynamical systems* in which these equations do not involve  $t$ , i.e.,

$$x^i = x^i(q^i), \quad (1.6)$$

then differentiating (1.6) with respect to the time  $t$  gives

$$\dot{x}^i = \frac{\partial x^i}{\partial q^j} \dot{q}^j. \quad (1.7)$$

The quantities  $\dot{q}^i$ , which form a vector with reference to coordinate transformations (1.3), we shall call the *generalized velocity vector*. We see from (1.7) that when the generalized velocity vector is given we know the velocity of each point of our system. Further, this gives us the system's *kinetic energy*,

$$E_{kin} = \frac{1}{2} M_\alpha g_{mn} \dot{x}_\alpha^m \dot{x}_\alpha^n = \frac{1}{2} M_\alpha g_{mn} \frac{\partial x_\alpha^m}{\partial q^i} \frac{\partial x_\alpha^n}{\partial q^j} \dot{q}^i \dot{q}^j. \quad (1.8)$$

Now, if we use the Euclidean metric tensor  $g_{ij}$  to define the *material metric tensor*  $G_{ij}$ , including the distribution of all the masses  $M_\alpha$  of our system, as

$$G_{ij} = M_\alpha g_{mn} \frac{\partial x_\alpha^m}{\partial q^i} \frac{\partial x_\alpha^n}{\partial q^j}, \quad (1.9)$$

the kinetic energy (1.8) becomes a *homogenous quadratic form* in the generalized system's velocities  $\dot{q}^i$ ,

$$E_{kin} = \frac{1}{2} G_{ij} \dot{q}^i \dot{q}^j. \quad (1.10)$$

From the transformation relation (1.9) we see that the material metric tensor  $G_{ij}$  is symmetric in  $i$  and  $j$ . Also, since  $E_{kin}$  is an invariant for all transformations of generalized coordinates, from (1.10) we conclude that  $G_{ij}$  is a double symmetric tensor. Clearly, this is the central quantity in classical tensor system dynamics. We will see later, that  $G_{ij}$  defines the Riemannian geometry of the system dynamics. For simplicity reasons,  $G_{ij}$  is often denoted by purely geometric symbol  $g_{ij}$ , either assuming or neglecting the material properties of the system.

Now, let us find the equations of motion of our system. According to the *D'Alembert's Principle of virtual displacements*, the equations of motion in Cartesian coordinates  $x^i$  in  $\mathbb{R}^n$  are embodied in the single tensor equation

$$g_{mn}(M_\alpha \ddot{x}_\alpha^m - X_\alpha^m) \delta x_\alpha^n = 0, \quad (1.11)$$

where  $X_\alpha^i$  is the total force vector acting on the particle  $M_\alpha$ , while  $\delta x_\alpha^i$  is the associated *virtual displacement* vector, so that the product  $g_{ij} X_\alpha^i \delta x_\alpha^j$  is the *virtual work* of the system, and we can neglect in  $X_\alpha^i$  all the internal or external forces which do not work in the displacement  $\delta x_\alpha^i$ . If we give the system a small displacement compatible to with the constraints of the system, we see that this displacement may be effected by giving increments  $\delta q^i$  to the generalized coordinates  $q^i$  of the system, and these are related to the  $\delta x^i$  in accordance with the transformation formulae  $\delta x_\alpha^i = \frac{\partial x_\alpha^i}{\partial q^j} \delta q^j$ .

Furthermore, in this displacement the internal forces due to the constraints of the system will do no work, since these constraints are preserved, and consequently only the external forces will appear in (1.11), so it becomes

$$g_{mn} \left[ M_\alpha \frac{d}{dt} \left( \frac{\partial x_\alpha^m}{\partial q^j} \dot{q}^j \right) \frac{\partial x_\alpha^n}{\partial q^i} - X_\alpha^m \frac{\partial x_\alpha^n}{\partial q^i} \right] \delta q^i = 0. \quad (1.12)$$

Now, using (1.8–1.10), we derive

$$M_\alpha g_{mn} \frac{d}{dt} \left( \frac{\partial x_\alpha^m}{\partial q^j} \dot{q}^j \right) \frac{\partial x_\alpha^n}{\partial q^i} = \frac{d}{dt} (G_{ij} \dot{q}^j) - \frac{1}{2} \frac{\partial G_{st}}{\partial q^i} \dot{q}^j \dot{q}^k = \frac{d}{dt} \left( \frac{\partial E_{kin}}{\partial \dot{q}^i} \right) - \frac{\partial E_{kin}}{\partial q^i}.$$

Also, if we put

$$F_i = g_{mn} X_\alpha^m \frac{\partial x_\alpha^n}{\partial q^i},$$

we get

$$F_i \delta q^i = g_{mn} X_\alpha^m \delta x_\alpha^n = \delta W, \quad (1.13)$$

where  $\delta W$  is the virtual work done by the external forces in the small displacement  $\delta q^i$ , which shows that  $F_i$  is the covariant vector, called the *generalized force vector*. Now (1.12) takes the form

$$\left[ \frac{d}{dt} \left( \frac{\partial E_{kin}}{\partial \dot{q}^i} \right) - \frac{\partial E_{kin}}{\partial q^i} - F_i \right] \delta q^i = 0.$$

Since the coordinates  $q^i$  are independent this equation is true for all variations  $\delta q^i$  and we get as a final result the *covariant Lagrangian equations of motion*,

$$\frac{d}{dt} \left( \frac{\partial E_{kin}}{\partial \dot{q}^i} \right) - \frac{\partial E_{kin}}{\partial q^i} = F_i.$$

If the force system is conservative and  $E_{pot}$  is the system's *potential energy* given by

$$F_i = - \frac{\partial E_{pot}}{\partial q^i},$$

then, using (1.13) the Lagrangian equations take the standard form

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^i} \right) = \frac{\partial L}{\partial q^i}, \quad (1.14)$$

where the *Lagrangian function*  $L = L(q, \dot{q})$  of the system is given by  $L = E_{kin} - E_{pot}$  (since  $E_{pot}$  does not contain  $\dot{q}^i$ ).

Now, the kinetic energy  $E_{kin}$  of the system, given by quadratic form (1.10), is always positive except when  $\dot{q}^i$  is zero in which case  $E_{kin}$  vanishes. In other words, the quadratic form (1.10) is positive definite. Consequently, we can always find the *line* (or *arc*) *element*, defined by

$$ds^2 = G_{ij} dq^i dq^j. \quad (1.15)$$

A manifold in which  $ds^2$  is given by relation of the type of (1.15), geometrically with  $g_{ij}$  instead of  $G_{ij}$ , is called a *Riemannian manifold*.

### Riemannian Curvature Tensor

Every Riemannian manifold is characterized by the *Riemann curvature tensor*. In physical literature (see, e.g., [MTW73]) it is usually introduced through the *Jacobi equation of geodesic deviation*, showing the acceleration of the relative separation of nearby geodesics (the shortest, straight lines on the manifold). For simplicity, consider a sphere of radius  $a$  in  $\mathbb{R}^3$ . Here, Jacobi equation is pretty simple,

$$\frac{d^2 \xi}{ds^2} + R\xi = 0,$$

where  $\xi$  is the *geodesic separation vector* (the so-called Jacobi vector-field),  $s$  denotes the geodesic arc parameter given by (1.15) and  $R = 1/a^2$  is the *Gaussian curvature* of the surface.

In case of a higher-dimensional manifold  $M$ , the situation is naturally more complex, but the main structure of the Jacobi equation remains similar,

$$\frac{D^2 \xi}{ds^2} + R(u, \xi, u) = 0,$$

where  $D$  denotes the covariant derivative and  $R(u, \xi, u)$  is the curvature tensor, a three-slot linear machine. In components defined in a local coordinate chart  $(x^i)$  on  $M$ , this equation reads

$$\frac{D^2 \xi^i}{ds^2} + R_{jkl}^i \frac{dx^j}{ds} \xi^k \frac{dx^l}{ds} = 0,$$

where  $R_{jkl}^i$  are the components of the Riemannian curvature tensor.

### Exterior Differential Forms

Recall that *exterior differential forms* are a special kind of antisymmetrical covariant tensors (see, e.g., [DRh84, Fla63]). Such tensor-fields arise in many

applications in physics, engineering, and differential geometry. The reason for this is the fact that the classical vector operations of **grad**, **div**, and **curl** as well as the theorems of Green, Gauss, and Stokes can all be expressed concisely in terms of differential forms and the main operator acting on them, the exterior derivative  $d$ . Differential forms inherit all geometric properties of the general tensor calculus and add to it their own powerful geometric, algebraic and topological machinery (see Figures 1.2 and 1.3). Differential  $p$ -forms formally occur as *integrands* under ordinary integral signs in  $\mathbb{R}^3$ :

- a *line integral*  $\int P dx + Q dy + R dz$  has as its integrand the *one-form*  $\omega = P dx + Q dy + R dz$ ;
- a *surface integral*  $\iint A dydz + B dzdx + C dxdy$  has as its integrand the *two-form*  $\alpha = A dydz + B dzdx + C dxdy$ ;
- a *volume integral*  $\iiint K dxdydz$  has as its integrand the *three-form*  $\lambda = K dxdydz$ .

By means of an *exterior derivative*  $d$ , a *derivation* that transforms  $p$ -forms into  $(p + 1)$ -forms, these geometric objects generalize ordinary vector differential operators in  $\mathbb{R}^3$ :

- a *scalar function*  $f = f(x)$  is a zero-form;
- its *gradient*  $df$ , is a one-form<sup>2</sup>

$$df = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz;$$

- a *curl*  $d\omega$ , of a one-form  $\omega$  above, is a two-form

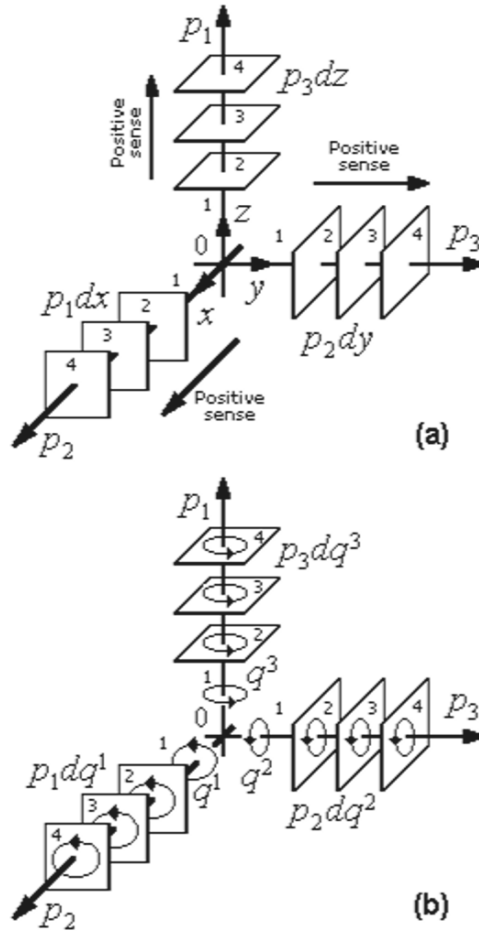
$$d\omega = \left( \frac{\partial R}{\partial y} - \frac{\partial Q}{\partial z} \right) dydz + \left( \frac{\partial P}{\partial z} - \frac{\partial R}{\partial x} \right) dzdx + \left( \frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} \right) dxdy;$$

- a *divergence*  $d\alpha$ , of the two-form  $\alpha$  above, is a three-form

$$d\alpha = \left( \frac{\partial A}{\partial x} + \frac{\partial B}{\partial y} + \frac{\partial C}{\partial z} \right) dxdydz.$$

Now, although visually intuitive, our Euclidean 3D space  $\mathbb{R}^3$  is not sufficient for thorough biomechanical analysis. The fundamental concept of a *smooth manifold*, locally topologically equivalent to the Euclidean  $n$ D space  $\mathbb{R}^n$ , is required (with or without Riemannian metric tensor defined on it). In general, a proper definition of exterior derivative  $d$  for a  $p$ -form  $\beta$  on a smooth manifold  $M$ , includes the *Poincaré lemma*:  $d(d\beta) = 0$ , and validates the general integral *Stokes formula*

<sup>2</sup> We use the same symbol,  $d$ , to denote both ordinary and exterior derivation, in order to avoid extensive use of the boldface symbols. It is clear from the context which derivative (differential) is in place: exterior derivative operates only on differential forms, while the ordinary differential operates mostly on coordinates.



**Fig. 1.2.** Basis vectors and one-forms in Euclidean  $\mathbb{R}^3$ -space: (a) Translational case; and (b) Rotational case.

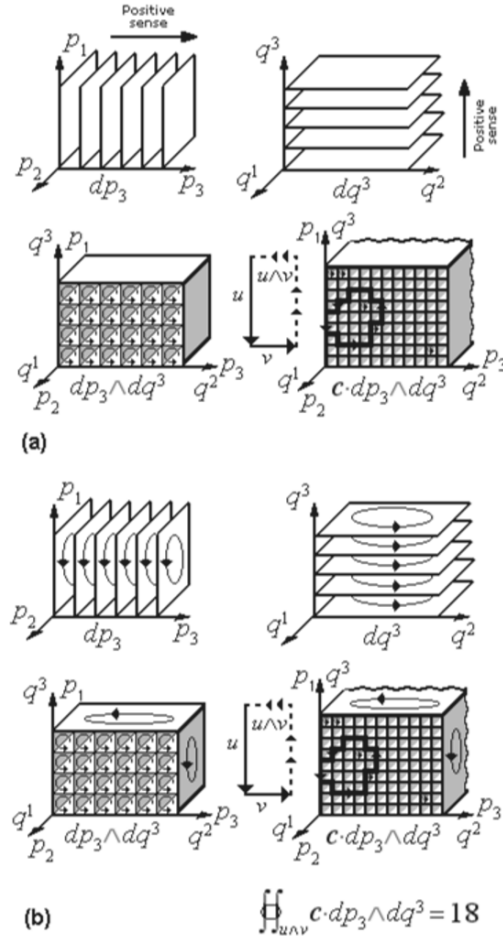
$$\int_{\partial M} \beta = \int_M d\beta,$$

where  $M$  is a  $p$ -dimensional *manifold with a boundary* and  $\partial M$  is its  $(p - 1)$ -dimensional *boundary*, while the integrals have appropriate dimensions.

A  $p$ -form  $\beta$  is called *closed* if its exterior derivative is equal to zero,

$$d\beta = 0.$$

From this condition one can see that the closed form (the *kernel* of the exterior derivative operator  $d$ ) is conserved quantity. Therefore, closed  $p$ -forms possess certain invariant properties, physically corresponding to the conservation laws.



**Fig. 1.3.** Fundamental two-form and its flux in  $\mathbb{R}^3$ : (a) Translational case; (b) Rotational case. In both cases the flux through the plane  $u \wedge v$  is defined as  $\int \int_{u \wedge v} c \, dp_i dq^i$  and measured by the number of tubes crossed by the circulation oriented by  $u \wedge v$ .

A  $p$ -form  $\beta$  that is an exterior derivative of some  $(p - 1)$ -form  $\alpha$ ,

$$\beta = d\alpha,$$

is called *exact* (the *image* of the exterior derivative operator  $d$ ). By Poincaré Lemma, exact forms prove to be closed automatically,

$$d\beta = d(d\alpha) = 0.$$

Similarly to the components of a 3D vector  $v$  defined above, a one-form  $\theta$  defined on an  $n$ D manifold  $M$  can also be expressed in components, using

the coordinate basis  $\{dx^i\}$  along the local  $n$ D coordinate chart  $\{x^i\} \in M$ , as

$$\theta = \theta_i dx^i.$$

Now, the components of the exterior derivative of  $\theta$  are equal to the components of its *commutator* defined on  $M$  by

$$d\theta = \omega_{ij} dx^i dx^j,$$

where the components of the *form commutator*  $\omega_{ij}$  are given by

$$\omega_{ij} = \left( \frac{\partial \theta_i}{\partial x^j} - \frac{\partial \theta_j}{\partial x^i} \right).$$

The space of all smooth  $p$ -forms on a smooth manifold  $M$  is denoted by  $\Omega^p(M)$ . The *wedge*, or *exterior product* of two differential forms, a  $p$ -form  $\alpha \in \Omega^p(M)$  and a  $q$ -form  $\beta \in \Omega^q(M)$  is a  $(p+q)$ -form  $\alpha \wedge \beta$ . For example, if  $\theta = a_i dx^i$ , and  $\eta = b_j dx^j$ , their wedge product  $\theta \wedge \eta$  is given by

$$\theta \wedge \eta = a_i b_j dx^i dx^j,$$

so that the coefficients  $a_i b_j$  of  $\theta \wedge \eta$  are again smooth functions, being polynomials in the coefficients  $a_i$  of  $\theta$  and  $b_j$  of  $\eta$ . The exterior product  $\wedge$  is related to the exterior derivative  $d : \Omega^p(M) \rightarrow \Omega^{p+1}(M)$ , by

$$d(\alpha \wedge \beta) = d\alpha \wedge \beta + (-1)^p \alpha \wedge d\beta.$$

Another important linear operator is the *Hodge star*  $*$  :  $\Omega^p(M) \rightarrow \Omega^{n-p}(M)$ , where  $n$  is the dimension of the manifold  $M$ . This operator depends on the inner product (i.e., Riemannian metric) on  $M$  and also depends on the orientation (reversing orientation will change the sign). For any  $p$ -forms  $\alpha$  and  $\beta$ ,

$$**\alpha = (-1)^{p(n-p)}\alpha, \quad \text{and} \quad \alpha \wedge *\beta = \beta \wedge *\alpha.$$

Hodge star is generally used to define *dual*  $(n-p)$ -forms on  $n$ D smooth manifolds.

For example, in  $\mathbb{R}^3$  with the ordinary Euclidean metric, if  $f$  and  $g$  are functions then (compare with the 3D forms of gradient, curl and divergence defined above)

$$\begin{aligned} df &= \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz, \\ *df &= \frac{\partial f}{\partial x} dydz + \frac{\partial f}{\partial y} dzdx + \frac{\partial f}{\partial z} dxdy, \\ df \wedge *dg &= \left( \frac{\partial f}{\partial x} \frac{\partial g}{\partial x} + \frac{\partial f}{\partial y} \frac{\partial g}{\partial y} + \frac{\partial f}{\partial z} \frac{\partial g}{\partial z} \right) dxdydz = \Delta f dxdydz, \end{aligned}$$

where  $\Delta f$  is the *Laplacian* on  $\mathbb{R}^3$ . Therefore the three-form  $df \wedge *dg$  is the Laplacian multiplied by the volume element, which is valid, more generally, in any local orthogonal coordinate system in any smooth domain  $U \in \mathbb{R}^3$ .

The subspace of all closed  $p$ -forms on  $M$  we will denote by  $Z^p(M) \subset \Omega^p(M)$ , and the sub-subspace of all exact  $p$ -forms on  $M$  we will denote by  $B^p(M) \subset Z^p(M)$ . Now, the quotient space

$$H^p(M) = \frac{Z^p(M)}{B^p(M)} = \frac{\text{Ker}(d : \Omega^p(M) \rightarrow \Omega^{p+1}(M))}{\text{Im}(d : \Omega^{p-1}(M) \rightarrow \Omega^p(M))}$$

is called the  $p$ th *De Rham cohomology group* (or vector space) of a manifold  $M$ . Two  $p$ -forms  $\alpha$  and  $\beta$  on  $M$  are equivalent, or belong to the same *cohomology class*  $[\alpha] \in H^p(M)$ , if their difference equals  $\alpha - \beta = d\theta$ , where  $\theta$  is a  $(p-1)$ -form on  $M$ .

### 1.1.3 Lagrangian Action and Feynman Path Integral

Recall that all the fundamental laws of classical physics can be understood in terms of one mathematical construct, the *action principle*, as well as all the fundamental laws of quantum physics can be understood in terms of associated construct, the *Feynman path integral* (see, e.g., [Ram90]).

In 1746 Maupertuis formulated the Principle of Least Action, which is all too commonly credited to one of the three great mathematicians, Euler, Lagrange, and Hamilton, who further developed it. This principle is one of the greatest generalizations in all physical science, although not fully appreciated until the advent of quantum mechanics and Feynman path integral in the mid 20th century.

In particular, all Newtonian particle mechanics is contained in the *Hamilton's principle of least action*, which demands that the true trajectory  $x = x(t)$  of a particle is that function which *minimizes the action*  $S[x(t)]$ , given as a temporal integral of the autonomous *Lagrangian function*  $L = L(x, \dot{x})$ ,

$$S[x] = \int_{t_0}^{t_1} L(x, \dot{x}) dt \longrightarrow \min, \quad \text{or,} \quad \delta S[x] = 0,$$

where the second expression reads: ‘variation of the action equals zero’ and implies using techniques from the *calculus of variations* (see e.g., [For60]).

Now, associated to the least action principle is the path integral, or Feynman’s *sum-over-histories*.<sup>3</sup> While Nature’s command for the classical particle is: “Follow the path of least action,” to the elementary particle it commands: “Explore all possible paths!”

<sup>3</sup> Here we quote F. Dyson: “Dick Feynman told me about his sum-over-histories version of quantum mechanics. “The electron does anything it likes,” he said. “It just goes in any direction at any speed, forward or backward in time, however it likes, and then you add up the amplitudes and it gives you the wave-function.” I said to him, “You’re crazy.” But he wasn’t.”

According to this general *action principle – path integral* formalism (see section 3.3 as well as Appendix, section A.3), we first formulate the acceptable *action functional* (AF, denoted by square brackets [...]), from which we derive *Euler–Lagrangian equations* of motion, and subsequently we perform the *quantization* of the system and find its *transition amplitude*, by evaluating the *associate path integral*.

In mechanics, the *Lagrangian action formalism* is a four-step algorithm with a purpose of finding the *true*, or *straight path*  $x^i = x^i(t)$ , ( $i = 1, \dots, N$ ) of an  $N$ -degree-of-freedom autonomous dynamical system:

1. Formulate the *Lagrangian function*  $L = L(x, \dot{x})$  of the system, e.g., as a function  $L(x, \dot{x}) = E_{kin}(\dot{x}) - E_{pot}(x)$ ;
2. Write down the AF, as a temporal integral,

$$S[x] = \int_{t_0}^{t_1} L dt;$$

3. Formulate the *action principle*, as a vanishing variation of the AF,

$$\delta S[x] = \delta \int_{t_0}^{t_1} L dt = \int_{t_0}^{t_1} \delta L dt = 0,$$

with zero initial and final path variations,  $\delta x(t_0) = \delta x(t_1) = 0$ ;

4. Derive the *Euler–Lagrangian equations* of motion,

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}^i} \right) = \frac{\partial L}{\partial x^i}, \quad (i = 1, \dots, N),$$

using the vanishing *functional derivative*,  $\frac{\delta S}{\delta x^i} = 0$ , given by (using standard variational techniques)

$$\frac{\delta S}{\delta x^i} \equiv \frac{\partial L}{\partial x^i} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}^i} \right).$$

For illustration, take the simple example of a single *point particle* moving in Euclidean 3D space, with position vector  $x^i = x^i(t)$  ( $i = 1, 2, 3$ ), at time  $t$ , within a time independent *potential field*  $V(x^i)$ . The corresponding AF is given by

$$S([x^i], t_0, t_1) = \int_{t_0}^{t_1} dt \left( \frac{1}{2} m \frac{dx^i}{dt} \frac{dx^i}{dt} - V(x^i) \right). \quad (1.16)$$

The AF (1.16) is a *function* of the initial and final times,  $t_0$  and  $t_1$  (which we write  $S(t_0, t_1)$ ), and at the same time a *functional of the path*  $x^i(t)$  (which we write  $S[x^i]$ ) for  $t_0 < t_1$ .<sup>4</sup> To build the AF, we consider a small deformation of the path,

$$x^i(t) \rightarrow x^i(t) + \delta x^i(t).$$

<sup>4</sup> For example, the length of a path is a functional of the path.

The  $S$ -response to the small path deformation is given by

$$\begin{aligned} S[x^i + \delta x^i] &= \int_{t_0}^{t_1} dt \left( \frac{1}{2} m \frac{d(x^i + \delta x^i)}{dt} \frac{d(x^i + \delta x^i)}{dt} - V(x^i + \delta x^i) \right) \quad (1.17) \\ &= S[x^i] + \int_{t_0}^{t_1} dt \delta x^i (-\partial_i V(x^i) - m\ddot{x}^i) + m \int_{t_0}^{t_1} dt \frac{d}{dt} (\delta x^i \dot{x}^i), \end{aligned}$$

where  $\partial_i \equiv \partial_{x^i} \equiv \frac{\partial}{\partial x^i}$ , and

$$V(x^i + \delta x^i) = V(x^i) + \delta x^i \partial_i V(x^i).$$

According to the standard variation techniques, the last term in (1.17) is just a ‘surface’ term, which is usually eliminated by restricting the variations to paths which vanish at the end points,

$$\delta x^i(t_0) = \delta x^i(t_1) = 0.$$

In this way, (1.17) becomes

$$S[x^i + \delta x^i] = S[x^i] + \int_{t_0}^{t_1} dt \delta x^i \frac{\delta S}{\delta x^i},$$

where the functional derivative  $\frac{\delta S}{\delta x^i}$  is defined by

$$\frac{\delta S}{\delta x^i} = -(m\ddot{x}^i + \partial_i V(x^i)). \quad (1.18)$$

Therefore, the minimization of the AF (1.16) is, according to the Hamilton action principle, equivalent to the vanishing functional derivative, which leads to the equations of motion

$$\frac{\delta S}{\delta x^i} \equiv -(m\ddot{x}^i + \partial_i V(x^i)) = 0, \quad \text{or,} \quad m\ddot{x}^i = \partial_i V(x^i).$$

Note, however, that minimization of  $S$  only leads to a *class of possible paths*. Which of those is followed depends on the boundary conditions, given as initial values of positions  $x^i(t_0)$  and velocities  $\dot{x}^i(t_0) \equiv \frac{dx^i(t_0)}{dt}$ .

More generally, in *field theory*, the four-step Lagrangian action formalism is the following algorithm:

1. Formulate the *Lagrangian density*  $\mathcal{L} = \mathcal{L}(\varphi^i, \partial_\mu \varphi^i)$  of the system as a function of  $m$  field variables  $\varphi^i = \varphi^i(x^\mu)$  and their first partial derivatives  $\partial_\mu \varphi^i$  over the  $n$  system coordinates  $x^\mu$  (e.g., 4 space-time coordinates);
2. Write down the AF, as an  $n$ D integral,

$$S[x] = \int \mathcal{L}(\varphi^i, \partial_\mu \varphi^i) dx, \quad dx = \prod_{\mu=1}^n dx^\mu;$$

3. Formulate the *action principle*, as a vanishing variation of the AF,

$$\delta S[x] = \delta \int \mathcal{L} dx = \int \delta \mathcal{L} dx = 0,$$

with zero boundary field variations;

4. Derive the *Euler-Lagrangian equations* of motion, using the vanishing *functional derivative*,  $\frac{\delta S}{\delta x^i} = 0$ , given by

$$\frac{\delta S}{\delta \varphi^i} \equiv \frac{\partial \mathcal{L}}{\partial \varphi^i} - \partial_\mu \left( \frac{\partial \mathcal{L}}{\partial_\mu \varphi^i} \right).$$

Now, once we have an acceptable AF, we can formulate the associated Feynman path integral, according to the procedures developed in Appendix. In case of a single point particle, the path integral corresponding to the AF (1.16) is formally written as (we use the normal units with  $\hbar = 1$ ; also,  $i \equiv \sqrt{-1}$ )

$$\int \mathcal{D}[x] e^{iS([x], t_0, t_1)} = \int \mathcal{D}[x] \exp \left[ i \int_{t_0}^{t_1} dt \left( \frac{1}{2} m \dot{x}^i \dot{x}^i - V(x^i) \right) \right], \quad (1.19)$$

where

$$\int \mathcal{D}[x] \approx \int \prod_{k=1}^N \frac{dx_k^i}{\sqrt{2\pi k dt}}$$

is the *Lebesgue integration over all possible complex-valued trajectories*  $x^i = x^i(t)$  between  $t_0$  and  $t_1$ , performed by splitting the time interval  $[t_0, t_1]$  into  $N$  subintervals (see Appendix for details). Integral (1.19) represents the *transition amplitude*  $\langle X_1^i | X_0^i \rangle$  for the particle ‘jumping’ from point  $x^i(t_0)$  to point  $x^i(t_1)$ , where  $X^i = X^i(t)$  is the *Hermitian position operator* corresponding to the coordinate  $x^i$  such that the boundary condition for  $x^i$  at point  $t_0$  is  $X_0^i$  and  $x^i$  at point  $t_1$  is  $X_1^i$ . The transition amplitude is then given by

$$\langle X_1^i | X_0^i \rangle = \int \mathcal{D}[x] e^{iS([x], t_0, t_1)}.$$

In case of external driving forces,  $F_i = F_i(t)$ , the AF (1.16) is expanded into

$$S([x], t_0, t_1) = \int_{t_0}^{t_1} dt \left( \frac{1}{2} m \dot{x}^i \dot{x}^i - V(x^i) + F_i(t) x^i(t) \right),$$

and the corresponding *forced transition amplitude* becomes (see, e.g., [Ram90])

$$\langle X_1^i | X_0^i \rangle_F = \int \mathcal{D}[x] \exp \left[ i \int_{t_0}^{t_1} dt \left( \frac{1}{2} m \dot{x}^i \dot{x}^i - V(x^i) + F_i(t) x^i(t) \right) \right].$$

For the derivation of the path integral, see Appendix. In Chapter 5 we will formulate the path-integral model for the neural control of human motion. In Chapter 6 we will use more general actions and path integrals to explore biophysics of electro-muscular stimulation.

### 1.1.4 Noether Theorem

Recall that the ‘surface term’  $G$  of the general action functional (AF)

$$S([x^i], t_0, t_1) = \int_{t_1}^{t_2} L(x^i, \dot{x}^i) dt, \quad (i = 1, \dots, N) \quad (1.20)$$

offers a connection between the *conservation laws* and the *invariants of the dynamical system*, governed by the celebrated *Noether theorem* (see [Ram90, AM78, Arn89, MR99]).

Noether’s theorem relates pairs of basic ideas of physics, one being the invariance of the form that a physical law takes with respect to any (generalized) transformation that preserves the coordinate system (both spatial and temporal aspects taken into consideration), and the other being a conservation law of a physical quantity. Informally, Noether’s theorem can be stated as: *There is a one-to-one correspondence between continuous symmetries of the laws of physics, and conservation laws in physics.* More precisely, yet still informal: *To every differentiable symmetry which is generated by local actions, there corresponds a conservation law, defining a conserved current, and vice versa.* The formal statement of the theorem derives an expression for the physical quantity that is conserved (and hence also defines it (actually, its current)), from the condition of invariance alone. For example: (i) Invariance of physical systems with respect to *translation* gives the law of *conservation of linear momentum* (when simply stated, it is just that the laws of physics don’t vary with location in space); (ii) Invariance with respect to *rotation* gives law of *conservation of angular momentum*; (iii) Invariance with respect to *time* gives the well known law of *conservation of energy*, etc.

To get some ‘feeling’ for the Noether’s theorem, recall that the *Lagrangian equations* corresponding to the action (1.20) read

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}^i} \right) = \frac{\partial L}{\partial x^i}.$$

These equations signify that if the expression on the r.h.s *is zero*,  $\frac{\partial L}{\partial x^i} = 0$ , meaning that  $L$  is symmetrical over the coordinates  $x^i = x^i(t)$ , then the *rate of change* of the expression in parentheses on the l.h.s *is also zero*,  $\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}^i} \right) = 0$ , and therefore, the  $N$  *generalized momenta*,  $p_i = \frac{\partial L}{\partial \dot{x}^i}$ , are *conserved quantities*.

Despite the fact that the classical Lagrangian equation,  $\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}^i} \right) = \frac{\partial L}{\partial x^i}$ , is essentially an explicit statement of this proposition, it seems not to have been discussed and formalized as a theorem until 1918, by Emmy Noether (1882–1935), so it is now called Noether’s Theorem. This theorem was praised by Einstein as a piece of “penetrating mathematical thinking”. It is now a standard workhorse in theoretical physics.

More precisely, let us assume that our variation of the AF vanishes under certain circumstances:  $\delta S[x] = 0$ . We then say that the action, which remains

unchanged, is invariant under that particular variation of the path. Recall that the principle of stationary action then states:

$$\delta S[x] = 0 = G_2 - G_1,$$

i.e.,  $G$  has the same value, independent of the initial and final configurations.

In particular, let us assume that the AF (in Hamiltonian formulation) is invariant for a variation around the actual path for which it holds that

$$\delta x^i(t_{1,2}) = 0, \quad \frac{d}{dt}(\delta t) = 0, \quad \text{therefore} \quad \delta t = \text{const} = \varepsilon.$$

Then it follows from the invariance of the AF under infinitesimal constant time translation:

$$\delta S = 0 = G_2 - G_1 = -H(t_2)\delta t_2 + H(t_1)\delta t_1 = -(H_2 - H_1)\varepsilon,$$

the conservation of energy:

$$H(t_2) = H(t_1), \quad \text{meaning} \quad \dot{H} = 0.$$

Similarly, the conservation law for linear momentum follows if we assume that the AF is invariant under constant space translation and the change of the terminal times vanishes:

$$\begin{aligned} \delta x^i &= \delta \varepsilon_i = \text{const}, & \delta t(t_{1,2}) &= 0, \\ \delta S = 0 &= G_2 - G_1 = (p_i \delta x^i)_2 - (p_i \delta x^i)_1 = (p_{i_2} - p_{i_1})\delta \varepsilon_i, \\ \text{or} \quad p_i(t_2) &= p_i(t_1), & \text{meaning} \quad \dot{p}_i &= 0. \end{aligned}$$

Now let

$$H = \frac{p_i^2}{2m} + V(r),$$

i.e., potential may only depend on the distance  $r = \sqrt{(x^i)^2}$ . Then no space direction is distinguished, and with respect to rigid rotations  $\delta \omega_i = \text{const}$  and

$$\delta t(t_{1,2}) = 0, \quad \delta x^i = \varepsilon_k^{ij} \delta \omega_j x^k,$$

it can be proved that

$$\delta S = \delta \int_{t_1}^{t_2} dt \left[ p_i \dot{x}^i - \frac{p_i^2}{2m} - V(\sqrt{x^i}) \right] = 0.$$

Because

$$\begin{aligned} \delta S = 0 &= G_2 - G_1 = (p_i \delta x^i)_2 - (p_i \delta x^i)_1 \\ &= (p_i \varepsilon_k^{ij} \delta \omega_j x^k)_2 - (p_i \varepsilon_k^{ij} \delta \omega_j x^k)_1 \\ &= \delta \omega_i \{ [(r \times p)_i]_2 - [(r \times p)_i]_1 \} \end{aligned}$$

this implies the conservation for angular momentum:

$$L(t_2) = L(t_1), \quad \text{meaning} \quad \dot{L} = 0.$$

Conversely, the conservation for angular momentum corresponds to the invariance,  $\delta S = 0$ , under rigid rotation in space. The generalization of this statement is this: if a conservation law exists, then the AF is stationary with respect to the infinitesimal transformation of a corresponding variable. The converse of this statement is also true: If the AF is invariant with respect to an infinitesimal transformation,  $\delta S = 0$ , then the corresponding conservation is valid.

Emmy Noether was primarily an algebraist, but when she came to Göttingen in 1915, she was asked by David Hilbert for help in trying to understand the status of *energy conservation* in general relativity. As we have seen, the conservation of energy in classical physics is closely related to the time-invariance of physical laws, but in general relativity there is not necessarily a global time coordinate, so the classical invariance cannot be invoked to establish the conservation of energy. Nevertheless, if spacetime in the region of interest is regarded as asymptotically flat, it is possible to define a conserved energy. This important aspect of general relativity was greatly clarified by Noether's Theorem in 1918. Subsequently the theorem has found important applications in many branches of physics. For example, in quantum mechanics the phase of the wave function can be incremented without affecting any observables, and this *gauge symmetry* corresponds to the *conservation of electric charge*. Moreover, Noether's approach of identifying symmetries with conserved quantities forms the basis of the Standard Model of particle physics.

A proper mathematical exposition of the Noether's theorem is founded on the theory of Sophus Lie: groups, algebras, symmetries and general invariance (see section 2.4.1 below).

### 1.1.5 Symplectic Mechanics

In general mechanics on smooth manifolds, one first defines the configuration manifold  $Q$  of the system in consideration, and then proceeds either using Lagrangian formalism on the tangent bundle  $TQ$  or Hamiltonian formalism on the cotangent bundle  $T^*Q$ . In case of Hamiltonian formalism,  $T^*Q$  is called the (momentum) phase space, admitting a natural symplectic structure that is usually defined as follows (see [AMR88, Arn89, Put93, MR99]). Let  $Q$  be a smooth  $n$ -dimensional manifold and pick local coordinates  $\{dq^1, \dots, dq^n\}$ . Then  $\{dq^1, \dots, dq^n\}$  defines a basis of the cotangent space  $T_q^*Q$ , and by writing the canonical one-form  $\theta \in T_q^*Q$  as

$$\theta = p_i dq^i, \tag{1.21}$$

we get local coordinates  $\{q^1, \dots, q^n, p_1, \dots, p_n\}$  on  $T^*Q$  (see Figure 1.2 for the basis of Euclidean  $\mathbb{R}^3$ -space). Now, define the canonical symplectic two-form  $\omega$  on  $T^*Q$  by

$$\omega = d\theta = dp_i \wedge dq^i. \quad (1.22)$$

This two-form  $\omega$  is obviously independent of the choice of coordinates  $\{q^1, \dots, q^n \in Q\}$  and independent of the base point  $\{q^1, \dots, q^n, p_1, \dots, p_n\} \in T_q^*Q$ ; therefore, it is locally constant, and so  $d\omega = 0$  (see Figure 1.3 for the fundamental two-form in Euclidean  $\mathbb{R}^3$ -space).

Let  $(M, \omega)$  be a symplectic manifold and  $H \in C^\infty(M, \mathbb{R})$  a smooth real valued function on  $M$ . Hamiltonian vector field  $X_H$ , corresponding to the total energy function  $H$ , is the smooth vector field on  $M$ , determined by the condition

$$i_{X_H}\omega + dH = 0,$$

where  $i_{X_H}$  denotes the contraction (or inner product) of the vector field  $X_H$  and the symplectic form  $\omega$ . A triple  $(M, \omega, H)$  is called a Hamiltonian mechanical system. Nondegeneracy of  $\omega$  guarantees that  $X_H$  exists (see [Put93]).

Let  $\{q^1, \dots, q^n, p_1, \dots, p_n\}$  be canonical coordinates on  $M$ , i.e., relation (1.22) is valid. Then in these coordinates Hamiltonian vector field  $X_H$  is defined by

$$X_H = \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q^i} - \frac{\partial H}{\partial q^i} \frac{\partial}{\partial p_i}. \quad (1.23)$$

As a consequence,  $((q^i(t)), (p_i(t)))$  is an integral curve of  $X_H$  (for  $i = 1, \dots, n$ ) iff Hamilton's equations (3.10) hold.

In this way, the Newton's law of motion (1.1), for  $n$  conservative particles, has the following symplectic formulation on  $\mathbb{R}^{3n}$  (see [AMR88, Put93]):

$$M = T^*\mathbb{R}^{3n} \simeq \mathbb{R}^{6n}, \quad \omega = dp_i \wedge dq^i, \quad H = \sum_{i=1}^{3n} \frac{p_i^2}{2m_i} + U.$$

The Hamiltonian vector field (1.23) is

$$X_H = \frac{p_i}{m_i} \frac{\partial}{\partial q^i} - \frac{\partial U}{\partial q^i} \frac{\partial}{\partial p_i},$$

and the Hamilton's equations (3.10) become

$$\dot{q}^i = \frac{p_i}{m_i}, \quad \dot{p}_i = -\frac{\partial U}{\partial q^i}, \quad (i = 1, \dots, n).$$

### 1.1.6 Modern Rotational Biomechanics

Despite the elegance of translational symplectic geometry/mechanics outlined above, the most suitable formalism to deal with the full complexity of modern biomechanics of human motion and its robotics application, is *rotational symplectic geometry/mechanics*. Namely, as human joints are by nature rotational, combined muscular force vectors are transformed by joint geometry into *driving torque one-forms*,  $T_i(t, q^i, p_i)$  (see Figure 1.4).

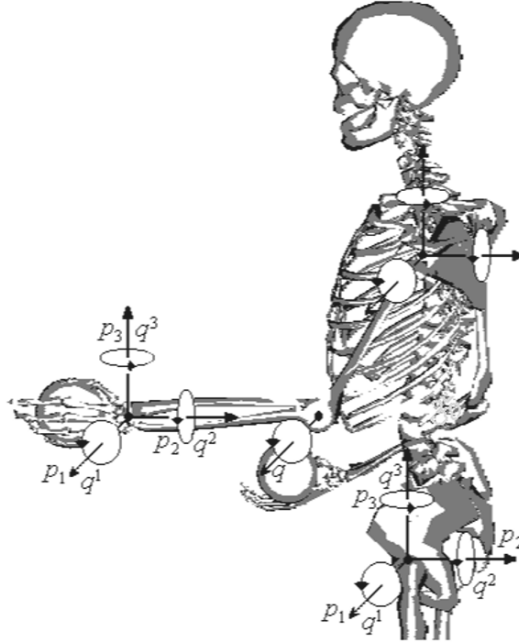
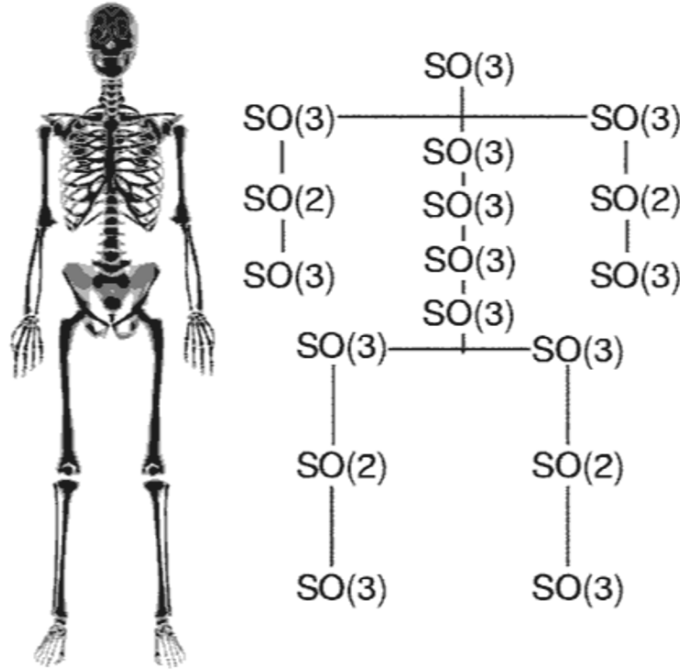


Fig. 1.4. Rotational synovial joints in human body.

Joint rotations are in modern biomechanics described in the language of constrained rotational Lie groups,  $SO(2)$  and  $SO(3)$ , where constrained rotation is for each human joint separately defined in anatomical terms, so that the rotational joint amplitude is always less than the full circle. Nevertheless, the formalism of rotational Lie groups still works, just bearing in mind the imposed anatomical joint restrictions (see [Iva04, ILI95]).

All active joint-angles  $q^i$  ( $i = 1, \dots, N \equiv \text{DOF}$ ), constitute a smooth configuration manifold  $Q^N$ , defined as a direct product of constrained rotational joint Lie groups  $SO(3) \times SO(2) \times SO(3) \times \dots$  for all rotational joints considered (see Figure 1.5). Uniaxial, ‘hinge’ joints represent constrained, classical, rotational groups  $SO(2)^i$ , parameterized by constrained angles  $q^i \equiv q^i \in [q_{\min}^i, q_{\max}^i]$ . Their associated velocities are defined by the corresponding Lie algebras  $\mathfrak{so}(2)^i$ . Three-axial, ‘ball-and-socket’ joints represent constrained rotational groups  $SO(3)^i$ , usually parameterized by constrained Euler angles  $q_{1,2,3}^i = \{\phi, \psi, \theta\}^i$ . Their associated velocities are defined by the corresponding Lie algebras  $\mathfrak{so}(3)^i$ .

We refer to the tangent bundle  $TQ^N$  of the configuration manifold  $Q^N$  as the *velocity phase-space* manifold, and to its cotangent bundle  $T^*Q^N$  as the *momentum phase-space* manifold. In this way, rotational biomechanics uses the full power of symplectic mechanics outlined above.



**Fig. 1.5.** Basic structure of the biomechanical configuration manifold  $Q^n$  composed as a direct product of constrained rotational Lie groups of human ‘ball-end-socket joints’.

**Passive Joint Dynamics**

Recall that all biological systems are *dissipative structures*, emphasizing *irreversible processes* inefficient energetically, but highly efficient in terms of information and control (see [NP77]). In case of biomechanics, we have the passive joint damping contribution to *driving torque one-forms*,  $T_i(t, q^i, p_i)$ , which has the basic stabilizing effect to the complex human movement. This effect can be described by  $(q, p)$ -quadratic form of the *Rayleigh – Van der Pol’s dissipation function* (see [BR78])

$$R = \frac{1}{2} \sum_{i=1}^9 p_i^2 [a_i + b_i(q^i)^2], \tag{1.24}$$

where  $a_i$  and  $b_i$  denote dissipation parameters. Its partial derivatives  $\partial R/\partial p$  give rise to viscous forces in the joints which are linear in  $p_i$  and quadratic in  $q^i$ . It is based on the unforced Van der Pol’s oscillator

$$\ddot{x} - (a + b x^2) \dot{x} + x = 0,$$

where the damping force  $F^{dmp}(\dot{x}) = -\partial R/\partial \dot{x}$  is given by the Rayleigh's dissipation function  $R = \frac{1}{2}(a + b x^2) \dot{x}^2$  – with the velocity term  $\dot{x}$  replaced by our momentum term  $p^2$  (see [Iva04, ILI95]).

Using (1.24) we get the *dissipative Hamiltonian biomechanics*

$$\begin{aligned} \dot{q}^i &= \frac{\partial H(q, p)}{\partial p_i} + \frac{\partial R(q, p)}{\partial p_i}, \\ \dot{p}_i &= -\frac{\partial H(q, p)}{\partial q^i} + \frac{\partial R(q, p)}{\partial q^i}, \quad (i = 1, \dots, N), \end{aligned} \quad (1.25)$$

which reduces to the gradient system in case  $H = 0$  (as well as to the conservative system in case  $R = 0$ ).

### 1.1.7 Muscular Dynamics and Control

#### Muscular Dynamics

Muscular dynamics describes the internal *excitation* and *contraction* dynamics [Hat78, Iva04] of *equivalent muscular actuators*, anatomically represented by resulting action of *antagonistic muscle-pairs* for each uniaxial joint. We attempt herein to describe the equivalent muscular dynamics in the simplest possible way (for example, Hatze used 51 nonlinear differential equations of the first order to derive his, arguably most elaborate, myocybernetic model [Hat78]), and yet to include the main excitation and contraction relations.

The active muscular-control contribution to the torque one-forms,  $T_i = T_i(t, q^i, p_i)$ , should describe the internal *excitation* and *contraction* dynamics [IS01, Iva04, Iva91, IP01a]) of *equivalent muscular actuators*, anatomically represented by resulting action of *antagonistic muscle-pairs* per each active degree-of-freedom.

(a) *Excitation dynamics* can be described by impulse *torque-time* relation

$$\begin{aligned} T_i^{imp} &= T_i^0(1 - e^{-t/\tau_i}) && \text{if stimulation} > 0 \\ T_i^{imp} &= T_i^0 e^{-t/\tau_i} && \text{if stimulation} = 0, \end{aligned}$$

where  $F_i^0$  denote the maximal isometric muscular torques applied at  $i$ -th joint, while  $\tau_i$  denote the time characteristics of particular muscular actuators. This is a rotational-joint form of the solution of the Wilkie's *muscular active-state element equation* [Wil56]

$$\dot{x} + \beta x = \beta S A, \quad x(0) = 0, \quad 0 < S < 1,$$

where  $x = x(t)$  represents the active state of the muscle,  $\beta$  denotes the element gain,  $A$  corresponds to the maximum tension the element can develop, and  $S = S(r)$  is the 'desired' active state as a function of motor unit stimulus rate  $r$ .

(b) *Contraction dynamics* has classically been described by the Hill's *hyperbolic force-velocity* relation [Hil38], which we propose here in the rotational  $(q, p)$ -form

$$T_i^{Hill} = \frac{(T_i^0 b_i - a_i p_i)}{(p_i - b_i)},$$

where  $a_i$  (having dimension of torque) and  $b_i$  (having dimension of momentum) denote the *rotational Hill's parameters* (see [IS01, Iva04]), corresponding to the energy dissipated during the contraction and the phosphagenic energy conversion rate, respectively.

Therefore, we can describe the excitation/contraction dynamics for the  $i$ th equivalent muscle-joint actuator, i.e., antagonistic muscle pair, by the simple impulse-hyperbolic product-relation

$$T_i(t, q, p) = T_i^{imp} \times T_i^{Hill}, \quad (i = 1, \dots, N). \quad (1.26)$$

Using (1.26) we get the *forced dissipative Hamiltonian biomechanics*, in the form

$$\begin{aligned} \dot{q}^i &= \frac{\partial H(q, p)}{\partial p_i} + \frac{\partial R(q, p)}{\partial p_i}, & (i = 1, \dots, N), \\ \dot{p}_i &= T_i(t, q, p) - \frac{\partial H(q, p)}{\partial q^i} + \frac{\partial R(q, p)}{\partial q^i}. \end{aligned} \quad (1.27)$$

### Muscular Control

We introduce the *control Hamiltonian function*  $H_c : T^*M^N \rightarrow \mathbb{R}$ , in local canonical coordinates on  $T^*M^N$  defined by [NS90]

$$H_c(q, p, u) = H_0(q, p) - q^i u_i, \quad (i = 1, \dots, N), \quad (1.28)$$

where  $u_i = u_i(t, q, p)$  are feedback-control one-forms, representing the corrections to the torque one-forms  $T_i(t, q, p)$ .

Using (1.28), the affine Hamiltonian system can be defined as

$$\begin{aligned} \dot{q}^i &= \frac{\partial H_c(q, p, u)}{\partial p_i} + \frac{\partial R(q, p)}{\partial p_i}, & (i = 1, \dots, N) \\ \dot{p}_i &= T_i(t, q, p) - \frac{\partial H_c(q, p, u)}{\partial q^i} + \frac{\partial R(q, p)}{\partial q^i}, \\ o^i &= -\frac{\partial H_c(q, p, u)}{\partial u_i}, & q^i(0) = q_0^i, \quad p_i(0) = p_i^0, \end{aligned} \quad (1.29)$$

where  $o^i = o^i(t)$  represent the natural outputs which can be different from commonly used joint angles.

If nominal reference outputs  $o_R^i = o_R^i(t)$  are known, the simple PD *stiffness-servo* [Whi87] could be formulated, via *error function*  $e(t) = o^j - o_R^j$ , in covariant form

$$u_i = K_o \delta_{ij} (o^j - o_R^j) + K_{\dot{o}} \delta_{ij} (\dot{o}^j - \dot{o}_R^j), \quad (1.30)$$

where  $K$ s are the control-gains and  $\delta_{ij}$  is the Kronecker tensor.

If natural outputs  $o^i$  *actually are* the joint angles and nominal canonical trajectories ( $q_R^i = q_R^i(t)$ ,  $p_i^R = p_i^R(t)$ ) are known, then the stiffness-servo (1.30) could be formulated in canonical form as

$$u_i = K_q \delta_{ij} (q^i - q_R^i) + K_p (p_i - p_i^R). \quad (1.31)$$

In this way formulated affine Hamiltonian control system (1.29–1.31) resembles the physiological *autogenetic motor servo* [Hou79], acting on the spinal-reflex level of the human locomotor control in the following way. Voluntary contraction force  $\Phi$  of human skeletal muscle is reflexly excited (positive feedback  $+\Phi^{-1}$ ) by responses of its *spindle receptors* to stretch and is reflexly inhibited (negative feedback  $-\Phi^{-1}$ ) by responses of its *Golgi tendon organs* to contraction. Stretch and unloading reflexes are mediated by combined actions of several autogenetic neural pathways, forming the so-called ‘motor-servo’. Term ‘*autogenetic*’ means that the stimulus excites receptors located in the same muscle that is the target of the reflex response. The most important of these muscle receptors are the primary and secondary endings in muscle-spindles, sensitive to length change – positive length feedback  $+\Phi^{-1}$ , and the Golgi tendon organs, sensitive to contractile force – negative force feedback  $-\Phi^{-1}$ .

The gain  $G$  of the length feedback  $+\Phi^{-1}$  can be expressed as the *positional stiffness* (the ratio  $G \approx S = d\Phi/dx$  of the force- $\Phi$  change to the length- $x$  change) of the muscle system. The greater the stiffness  $S$ , the less will the muscle be disturbed by a change in load and the more reliable will be the performance of the muscle system in executing controlled changes in length  $+\Phi^{-1}$ .

The autogenetic circuits  $+\Phi^{-1}$  and  $-\Phi^{-1}$  appear to function as *servoregulatory loops* that convey continuously graded amounts of excitation and inhibition to the large (*alpha*) skeletomotor neurons. Small (*gamma*) fusimotor neurons innervate the contractile poles of muscle spindles and function to modulate spindle-receptor discharge (for further details, see section 5.4 below).

## 1.2 Global Functorial Language of Human-Like Biomechanics

In modern mathematical sciences whenever one defines a new class of mathematical objects, one proceeds almost in the next breath to say what kinds of maps between objects will be considered [Swi75]. A general framework for dealing with situations where we have some *objects* and *maps between objects*, like sets and functions, vector spaces and linear operators, points in a

space and paths between points, etc. – provides the modern metalanguage of categories and functors. Categories are mathematical universes and functors are ‘projectors’ from one universe onto another. For this reason, in this book we extensively use this language, mainly following its founder, S. MacLane [MacL71].

### 1.2.1 Preliminaries from Calculus, Algebra and Topology

Before defining categories, functors and their natural transformations, we give the necessary preliminaries from calculus, algebra and point–set topology.

#### Notes From Calculus

##### *Functions*

Recall that a *function*  $f$  is a *rule* that assigns to each element  $x$  in a set  $A$  exactly one element, called  $f(x)$ , in a set  $B$ . A function could be thought of as a *machine*  $[[f]]$  with  $x$ –input (the *domain* of  $f$  is the set of all possible inputs) and  $f(x)$ –output (the *range* of  $f$  is the set of all possible outputs) [Stu99]

$$x \rightarrow [[f]] \rightarrow f(x)$$

There are four possible ways to represent a function: (i) verbally (by a description in words); (ii) numerically (by a table of values); (iii) visually (by a graph); and (iv) algebraically (by an explicit formula). The most common method for visualizing a function is its graph. If  $f$  is a function with domain  $A$ , then its *graph* is the set of ordered input–output pairs

$$\{(x, f(x)) : x \in A\}.$$

##### *Algebra of Functions*

Let  $f$  and  $g$  be functions with domains  $A$  and  $B$ . Then the functions  $f + g$ ,  $f - g$ ,  $fg$ , and  $f/g$  are defined as follows [Stu99]

$$\begin{aligned} (f + g)(x) &= f(x) + g(x) & \text{domain} &= A \cap B, \\ (f - g)(x) &= f(x) - g(x) & \text{domain} &= A \cap B, \\ (fg)(x) &= f(x)g(x) & \text{domain} &= A \cap B, \\ \left(\frac{f}{g}\right)(x) &= \frac{f(x)}{g(x)} & \text{domain} &= \{x \in A \cap B : g(x) \neq 0\}. \end{aligned}$$

*Compositions of Functions*

Given two functions  $f$  and  $g$ , the composite function  $f \circ g$  (also called the *composition* of  $f$  and  $g$ ) is defined by

$$(f \circ g)(x) = f(g(x)).$$

The  $(f \circ g)$ -machine is composed of the  $g$ -machine (first) and then the  $f$ -machine [Stu99],

$$x \rightarrow [[g]] \rightarrow g(x) \rightarrow [[f]] \rightarrow f(g(x))$$

For example, suppose that  $y = f(u) = \sqrt{u}$  and  $u = g(x) = x^2 + 1$ . Since  $y$  is a function of  $u$  and  $u$  is a function of  $x$ , it follows that  $y$  is ultimately a function of  $x$ . We compute this by substitution

$$y = f(u) = f \circ g = f(g(x)) = f(x^2 + 1) = \sqrt{x^2 + 1}.$$

*The Chain Rule*

If  $f$  and  $g$  are both differentiable and  $h = f \circ g$  is the composite function defined by  $h(x) = f(g(x))$ , then  $h$  is differentiable and  $h'$  is given by the product [Stu99]

$$h'(x) = f'(g(x)) g'(x).$$

In Leibniz notation, if  $y = f(u)$  and  $u = g(x)$  are both differentiable functions, then

$$\frac{dy}{dx} = \frac{dy}{du} \frac{du}{dx}.$$

The reason for the name *chain rule* becomes clear if we add another link to the chain. Suppose that we have one more differentiable function  $x = h(t)$ . Then, to compute the derivative of  $y$  with respect to  $t$ , we use the chain rule twice,

$$\frac{dy}{dt} = \frac{dy}{du} \frac{du}{dx} \frac{dx}{dt}.$$

*Integration and Change of Variables*

Based on the chain rule, under the certain hypotheses (such as a one-to-one  $C^0$  map  $T$  with a nonzero *Jacobian*  $\left| \frac{\partial(x, \dots)}{\partial(u, \dots)} \right|$  that maps a region  $S$  onto a region  $R$ , see [Stu99]) we have the following substitution formulas:

1. for a single integral,

$$\int_R f(x) dx = \int_S f(x(u)) \frac{\partial x}{\partial u} du,$$

2. for a double integral,

$$\iint_R f(x, y) dA = \iint_S f(x(u, v), y(u, v)) \left| \frac{\partial(x, y)}{\partial(u, v)} \right| dudv,$$

3. for a triple integral,

$$\iiint_R f(x, y, z) dV = \iiint_S f(x(u, v, w), y(u, v, w), z(u, v, w)) \left| \frac{\partial(x, y, z)}{\partial(u, v, w)} \right| dudvdw,$$

4. similarly for  $n$ -tuple integrals.

### Notes from Set Theory

Given a function  $f : A \rightarrow B$ , the set  $A$  is called the *domain* of  $f$ , and denoted  $\text{Dom } f$ . The set  $B$  is called the *codomain* of  $f$ , and denoted  $\text{Cod } f$ . The codomain is not to be confused with the *range* of  $f(A)$ , which is in general only a subset of  $B$ .

A function  $f : X \rightarrow Y$  is called *injective* or *one-to-one* or an *injection* if for every  $y$  in the codomain  $Y$  there is at most one  $x$  in the domain  $X$  with  $f(x) = y$ . Put another way, given  $x$  and  $x'$  in  $X$ , if  $f(x) = f(x')$ , then it follows that  $x = x'$ . A function  $f : X \rightarrow Y$  is called *surjective* or *onto* or a *surjection* if for every  $y$  in the codomain  $\text{Cod } f$  there is at least one  $x$  in the domain  $X$  with  $f(x) = y$ . Put another way, the *range*  $f(X)$  is equal to the codomain  $Y$ . A function is *bijective* iff it is both injective and surjective. Injective functions are called the *monomorphisms*, and surjective functions are called the *epimorphisms* in the *category of sets* (see below).

A *relation* is any subset of a *Cartesian product* (see below). By definition, an *equivalence relation*  $\alpha$  on a set  $X$  is a relation which is *reflexive*, *symmetrical* and *transitive*, i.e., relation that satisfies the following three conditions:

1. *Reflexivity*: each element  $x \in X$  is equivalent to itself, i.e.,  $x\alpha x$ ,
2. *Symmetry*: for any two elements  $x, x' \in X$ ,  $x\alpha x'$  implies  $x'\alpha x$ , and
3. *Transitivity*:  $a \leq b$  and  $b \leq c$  implies  $a \leq c$ .

Similarly, a relation  $\leq$  defines a *partial order* on a set  $S$  if it has the following properties:

1. *Reflexivity*:  $a \leq a$  for all  $a \in S$ ,
2. *Antisymmetry*:  $a \leq b$  and  $b \leq a$  implies  $a = b$ , and
3. *Transitivity*:  $a \leq b$  and  $b \leq c$  implies  $a \leq c$ .

A *partially ordered set* (or *poset*) is a set taken together with a partial order on it. Formally, a partially ordered set is defined as an ordered pair  $P = (X, \leq)$ , where  $X$  is called the *ground set* of  $P$  and  $\leq$  is the partial order of  $P$ .

### Notes from General Topology

*Topology* is a kind of *abstraction* of Euclidean geometry, and also a natural framework for the study of *continuity*. Euclidean geometry is abstracted by regarding triangles, circles, and squares as being the same basic object. Continuity enters because in saying this one has in mind a *continuous deformation* of a triangle into a square or a circle, or any arbitrary shape. On the other hand, a disk with a hole in the center is topologically different from a circle or a square because one cannot create or destroy holes by continuous deformations. Thus using topological methods one does not expect to be able to identify a geometric figure as being a triangle or a square. However, one does expect to be able to detect the presence of gross features such as holes or the fact that the figure is made up of two disjoint pieces etc. In this way topology produces theorems that are usually qualitative in nature – they may assert, for example, the existence or non-existence of an object. They will not in general, provide the means for its construction [Nas83].

Let  $X$  be any set and  $Y = \{X_\alpha\}$  denote a collection, finite or infinite of subsets of  $X$ . Then  $X$  and  $Y$  form a *topological space* provided the  $X_\alpha$  and  $Y$  satisfy:

1. Any finite or infinite subcollection  $\{Z_\alpha\} \subset X_\alpha$  has the property that  $\cup Z_\alpha \in Y$ , and
2. Any *finite subcollection*  $\{Z_{\alpha_1}, \dots, Z_{\alpha_n}\} \subset X_\alpha$  has the property that  $\cap Z_{\alpha_i} \in Y$ .

The set  $X$  is then called a topological space and the  $X_\alpha$  are called *open sets*. The choice of  $Y$  satisfying (2) is said to give a topology to  $X$ .

Now, given two topological spaces  $X$  and  $Y$ , a *function* (or, a *map*)  $f : X \rightarrow Y$  is *continuous* if the inverse image of an open set in  $Y$  is an open set in  $X$ .

The main general idea in topology is to study spaces which can be continuously deformed into one another, namely the idea of *homeomorphism*. If we have two topological spaces  $X$  and  $Y$ , then a map  $f : X \rightarrow Y$  is called a homeomorphism iff

1.  $f$  is continuous, and
2. There exists an inverse of  $f$ , denoted  $f^{-1}$ , which is also continuous.

Definition (2) implies that if  $f$  is a homeomorphism then so is  $f^{-1}$ . Homeomorphism is the main topological example of *reflexive*, *symmetrical* and *transitive relation*, i.e., *equivalence relation*. Homeomorphism divides all topological spaces up into *equivalence classes*. In other words, a pair of topological spaces,  $X$  and  $Y$ , belong to the same equivalence class if they are homeomorphic.

The second example of topological equivalence relation is *homotopy*. While homeomorphism generates equivalence classes whose members are topological spaces, homotopy generates equivalence classes whose members are continuous maps (or,  $C^0$ -maps). Consider two continuous maps  $f, g : X \rightarrow Y$  between

topological spaces  $X$  and  $Y$ . Then the map  $f$  is said to be *homotopic* to the map  $g$  if  $f$  can be continuously deformed into  $g$  (see below for the precise definition of homotopy). Homotopy is an equivalence relation which divides the space of continuous maps between two topological spaces into equivalence classes [Nas83].

Another important notions in topology are *covering*, *compactness* and *connectedness*. Given a family of sets  $\{X_\alpha\} = X$  say, then  $X$  is a *cover* of another set  $Y$  if  $\cup X_\alpha$  contains  $Y$ . If all the  $X_\alpha$  happen to be open sets the cover is called an *open cover*. Now consider the set  $Y$  and all its possible open coverings. The set  $Y$  is *compact* if for every open covering  $\{X_\alpha\}$  with  $\cup X_\alpha \supset Y$  there always exists a finite subcovering  $\{X_1, \dots, X_n\}$  of  $Y$  with  $X_1 \cup \dots \cup X_n \supset Y$ .<sup>5</sup> Again, we define a set  $Z$  to be *connected* if it cannot be written as  $Z = Z_1 \cup Z_2$ , where  $Z_1$  and  $Z_2$  are both open and  $Z_1 \cap Z_2$  is an empty set.

Let  $A_1, A_2, \dots, A_n$  be closed subspaces of a topological space  $X$  such that  $X = \cup_{i=1}^n A_i$ . Suppose  $f_i : A_i \rightarrow Y$  is a function,  $1 \leq i \leq n$ , iff

$$f_i|_{A_i \cap A_j} = f_j|_{A_i \cap A_j}, 1 \leq i, j \leq n. \quad (1.32)$$

In this case  $f$  is continuous iff each  $f_i$  is. Using this procedure we can define a  $C^0$ -function  $f : X \rightarrow Y$  by cutting up the space  $X$  into closed subsets  $A_i$  and defining  $f$  on each  $A_i$  separately in such a way that  $f|_{A_i}$  is obviously continuous; we then have only to check that the different definitions agree on the *overlaps*  $A_i \cap A_j$ .

The *universal property of the Cartesian product*: let  $p_X : X \times Y \rightarrow X$ , and  $p_Y : X \times Y \rightarrow Y$  be the *projections* onto the first and second factors, respectively. Given any pair of functions  $f : Z \rightarrow X$  and  $g : Z \rightarrow Y$  there is a unique function  $h : Z \rightarrow X \times Y$  such that  $p_X \circ h = f$ , and  $p_Y \circ h = g$ . Function  $h$  is continuous iff both  $f$  and  $g$  are. This property characterizes  $X/\alpha$  up to homeomorphism. In particular, to check that a given function  $h : Z \rightarrow X$  is continuous it will suffice to check that  $p_X \circ h$  and  $p_Y \circ h$  are continuous.

The *universal property of the quotient*: let  $\alpha$  be an equivalence relation on a topological space  $X$ , let  $X/\alpha$  denote the *space of equivalence classes* and  $p_\alpha : X \rightarrow X/\alpha$  the *natural projection*. Given a function  $f : X \rightarrow Y$ , there is a function  $f' : X/\alpha \rightarrow Y$  with  $f' \circ p_\alpha = f$  iff  $x\alpha x'$  implies  $f(x) = f(x')$ , for all  $x \in X$ . In this case  $f'$  is continuous iff  $f$  is. This property characterizes  $X/\alpha$  up to homeomorphism.

Now we return to the fundamental notion of homotopy. Let  $I$  be a compact unit interval  $I = [0, 1]$ . A *homotopy* from  $X$  to  $Y$  is a continuous function

<sup>5</sup> The notion of compactness is fundamental for biomechanical control. Namely, the basic (kinematic) unit of the biomechanical manifold is the special Euclidean group  $SE(3)$ . This group is non-compact, which means that it does not admit a natural metric generated by the segment's kinetic energy, and therefore there is not a natural control. However, its two subgroups, the group of rotations  $SE(3)$  and the group of translations  $\mathbb{R}^3$  are both compact, admitting the natural quadratic metric forms given by the kinetic energy. This implies the existence of (muscular-like) optimal controls in the sense of geodesics (see Chapter 2).

$F : X \times I \rightarrow Y$ . For each  $t \in I$  one has  $F_t : X \rightarrow Y$  defined by  $F_t(x) = F(x, t)$  for all  $x \in X$ . The functions  $F_t$  are called the ‘stages’ of the homotopy. If  $f, g : X \rightarrow Y$  are two continuous maps, we say  $f$  is homotopic to  $g$ , and write  $f \simeq g$ , if there is a homotopy  $F : X \times I \rightarrow Y$  such that  $F_0 = f$  and  $F_1 = g$ . In other words,  $f$  can be continuously deformed into  $g$  through the stages  $F_t$ . If  $A \subset X$  is a subspace, then  $F$  is a homotopy relative to  $A$  if  $F(a, t) = F(a, 0)$ , for all  $a \in A, t \in I$ .

The homotopy relation  $\simeq$  is an equivalence relation. To prove that we have  $f \simeq f$  is obvious; take  $F(x, t) = f(x)$ , for all  $x \in X, t \in I$ . If  $f \simeq g$  and  $F$  is a homotopy from  $f$  to  $g$ , then  $G : X \times I \rightarrow Y$  defined by  $G(x, t) = F(x, 1 - t)$ , is a homotopy from  $g$  to  $f$ , i.e.,  $g \simeq f$ . If  $f \simeq g$  with homotopy  $F$  and  $g \simeq h$  with homotopy  $G$ , then  $f \simeq h$  with homotopy  $H$  defined by

$$H(x, t) = \begin{cases} F(x, t), & 0 \leq t \leq 1/2 \\ G(x, 2t - 1), & 1/2 \leq t \leq 1 \end{cases}.$$

To show that  $H$  is continuous we use the relation (1.32).

In this way, the set of all  $C^0$ -functions  $f : X \rightarrow Y$  between two topological spaces  $X$  and  $Y$ , called the *function space* and denoted by  $Y^X$ , is partitioned into equivalence classes under the relation  $\simeq$ . The equivalence classes are called *homotopy classes*, the homotopy class of  $f$  is denoted by  $[f]$ , and the set of all homotopy classes is denoted by  $[X; Y]$ .

If  $\alpha$  is an equivalence relation on a topological space  $X$  and  $F : X \times I \rightarrow Y$  is a homotopy such that each stage  $F_t$  factors through  $X/\alpha$ , i.e.,  $x\alpha x'$  implies  $F_t(x) = F_t(x')$ , then  $F$  induces a homotopy  $F' : (X/\alpha) \times I \rightarrow Y$  such that  $F' \circ (p_\alpha \times 1) = F$ .

Homotopy theory has a range of applications of its own, outside topology and geometry, as for example in proving Cauchy theorem in complex variable theory, or in solving nonlinear equations of artificial neural networks.

A *pointed set*  $(S, s_0)$  is a set  $S$  together with a distinguished point  $s_0 \in S$ . Similarly, a *pointed topological space*  $(X, x_0)$  is a space  $X$  together with a distinguished point  $x_0 \in X$ . When we are concerned with pointed spaces  $(X, x_0), (Y, y_0)$ , etc., we always require that all functions  $f : X \rightarrow Y$  shell preserve base points, i.e.,  $f(x_0) = y_0$ , and that all homotopies  $F : X \times I \rightarrow Y$  be relative to the base point, i.e.,  $F(x_0, t) = y_0$ , for all  $t \in I$ . We denote the homotopy classes of base point-preserving functions by  $[X, x_0; Y, y_0]$  (where homotopies are relative to  $x_0$ ).  $[X, x_0; Y, y_0]$  is a pointed set with base point  $f_0$ , the constant function:  $f_0(x) = y_0$ , for all  $x \in X$ .

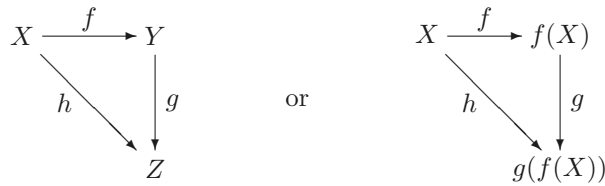
A *path*  $\gamma(t)$  from  $x_0$  to  $x_1$  in a topological space  $X$  is a continuous map  $\gamma : I \rightarrow X$  with  $\gamma(0) = x_0$  and  $\gamma(1) = x_1$ . Thus  $X^I$  is the space of all paths in  $X$  with the compact-open topology. We introduce a relation  $\sim$  on  $X$  by saying  $x_0 \sim x_1$  iff there is a path  $\gamma : I \rightarrow X$  from  $x_0$  to  $x_1$ .  $\sim$  is clearly an equivalence relation, and the set of equivalence classes is denoted by  $\pi_0(X)$ . The elements of  $\pi_0(X)$  are called the *path components*, or *0-components* of  $X$ . If  $\pi_0(X)$  contains just one element, then  $X$  is called *path connected*, or *0-connected*. A *closed path*, or *loop* in  $X$  at the point  $x_0$  is a path  $\gamma(t)$  for

which  $\gamma(0) = \gamma(1) = x_0$ . The *inverse loop*  $\gamma^{-1}(t)$  based at  $x_0 \in X$  is defined by  $\gamma^{-1}(t) = \gamma(1 - t)$ , for  $0 \leq t \leq 1$ . The *homotopy of loops* is the particular case of the above defined homotopy of continuous maps.

If  $(X, x_0)$  is a pointed space, then we may regard  $\pi_0(X)$  as a pointed set with the 0-component of  $x_0$  as a base point. We use the notation  $\pi_0(X, x_0)$  to denote  $p_0(X, x_0)$  thought of as a pointed set. If  $f : X \rightarrow Y$  is a map then  $f$  sends 0-components of  $X$  into 0-components of  $Y$  and hence defines a function  $\pi_0(f) : \pi_0(X) \rightarrow \pi_0(Y)$ . Similarly, a base point-preserving map  $f : (X, x_0) \rightarrow (Y, y_0)$  induces a map of pointed sets  $\pi_0(f) : \pi_0(X, x_0) \rightarrow \pi_0(Y, y_0)$ . In this way defined  $\pi_0$  represents a ‘functor’ from the ‘category’ of topological (point) spaces to the underlying category of (point) sets (see the next section).

### Commutative Diagrams

S. MacLane says that the category theory was born with an observation that many properties of mathematical systems can be unified and simplified by a presentation with *commutative diagrams of arrows* [MacL71]. Each arrow  $f : X \rightarrow Y$  represents a function (i.e., a map, transformation, operator); that is, a source (domain) set  $X$ , a target (codomain) set  $Y$ , and a rule  $x \mapsto f(x)$  which assigns to each element  $x \in X$  an element  $f(x) \in Y$ . A typical diagram of sets and functions is

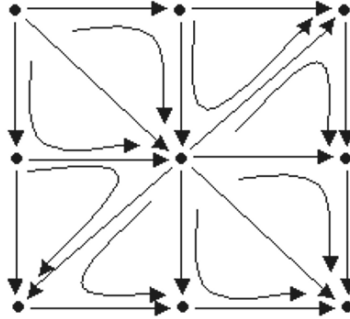


This diagram is *commutative* iff  $h = g \circ f$ , where  $g \circ f$  is the usual composite function  $g \circ f : X \rightarrow Z$ , defined by  $x \mapsto g(f(x))$ .

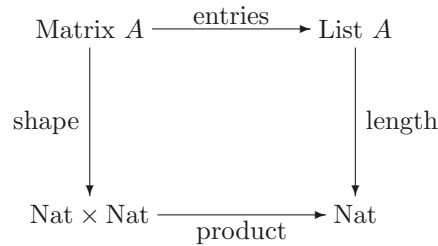
Similar commutative diagrams apply in other mathematical, physical and computing contexts; e.g., in the ‘category’ of all topological spaces, the letters  $X, Y$ , and  $Z$  represent topological spaces while  $f, g$ , and  $h$  stand for continuous maps. Again, in the category of all groups,  $X, Y$ , and  $Z$  stand for groups,  $f, g$ , and  $h$  for homomorphisms.

Less formally, composing maps is like following directed paths from one object to another (e.g., from set to set). In general, a diagram is commutative iff any two paths along arrows that start at the same point and finish at the same point yield the same ‘homomorphism’ via compositions along successive arrows. Commutativity of the whole diagram follows from commutativity of its triangular components (depicting a ‘commutative flow’, see Figure 1.6). Study of commutative diagrams is popularly called ‘diagram chasing’, and provides a powerful tool for mathematical thought.

As an example from linear algebra, consider an elementary diagrammatic description of matrices, using the following *pull-back diagram* [Bar93]:

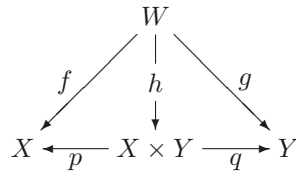


**Fig. 1.6.** A commutative flow (denoted by curved arrows) on a triangulated digraph. Commutativity of the whole diagram follows from commutativity of its triangular components.



asserts that a matrix is determined by its shape, given by a pair of natural numbers representing the number of rows and columns, and its data, given by the matrix entries listed in some specified order.

Many properties of mathematical constructions may be represented by *universal properties* of diagrams [MacL71]. Consider the *Cartesian product*  $X \times Y$  of two sets, consisting as usual of all ordered pairs  $\langle x, y \rangle$  of elements  $x \in X$  and  $y \in Y$ . The projections  $\langle x, y \rangle \mapsto x$ ,  $\langle x, y \rangle \mapsto y$  of the product on its ‘axes’  $X$  and  $Y$  are functions  $p : X \times Y \rightarrow X$ ,  $q : X \times Y \rightarrow Y$ . Any function  $h : W \rightarrow X \times Y$  from a third set  $W$  is uniquely determined by its composites  $p \circ h$  and  $q \circ h$ . Conversely, given  $W$  and two functions  $f$  and  $g$  as in the diagram below, there is a unique function  $h$  which makes the following diagram commute:



This property describes the Cartesian product  $X \times Y$  uniquely; the same diagram, read in the category of topological spaces or of groups, describes uniquely the Cartesian product of spaces or of the direct product of groups.

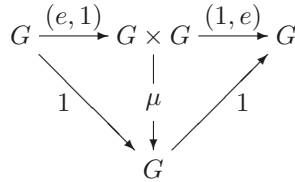
The construction ‘Cartesian product’ is technically called a ‘functor’ because it applies suitably both to the sets and to the functions between them; two functions  $k : X \rightarrow X'$  and  $l : Y \rightarrow Y'$  have a function  $k \times l$  as their Cartesian product:

$$k \times l : X \times Y \rightarrow X' \times Y', \quad \langle x, y \rangle \mapsto \langle kx, ly \rangle.$$

### Groups and Related Algebraic Structures

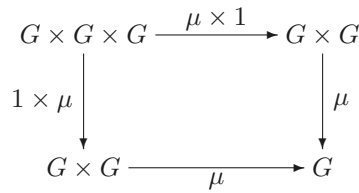
As already stated, the basic functional unit of lower biomechanics is the special Euclidean group  $SE(3)$  of rigid body motions. In general, a *group* is a pointed set  $(G, e)$  with a *multiplication*  $\mu : G \times G \rightarrow G$  and an *inverse*  $\nu : G \rightarrow G$  such that the following diagrams commute [Swi75]:

1.



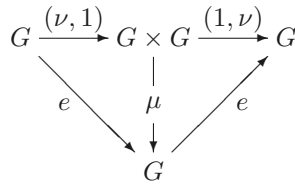
( $e$  is a two-sided identity)

2.



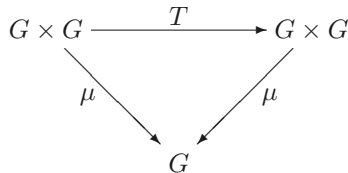
(associativity)

3.



(inverse).

Here  $e : G \rightarrow G$  is the constant map  $e(g) = e$  for all  $g \in G$ .  $(e, 1)$  means the map such that  $(e, 1)(g) = (e, g)$ , etc. A group  $G$  is called *commutative* or *Abelian group* if in addition the following diagram commutes



where  $T : G \times G \rightarrow G \times G$  is the switch map  $T(g_1, g_2) = (g_2, g_1)$ , for all  $(g_1, g_2) \in G \times G$ .

A group  $G$  *acts* (on the left) on a set  $A$  if there is a function  $\alpha : G \times A \rightarrow A$  such that the following diagrams commute [Swi75]:

1.

$$\begin{array}{ccc} A & \xrightarrow{(e, 1)} & G \times A \\ & \searrow 1 & \downarrow \alpha \\ & & A \end{array}$$

2.

$$\begin{array}{ccc} G \times G \times A & \xrightarrow{1 \times \alpha} & G \times A \\ \mu \times 1 \downarrow & & \downarrow \alpha \\ G \times A & \xrightarrow{\alpha} & A \end{array}$$

where  $(e, 1)(x) = (e, x)$  for all  $x \in A$ . The *orbits* of the action are the sets  $Gx = \{gx : g \in G\}$  for all  $x \in A$ .

Given two groups  $(G, *)$  and  $(H, \cdot)$ , a *group homomorphism* from  $(G, *)$  to  $(H, \cdot)$  is a function  $h : G \rightarrow H$  such that for all  $x$  and  $y$  in  $G$  it holds that

$$h(x * y) = h(x) \cdot h(y).$$

From this property, one can deduce that  $h$  maps the identity element  $e_G$  of  $G$  to the identity element  $e_H$  of  $H$ , and it also maps inverses to inverses in the sense that  $h(x^{-1}) = h(x)^{-1}$ . Hence one can say that  $h$  is *compatible* with the *group structure*.

The *kernel*  $\text{Ker } h$  of a group homomorphism  $h : G \rightarrow H$  consists of all those elements of  $G$  which are sent by  $h$  to the identity element  $e_H$  of  $H$ , i.e.,

$$\text{Ker } h = \{x \in G : h(x) = e_H\}.$$

The *image*  $\text{Im } h$  of a group homomorphism  $h : G \rightarrow H$  consists of all elements of  $H$  which are sent by  $h$  to  $H$ , i.e.,

$$\text{Im } h = \{h(x) : x \in G\}.$$

The kernel is a *normal subgroup* of  $G$  and the image is a *subgroup* of  $H$ . The homomorphism  $h$  is *injective* (and called a *group monomorphism*) iff  $\text{Ker } h = e_G$ , i.e., iff the kernel of  $h$  consists of the identity element of  $G$  only.

Similarly, a *ring* is a set  $S$  together with two binary operators  $+$  and  $*$  (commonly interpreted as addition and multiplication, respectively) satisfying the following conditions:

1. Additive associativity: For all  $a, b, c \in S$ ,  $(a + b) + c = a + (b + c)$ ,
2. Additive commutativity: For all  $a, b \in S$ ,  $a + b = b + a$ ,
3. Additive identity: There exists an element  $0 \in S$  such that for all  $a \in S$ ,  $0 + a = a + 0 = a$ ,
4. Additive inverse: For every  $a \in S$  there exists  $-a \in S$  such that  $a + (-a) = (-a) + a = 0$ ,
5. Multiplicative associativity: For all  $a, b, c \in S$ ,  $(a * b) * c = a * (b * c)$ ,
6. Left and right distributivity: For all  $a, b, c \in S$ ,  $a * (b + c) = (a * b) + (a * c)$  and  $(b + c) * a = (b * a) + (c * a)$ .

A ring (the term introduced by *D. Hilbert*) is therefore an Abelian group under addition and a semigroup under multiplication. A ring that is commutative under multiplication, has a unit element, and has no divisors of zero is called an *integral domain*. A ring which is also a commutative multiplication group is called a *field*. The simplest rings are the integers  $\mathbb{Z}$ , polynomials  $\mathbb{R}[x]$  and  $\mathbb{R}[x, y]$  in one and two variables, and square  $n \times n$  real matrices.

An *ideal* is a subset  $\mathfrak{I}$  of elements in a ring  $R$  which forms an additive group and has the property that, whenever  $x$  belongs to  $R$  and  $y$  belongs to  $\mathfrak{I}$ , then  $xy$  and  $yx$  belong to  $\mathfrak{I}$ . For example, the set of even integers is an ideal in the ring of integers  $\mathbb{Z}$ . Given an ideal  $\mathfrak{I}$ , it is possible to define a factor ring  $R/\mathfrak{I}$ .

A ring is called *left* (respectively, *right*) *Noetherian* if it does not contain an infinite ascending chain of left (respectively, right) ideals. In this case, the ring in question is said to satisfy the ascending chain condition on left (respectively, right) ideals. A *ring* is said to be *Noetherian* if it is both left and right Noetherian. If a ring  $R$  is Noetherian, then the following are equivalent:

1.  $R$  satisfies the ascending chain condition on ideals.
2. Every ideal of  $R$  is finitely generated.
3. Every set of ideals contains a maximal element.

A *module* is a mathematical object in which things can be added together commutatively by multiplying coefficients and in which most of the rules of manipulating vectors hold. A module is abstractly very similar to a vector space, although in modules, coefficients are taken in rings which are much more general algebraic objects than the fields used in vector spaces. A module taking its coefficients in a ring  $R$  is called a module over  $R$  or  $R$ -module. Modules are the basic tool of homological algebra.

Examples of modules include the set of integers  $\mathbb{Z}$ , the cubic lattice in  $d$  dimensions  $\mathbb{Z}^d$ , and the group ring of a group.  $\mathbb{Z}$  is a module over itself. It is closed under addition and subtraction. Numbers of the form  $n\alpha$  for  $n \in \mathbb{Z}$  and  $\alpha$  a fixed integer form a submodule since, for  $(n, m) \in \mathbb{Z}$ ,  $n\alpha \pm m\alpha = (n \pm m)\alpha$  and  $(n \pm m)$  is still in  $\mathbb{Z}$ . Also, given two integers  $a$  and  $b$ , the smallest module containing  $a$  and  $b$  is the module for their greatest common divisor,  $\alpha = GCD(a, b)$ .

A module  $M$  is a *Noetherian module* if it obeys the ascending chain condition with respect to inclusion, i.e., if every set of increasing sequences of submodules eventually becomes constant. If a module  $M$  is Noetherian, then the following are equivalent:

1.  $M$  satisfies the ascending chain condition on submodules.
2. Every submodule of  $M$  is finitely generated.
3. Every set of submodules of  $M$  contains a maximal element.

Let  $I$  be a partially ordered set. A *direct system* of  $R$ -modules over  $I$  is an ordered pair  $\{M_i, \varphi_j^i\}$  consisting of an indexed family of modules  $\{M_i : i \in I\}$  together with a family of homomorphisms  $\{\varphi_j^i : M_i \rightarrow M_j\}$  for  $i \leq j$ , such that  $\varphi_i^i = 1_{M_i}$  for all  $i$  and such that the following diagram commutes whenever  $i \leq j \leq k$

$$\begin{array}{ccc} M_i & \xrightarrow{\varphi_k^i} & M_k \\ & \searrow \varphi_k^j & \nearrow \varphi_j^i \\ & M_j & \end{array}$$

Similarly, an *inverse system* of  $R$ -modules over  $I$  is an ordered pair  $\{M_i, \psi_j^i\}$  consisting of an indexed family of modules  $\{M_i : i \in I\}$  together with a family of homomorphisms  $\{\psi_j^i : M_j \rightarrow M_i\}$  for  $i \leq j$ , such that  $\psi_i^i = 1_{M_i}$  for all  $i$  and such that the following diagram commutes whenever  $i \leq j \leq k$

$$\begin{array}{ccc} M_k & \xrightarrow{\psi_i^k} & M_i \\ & \searrow \psi_j^k & \nearrow \psi_i^j \\ & M_j & \end{array}$$

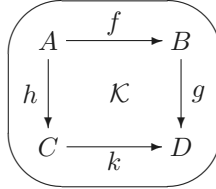
### 1.2.2 Categories

A category is a generic mathematical structure consisting of a collection of *objects* (sets with possibly additional structure), with a corresponding collection of *arrows*, or *morphisms*, between objects (agreeing with this additional structure). A category  $\mathcal{K}$  is defined as a pair  $(\text{Ob}(\mathcal{K}), \text{Mor}(\mathcal{K}))$  of generic objects  $A, B, \dots$  in  $\text{Ob}(\mathcal{K})$  and generic arrows  $f : A \rightarrow B, g : B \rightarrow C, \dots$  in  $\text{Mor}(\mathcal{K})$  between objects, with *associative composition*:

$$A \xrightarrow{f} B \xrightarrow{g} C = A \xrightarrow{f \circ g} C,$$

and *identity (loop) arrow*. (Note that in topological literature,  $\text{Hom}(\mathcal{K})$  or  $\text{hom}(\mathcal{K})$  is used instead of  $\text{Mor}(\mathcal{K})$ ; see [Swi75]).

A category  $\mathcal{K}$  is usually depicted as a *commutative diagram* (i.e., a diagram with a common *initial object*  $A$  and *final object*  $D$ ):



To make this more precise, we say that a *category*  $\mathcal{K}$  is defined if we have:

1. A *class of objects*  $\{A, B, C, \dots\}$  of  $\mathcal{K}$ , denoted by  $\text{Ob}(\mathcal{K})$ ;
2. A *set of morphisms*, or *arrows*  $\text{Mor}_{\mathcal{K}}(A, B)$ , with elements  $f : A \rightarrow B$ , defined for any *ordered pair*  $(A, B) \in \mathcal{K}$ , such that for two different pairs  $(A, B) \neq (C, D)$  in  $\mathcal{K}$ , we have  $\text{Mor}_{\mathcal{K}}(A, B) \cap \text{Mor}_{\mathcal{K}}(C, D) = \emptyset$ ;
3. For any *triplet*  $(A, B, C) \in \mathcal{K}$  with  $f : A \rightarrow B$  and  $g : B \rightarrow C$ , there is a *composition* of morphisms

$$\text{Mor}_{\mathcal{K}}(B, C) \times \text{Mor}_{\mathcal{K}}(A, B) \ni (g, f) \rightarrow g \circ f \in \text{Mor}_{\mathcal{K}}(A, C),$$

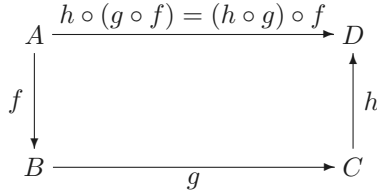
written schematically as

$$\frac{f : A \rightarrow B, \quad g : B \rightarrow C}{g \circ f : A \rightarrow C}.$$

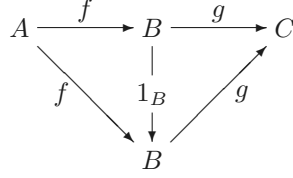
If we have a morphism  $f \in \text{Mor}_{\mathcal{K}}(A, B)$ , (otherwise written  $f : A \rightarrow B$ , or  $A \xrightarrow{f} B$ ), then  $A = \text{dom}(f)$  is a *domain* of  $f$ , and  $B = \text{cod}(f)$  is a *codomain* of  $f$  (of which *range* of  $f$  is a subset) and denoted  $B = \text{ran}(f)$ .

To make  $\mathcal{K}$  a category, it must also fulfill the following two properties:

1. *Associativity of morphisms*: for all  $f \in \text{Mor}_{\mathcal{K}}(A, B)$ ,  $g \in \text{Mor}_{\mathcal{K}}(B, C)$ , and  $h \in \text{Mor}_{\mathcal{K}}(C, D)$ , we have  $h \circ (g \circ f) = (h \circ g) \circ f$ ; in other words, the following diagram is commutative



2. *Existence of identity morphism*: for every object  $A \in \text{Ob}(\mathcal{K})$  exists a unique identity morphism  $1_A \in \text{Mor}_{\mathcal{K}}(A, A)$ ; for any two morphisms  $f \in \text{Mor}_{\mathcal{K}}(A, B)$ , and  $g \in \text{Mor}_{\mathcal{K}}(B, C)$ , compositions with identity morphism  $1_B \in \text{Mor}_{\mathcal{K}}(B, B)$  give  $1_B \circ f = f$  and  $g \circ 1_B = g$ , i.e., the following diagram is commutative:



The set of all morphisms of the category  $\mathcal{K}$  is denoted

$$\text{Mor}(\mathcal{K}) = \bigcup_{A, B \in \text{Ob}(\mathcal{K})} \text{Mor}_{\mathcal{K}}(A, B).$$

If for two morphisms  $f \in \text{Mor}_{\mathcal{K}}(A, B)$  and  $g \in \text{Mor}_{\mathcal{K}}(B, A)$  the equality  $g \circ f = 1_A$  is valid, then the morphism  $g$  is said to be *left inverse* (or *retraction*), of  $f$ , and  $f$  *right inverse* (or *section*) of  $g$ . A morphism which is both right and left inverse of  $f$  is said to be *two-sided inverse* of  $f$ .

A morphism  $m : A \rightarrow B$  is called *monomorphism* in  $\mathcal{K}$  (i.e., *one-to-one*, or *injection* map), if for any two parallel morphisms  $f_1, f_2 : C \rightarrow A$  in  $\mathcal{K}$  the equality  $m \circ f_1 = m \circ f_2$  implies  $f_1 = f_2$ ; in other words,  $m$  is monomorphism if it is *left cancellable*. Any morphism with a left inverse is monomorphism.

A morphism  $e : A \rightarrow B$  is called *epimorphism* in  $\mathcal{K}$  (i.e., *onto*, or *surjection* map), if for any two morphisms  $g_1, g_2 : B \rightarrow C$  in  $\mathcal{K}$  the equality  $g_1 \circ e = g_2 \circ e$  implies  $g_1 = g_2$ ; in other words,  $e$  is epimorphism if it is *right cancellable*. Any morphism with a right inverse is epimorphism.

A morphism  $f : A \rightarrow B$  is called *isomorphism* in  $\mathcal{K}$  (denoted as  $f : A \cong B$ ) if there exists a morphism  $f^{-1} : B \rightarrow A$  which is a two-sided inverse of  $f$  in  $\mathcal{K}$ . The relation of isomorphism is reflexive, symmetric, and transitive, i.e., equivalence relation.

For example, an isomorphism in the category of sets is called a *set-isomorphism*, or a *bijection*, in the category of topological spaces is called a *topological isomorphism*, or a *homeomorphism*, in the category of differentiable manifolds is called a *differentiable isomorphism*, or a *diffeomorphism*.

A morphism  $f \in \text{Mor}_{\mathcal{K}}(A, B)$  is *regular* if there exists a morphism  $g : B \rightarrow A$  in  $\mathcal{K}$  such that  $f \circ g \circ f = f$ . Any morphism with either a left or a right inverse is regular.

An object  $T$  is a *terminal object* in  $\mathcal{K}$  if to each object  $A \in \text{Ob}(\mathcal{K})$  there is exactly one arrow  $A \rightarrow T$ . An object  $S$  is an *initial object* in  $\mathcal{K}$  if to each object  $A \in \text{Ob}(\mathcal{K})$  there is exactly one arrow  $S \rightarrow A$ . A *null object*  $Z \in \text{Ob}(\mathcal{K})$  is an object which is both initial and terminal; it is unique up to isomorphism. For any two objects  $A, B \in \text{Ob}(\mathcal{K})$  there is a unique morphism  $A \rightarrow Z \rightarrow B$  (the composite through  $Z$ ), called the *zero morphism* from  $A$  to  $B$ .

A notion of subcategory is analogous to the notion of subset. A subcategory  $\mathcal{L}$  of a category  $\mathcal{K}$  is said to be a *complete subcategory* iff for any objects  $A, B \in \mathcal{L}$ , every morphism  $A \rightarrow B$  of  $\mathcal{L}$  is in  $\mathcal{K}$ .

The standard categories that we will use in this book are:

- $\mathcal{S}$  – all sets as objects and all functions between them as morphisms;

- $\mathcal{PS}$  – all pointed sets as objects and all functions between them preserving base point as morphisms;
- $\mathcal{V}$  – all vector spaces as objects and all linear maps between them as morphisms;
- $\mathcal{B}$  – Banach spaces over  $\mathbb{R}$  as objects and bounded linear maps between them as morphisms;
- $\mathcal{G}$  – all groups as objects, all homomorphisms between them as morphisms;
- $\mathcal{A}$  – Abelian groups as objects, homomorphisms between them as morphisms;
- $\mathcal{AL}$  – all algebras (over a given field  $\mathbb{K}$ ) as objects, all their homomorphisms between them as morphisms;
- $\mathcal{T}$  – all topological spaces as objects, all continuous functions between them as morphisms;
- $\mathcal{PT}$  – pointed topological spaces as objects, continuous functions between them preserving base point as morphisms;
- $\mathcal{TG}$  – all topological groups as objects, their continuous homomorphisms as morphisms;
- $\mathcal{M}$  – all smooth manifolds as objects, all smooth maps between them as morphisms;
- $\mathcal{M}_n$  –  $n$ D manifolds as objects, their local diffeomorphisms as morphisms;
- $\mathcal{LG}$  – all Lie groups as objects, all smooth homomorphisms between them as morphisms;
- $\mathcal{LAL}$  – all Lie algebras (over a given field  $\mathbb{K}$ ) as objects, all smooth homomorphisms between them as morphisms;
- $\mathcal{TB}$  – all tangent bundles as objects, all smooth tangent maps between them as morphisms;
- $\mathcal{T^*B}$  – all cotangent bundles as objects, all smooth cotangent maps between them as morphisms;
- $\mathcal{VB}$  – all smooth vector bundles as objects, all smooth homomorphisms between them as morphisms;
- $\mathcal{FB}$  – all smooth fibre bundles as objects, all smooth homomorphisms between them as morphisms;

A *groupoid* is a category in which every morphism is invertible. A typical groupoid is the *fundamental groupoid*  $\Pi_1(X)$  of a topological space  $X$ . An object of  $\Pi_1(X)$  is a point  $x \in X$ , and a morphism  $x \rightarrow x'$  of  $\Pi_1(X)$  is a homotopy class of paths  $f$  from  $x$  to  $x'$ . The *composition* of paths  $g : x' \rightarrow x''$  and  $f : x \rightarrow x'$  is the path  $h$  which is ‘ $f$  followed by  $g$ ’. Composition applies also to homotopy classes, and makes  $\Pi_1(X)$  a category and a groupoid (the inverse of any path is the same path traced in the opposite direction).

A *group* is a groupoid with one object, i.e., a *category with one object* in which *all morphisms are isomorphisms*. Therefore, if we try to generalize the concept of a group, keeping associativity as an essential property, we get the notion of a category.

A category is *discrete* if every morphism is an identity. A *monoid* is a category with one object. A *group* is a category with one object in which every morphism has a two-sided inverse under composition.

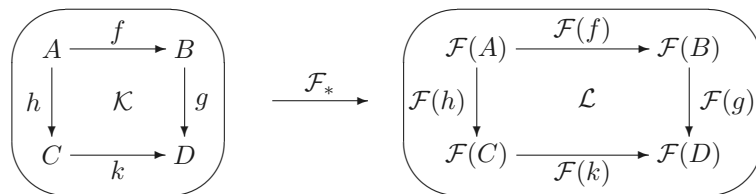
*Homological algebra* was the progenitor of category theory (see e.g., [Die88]). Generalizing L. Euler’s formula  $f + v = e + 2$  for the faces, vertices and edges of a convex polyhedron, E. Betti defined *numerical invariants of spaces* by formal addition and subtraction of faces of various dimensions; H. Poincaré formalized these and introduced homology. E. Noether stressed the fact that these calculations go on in Abelian groups, and that the operation  $\partial_n$  taking a face of dimension  $n$  to the alternating sum of faces of dimension  $n - 1$  which form its boundary is a homomorphism, and it also satisfies  $\partial_n \cdot \partial_{n+1} = 0$ . There are many ways of approximating a given space by polyhedra, but the quotient  $H_n = \text{Ker } \partial_n / \text{Im } \partial_{n+1}$  is an invariant, the *homology group*. Since Noether, the groups have been the object of study instead of their dimensions, which are the *Betti numbers* (see Chapter 4 for details).

### 1.2.3 Functors

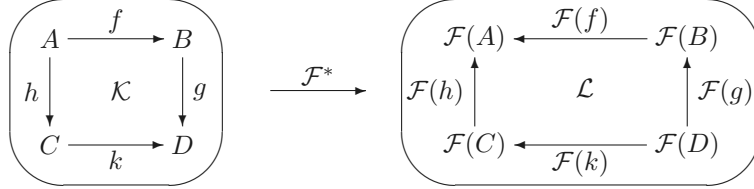
In algebraic topology, one attempts to assign to every topological space  $X$  some algebraic object  $\mathcal{F}(X)$  in such a way that to every  $C^0$ -function  $f : X \rightarrow Y$  there is assigned a homomorphism  $\mathcal{F}(f) : \mathcal{F}(X) \rightarrow \mathcal{F}(Y)$  (see [Swi75, DP97]). One advantage of this procedure is, e.g., that if one is trying to prove the non-existence of a  $C^0$ -function  $f : X \rightarrow Y$  with certain properties, one may find it relatively easy to prove the non-existence of the corresponding algebraic function  $\mathcal{F}(f)$  and hence deduce that  $f$  could not exist. In other words,  $\mathcal{F}$  is to be a ‘homomorphism’ from one category (e.g.,  $\mathcal{T}$ ) to another (e.g.,  $\mathcal{G}$  or  $\mathcal{A}$ ). Formalization of this notion is a *functor*.

A functor is a generic *picture* projecting one category into another. Let  $\mathcal{K} = (\text{Ob}(\mathcal{K}), \text{Mor}(\mathcal{K}))$  be a *source* (or domain) *category* and  $\mathcal{L} = (\text{Ob}(\mathcal{L}), \text{Mor}(\mathcal{L}))$  be a *target* (or codomain) *category*. A functor  $\mathcal{F} = (\mathcal{F}_O, \mathcal{F}_M)$  is defined as a pair of maps,  $\mathcal{F}_O : \text{Ob}(\mathcal{K}) \rightarrow \text{Ob}(\mathcal{L})$  and  $\mathcal{F}_M : \text{Mor}(\mathcal{K}) \rightarrow \text{Mor}(\mathcal{L})$ , preserving categorical symmetry (i.e., commutativity of all diagrams) of  $\mathcal{K}$  in  $\mathcal{L}$ .

More precisely, a *covariant functor*, or simply a *functor*,  $\mathcal{F}_* : \mathcal{K} \rightarrow \mathcal{L}$  is a *picture* in the target category  $\mathcal{L}$  of (all objects and morphisms of) the source category  $\mathcal{K}$ :



Similarly, a *contravariant functor*, or a *cofunctor*,  $\mathcal{F}^* : \mathcal{K} \rightarrow \mathcal{L}$  is a *dual picture* with reversed arrows:



In other words, a *functor*  $\mathcal{F} : \mathcal{K} \rightarrow \mathcal{L}$  from a *source* category  $\mathcal{K}$  to a *target* category  $\mathcal{L}$ , is a pair  $\mathcal{F} = (\mathcal{F}_O, \mathcal{F}_M)$  of maps  $\mathcal{F}_O : \text{Ob}(\mathcal{K}) \rightarrow \text{Ob}(\mathcal{L})$ ,  $\mathcal{F}_M : \text{Mor}(\mathcal{K}) \rightarrow \text{Mor}(\mathcal{L})$ , such that

1. If  $f \in \text{Mor}_{\mathcal{K}}(A, B)$  then  $\mathcal{F}_M(f) \in \text{Mor}_{\mathcal{L}}(\mathcal{F}_O(A), \mathcal{F}_O(B))$  in case of the *covariant* functor  $\mathcal{F}_*$ , and  $\mathcal{F}_M(f) \in \text{Mor}_{\mathcal{L}}(\mathcal{F}_O(B), \mathcal{F}_O(A))$  in case of the *contravariant* functor  $\mathcal{F}^*$ ;
2. For all  $A \in \text{Ob}(\mathcal{K}) : \mathcal{F}_M(1_A) = 1_{\mathcal{F}_O(A)}$ ;
3. For all  $f, g \in \text{Mor}(\mathcal{K})$ : if  $\text{cod}(f) = \text{dom}(g)$ , then  $\mathcal{F}_M(g \circ f) = \mathcal{F}_M(g) \circ \mathcal{F}_M(f)$  in case of the *covariant* functor  $\mathcal{F}_*$ , and  $\mathcal{F}_M(g \circ f) = \mathcal{F}_M(f) \circ \mathcal{F}_M(g)$  in case of the *contravariant* functor  $\mathcal{F}^*$ .

Category theory originated in algebraic topology, which tried to assign algebraic invariants to topological structures. The golden rule of such *invariants* is that they should be *functors*. For example, the *fundamental group*  $\pi_1$  is a functor. Algebraic topology constructs a group called the *fundamental group*  $\pi_1(X)$  from any topological space  $X$ , which keeps track of how many holes the space  $X$  has. But also, any map between topological spaces determines a homomorphism  $\phi : \pi_1(X) \rightarrow \pi_1(Y)$  of the fundamental groups. So the fundamental group is really a functor  $\pi_1 : \mathcal{T} \rightarrow \mathcal{G}$ . This allows us to completely transpose any situation involving *spaces* and *continuous maps* between them to a parallel situation involving *groups* and *homomorphisms* between them, and thus reduce some topology problems to algebra problems.

Also, singular homology in a given dimension  $n$  assigns to each topological space  $X$  an Abelian group  $H_n(X)$ , its *nth homology group* of  $X$ , and also to each continuous map  $f : X \rightarrow Y$  of spaces a corresponding homomorphism  $H_n(f) : H_n(X) \rightarrow H_n(Y)$  of groups, and this in such a way that  $H_n(X)$  becomes a functor  $H_n : \mathcal{T} \rightarrow \mathcal{A}$ .

The leading idea in the *use of functors in topology* is that  $H_n$  or  $\pi_n$  gives an algebraic picture or image not just of the topological spaces  $X, Y$  but also of all the continuous maps  $f : X \rightarrow Y$  between them.

Similarly, there is a functor  $\Pi_1 : \mathcal{T} \rightarrow \mathcal{G}$ , called the ‘fundamental groupoid functor’, which plays a very basic role in algebraic topology. Here’s how we get from any space  $X$  its ‘fundamental groupoid’  $\Pi_1(X)$ . To say what the groupoid  $\Pi_1(X)$  is, we need to say what its objects and morphisms are. The objects in  $\Pi_1(X)$  are just the *points* of  $X$  and the morphisms are just certain equivalence classes of *paths* in  $X$ . More precisely, a morphism  $f : x \rightarrow y$  in  $\Pi_1(X)$  is just an equivalence class of continuous paths from  $x$  to  $y$ , where two

paths from  $x$  to  $y$  are decreed equivalent if one can be continuously deformed to the other while not moving the endpoints. (If this equivalence relation holds we say the two paths are ‘homotopic’, and we call the equivalence classes ‘homotopy classes of paths’ (see [MacL71, Swi75]).

Another examples are covariant *forgetful* functors:

- From the category of topological spaces to the category of sets; it ‘forgets’ the topology–structure.
- From the category of metric spaces to the category of topological spaces with the topology induced by the metrics; it ‘forgets’ the metric.

For each category  $\mathcal{K}$ , the *identity functor*  $I_{\mathcal{K}}$  takes every  $\mathcal{K}$ –object and every  $\mathcal{K}$ –morphism to itself.

Given a category  $\mathcal{K}$  and its subcategory  $\mathcal{L}$ , we have an *inclusion functor*  $\text{In} : \mathcal{K} \rightarrow \mathcal{L}$ .

Given a category  $\mathcal{K}$ , a *diagonal functor*  $\Delta : \mathcal{K} \rightarrow \mathcal{K} \times \mathcal{K}$  takes each object  $A \in \mathcal{K}$  to the object  $(A, A)$  in the product category  $\mathcal{K} \times \mathcal{K}$ .

Given a category  $\mathcal{K}$  and a category of sets  $\mathcal{S}$ , each object  $A \in \mathcal{K}$  determines a *covariant Hom–functor*  $\mathcal{K}[A, \_] : \mathcal{K} \rightarrow \mathcal{S}$ , a *contravariant Hom–functor*  $\mathcal{K}[\_, A] : \mathcal{K} \rightarrow \mathcal{S}$ , and a *Hom–bifunctor*  $\mathcal{K}[\_, \_] : \mathcal{K}^{op} \times \mathcal{K} \rightarrow \mathcal{S}$ .

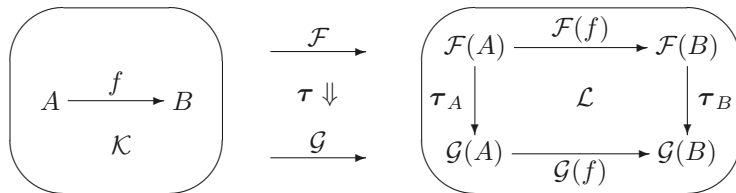
A functor  $\mathcal{F} : \mathcal{K} \rightarrow \mathcal{L}$  is a *faithful functor* if for all  $A, B \in \text{Ob}(\mathcal{K})$  and for all  $f, g \in \text{Mor}_{\mathcal{K}}(A, B)$ ,  $\mathcal{F}(f) = \mathcal{F}(g)$  implies  $f = g$ ; it is a *full functor* if for every  $h \in \text{Mor}_{\mathcal{L}}(\mathcal{F}(A), \mathcal{F}(B))$ , there is  $g \in \text{Mor}_{\mathcal{K}}(A, B)$  such that  $h = \mathcal{F}(g)$ ; it is a *full embedding* if it is both full and faithful.

A *representation of a group* is a functor  $\mathcal{F} : \mathcal{G} \rightarrow \mathcal{V}$ .

Similarly, we can define a *representation of a category* to be a functor  $\mathcal{F} : \mathcal{K} \rightarrow \mathcal{V}$  from the 2–category  $\mathcal{K}$  (a ‘big’ category including all ordinary, or ‘small’ categories, see subsection (1.2.7) below) to the category of vector spaces  $\mathcal{V}$ . In this way, a category is a generalization of a group and group representations are a special case of category representations.

### 1.2.4 Natural Transformations

A *natural transformation* (i.e., a *functor morphism*)  $\tau : \mathcal{F} \rightarrow \mathcal{G}$  is a map between two functors of the same variance,  $(\mathcal{F}, \mathcal{G}) : \mathcal{K} \rightrightarrows \mathcal{L}$ , preserving categorical symmetry:



More precisely, all functors of the same variance from a source category  $\mathcal{K}$  to a target category  $\mathcal{L}$  form themselves objects of the *functor category*  $\mathcal{L}^{\mathcal{K}}$ . Morphisms of  $\mathcal{L}^{\mathcal{K}}$ , called *natural transformations*, are defined as follows.

Let  $\mathcal{F} : \mathcal{K} \rightarrow \mathcal{L}$  and  $\mathcal{G} : \mathcal{K} \rightarrow \mathcal{L}$  be two functors of the same variance from a category  $\mathcal{K}$  to a category  $\mathcal{L}$ . Natural transformation  $\mathcal{F} \xrightarrow{\tau} \mathcal{G}$  is a family of morphisms such that for all  $f \in \text{Mor}_{\mathcal{K}}(A, B)$  in the source category  $\mathcal{K}$ , we have  $\mathcal{G}(f) \circ \tau_A = \tau_B \circ \mathcal{F}(f)$  in the target category  $\mathcal{L}$ . Then we say that the *component*  $\tau_A : \mathcal{F}(A) \rightarrow \mathcal{G}(A)$  is *natural in A*.

If we think of a functor  $\mathcal{F}$  as giving a *picture* in the target category  $\mathcal{L}$  of (all the objects and morphisms of) the source category  $\mathcal{K}$ , then a natural transformation  $\tau$  represents a set of morphisms mapping the picture  $\mathcal{F}$  to another picture  $\mathcal{G}$ , preserving the commutativity of all diagrams.

An invertible natural transformation, such that all components  $\tau_A$  are isomorphisms) is called a *natural equivalence* (or, *natural isomorphism*). In this case, the inverses  $(\tau_A)^{-1}$  in  $\mathcal{L}$  are the components of a natural isomorphism  $(\tau)^{-1} : \mathcal{G} \xrightarrow{*} \mathcal{F}$ . Natural equivalences are among the most important *metamathematical constructions* in algebraic topology (see [Swi75]).

For example, let  $\mathcal{B}$  be the category of Banach spaces over  $\mathbb{R}$  and bounded linear maps. Define  $D : \mathcal{B} \rightarrow \mathcal{B}$  by taking  $D(X) = X^*$  = Banach space of bounded linear functionals on a space  $X$  and  $D(f) = f^*$  for  $f : X \rightarrow Y$  a bounded linear map. Then  $D$  is a cofunctor.  $D^2 = D \circ D$  is also a functor. We also have the identity functor  $1 : \mathcal{B} \rightarrow \mathcal{B}$ . Define  $T : 1 \rightarrow D \circ D$  as follows: for every  $X \in \mathcal{B}$  let  $T(X) : X \rightarrow D^2X = X^{**}$  be the *natural inclusion* – that is, for  $x \in X$  we have  $[T(X)(x)](f) = f(x)$  for every  $f \in X^*$ .  $T$  is a natural transformation. On the subcategory of finite–dimensional Banach spaces  $T$  is even a natural equivalence. The largest subcategory of  $\mathcal{B}$  on which  $T$  is a natural equivalence is called the category of reflexive Banach spaces [Swi75].

As S. Eilenberg and S. MacLane first observed, ‘category’ has been defined in order to define ‘functor’ and ‘functor’ has been defined in order to define ‘natural transformation’ [MacL71]).

### Compositions of Natural Transformations

Natural transformations can be *composed* in two different ways. First, we have an ‘ordinary’ composition: if  $\mathcal{F}, \mathcal{G}$  and  $\mathcal{H}$  are three functors from the source category  $\mathcal{A}$  to the target category  $\mathcal{B}$ , and then  $\alpha : \mathcal{F} \rightarrow \mathcal{G}$ ,  $\beta : \mathcal{G} \rightarrow \mathcal{H}$  are two natural transformations, then the formula

$$(\beta \circ \alpha)_A = \beta_A \circ \alpha_A, \quad \text{for all } A \in \mathcal{A}, \quad (1.33)$$

defines a new natural transformation  $\beta \circ \alpha : \mathcal{F} \rightarrow \mathcal{H}$ . This composition law is clearly associative and possesses a unit  $1_{\mathcal{F}}$  at each functor  $\mathcal{F}$ , whose  $A$ –component is  $1_{\mathcal{F}A}$ .

Second, we have the *Godement product* of natural transformations, usually denoted by  $*$ . Let  $\mathcal{A}, \mathcal{B}$  and  $\mathcal{C}$  be three categories,  $\mathcal{F}, \mathcal{G}, \mathcal{H}$  and  $\mathcal{K}$  be four

functors such that  $(\mathcal{F}, \mathcal{G}) : \mathcal{A} \rightrightarrows \mathcal{B}$  and  $(\mathcal{H}, \mathcal{K}) : \mathcal{B} \rightrightarrows \mathcal{C}$ , and  $\alpha : \mathcal{F} \xrightarrow{\cdot} \mathcal{G}$ ,  $\beta : \mathcal{H} \xrightarrow{\cdot} \mathcal{K}$  be two natural transformations. Now, instead of (1.33), the Godement composition is given by

$$(\beta * \alpha)_A = \beta_{GA} \circ H(\alpha_A) = K(\alpha_A) \circ \beta_{FA}, \quad \text{for all } A \in \mathcal{A}, \quad (1.34)$$

which defines a new natural transformation  $\beta * \alpha : \mathcal{H} \circ \mathcal{F} \xrightarrow{\cdot} \mathcal{K} \circ \mathcal{G}$ .

Finally, the two compositions (1.33) and (1.33) of natural transformations can be combined as

$$(\delta * \gamma) \circ (\beta * \alpha) = (\delta \circ \beta) * (\gamma \circ \alpha),$$

where  $\mathcal{A}, \mathcal{B}$  and  $\mathcal{C}$  are three categories,  $\mathcal{F}, \mathcal{G}, \mathcal{H}, \mathcal{K}, \mathcal{L}, \mathcal{M}$  are six functors, and  $\alpha : \mathcal{F} \xrightarrow{\cdot} \mathcal{H}$ ,  $\beta : \mathcal{G} \xrightarrow{\cdot} \mathcal{K}$ ,  $\gamma : \mathcal{H} \xrightarrow{\cdot} \mathcal{L}$ ,  $\delta : \mathcal{K} \xrightarrow{\cdot} \mathcal{M}$  are four natural transformations.

### Dinatural Transformations

Double natural transformations are called *dinatural transformations*. An end of a functor  $S : C^{op} \times C \rightarrow X$  is a universal dinatural transformation from a constant  $e$  to  $S$ . In other words, an end of  $S$  is a pair  $\langle e, \omega \rangle$ , where  $e$  is an object of  $X$  and  $\omega : e \xrightarrow{\cdot} S$  is a *wedge (dinatural) transformation* with the property that to every wedge  $\beta : x \xrightarrow{\cdot} S$  there is a unique arrow  $h : x \rightarrow e$  of  $B$  with  $\beta_c = \omega_c h$  for all  $a \in C$ . We call  $\omega$  the *ending wedge* with *components*  $\omega_c$ , while the object  $e$  itself, by abuse of language, is called the end of  $S$  and written with integral notation as  $\int_c S(c, c)$ ; thus

$$S(c, c) \xrightarrow{\omega_c} \int_c S(c, c) = e.$$

Note that the ‘variable of integration’  $c$  appears twice under the integral sign (once contravariant, once covariant) and is ‘bound’ by the integral sign, in that the result no longer depends on  $c$  and so is unchanged if ‘ $c$ ’ is replaced by any other letter standing for an object of the category  $C$ . These properties are like those of the letter  $x$  under the usual integral symbol  $\int f(x) dx$  of calculus.

Every end is manifestly a limit – specifically, a limit of a suitable diagram in  $X$  made up of pieces like  $S(b, b) \rightarrow S(b, c) \rightarrow S(c, c)$ .

For each functor  $T : C \rightarrow X$  there is an isomorphism

$$\int_c S(c, c) = \int_c Tc \cong \text{Lim } T,$$

valid when either the end of the limit exists, carrying the ending wedge to the limiting cone; the indicated notation thus allows us to write any limit as an

integral (an end) without explicitly mentioning the dummy variable (the first variable  $c$  of  $S$ ).

A functor  $H : X \rightarrow Y$  is said to *preserve the end* of a functor  $S : C^{op} \times C \rightarrow X$  when  $\omega : e \rightrightarrows S$  an end of  $S$  in  $X$  implies that  $H\omega : He \rightrightarrows HS$  is an end for  $HS$ ; in symbols

$$H \int_c S(c, c) = \int_c HS(c, c).$$

Similarly,  $H$  *creates* the end of  $S$  when to each end  $v : y \rightrightarrows HS$  in  $Y$  there is a unique wedge  $\omega : e \rightrightarrows S$  with  $H\omega = v$ , and this wedge  $\omega$  is an end of  $S$ .

The definition of the coend of a functor  $S : C^{op} \times C \rightarrow X$  is dual to that of an end. A *coend* of  $S$  is a pair  $\langle d, \zeta \rangle$ , consisting of an object  $d \in X$  and a wedge  $\zeta : S \rightrightarrows d$ . The object  $d$  (when it exists, unique up to isomorphism) will usually be written with an integral sign and with the bound variable  $c$  as superscript; thus

$$S(c, c) \xrightarrow{\zeta} \int_c S(c, c) = d.$$

The formal properties of coends are dual to those of ends. Both are much like those for integrals in calculus (see [MacL71], for technical details).

### 1.2.5 Limits and Colimits

In abstract algebra constructions are often defined by an abstract property which requires the existence of unique morphisms under certain conditions. These properties are called *universal properties*. The *limit* of a functor generalizes the notions of inverse limit and product used in various parts of mathematics. The dual notion, *colimit*, generalizes direct limits and direct sums. Limits and colimits are defined via universal properties and provide many examples of *adjoint functors*.

A *limit* of a covariant functor  $\mathcal{F} : \mathcal{J} \rightarrow \mathcal{C}$  is an object  $L$  of  $\mathcal{C}$ , together with morphisms  $\phi_X : L \rightarrow \mathcal{F}(X)$  for every object  $X$  of  $\mathcal{J}$ , such that for every morphism  $f : X \rightarrow Y$  in  $\mathcal{J}$ , we have  $\mathcal{F}(f)\phi_X = \phi_Y$ , and such that the following *universal property* is satisfied: for any object  $N$  of  $\mathcal{C}$  and any set of morphisms  $\psi_X : N \rightarrow \mathcal{F}(X)$  such that for every morphism  $f : X \rightarrow Y$  in  $\mathcal{J}$ , we have  $\mathcal{F}(f)\psi_X = \psi_Y$ , there exists precisely one morphism  $u : N \rightarrow L$  such that  $\phi_X u = \psi_X$  for all  $X$ . If  $\mathcal{F}$  has a limit (which it need not), then the limit is defined up to a unique isomorphism, and is denoted by  $\lim \mathcal{F}$ .

Analogously, a *colimit* of the functor  $\mathcal{F} : \mathcal{J} \rightarrow \mathcal{C}$  is an object  $L$  of  $\mathcal{C}$ , together with morphisms  $\phi_X : \mathcal{F}(X) \rightarrow L$  for every object  $X$  of  $\mathcal{J}$ , such that for every morphism  $f : X \rightarrow Y$  in  $\mathcal{J}$ , we have  $\phi_Y \mathcal{F}(X) = \phi_X$ , and such that the following universal property is satisfied: for any object  $N$  of  $\mathcal{C}$  and any set of morphisms  $\psi_X : \mathcal{F}(X) \rightarrow N$  such that for every morphism  $f : X \rightarrow Y$  in  $\mathcal{J}$ , we have  $\psi_Y \mathcal{F}(X) = \psi_X$ , there exists precisely one morphism  $u : L \rightarrow N$  such

that  $u\phi_X = \psi_X$  for all  $X$ . The colimit of  $\mathcal{F}$ , unique up to unique isomorphism if it exists, is denoted by  $\text{colim } \mathcal{F}$ .

Limits and colimits are related as follows: A functor  $\mathcal{F} : \mathcal{J} \rightarrow \mathcal{C}$  has a colimit iff for every object  $N$  of  $\mathcal{C}$ , the functor  $X \mapsto \text{Mor}_{\mathcal{C}}(\mathcal{F}(X), N)$  (which is a covariant functor on the dual category  $\mathcal{J}^{op}$ ) has a limit. If that is the case, then  $\text{Mor}_{\mathcal{C}}(\text{colim } \mathcal{F}, N) = \lim \text{Mor}_{\mathcal{C}}(\mathcal{F}(-), N)$  for every object  $N$  of  $\mathcal{C}$ .

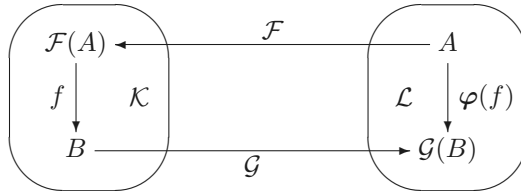
### 1.2.6 The Adjunction

The most important functorial operation is adjunction; as S. MacLane once said, “Adjoint functors arise everywhere” [MacL71].

The *adjunction*  $\varphi : \mathcal{F} \dashv \mathcal{G}$  between two functors  $(\mathcal{F}, \mathcal{G}) : \mathcal{K} \rightleftarrows \mathcal{L}$  of *opposite variance* [Kan58], represents a *weak functorial inverse*

$$\frac{f : \mathcal{F}(A) \rightarrow B}{\varphi(f) : A \rightarrow \mathcal{G}(B)}$$

forming a *natural equivalence*  $\varphi : \text{Mor}_{\mathcal{K}}(\mathcal{F}(A), B) \xrightarrow{\varphi} \text{Mor}_{\mathcal{L}}(A, \mathcal{G}(B))$ . The adjunction isomorphism is given by a *bijective correspondence* (a one-to-one and onto map on objects)  $\varphi : \text{Mor}(\mathcal{K}) \ni f \rightarrow \varphi(f) \in \text{Mor}(\mathcal{L})$  of isomorphisms in the two categories,  $\mathcal{K}$  (with a representative object  $A$ ), and  $\mathcal{L}$  (with a representative object  $B$ ). It can be depicted as a (non-commutative) diagram



In this case  $\mathcal{F}$  is called *left adjoint*, while  $\mathcal{G}$  is called *right adjoint*.

In other words, an *adjunction*  $\mathcal{F} \dashv \mathcal{G}$  between two functors  $(\mathcal{F}, \mathcal{G})$  of opposite variance, from a source category  $\mathcal{K}$  to a target category  $\mathcal{L}$ , is denoted by  $(\mathcal{F}, \mathcal{G}, \eta, \varepsilon) : \mathcal{K} \rightleftarrows \mathcal{L}$ . Here,  $\mathcal{F} : \mathcal{L} \rightarrow \mathcal{K}$  is the *left (upper) adjoint functor*,  $\mathcal{G} : \mathcal{K} \rightarrow \mathcal{L}$  is the *right (lower) adjoint functor*,  $\eta : 1_{\mathcal{L}} \rightarrow \mathcal{G} \circ \mathcal{F}$  is the *unit natural transformation* (or, *front adjunction*), and  $\varepsilon : \mathcal{F} \circ \mathcal{G} \rightarrow 1_{\mathcal{K}}$  is the *counit natural transformation* (or, *back adjunction*).

For example,  $\mathcal{K} = \mathcal{S}$  is the category of sets and  $\mathcal{L} = \mathcal{G}$  is the category of groups. Then  $\mathcal{F}$  turns any set into the *free group* on that set, while the ‘forgetful’ functor  $\mathcal{F}^*$  turns any group into the *underlying set* of that group. Similarly, all sorts of other ‘free’ and ‘underlying’ constructions are also left and right adjoints, respectively.

Right adjoints preserve *limits*, and left adjoints preserve *colimits*.

The category  $\mathcal{C}$  is called a *cocomplete category* if every functor  $\mathcal{F} : \mathcal{J} \rightarrow \mathcal{C}$  has a colimit. The following categories are cocomplete:  $\mathcal{S}, \mathcal{G}, \mathcal{A}, \mathcal{T}$ , and  $\mathcal{PT}$ .

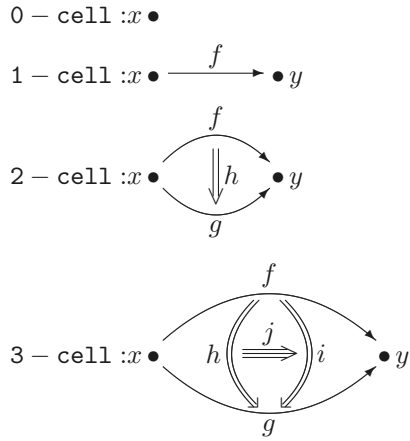
The importance of adjoint functors lies in the fact that every functor which has a left adjoint (and therefore is a right adjoint) is continuous. In the category  $\mathcal{A}$  of Abelian groups, this e.g., shows that the kernel of a product of homomorphisms is naturally identified with the product of the kernels. Also, limit functors themselves are continuous. A covariant functor  $\mathcal{F} : \mathcal{J} \rightarrow \mathcal{C}$  is *cocontinuous* if it transforms colimits into colimits. Every functor which has a right adjoint (and is a left adjoint) is cocontinuous.

The *analogy* between *adjoint functors* and *adjoint linear operators* relies upon a deeper analogy: just as in quantum theory the inner product  $\langle \phi, \psi \rangle$  represents the *amplitude* to pass from  $\phi$  to  $\psi$ , in category theory  $\text{Mor}(A, B)$  represents the *set of ways* to go from  $A$  to  $B$ . These are to Hilbert spaces as categories are to sets. The analogues of adjoint linear operators between Hilbert spaces are certain adjoint functors between 2–Hilbert spaces [Bae97, BD98]. Similarly, the *adjoint representation* of a Lie group  $G$  is the linearized version of the action of  $G$  on itself by conjugation, i.e., for each  $g \in G$ , the inner automorphism  $x \mapsto gxg^{-1}$  gives a linear transformation  $Ad(g) : \mathfrak{g} \rightarrow \mathfrak{g}$ , from the Lie algebra  $\mathfrak{g}$  of  $G$  to itself.

### 1.2.7 $n$ –Categories

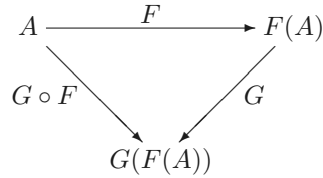
#### Generalization from ‘Small’ Categories to ‘Big’ $n$ –Categories

If we think of a point in geometric space (either natural, or abstract) as an *object* (or, a 0–cell), and a path between two points as an *arrow* (or, a 1–*morphism*, or a 1–cell), we could think of a ‘path of paths’ as a 2–arrow (or, a 2–morphism, or a 2–cell), and a ‘path of paths of paths’ (or, a 3–morphism, or a 3–cell), etc. Here a ‘path of paths’ is just a continuous 1–parameter family of paths from between source and target points, which we can think of as tracing out a 2D surface, etc. In this way we get a ‘skeleton’ of an  $n$ –category, where a 1–category operates with 0–cells (objects) and 1–cells (arrows, causally connecting *source* objects with *target* ones), a 2–category operates with all the cells up to 2–cells [Ben67], a 3–category operates with all the cells up to 3–cells, etc. This skeleton clearly demonstrates the *hierarchical self-similarity* of  $n$ –categories:

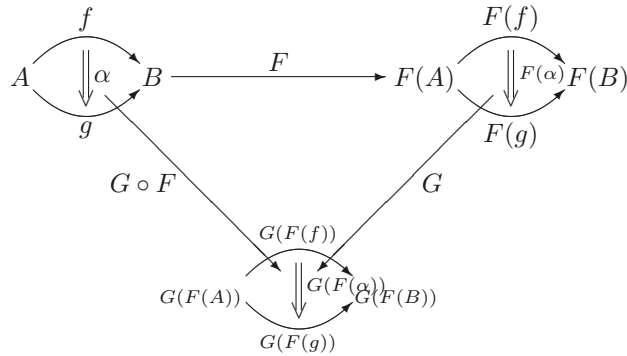


where triple arrow goes in the third direction, perpendicular to both single and double arrows. Categorical composition is defined by pasting arrows.

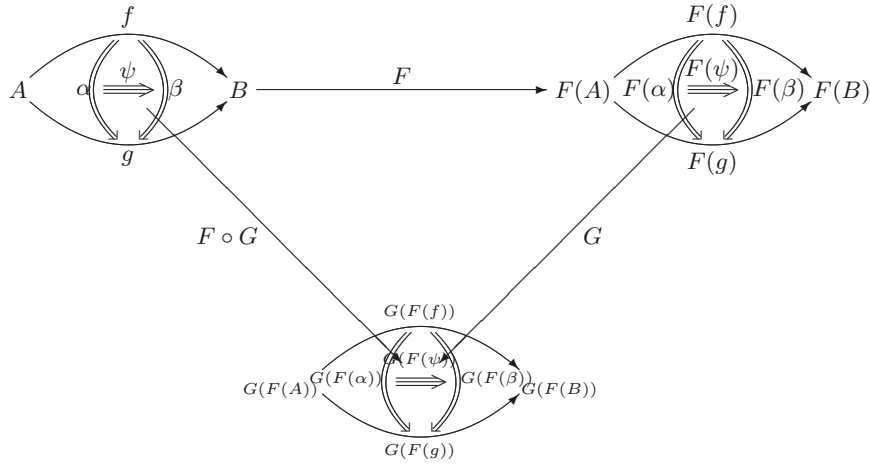
In this way defined, a 1–category can be depicted as a commutative triangle:



a 2–category is a commutative triangle:



a 3–category is a commutative triangle:



etc., up to  $n$ -categories.

Many deep-sounding results in mathematical sciences are obtained by the process of *categorification*<sup>6</sup> of the high school mathematics [CF94, BD98].

An  $n$ -category is a generic mathematical structure consisting of a collection of objects, a collection of arrows between objects, a collection of 2-arrows between arrows [Ben67], a collection of 3-arrows between 2-arrows, and so on up to  $n$  [Bae97, BD98, Lei02, Lei03, Lei04].

More precisely, an  $n$ -category (for  $n \geq 0$ ) consists of:

- 0-cells, or objects,  $A, B, \dots$
- 1-cells, or arrows,  $A \xrightarrow{f} B$ , with a composition

$$A \xrightarrow{f} B \xrightarrow{g} C = A \xrightarrow{g \circ f} C$$

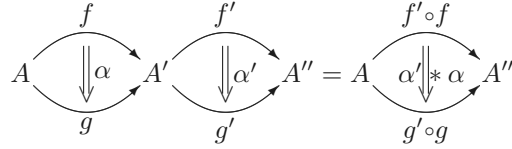
- 2-cells, ‘arrows between arrows’,  $A \begin{array}{c} \xrightarrow{f} \\ \Downarrow \alpha \\ \xrightarrow{g} \end{array} B$ , with vertical compositions

(denoted by  $\circ$ ) and horizontal compositions (denoted by  $*$ ), respectively given by

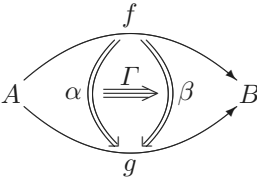
$$A \begin{array}{c} \xrightarrow{f} \\ \Downarrow \alpha \\ \xrightarrow{g} \\ \Downarrow \beta \\ \xrightarrow{h} \end{array} B = A \begin{array}{c} \xrightarrow{f} \\ \Downarrow \beta \circ \alpha \\ \xrightarrow{h} \end{array} B$$

<sup>6</sup> Categorification means replacing sets with categories, functions with functors, and equations between functions by natural equivalences between functors. Iterating this process requires a theory of  $n$ -categories.

and



- 3-cells, ‘arrows between arrows between arrows’,

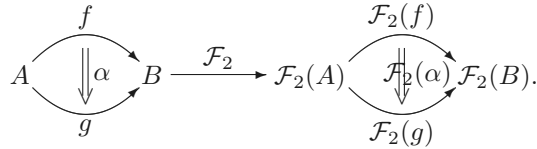


(where the  $\Gamma$ -arrow goes in a direction perpendicular to  $f$  and  $\alpha$ ), with various kinds of vertical, horizontal and mixed compositions,

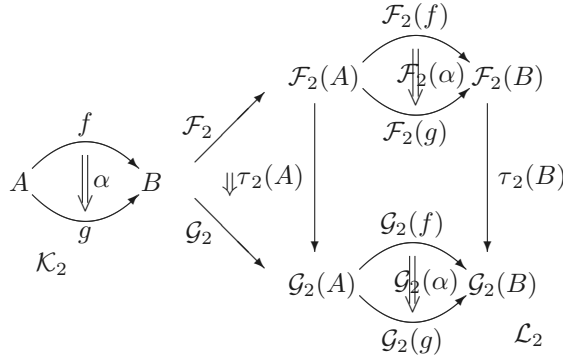
- etc., up to  $n$ -cells.

Calculus of  $n$ -categories has been developed as follows. First, there is  $\mathcal{K}_2$ , the 2-category of all ordinary (or small) categories.  $\mathcal{K}_2$  has categories  $\mathcal{K}, \mathcal{L}, \dots$  as objects, functors  $\mathcal{F}, \mathcal{G} : \mathcal{K} \rightleftarrows \mathcal{L}$  as arrows, and natural transformations, like  $\tau : \mathcal{F} \rightarrow \mathcal{G}$  as 2-arrows.

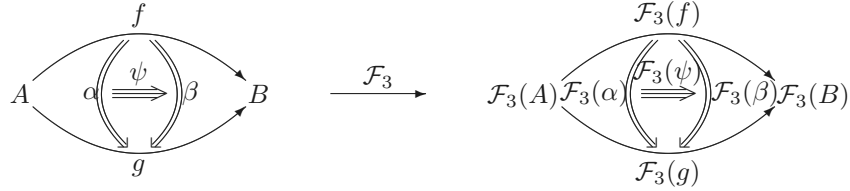
In a similar way, the arrows in a 3-category  $\mathcal{K}_3$  are 2-functors  $\mathcal{F}_2, \mathcal{G}_2, \dots$  sending objects in  $\mathcal{K}_2$  to objects in  $\mathcal{L}_2$ , arrows to arrows, and 2-arrows to 2-arrows, strictly preserving all the structure of  $\mathcal{K}_2$



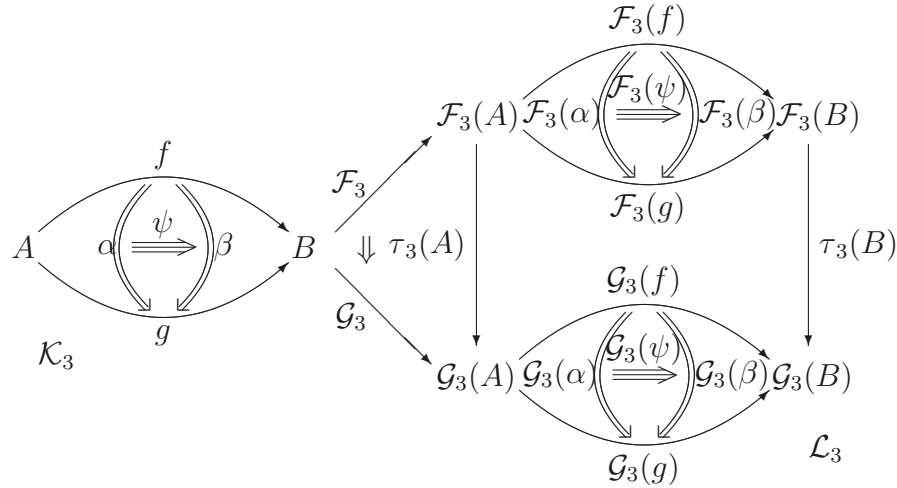
The 2-arrows in  $\mathcal{K}_3$  are 2-natural transformations, like  $\tau_2 : \mathcal{F}_2 \xrightarrow{\cong} \mathcal{G}_2$  between 2-functors  $\mathcal{F}_2, \mathcal{G}_2 : \mathcal{K}_2 \rightarrow \mathcal{L}_2$  that sends each object in  $\mathcal{K}_2$  to an arrow in  $\mathcal{L}_2$  and each arrow in  $\mathcal{K}_2$  to a 2-arrow in  $\mathcal{L}_2$ , and satisfies natural transformation-like conditions. We can visualize  $\tau_2$  as a prism going from one functorial picture of  $\mathcal{K}_2$  in  $\mathcal{L}_2$  to another, built using commutative squares:



Similarly, the arrows in a 4-category  $\mathcal{K}_4$  are 3-functors  $\mathcal{F}_3, \mathcal{G}_3, \dots$  sending objects in  $\mathcal{K}_3$  to objects in  $\mathcal{L}_3$ , arrows to arrows, and 2-arrows to 2-arrows, strictly preserving all the structure of  $\mathcal{K}_3$



The 2-arrows in  $\mathcal{K}_4$  are 3-natural transformations, like  $\tau_3 : \mathcal{F} \overset{3}{\rightrightarrows} \mathcal{G}$  between 3-functors  $\mathcal{F}_3, \mathcal{G}_3 : \mathcal{K}_3 \rightarrow \mathcal{L}_3$  that sends each object in  $\mathcal{K}_3$  to a arrow in  $\mathcal{L}_3$  and each arrow in  $\mathcal{K}_3$  to a 2-arrow in  $\mathcal{L}_3$ , and satisfies natural transformation-like conditions. We can visualize  $\tau_3$  as a prism going from one picture of  $\mathcal{K}_3$  in  $\mathcal{L}_3$  to another, built using commutative squares:



### Topological Structure of $n$ -Categories

We already emphasized the topological nature of ordinary category theory. This fact is even more obvious in the general case of  $n$ -categories (see [Lei02, Lei03, Lei04]).

#### Homotopy Theory

Any topological manifold  $M$  gives rise to an  $n$ -category  $\Pi_n(M)$  (its *fundamental  $n$ -groupoid*), in which 0-cells are *points* in  $M$ ; 1-cells are *paths* in  $M$  (i.e., parameterized continuous maps  $f : [0, 1] \rightarrow M$ ); 2-cells are *homotopies* (denoted by  $\simeq$ ) *of paths* relative to endpoints (i.e., parameterized continuous

maps  $h : [0, 1] \times [0, 1] \rightarrow M$ ); 3-cells are *homotopies of homotopies* of paths in  $M$  (i.e., parameterized continuous maps  $j : [0, 1] \times [0, 1] \times [0, 1] \rightarrow M$ ); categorical *composition* is defined by *pasting* paths and homotopies. In this way the following ‘homotopy skeleton’ emerges:

0-cell:  $x \bullet \quad x \in M$ ;

1-cell:  $x \bullet \xrightarrow{f} \bullet y \quad f : x \simeq y \in M,$   
 $f : [0, 1] \rightarrow M, f : x \mapsto y, y = f(x), f(0) = x, f(1) = y;$   
 e.g., linear path:  $f(t) = (1 - t)x + ty$ ;

2-cell:  $x \bullet \begin{array}{c} \xrightarrow{f} \\ \Downarrow h \\ \xrightarrow{g} \end{array} \bullet y \quad h : f \simeq g \in M,$

$h : [0, 1] \times [0, 1] \rightarrow M, h : f \mapsto g, g = h(f(x)),$   
 $h(x, 0) = f(x), h(x, 1) = g(x), h(0, t) = x, h(1, t) = y$   
 e.g., linear homotopy:  $h(x, t) = (1 - t)f(x) + tg(x)$ ;

3-cell:  $x \bullet \begin{array}{c} \xrightarrow{f} \\ \left( \begin{array}{c} \left( \begin{array}{c} \xrightarrow{h} \\ \Downarrow j \\ \xrightarrow{i} \end{array} \right) \\ \Downarrow \\ \xrightarrow{g} \end{array} \right) \\ \xrightarrow{g} \end{array} \bullet y \quad j : h \simeq i \in M,$

$j : [0, 1] \times [0, 1] \times [0, 1] \rightarrow M, j : h \mapsto i, i = j(h(f(x)))$   
 $j(x, t, 0) = h(f(x)), j(x, t, 1) = i(f(x)),$   
 $j(x, 0, s) = f(x), j(x, 1, s) = g(x),$   
 $j(0, t, s) = x, j(1, t, s) = y$   
 e.g., linear composite homotopy:  $j(x, t, s) = (1 - t)h(f(x)) + ti(f(x)).$

If  $M$  is a *smooth* manifold, then all included paths and homotopies need to be *smooth*. Recall that a *groupoid* is a category in which every morphism is invertible; its special case with only one object is a *group*.

*Category TT*

Topological  $n$ -category  $\mathcal{TT}$  has:

- 0-cells: topological spaces  $X$
- 1-cells: continuous maps  $X \xrightarrow{f} Y$

- 2-cells: homotopies  $h$  between  $f$  and  $g : X \begin{array}{c} \xrightarrow{f} \\ \Downarrow h \\ \xrightarrow{g} \end{array} Y$   
 i.e., continuous maps  $h : X \times [0, 1] \rightarrow Y$ , such that  $\forall x \in X, h(x, 0) = f(x)$  and  $h(x, 1) = g(x)$

- 3-cells: homotopies between homotopies :  $X \begin{array}{c} \xrightarrow{f} \\ \left( \begin{array}{c} \Downarrow h \\ \Downarrow i \end{array} \right) \\ \xrightarrow{g} \end{array} Y$   
 i.e., continuous maps  $j : X \times [0, 1] \times [0, 1] \rightarrow Y$ .

*Category  $\mathcal{CK}$*

Consider an  $n$ -category  $\mathcal{CK}$ , which has:

- 0-cells: chain complexes  $A$  (of Abelian groups, say)
- 1-cells: chain maps  $A \xrightarrow{f} B$
- 2-cells: chain homotopies  $A \begin{array}{c} \xrightarrow{f} \\ \Downarrow \alpha \\ \xrightarrow{g} \end{array} B$ ,  
 i.e., maps  $\alpha : A \rightarrow B$  of degree 1
- 3-cells  $A \begin{array}{c} \xrightarrow{f} \\ \left( \begin{array}{c} \Downarrow \alpha \\ \Downarrow \beta \end{array} \right) \\ \xrightarrow{g} \end{array} B$ : homotopies between homotopies,  
 i.e., maps  $\Gamma : A \rightarrow B$  of degree 2 such that  $d\Gamma - \Gamma d = \beta - \alpha$ .

There ought to be some kind of map  $\mathcal{CC} : \mathcal{TT} \Rightarrow \mathcal{CK}$  (see [Lei02, Lei03, Lei04]).

*Categorification*

Categorification is the process of finding category-theoretic analogs of set-theoretic concepts by replacing sets with categories, functions with functors, and equations between functions by natural isomorphisms between functors, which in turn should satisfy certain equations of their own, called ‘coherence laws’. Iterating this process requires a theory of  $n$ -categories.

Categorification uses the following analogy between set theory and category theory [CF94, BD98]:

Set Theory	Category Theory
elements	objects
equations between elements	isomorphisms between objects
sets	categories
functions	functors
equations between functions	natural isomorphisms between functors

Just as sets have elements, categories have objects. Just as there are functions between sets, there are functors between categories. Now, the proper analog of an equation between elements is not an equation between objects, but an isomorphism. Similarly, the analog of an equation between functions is a natural isomorphism between functors.

### 1.2.8 Abelian Functorial Algebra

An *Abelian category* is a certain kind of category in which morphisms and objects can be added and in which kernels and cokernels exist and have the usual properties. The motivating prototype example of an Abelian category is the category of Abelian groups  $\mathcal{A}$ . Abelian categories are the framework for homological algebra (see [Die88]).

Given a homomorphism  $f : A \rightarrow B$  between two objects  $A \equiv \text{Dom } f$  and  $B \equiv \text{Cod } f$  in an Abelian category  $\mathcal{A}$ , then its *kernel*, *image*, *cokernel* and *coimage* in  $\mathcal{A}$  are defined respectively as:

$$\begin{aligned} \text{Ker } f &= f^{-1}(e_B), & \text{Coker } f &= \text{Cod } f / \text{Im } f, \\ \text{Im } f &= f(A), & \text{Coim } f &= \text{Dom } f / \text{Ker } f, \end{aligned}$$

where  $e_B$  is a unit of  $B$  [DP97].

In an Abelian category  $\mathcal{A}$  a *composable* pair of arrows,

$$\bullet \xrightarrow{f} B \xrightarrow{g} \bullet$$

is *exact* at  $B$  iff  $\text{Im } f \equiv \text{Ker } g$  (equivalence as subobjects of  $B$ ) – or, equivalently, if  $\text{Coker } f \equiv \text{Coim } g$  [MacL71].

For each arrow  $f$  in an Abelian category  $\mathcal{A}$  the *triangular identities* read

$$\text{Ker}(\text{Coker}(\text{Ker } f)) = \text{Ker } f, \quad \text{Coker}(\text{Ker}(\text{Coker } f)) = \text{Coker } f.$$

The diagram (with  $0$  the null object)

$$0 \longrightarrow A \xrightarrow{f} B \xrightarrow{g} C \longrightarrow 0 \quad (1.35)$$

is a *short exact sequence* when it is exact at  $A$ , at  $B$ , and at  $C$ .

Since  $0 \rightarrow a$  is the zero arrow, exactness at  $A$  means just that  $f$  is *monic* (i.e., one-to-one, or injective map); dually, exactness at  $C$  means that  $g$  is *epic* (i.e., onto, or surjective map). Therefore, (1.35) is equivalent to

$$f = \text{Ker } g, \quad g = \text{Coker } f.$$

Similarly, the statement that  $h = \text{Coker } f$  becomes the statement that the sequence

$$A \xrightarrow{f} B \xrightarrow{g} C \longrightarrow 0$$

is exact at  $B$  and at  $C$ . Classically, such a sequence was called a short right exact sequence. Similarly,  $k = \text{Ker } f$  is expressed by a short left exact sequence

$$0 \longrightarrow A \xrightarrow{f} B \xrightarrow{g} C.$$

If  $\mathcal{A}$  and  $\mathcal{A}'$  are Abelian categories, an *additive functor*  $\mathcal{F} : \mathcal{A} \rightarrow \mathcal{A}'$  is a functor from  $\mathcal{A}$  to  $\mathcal{A}'$  with

$$\mathcal{F}(f + f') = \mathcal{F}f + \mathcal{F}f',$$

for any parallel pair of arrows  $f, f' : b \rightarrow c$  in  $\mathcal{A}$ . It follows that  $\mathcal{F}0 = 0$ .

A functor  $\mathcal{F} : \mathcal{A} \rightarrow \mathcal{A}'$  between Abelian categories  $\mathcal{A}$  and  $\mathcal{A}'$  is, by definition, *exact* when it preserves all finite limits and all finite colimits. In particular, an exact functor preserves kernels and cokernels, which means that

$$\text{Ker}(\mathcal{F}f) = \mathcal{F}(\text{Ker } f) \quad \text{and} \quad \text{Coker}(\mathcal{F}f) = \mathcal{F}(\text{Coker } f);$$

then  $\mathcal{F}$  also preserves images, coimages, and carries exact sequences to exact sequences. By construction of limits from products and equalizers and dual constructions,  $\mathcal{F} : \mathcal{A} \rightarrow \mathcal{A}'$  is exact iff it is additive and preserves kernels and cokernels.

A functor  $\mathcal{F}$  is *left exact* when it preserves all finite limits. In other words,  $\mathcal{F}$  is left exact iff it is additive and  $\text{Ker}(\mathcal{F}f) = \mathcal{F}(\text{Ker } f)$  for all  $f$ : the last condition is equivalent to the requirement that  $\mathcal{F}$  preserves short left exact sequences.

Similarly, a functor  $\mathcal{F}$  is *right exact* when it preserves all finite colimits. In other words,  $\mathcal{F}$  is right exact iff it is additive and  $\text{Coker}(\mathcal{F}f) = \mathcal{F}(\text{Coker } f)$  for all  $f$ : the last condition is equivalent to the requirement that  $\mathcal{F}$  preserves short right exact sequences.

In an Abelian category  $\mathcal{A}$ , a *chain complex* is a sequence

$$\dots \longrightarrow c_{n+1} \xrightarrow{\partial_{n+1}} c_n \xrightarrow{\partial_n} c_{n-1} \longrightarrow \dots$$

of composable arrows, with  $\partial_n \partial_{n+1} = 0$  for all  $n$ . The sequence need not be exact at  $c_n$ ; the deviation from exactness is measured by the *nth homology object*

$$H_n c = \text{Ker}(\partial_n : c_n \longrightarrow c_{n-1}) / \text{Im}(\partial_{n+1} : c_{n+1} \longrightarrow c_n).$$

Similarly, a *cochain complex* in an Abelian category  $\mathcal{A}$  is a sequence

$$\dots \longrightarrow w_{n+1} \xrightarrow{d_{n+1}} w_n \xrightarrow{d_n} w_{n-1} \longrightarrow \dots$$

of composable arrows, with  $d_n d_{n+1} = 0$  for all  $n$ . The sequence need not be exact at  $w_n$ ; the deviation from exactness is measured by the  $n$ th *cohomology object*

$$H^n w = \text{Ker}(d_{n+1} : w_n \longrightarrow w_{n+1}) / \text{Im}(d_n : w_{n-1} \longrightarrow w_n).$$

A *cycle* is a chain  $C$  such that  $\partial C = 0$ . A *boundary* is a chain  $C$  such that  $C = \partial B$ , for any other chain  $B$ .

A *cocycle* (a *closed form*) is a cochain  $\omega$  such that  $d\omega = 0$ . A *coboundary* (an *exact form*) is a cochain  $\omega$  such that  $\omega = d\theta$ , for any other cochain  $\theta$ .

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## Geometric Basis of Human–Like Biomechanics

In this Chapter we develop the geometric structure of modern biomechanics.

### 2.1 Biomechanical Manifold $M$

The core of geometrodynamics is the concept of the *manifold*, the stage where our *covariant force law*,  $F_i = mg_{ij}a^j$ , works. To get some dynamical feeling before we dive into more serious geometry, let us consider a simple 3DOF biomechanical system (e.g., a representative point of the center of mass of the human body) determined by three *generalized coordinates*  $q^i = \{q^1, q^2, q^3\}$ . There is a unique way to represent this system as a 3D manifold, such that to each point of the manifold there corresponds a definite configuration of the biomechanical system with coordinates  $q^i$ ; therefore, we have a geometric representation of the configurations of our biomechanical system. For this reason, the manifold is called the *configuration manifold*. If the biomechanical system moves in any way, its coordinates are given as the functions of the time. Thus, the motion is given by equations of the form:  $q^i = q^i(t)$ . As  $t$  varies we observe that the system's *representative point* in the configuration manifold describes a *curve* and  $q^i = q^i(t)$  are the equations of this curve.

On the other hand, a *topological manifold* is a separable Hausdorff space  $M$  which is locally homeomorphic to  $\mathbb{R}^n$  (see, e.g., [Tho79, Hir76, Hel01, Lee00, Lee02]). So, a topological manifold has the following properties:

1.  $M$  is a *Hausdorff space*: For every pair of points  $m_1, m_2 \in M$ , there are disjoint open subsets  $U, V \subset M$  such that  $m_1 \in U$  and  $m_2 \in V$ .
2.  $M$  is *second countable*: There exists a countable basis for the topology of  $M$ .
3.  $M$  is *locally Euclidean of dimension  $n$* : Every point of  $M$  has a neighborhood that is homeomorphic to an open subset of  $\mathbb{R}^n$ .

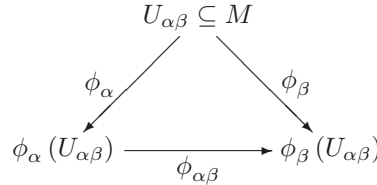
This further implies that for any point  $m \in M$  there is a homeomorphism  $\phi : U \rightarrow \phi(U) \subseteq \mathbb{R}^n$ , where  $U$  is an open neighborhood of  $m$  in  $M$  and  $\phi(U)$

is an open subset in  $\mathbb{R}^n$ . The pair  $(U, \phi)$  is called a *coordinate chart* at a point  $m \in M$ .

**2.1.1 Definition of the Manifold  $M$**

Given a chart  $(U, \phi)$ , we call the set  $U$  a *coordinate domain*, or a coordinate neighborhood of each of its points. If in addition  $\phi(U)$  is an open ball in  $\mathbb{R}^n$ , then  $U$  is called a *coordinate ball*. The map  $\phi$  is called a (*local*) *coordinate map*, and the component functions  $(x^1, \dots, x^n)$  of  $\phi$ , defined by  $\phi(m) = (x^1(m), \dots, x^n(m))$ , are called *local coordinates* on  $U$ .

Two charts  $(U_1, \phi_1)$  and  $(U_2, \phi_2)$  such that  $U_1 \cap U_2 \neq \emptyset$  are called *compatible* if  $\phi_1(U_1 \cap U_2)$  and  $\phi_2(U_2 \cap U_1)$  are open subsets of  $\mathbb{R}^n$ . A family  $(U_\alpha, \phi_\alpha)_{\alpha \in A}$  of compatible charts on  $M$  such that the  $U_\alpha$  form a *cover* of  $M$  is called an *atlas*. The maps  $\phi_{\alpha\beta} = \phi_\beta \circ \phi_\alpha^{-1} : \phi_\alpha(U_{\alpha\beta}) \rightarrow \phi_\beta(U_{\alpha\beta})$  are called the *chart changings*, or *transition maps*, for the atlas  $(U_\alpha, \phi_\alpha)_{\alpha \in A}$ , where  $U_{\alpha\beta} = U_\alpha \cap U_\beta$ , so that we have a commutative triangle:



An atlas  $(U_\alpha, \phi_\alpha)_{\alpha \in A}$  for a manifold  $M$  is said to be a  $C^k$ -*atlas*, if all transition maps  $\phi_{\alpha\beta} : \phi_\alpha(U_{\alpha\beta}) \rightarrow \phi_\beta(U_{\alpha\beta})$  are differentiable of class  $C^k$ . Two  $C^k$  atlases are called  $C^k$ -*equivalent*, if their union is again a  $C^k$ -atlas for  $M$ . An equivalence class of  $C^k$ -atlases is called a  $C^k$ -*structure* on  $M$ . In other words, a smooth structure on  $M$  is a *maximal* smooth atlas on  $M$ , i.e., such an atlas that is not contained in any strictly larger smooth atlas. By a  $C^k$ -*manifold*  $M$ , we mean a topological manifold together with a  $C^k$ -structure and a chart on  $M$  will be a chart belonging to some atlas of the  $C^k$ -structure. Smooth manifold means  $C^\infty$ -manifold, and the word ‘*smooth*’ is used synonymously for  $C^\infty$ . However, for most of our biomechanical needs, the weaker requirement,  $C^k$  would be sufficient. In case of any doubt, we can simply replace  $C^k$  with  $C^\infty$ .

Sometimes the terms ‘local coordinate system’ or ‘parametrization’ are used instead of charts. That  $M$  is not defined with any particular atlas, but with an equivalence class of atlases, is a mathematical formulation of the *general covariance* principle. Every suitable coordinate system is equally good. A Euclidean chart may well suffice for an open subset of  $\mathbb{R}^n$ , but this coordinate system is not to be preferred to the others, which may require many charts (as with polar coordinates), but are more convenient in other respects.

For example, the atlas of a  $n$ -sphere  $S^n$  has two charts. If  $N = (1, 0, \dots, 0)$  and  $S = (-1, \dots, 0, 0)$  are the north and south poles of  $S^n$  respectively, then the two charts are given by the stereographic projections from  $N$  and  $S$ :

$$\phi_1 : S^n \setminus \{N\} \rightarrow \mathbb{R}^n, \phi_1(x^1, \dots, x^{n+1}) = (x^2/(1 - x^1), \dots, x^{n+1}/(1 - x^1)),$$

and

$$\phi_2 : S^n \setminus \{S\} \rightarrow \mathbb{R}^n, \phi_2(x^1, \dots, x^{n+1}) = (x^2/(1 + x^1), \dots, x^{n+1}/(1 + x^1)),$$

and the overlap map  $\phi_2 \circ \phi_1^{-1} : \mathbb{R}^n \setminus \{0\} \rightarrow \mathbb{R}^n \setminus \{0\}$  is given by the diffeomorphism  $(\phi_2 \circ \phi_1^{-1})(z) = z/\|z\|^2$ , for  $z$  in  $\mathbb{R}^n \setminus \{0\}$ , from  $\mathbb{R}^n \setminus \{0\}$  to itself.

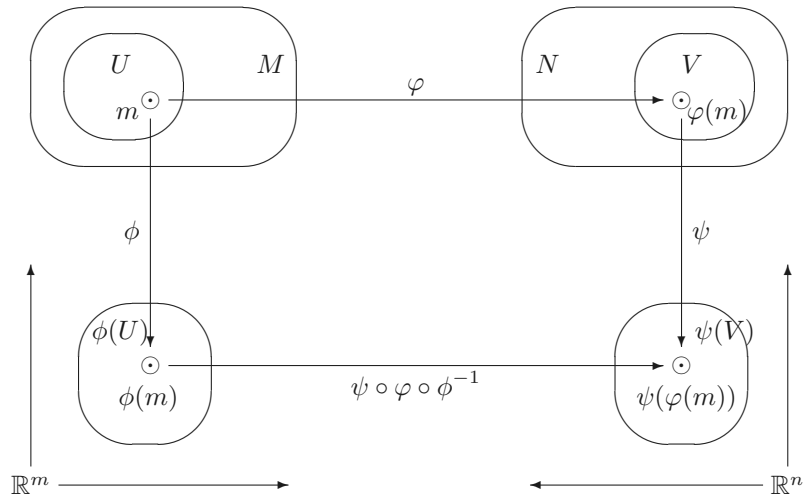
Various *additional structures* can be imposed on  $\mathbb{R}^n$ , and the corresponding manifold  $M$  will inherit them through its covering by charts. For example, if a covering by charts takes their values in a *Banach space*  $E$ , then  $E$  is called the *model space* and  $M$  is referred to as a  $C^k$ -*Banach manifold* modelled on  $E$ . Similarly, if a covering by charts takes their values in a *Hilbert space*  $\mathcal{H}$ , then  $\mathcal{H}$  is called the *model space* and  $M$  is referred to as a  $C^k$ -*Hilbert manifold* modelled on  $\mathcal{H}$ . If not otherwise specified, we will consider  $M$  to be an Euclidean manifold, with its covering by charts taking their values in  $\mathbb{R}^n$ .

For a Hausdorff  $C^k$ -manifold the following properties are equivalent [KMS93]:

1. It is paracompact.
2. It is metrizable.
3. It admits a Riemannian metric.
4. Each connected component is separable.

### 2.1.2 Smooth Maps Between Manifolds

A map  $\varphi : M \rightarrow N$  between two manifolds  $M$  and  $N$ , with  $M \ni m \mapsto \varphi(m) \in N$ , is called a *smooth map*, or  $C^k$ -map, if we have the following charting:



This means that for each  $m \in M$  and each chart  $(V, \psi)$  on  $N$  with  $\varphi(m) \in V$  there is a chart  $(U, \phi)$  on  $M$  with  $m \in U, \varphi(U) \subseteq V$ , and  $\Phi = \psi \circ \varphi \circ \phi^{-1}$  is  $C^k$ , that is, the following diagram commutes:

$$\begin{array}{ccc}
 M \supseteq U & \xrightarrow{\varphi} & V \subseteq N \\
 \downarrow \phi & & \downarrow \psi \\
 \phi(U) & \xrightarrow{\Phi} & \psi(V)
 \end{array}$$

Let  $M$  and  $N$  be smooth manifolds and let  $\varphi : M \rightarrow N$  be a smooth map. The map  $\varphi$  is called a *covering*, or equivalently,  $M$  is said to *cover*  $N$ , if  $\varphi$  is surjective and each point  $n \in N$  admits an open neighborhood  $V$  such that  $\varphi^{-1}(V)$  is a union of disjoint open sets, each diffeomorphic via  $\varphi$  to  $V$ .

A  $C^k$ -map  $\varphi : M \rightarrow N$  is called a  $C^k$ -*diffeomorphism* if  $\varphi$  is a bijection,  $\varphi^{-1} : N \rightarrow M$  exists and is also  $C^k$ . Two manifolds are called diffeomorphic if there exists a diffeomorphism between them.

All smooth manifolds and smooth maps between them form the category  $\mathcal{M}$ .

The most important examples of biomechanical manifolds have also an additional group structure and thus belong to the *category of Lie groups*  $\mathcal{G}$ .

## 2.2 Biomechanical Bundles

In this section we introduce secondary concepts of *biomechanical bundles*, derived from the primary concept of the manifold.

### 2.2.1 The Tangent Bundle of the Manifold $M$

Recall that if  $[a, b]$  is a closed interval, a  $C^0$ -map  $\gamma : [a, b] \rightarrow M$  is said to be *differentiable* at the endpoint  $a$  if there is a chart  $(U, \phi)$  at  $\gamma(a)$  such that the following limit exists and is finite [AMR88]:

$$\frac{d}{dt}(\phi \circ \gamma)(a) \equiv (\phi \circ \gamma)'(a) = \lim_{t \rightarrow a} \frac{(\phi \circ \gamma)(t) - (\phi \circ \gamma)(a)}{t - a}. \quad (2.1)$$

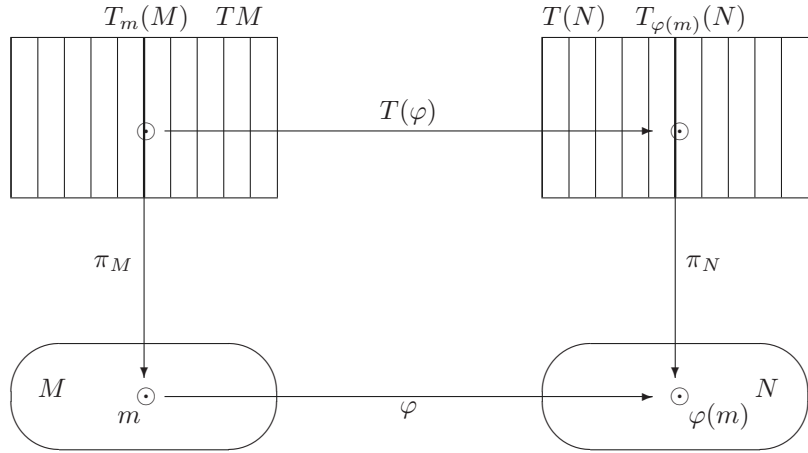
Generalizing (2.1), we get the notion of the *curve on a manifold*. For a smooth manifold  $M$  and a point  $m \in M$  a curve at  $m$  is a  $C^0$ -map  $\gamma : I \rightarrow M$  from an interval  $I \subset \mathbb{R}$  into  $M$  with  $0 \in I$  and  $\gamma(0) = m$ .

Two curves  $\gamma_1$  and  $\gamma_2$  passing through a point  $m \in U$  are *tangent at  $m$*  with respect to the chart  $(U, \phi)$  if  $(\phi \circ \gamma_1)'(0) = (\phi \circ \gamma_2)'(0)$ . Thus, two curves are tangent if they have identical tangent vectors (same direction and speed) in a local chart on a manifold.

For a smooth manifold  $M$  and a point  $m \in M$ , the *tangent space*  $T_m M$  to  $M$  at  $m$  is the *set of equivalence classes* of curves at  $m$ :

$$T_m M = \{[\gamma]_m : \gamma \text{ is a curve at a point } m \in M\}.$$

A  $C^k$ -map  $\varphi : M \ni m \mapsto \varphi(m) \in N$  between two manifolds  $M$  and  $N$  induces a linear map  $T_m \varphi : T_m M \rightarrow T_{\varphi(m)} N$  for each point  $m \in M$ , called a *tangent map*, if we have:



i.e., the following diagram commutes:

$$\begin{array}{ccc}
 T_m M & \xrightarrow{T_m \varphi} & T_{\varphi(m)} N \\
 \pi_M \downarrow & & \downarrow \pi_N \\
 M \ni m & \xrightarrow{\varphi} & \varphi(m) \in N
 \end{array}$$

with the *natural projection*, or *tangent bundle projection*,  $\pi_M : TM \rightarrow M$ , given by  $\pi_M(T_m M) = m$ , that takes a tangent vector  $v$  to the point  $m \in M$  at which the vector  $v$  is attached i.e.,  $v \in T_m M$ .

For a smooth manifold  $M$  of dimension  $n$ , its *tangent bundle*  $TM$  is the disjoint union of all its tangent spaces  $T_m M$  at all points  $m \in M$ , i.e.,  $TM = \bigsqcup_{m \in M} T_m M$ .

If  $M$  is an  $n$ -manifold, then  $TM$  is a  $2n$ -manifold. To define the smooth structure on  $TM$ , we need to specify how to construct local coordinates on  $TM$ . To do this, let  $(x^1(m), \dots, x^n(m))$  be local coordinates of a point  $m$  on  $M$  and let  $(v^1(m), \dots, v^n(m))$  be components of a tangent vector in this coordinate system. Then the  $2n$  numbers  $(x^1(m), \dots, x^n(m), v^1(m), \dots, v^n(m))$  give a local coordinate system on  $TM$ . This is the basic idea one uses to prove that indeed  $TM$  is a  $2n$ -manifold [MR99].

$TM = \bigsqcup_{m \in M} T_m M$  defines a family of vector spaces parameterized by  $M$ .

The inverse image  $\pi_M^{-1}(m)$  of a point  $m \in M$  under the natural projection  $\pi_M$  is the tangent space  $T_m M$ . This space is called the *fibre* of the tangent bundle over the point  $m \in M$  [Sti51].

A  $C^k$ -map  $\varphi : M \rightarrow N$  between two manifolds  $M$  and  $N$  induces a linear *tangent map*  $T\varphi : TM \rightarrow TN$  between their tangent bundles, i.e., the following diagram commutes:

$$\begin{array}{ccc}
 TM & \xrightarrow{T\varphi} & TN \\
 \pi_M \downarrow & & \downarrow \pi_N \\
 M & \xrightarrow{\varphi} & N
 \end{array}$$

All tangent bundles and their tangent maps form the category  $\mathcal{TB}$ . The category  $\mathcal{TB}$  is the natural framework for *Lagrangian biomechanics*.

Now, we can formulate the *global version of the chain rule*. If  $\varphi : M \rightarrow N$  and  $\psi : N \rightarrow P$  are two smooth maps, then we have  $T(\psi \circ \varphi) = T\psi \circ T\varphi$  (see [KMS93]). In other words, we have a functor  $T : \mathcal{M} \Rightarrow \mathcal{TB}$  from the category  $\mathcal{M}$  of smooth manifolds to the category  $\mathcal{TB}$  of their tangent bundles:

$$\begin{array}{ccc}
 M & & TM \\
 \varphi \swarrow & & \swarrow T\varphi \\
 N & \xrightarrow{\psi} & P \\
 & \searrow \psi \circ \varphi & \\
 & & TP \\
 & \swarrow T\psi & \\
 TN & & TP
 \end{array}
 \quad \xrightarrow{T}$$

### 2.2.2 The Cotangent Bundle of the Manifold $M$

The *dual* notion to the tangent space  $T_m M$  to a smooth manifold  $M$  at a point  $m$  is its *cotangent space*  $T_m^* M$  at the same point  $m$ . Similarly to the tangent bundle, for a smooth manifold  $M$  of dimension  $n$ , its *cotangent bundle*  $T^* M$  is the disjoint union of all its cotangent spaces  $T_m^* M$  at all points  $m \in M$ , i.e.,  $T^* M = \bigsqcup_{m \in M} T_m^* M$ . Therefore, the cotangent bundle of an  $n$ -manifold  $M$  is

the vector bundle  $T^* M = (TM)^*$ , the (real) dual of the tangent bundle  $TM$ .

If  $M$  is an  $n$ -manifold, then  $T^* M$  is a  $2n$ -manifold. To define the smooth structure on  $T^* M$ , we need to specify how to construct local coordinates on  $T^* M$ . To do this, let  $(x^1(m), \dots, x^n(m))$  be local coordinates of a point  $m$  on  $M$  and let  $(p_1(m), \dots, p_n(m))$  be components of a covector in this coordinate system. Then the  $2n$  numbers  $(x^1(m), \dots, x^n(m), p_1(m), \dots, p_n(m))$  give a local coordinate system on  $T^* M$ . This is the basic idea one uses to prove that indeed  $T^* M$  is a  $2n$ -manifold.

$T^* M = \bigsqcup_{m \in M} T_m^* M$  defines a family of vector spaces parameterized by  $M$ , with the *conatural projection*, or *cotangent bundle projection*,  $\pi_M^* : T^* M \rightarrow M$ , given by  $\pi_M^*(T_m^* M) = m$ , that takes a covector  $p$  to the point  $m \in M$  at which the covector  $p$  is attached i.e.,  $p \in T_m^* M$ . The inverse image  $\pi_M^{-1}(m)$  of a point  $m \in M$  under the conatural projection  $\pi_M^*$  is the cotangent space  $T_m^* M$ . This space is called the *fibre* of the cotangent bundle over the point  $m \in M$ .

In a similar way, a  $C^k$ -map  $\varphi : M \rightarrow N$  between two manifolds  $M$  and  $N$  induces a linear *cotangent map*  $T^* \varphi : T^* M \rightarrow T^* N$  between their cotangent

bundles, i.e., the following diagram commutes:

$$\begin{array}{ccc}
 T^*M & \xrightarrow{T^*\varphi} & T^*N \\
 \pi_M^* \downarrow & & \downarrow \pi_N^* \\
 M & \xrightarrow{\varphi} & N
 \end{array}$$

All cotangent bundles and their cotangent maps form the category  $\mathcal{T}^*\mathcal{B}$ . The category  $\mathcal{T}^*\mathcal{B}$  is the natural stage for *Hamiltonian biomechanics*.

Now, we can formulate the *dual version of the global chain rule*. If  $\varphi : M \rightarrow N$  and  $\psi : N \rightarrow P$  are two smooth maps, then we have  $T^*(\psi \circ \varphi) = T^*\psi \circ T^*\varphi$ . In other words, we have a cofunctor  $T^* : \mathcal{M} \Rightarrow \mathcal{T}^*\mathcal{B}$  from the category  $\mathcal{M}$  of smooth manifolds to the category  $\mathcal{T}^*\mathcal{B}$  of their cotangent bundles:

$$\begin{array}{ccc}
 & M & \\
 \varphi \swarrow & & \searrow (\psi \circ \varphi) \\
 N & \xrightarrow{\psi} & P
 \end{array}
 \xrightarrow{T^*}
 \begin{array}{ccc}
 & T^*M & \\
 T^*\varphi \swarrow & & \searrow T^*(\psi \circ \varphi) \\
 T^*N & \xleftarrow{T^*\psi} & T^*P
 \end{array}$$

### 2.2.3 Fibre Bundles

#### Vector Bundles

Both the tangent bundle  $(TM, \pi_M, M)$  and the cotangent bundle  $(T^*M, \pi_M^*, M)$  are examples of a more general notion of *vector bundle*  $(E, \pi, M)$  of a manifold  $M$ , which consists of manifolds  $E$  (the total space) and  $M$  (the base), as well as a smooth map  $\pi : E \rightarrow M$  (the projection) together with an equivalence class of vector bundle atlases (in this section we follow [KMS93]). A vector bundle atlas  $(U_\alpha, \phi_\alpha)_{\alpha \in A}$  for  $(E, \pi, M)$  is a set of pairwise compatible vector bundle charts  $(U_\alpha, \phi_\alpha)$  such that  $(U_\alpha)_{\alpha \in A}$  is an open cover of  $M$ . Two vector bundle atlases are called equivalent, if their union is again a vector bundle atlas.

On each fibre  $E_m = \pi^{-1}(m)$  corresponding to the point  $m \in M$  there is a unique structure of a real vector space, induced from any vector bundle chart  $(U_\alpha, \phi_\alpha)$  with  $m \in U_\alpha$ . A section  $u$  of  $(E, \pi, M)$  is a smooth map  $u : M \rightarrow E$  with  $\pi \circ u = Id_M$ .

Let  $(E, \pi_M, M)$  and  $(F, \pi_N, N)$  be vector bundles. A *vector bundle homomorphism*  $\Phi : E \rightarrow F$  is a fibre linear smooth map induced by the smooth map  $\varphi : M \rightarrow N$  between the base manifolds  $M$  and  $N$ , i.e., the following diagram commutes:

$$\begin{array}{ccc}
 E & \xrightarrow{\Phi} & F \\
 \pi_M \downarrow & & \downarrow \pi_N \\
 M & \xrightarrow{\varphi} & N
 \end{array}$$

We say that  $\Phi$  covers  $\varphi$ . If  $\Phi$  is invertible, it is called a *vector bundle isomorphism*.

All smooth vector bundles together with their homomorphisms form a category  $\mathcal{VB}$ .

If  $(E, \pi, M)$  is a vector bundle which admits a vector bundle atlas  $(U_\alpha, \phi_\alpha)_{\alpha \in A}$  with the given open cover, then, we have  $\phi_\alpha \circ \phi_\beta^{-1}(m, v) = (m, \phi_{\alpha\beta}(m)v)$  for  $C^k$ -transition functions  $\phi_{\alpha\beta} : U_{\alpha\beta} = U_\alpha \cap U_\beta \rightarrow GL(V)$  (where we have fixed a standard fibre  $V$ ). This family of transition maps satisfies the *cocycle condition*

$$\begin{cases} \phi_{\alpha\beta}(m) \cdot \phi_{\beta\gamma}(m) = \phi_{\alpha\gamma}(m) & \text{for each } m \in U_{\alpha\beta\gamma} = U_\alpha \cap U_\beta \cap U_\gamma, \\ \phi_{\alpha\alpha}(m) = e & \text{for all } m \in U_\alpha. \end{cases}$$

The family  $(\phi_{\alpha\beta})$  is called the *cocycle* of transition maps for the vector bundle atlas  $(U_\alpha, \phi_\alpha)$ .

Now, let us suppose that the same vector bundle  $(E, \pi, M)$  is described by an equivalent vector bundle atlas  $(U_\alpha, \psi_\alpha)_{\alpha \in A}$  with the same open cover  $(U_\alpha)$ . Then the vector bundle charts  $(U_\alpha, \phi_\alpha)$  and  $(U_\alpha, \psi_\alpha)$  are compatible for each  $\alpha$ , so  $\psi_\alpha \circ \phi_\beta^{-1}(m, v) = (m, \tau_\alpha(m)v)$  for some  $\tau_\alpha : U_\alpha \rightarrow GL(V)$ . We get

$$\tau_\alpha(m) \phi_{\alpha\beta}(m) = \phi_{\alpha\beta}(m) \tau_\beta(m) \quad \text{for all } m \in U_{\alpha\beta},$$

and we say that the two cocycles  $(\phi_{\alpha\beta})$  and  $(\psi_{\alpha\beta})$  of transition maps over the cover  $(U_\alpha)$  are *cohomologous*. If  $GL(V)$  is an Abelian group, i.e., if the standard fibre  $V$  is of real or complex dimension 1, then the cohomology classes of cocycles  $(\phi_{\alpha\beta})$  over the open cover  $(U_\alpha)$  form a usual cohomology group  $H^1(M, GL(V))$  with coefficients in the sheaf  $GL(V)$  [KMS93].

Let  $(E, \pi, M)$  be a vector bundle and let  $\varphi : N \rightarrow M$  be a smooth map between the base manifolds  $N$  and  $M$ . Then there exists the *pull-back vector bundle*  $(\varphi^*E, \varphi^*\pi, \varphi^*N)$  with the same typical fibre and a vector bundle homomorphism, given by the commutative diagram [KMS93]:

$$\begin{array}{ccc}
 \varphi^*E & \xrightarrow{\pi^*\varphi} & E \\
 \varphi^*\pi \downarrow & & \downarrow \pi \\
 N & \xrightarrow{\varphi} & M
 \end{array}$$

The vector bundle  $(\varphi^*E, \varphi^*\pi, \varphi^*N)$  is constructed as follows. Let  $E = VB(\phi_{\alpha\beta})$  denote that  $E$  is described by a cocycle  $(\phi_{\alpha\beta})$  of transition maps over

an open cover  $(U_\alpha)$  of  $M$ . Then  $(\phi_{\alpha\beta} \circ \varphi)$  is a cocycle of transition maps over the open cover  $(\varphi^{-1}(U_\alpha))$  of  $N$  and the bundle is given by  $\varphi^*E = VB(\phi_{\alpha\beta} \circ \varphi)$ .

### The Second Vector Bundle of the Manifold $M$

Let  $(E, \pi, M)$  be a vector bundle over the biomechanical manifold  $M$  with fibre addition  $+_E : E \times_M E \rightarrow E$  and fibre scalar multiplication  $m_t^E : E \rightarrow E$ . Then  $(TE, \pi_E, E)$ , the tangent bundle of the manifold  $E$ , is itself a vector bundle, with fibre addition denoted by  $+_{TE}$  and scalar multiplication denoted by  $m_t^{TE}$ . The *second vector bundle* structure on  $(TE, T\pi, TM)$ , is the ‘derivative’ of the original one on  $(E, \pi, M)$ . In particular, the space  $\{\Xi \in TE : T\pi \cdot \Xi = 0 \in TM\} = (Tp)^{-1}(0)$  is denoted by  $VE$  and is called the *vertical bundle* over  $E$ . Its main characteristics are *vertical lift* and *vertical projection* (see [KMS93] for details).

All of this is valid for the *second tangent bundle*  $T^2M = TTM$  of a manifold, but here we have one more natural structure at our disposal. The *canonical flip* or *involution*  $\kappa_M : T^2M \rightarrow T^2M$  is defined locally by

$$(T^2\phi \circ \kappa_M \circ T^2\phi^{-1})(x, \xi; \eta, \zeta) = (x, \eta; \xi, \zeta).$$

where  $(U, \phi)$  is a local chart on  $M$  (this definition is invariant under changes of charts). The flip  $\kappa_M$  has the following properties (see [KMS93]):

1.  $\kappa_M \circ T^2f = T^2f \circ \kappa_M$  for each  $f \in C^k(M, N)$ ;
2.  $T(\pi_M) \circ \kappa_M = \pi_{TM}$ ;
3.  $\pi_{TM} \circ \kappa_M = T(\pi_M)$ ;
4.  $\kappa_M^{-1} = \kappa_M$ ;
5.  $\kappa_M$  is a linear isomorphism from the bundle  $(TTM, T(\pi_M), TM)$  to  $(TTM, \pi_{TM}, TM)$ , so it interchanges the two vector bundle structures on  $TTM$ ;
6.  $\kappa_M$  is the unique smooth map  $TTM \rightarrow TTM$  which, for each  $\gamma : \mathbb{R} \rightarrow M$ , satisfies

$$\partial_t \partial_s \gamma(t, s) = \kappa_M \partial_t \partial_s \gamma(t, s).$$

In a similar way the second cotangent bundle of a manifold  $M$  can be defined. Even more, for every manifold there is a *geometric isomorphism* between the bundles  $TT^*M = T(T^*M)$  and  $T^*TM = T^*(TM)$  [MS78].

### General Fibre Bundles

A vector bundle is a special case of a more general structure, a *fibre bundle* [Sti51], a topological construction which itself is a class of *fibrations*.

Let  $I = [0, 1]$ . A map  $p : E \rightarrow B$  is said to have the *homotopy lifting property* (HLP) with respect to a topological space  $X$  if for every map  $f : X \rightarrow E$  and homotopy  $G : X \times I \rightarrow B$  of  $p \circ f$  there is a homotopy  $F : X \times I \rightarrow E$  with  $f = F_0$  and  $p \circ F = G$ .  $F$  is said to be a *lifting* of  $G$ .  $p$  is called a *fibration*

if it has the HLP for all spaces  $X$  and a weak fibration if it has the HLP for all disks  $D^n$ ,  $n \geq 0$ . If  $b_0 \in B$  is the base point, then the space  $F = p^{-1}(b_0)$  is called the *fibre* of  $p$ . The projection onto the first factor,  $p_B : B \times F \rightarrow B$ , is clearly a fibration and is called the *trivial fibration* over  $B$  with fibre  $F$  [Swi75].

A *fibre bundle* is a quadruple  $(B, p, E, F)$  where the space  $B$  is called the *base space*,  $E$  is the *total space*, and the vector spaces  $F = p^{-1}(b)$  are the fibers. Here the projection  $p : E \rightarrow B$  is such a map that  $B$  has an open covering  $\{U_\alpha\}_{\alpha \in A}$ , and for each  $\alpha \in A$  there is a homeomorphism  $\phi_\alpha : U_\alpha \times F \rightarrow p^{-1}U_\alpha$  such that  $p \circ \phi_\alpha = p_{U_\alpha} : U_\alpha \times F \rightarrow U_\alpha$  [Sti51]. In other words, locally  $p : E \rightarrow B$  looks like a trivial fibration. If  $B$  is paracompact, one can show that  $p : E \rightarrow B$  is a fibration. If  $(B, p, E, F)$  is a fibre bundle, then  $p : E \rightarrow B$  is a weak fibration [Swi75]. A map  $p : E \rightarrow B$  has a *local cross-section* at a point  $x \in B$  if there is a neighborhood  $U$  of  $x$  in  $B$  and a map  $\lambda : U \rightarrow E$  with  $p \circ \lambda = 1_U$ .

A fibre bundle  $(B, p, E, F)$  with  $F$  discrete is called a covering of  $B$ .  $p$  is called a *covering projection* and  $E$  a covering space over  $B$ . For example, the  $n$ -torus  $T^n$  is the  $n$ -fold Cartesian product  $S^1 \times S^1 \times \dots \times S^1$ . The map  $p : \mathbb{R}^n \rightarrow T^n$  defined by  $p(r_1, r_2, \dots, r_n) = (e^{2\pi i r_1}, e^{2\pi i r_2}, \dots, e^{2\pi i r_n})$  is a covering projection. The fibre is the set of integer lattice points in  $\mathbb{R}^n$ . Since  $\mathbb{R}^n$  is contractible, it follows that its  $k$ th homotopy group  $\pi_k(T^n) = 0$  for  $k \geq 2$  [Swi75].

All smooth fibre bundles together with their homomorphisms form a category  $\mathcal{FB}$ .

Our vector bundle defined above represents an important class of fibre bundles for which every fibre has the structure of a vector space in a way which is compatible on neighboring fibres. Let  $F$  denote  $\mathbb{R}, \mathbb{C}$  or  $\mathbb{H}$  – the real, complex or quaternionic numbers. An  $n$ D  $F$ -vector bundle is a fibre bundle  $\xi = (B, p, E, F^n)$  in which each fibre  $p^{-1}(b)$ ,  $b \in B$ , has the structure of a vector space over  $F$  such that there is an open covering  $\{U_\alpha : \alpha \in A\}$  of  $B$  and for each  $\alpha \in A$  a homeomorphism  $\phi_\alpha : U_\alpha \times F^n \rightarrow p^{-1}U_\alpha$  with  $p \circ \phi_\alpha = p_{U_\alpha}$  and  $(\phi_\alpha|_{\{b\} \times F^n}) : \{b\} \times F^n \rightarrow p^{-1}(b)$  a vector space isomorphism for each  $b \in U_\alpha$ . We speak of real, complex or quaternionic vector bundles according to whether  $F = \mathbb{R}, \mathbb{C}$  or  $\mathbb{H}$  [Swi75].

For example, for any space  $B$  the trivial  $n$ D  $F$ -vector bundle is  $(B, p_B, B \times F^n, F^n)$ .

If we let  $E$  be the quotient space of  $I \times \mathbb{R}$  under the identifications  $(0, t) \sim (1, -t)$ , then the projection  $I \times \mathbb{R} \rightarrow I$  induces a map  $p : E \rightarrow S^1$  which is a 1D vector bundle, or *line bundle*. Since  $E$  is homeomorphic to a Möbius band with its boundary circle deleted, we call this bundle the *Möbius bundle* [Hat02].

For any  $n \geq 1$  the *tangent bundle*  $TS^n$  of the unit  $n$ -sphere  $S^n = \{x \in \mathbb{R}^{n+1} : \|x\| = 1\}$  is the fibre bundle  $(S^n, p, E, \mathbb{R}^n)$ , where  $E = \{(x, y) \in \mathbb{R}^{n+1} \times \mathbb{R}^{n+1} : \|x\| = 1, x \cdot y = 0\}$  and  $p : E \rightarrow S^n$  is defined by  $p(x, y) = x$ .

For any  $n \geq 1$  the *normal bundle*  $NS^n$  of the  $n$ -sphere  $S^n$  is the fibre bundle  $(S^n, p', E', \mathbb{R}^1)$ , where  $E' = \{(x, y) \in \mathbb{R}^{n+1} \times \mathbb{R}^{n+1} : \|x\| = 1, y = \lambda x, \lambda \in \mathbb{R}^1\}$  and  $p' : E' \rightarrow S^n$  is defined by  $p'(x, y) = x$  [Swi75].

The only two vector bundles with base space  $B$  a circle and 1D fibre  $F$  are the Möbius band and the annulus, but the classification of all the different vector bundles over a given base space with fibre of a given dimension is quite difficult in general. For example, when the base space is a high-dimensional sphere and the dimension of the fibre is at least three, then the classification is of the same order of difficulty as the fundamental but still largely unsolved problem of computing the homotopy groups of spheres [Hat02].

Now, there is a natural direct sum operation for vector bundles over a fixed base space  $X$ , which in each fibre reduces just to direct sum of vector spaces. Using this, one can obtain a weaker notion of isomorphism of vector bundles by defining two vector bundles over the same base space  $X$  to be stably isomorphic if they become isomorphic after direct sum with product vector bundles  $X \times \mathbb{R}^n$  for some  $n$ , perhaps different  $n$ 's for the two given vector bundles. Then it turns out that the set of stable isomorphism classes of vector bundles over  $X$  forms an Abelian group under the direct sum operation, at least if  $X$  is compact Hausdorff. The traditional notation for this group is  $\widetilde{KO}(X)$ . In the case of spheres the groups  $\widetilde{KO}(S^n)$  have the quite unexpected property of being periodic in  $n$ . This is called *Bott periodicity*, and the values of  $\widetilde{KO}(S^n)$  are given by the following table [Hat02]:

$n \bmod 8$	1	2	3	4	5	6	7	8
$\widetilde{KO}(S^n)$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$

For example,  $\widetilde{KO}(S^1)$  is  $\mathbb{Z}_2$ , a cyclic group of order two, and a generator for this group is the Möbius bundle. This has order two since the direct sum of two copies of the Möbius bundle is the product  $S^1 \times \mathbb{R}^1$ , as one can see by embedding two Möbius bands in a solid torus so that they intersect orthogonally along the common core circle of both bands, which is also the core circle of the solid torus.

The complex version of  $\widetilde{KO}(X)$ , called  $\widetilde{K}(X)$ , is constructed in the same way as  $\widetilde{KO}(X)$  but using vector bundles whose fibers are vector spaces over  $\mathbb{C}$  rather than  $\mathbb{R}$ . The complex form of Bott Periodicity asserts simply that  $\widetilde{K}(S^n)$  is  $\mathbb{Z}$  for  $n$  even and 0 for  $n$  odd, so the period is two rather than eight.

The groups  $\widetilde{K}(X)$  and  $\widetilde{KO}(X)$  for varying  $X$  share certain formal properties with the cohomology groups studied in classical algebraic topology. Using a more general form of Bott periodicity, it is in fact possible to extend the groups  $\widetilde{K}(X)$  and  $\widetilde{KO}(X)$  to a full cohomology theory, families of Abelian groups  $\widetilde{K}^n(X)$  and  $\widetilde{KO}^n(X)$  for  $n \in \mathbb{Z}$  that are periodic in  $n$  of period two and eight, respectively. There is more algebraic structure here than just the additive group structure, however. Tensor products of vector spaces give rise to tensor products of vector bundles, which in turn give product operations

in both real and complex K-theory similar to cup product in ordinary cohomology. Furthermore, exterior powers of vector spaces give natural operations within K-theory [Hat02].

### Tensor Fields as Sections of the Vector Bundle

A *tensor-field*  $\tau \in \Gamma(\mathcal{F}(M))$  of type  $(p, q)$  (see Appendix) on a smooth  $n$ -manifold  $M$  is a *smooth section of the vector bundle*

$$\bigotimes^q T^*M \otimes \bigotimes^p TM = TM \overbrace{\otimes \dots \otimes TM}^{p \text{ times}} \otimes T^*M \overbrace{\otimes \dots \otimes T^*M}^{q \text{ times}}.$$

The coefficients of the tensor-field  $\tau$  are  $C^k$  functions on  $U$ , with  $p$  indices up and  $q$  indices down. The classical position of indices can be explained in modern terms as follows. If  $(U, \phi)$  is a chart at a point  $m \in M$  with local coordinates  $(x^1, \dots, x^n)$ , we have the *holonomous frame field*

$$\partial_{x^{i_1}} \otimes \partial_{x^{i_2}} \otimes \dots \otimes \partial_{x^{i_p}} \otimes dx^{j_1} \otimes dx^{j_2} \dots \otimes dx^{j_q},$$

for  $i \in \{1, \dots, n\}^p$ ,  $j = \{1, \dots, n\}^q$ , over  $U$  of this tensor bundle, and for any  $(p, q)$ -tensor-field  $\tau$  we have

$$\tau|U = \tau_{j_1 \dots j_q}^{i_1 \dots i_p} \partial_{x^{i_1}} \otimes \partial_{x^{i_2}} \otimes \dots \otimes \partial_{x^{i_p}} \otimes dx^{j_1} \otimes dx^{j_2} \dots \otimes dx^{j_q}.$$

For such tensor-fields the Lie derivative along any vector-field is defined, and it is a *derivation* (i.e., both linearity and Leibniz rules hold) with respect to the tensor product. This natural bundle admits many natural transformations. For example, a ‘contraction’ like the trace  $T^*M \otimes TM = L(TM, TM) \rightarrow M \times \mathbb{R}$ , but applied just to one specified factor of type  $T^*M$  and another one of type  $TM$ , is a natural transformation. And any ‘permutation of the same kind of factors’ is a natural transformation.

The tangent bundle  $\pi_M : TM \rightarrow M$  of a manifold  $M$  is a vector bundle over  $M$  such that, given an atlas  $\{(U_\alpha, \varphi_\alpha)\}$  of  $M$ ,  $TM$  is provided with the *holonomic atlas*

$$\Psi = \{(U_\alpha, \varphi_\alpha = T\varphi_\alpha)\}.$$

The associated linear bundle coordinates are the induced coordinates  $(\dot{x}^\lambda)$  at a point  $m \in M$  with respect to the *holonomic frames*  $\{\partial_\lambda\}$  in tangent spaces  $T_m M$ . Their transition functions read (see Appendix)

$$\dot{x}'^\lambda = \frac{\partial x'^\lambda}{\partial x^\mu} \dot{x}^\mu.$$

The tangent bundle  $TM$  is a fibre bundle with the structure group  $GL(\dim M, \mathbb{R})$ .

The cotangent bundle of  $M$  is the dual  $T^*M$  of  $TM$ . It is equipped with the induced coordinates  $(\dot{x}_\lambda)$  at a point  $m \in M$  with respect to *holonomic coframes*  $\{dx^\lambda\}$  dual of  $\{\partial_\lambda\}$ . Their transition functions read

$$\dot{x}'_\lambda = \frac{\partial x'^\mu}{\partial x^\lambda} \dot{x}_\mu.$$

The tensor products

$$(\otimes^m TX) \otimes (\otimes^k T^*X)$$

of the tangent and cotangent bundles are called *tensor bundles*.

### The Natural Vector Bundle

In this section we mainly follow [Mic01, KMS93].

A *vector bundle functor* or *natural vector bundle* is a functor  $\mathcal{F}$  which associates a vector bundle  $(\mathcal{F}(M), \pi_M, M)$  to each  $n$ -manifold  $M$  and a vector bundle homomorphism

$$\begin{array}{ccc} \mathcal{F}(M) & \xrightarrow{\mathcal{F}(\varphi)} & \mathcal{F}(N) \\ \pi_M \downarrow & & \downarrow \pi_N \\ M & \xrightarrow{\varphi} & N \end{array}$$

to each  $\varphi : M \rightarrow N$  in  $\mathcal{M}$ , which covers  $\varphi$  and is fiberwise a linear isomorphism. Two common examples of the vector bundle functor  $\mathcal{F}$  are tangent bundle functor  $T$  (subsection 2.2.1) and cotangent bundle functor  $T^*$  (subsection 2.2.2).

The space of all smooth sections of the vector bundle  $(E, \pi_M, M)$  is denoted by  $\Gamma(E, \pi_M, M)$ . Clearly, it is a vector space with fiberwise addition and scalar multiplication.

Let  $\mathcal{F}$  be a vector bundle functor on  $\mathcal{M}$ . Let  $M$  be a smooth manifold and let  $X \in \mathcal{X}(M)$  be a vector-field on  $M$ . Then the flow  $F_t$  of  $X$  for fixed  $t$ , is a diffeomorphism defined on an open subset of  $M$ . The map

$$\begin{array}{ccc} \mathcal{F}(M) & \xrightarrow{\mathcal{F}(F_t)} & \mathcal{F}(M) \\ \pi_M \downarrow & & \downarrow \pi_M \\ M & \xrightarrow{F_t} & M \end{array}$$

is then a vector bundle isomorphism, defined over an open subset of  $M$ .

We consider a tensor-field  $\tau$  (2.2.3), which is a section  $\tau \in \Gamma(\mathcal{F}(M))$  of the vector bundle  $(\mathcal{F}(M), \pi_M, M)$  and we define for  $t \in \mathbb{R}$

$$F_t^* \tau = \mathcal{F}(F_{-t}) \circ \tau \circ F_t,$$

a local section of the bundle  $\mathcal{F}(M)$ . For each point  $m \in M$  the value  $F_t^* \tau(x) \in \mathcal{F}(M)_m$  is defined, if  $t$  is small enough (depending on  $x$ ). So, in the vector space  $\mathcal{F}(M)_m$  the expression  $\frac{d}{dt} \Big|_{t=0} F_t^* \tau(x)$  makes sense and therefore the section

$$\mathcal{L}_X \tau = \frac{d}{dt} \Big|_{t=0} F_t^* \tau$$

is globally defined and is an element of  $\Gamma(\mathcal{F}(M))$ . It is called the *Lie derivative of the tensor-field  $\tau$  along a vector-field  $X \in \mathcal{X}(M)$*  (see subsection 2.4.1, for details on Lie derivative).

In this situation we have:

1.  $F_t^* F_r^* \tau = F_{t+r}^* \tau$ , whenever defined.
2.  $\frac{d}{dt} F_t^* \tau = F_t^* \mathcal{L}_X \tau = \mathcal{L}_X (F_t^* \tau)$ , so  
 $[\mathcal{L}_X, F_t^*] = \mathcal{L}_X \circ F_t^* - F_t^* \circ \mathcal{L}_X = 0$ , whenever defined.
3.  $F_t^* \tau = \tau$  for all relevant  $t$  iff  $\mathcal{L}_X \tau = 0$ .

Let  $\mathcal{F}_1$  and  $\mathcal{F}_2$  be two vector bundle functors on  $\mathcal{M}$ . Then the (fiberwise) tensor product  $(\mathcal{F}_1 \otimes \mathcal{F}_2)(M) = \mathcal{F}_1(M) \otimes \mathcal{F}_2(M)$  is again a vector bundle functor and for  $\tau_i \in \Gamma(\mathcal{F}_i(M))$  with  $i = 1, 2$ , there is a section  $\tau_1 \otimes \tau_2 \in \Gamma(\mathcal{F}_1 \otimes \mathcal{F}_2)(M)$ , given by the pointwise tensor product.

Also in this situation, for  $X \in \mathcal{X}(M)$  we have

$$\mathcal{L}_X (\tau_1 \otimes \tau_2) = \mathcal{L}_X \tau_1 \otimes \tau_2 + \tau_1 \otimes \mathcal{L}_X \tau_2.$$

In particular, for  $f \in C^k(M, \mathbb{R})$  we have  $\mathcal{L}_X (f \tau) = df(X) \tau + f \mathcal{L}_X \tau$ .

For any vector bundle functor  $\mathcal{F}$  on  $\mathcal{M}$  and  $X, Y \in \mathcal{X}(M)$  we have:

$$[\mathcal{L}_X, \mathcal{L}_Y] = \mathcal{L}_X \circ \mathcal{L}_Y - \mathcal{L}_Y \circ \mathcal{L}_X = \mathcal{L}_{[X, Y]} : \Gamma(\mathcal{F}(M)) \rightarrow \Gamma(\mathcal{F}(M)).$$

### The Pull-Back and Push-Forward

In this subsection we define two important operations, following [AMR88], which will be used in the further text.

Let  $\varphi : M \rightarrow N$  be a  $C^k$  map of manifolds and  $f \in C^k(N, \mathbb{R})$ . Define the *pull-back* of  $f$  by  $\varphi$  by

$$\varphi^* f = f \circ \varphi \in C^k(M, \mathbb{R}).$$

If  $f$  is a  $C^k$  diffeomorphism and  $X \in \mathcal{X}^k(M)$ , the *push-forward* of  $X$  by  $\varphi$  is defined by

$$\varphi_* X = T\varphi \circ X \circ \varphi^{-1} \in \mathcal{X}^k(N).$$

If  $x^i$  are local coordinates on  $M$  and  $y^j$  local coordinates on  $N$ , the preceding formula gives the components of  $\varphi_* X$  by

$$(\varphi_* X)^j(y) = \frac{\partial \varphi^j}{\partial x^i}(x) X^i(x), \quad \text{where } y = \varphi(x).$$

We can interchange pull-back and push-forward by changing  $\varphi$  to  $\varphi^{-1}$ , that is, defining  $\varphi_*$  (resp.  $\varphi^*$ ) by  $\varphi_* = (\varphi^{-1})^*$  (resp.  $\varphi^* = (\varphi^{-1})_*$ ). Thus the *push-forward* of a function  $f$  on  $M$  is  $\varphi_* f = f \circ \varphi^{-1}$  and the *pull-back* of a vector-field  $Y$  on  $N$  is  $\varphi^* Y = (T\varphi)^{-1} \circ Y \circ \varphi$ .

Notice that  $\varphi$  must be a diffeomorphism in order that the pull-back and push-forward operations make sense, the only exception being pull-back of functions. Thus vector-fields can only be pulled back and pushed forward by diffeomorphisms. However, even when  $\varphi$  is not a diffeomorphism we can talk about  $\varphi$ -related vector-fields as follows.

Let  $\varphi : M \rightarrow N$  be a  $C^k$  map of manifolds. The vector-fields  $X \in \mathcal{X}^{k-1}(M)$  and  $Y \in \mathcal{X}^{k-1}(N)$  are called  $\varphi$ -related, denoted  $X \sim_\varphi Y$ , if  $T\varphi \circ X = Y \circ \varphi$ .

Note that if  $\varphi$  is diffeomorphism and  $X$  and  $Y$  are  $\varphi$ -related, then  $Y = \varphi_* X$ . In general however,  $X$  can be  $\varphi$ -related to more than one vector-field on  $N$ .  $\varphi$ -relatedness means that the following diagram commutes:

$$\begin{array}{ccc}
 TM & \xrightarrow{T\varphi} & TN \\
 X \uparrow & & \uparrow Y \\
 M & \xrightarrow{\varphi} & N
 \end{array}$$

The behavior of flows under these operations is as follows: Let  $\varphi : M \rightarrow N$  be a  $C^k$ -map of manifolds,  $X \in \mathcal{X}^k(M)$  and  $Y \in \mathcal{X}^k(N)$ . Let  $F_t$  and  $G_t$  denote the flows of  $X$  and  $Y$  respectively. Then  $X \sim_\varphi Y$  iff  $\varphi \circ F_t = G_t \circ \varphi$ . In particular, if  $\varphi$  is a diffeomorphism, then the equality  $Y = \varphi_* X$  holds iff the flow of  $Y$  is  $\varphi \circ F_t \circ \varphi^{-1}$  (This is called the push-forward of  $F_t$  by  $\varphi$  since it is the natural way to construct a diffeomorphism on  $N$  out of one on  $M$ ). In particular,  $(F_t)_* X = X$ . Therefore, the flow of the push-forward of a vector-field is the push-forward of its flow.

### 2.2.4 Jet Bundles

Roughly speaking, two maps  $f, g : M \rightarrow N$  are said to determine the same  $r$ -jet at  $x \in M$ , if they have the  $r$ th order contact at  $x$  [KMS93]. To make this idea precise, we first define the  $r$ th order contact of two curves on a manifold. We recall that a smooth function  $\mathbb{R} \rightarrow \mathbb{R}$  is said to vanish to  $r$ th order at a point, if all its derivatives up to order  $r$  vanish at this point. Two curves  $\gamma, \delta : \mathbb{R} \rightarrow M$  have the  $r$ th contact at zero, if for every smooth function  $\varphi$  on  $M$  the difference  $\varphi \circ \gamma - \varphi \circ \delta$  vanishes to  $r$ th order at  $0 \in \mathbb{R}$ . In this case we write  $\gamma \sim_r \delta$ . Clearly,  $\sim_r$  is an equivalence relation. For  $r = 0$  this relation means  $\gamma(0) = \delta(0)$ . If  $\gamma \sim_r \delta$ , then  $f \circ \gamma \sim_r f \circ \delta$  for every map  $f : M \rightarrow N$ .

Two maps  $f, g : M \rightarrow N$  are said to determine the same  $r$ jet at  $x \in M$ , if for every curve  $\gamma : \mathbb{R} \rightarrow M$  with  $\gamma(0) = x$  the curves  $f$  and  $g$  have the  $r$ th order contact at zero. In such a case we write  $j_x^r f = j_x^r g$  or  $j^r f(x) = j^r g(x)$ .

An equivalence class of this relation is called an *rjet* of  $M$  into  $N$ . The set of all *rjets* of  $M$  into  $N$  is denoted by  $J^r(M, N)$ . For  $X = j_x^r f \in J^r(M, N)$ , the point  $x = \alpha X$  is the *source* of  $X$  and the point  $f(x) = \beta X$  is the *target* of  $X$ . We denote by  $\pi_s^r$ ,  $0 \leq s \leq r$ , the *projection*  $j_x^r f \mapsto j_x^s f$  of *rjets* into *sjets*. By  $J_x^r(M, N)$  or  $J^r(M, N)_y$  we mean the set of all *rjets* of  $M$  into  $N$  with source  $x \in M$  or target  $y \in N$ , respectively, and we write  $J_x^r(M, N)_y = J_x^r(M, N) \cap J^r(M, N)_y$ . The map  $j^r f : M \rightarrow J^r(M, N)$  is called the *rth jet prolongation* of  $f : M \rightarrow N$  [KMS93].

Since the composition of maps is associative, the same holds for *rjets*. Hence all *rjets* form a category  $\mathcal{J}$ , the units of which are the *rjets* of the identity maps of manifolds. Then also  $J^r$  is a *jet bifunctor* defined on the product category  $\mathcal{M}_n \times \mathcal{M}$ , with the values in the category of fibre bundles  $\mathcal{FB}$  i.e.,  $J^r : \mathcal{M}_n \times \mathcal{M} \rightarrow \mathcal{FB}$ .

Next, we are going to describe the coordinate expression of *r-jets*. By

$$D_\alpha f = \frac{\partial^{|\alpha|} f}{(\partial x^1)^{\alpha_1} \dots (\partial x^m)^{\alpha_m}},$$

where  $\alpha = (\alpha_1, \dots, \alpha_m)$  a multiindex of range  $m$ , we denote the partial derivative with respect to the multiindex  $\alpha$  of a function  $f : U \subset \mathbb{R}^m \rightarrow \mathbb{R}$ . Given a local coordinate system  $x^i$  on  $M$  in a neighborhood of  $x$  and a local coordinate system  $y^p$  on  $N$  in a neighborhood of  $f(x)$ , two maps  $f, g : M \rightarrow N$  satisfy  $j_x^r f = j_x^r g$  iff all the partial derivatives up to order  $r$  of the components  $f^p$  and  $g^p$  of their coordinate expressions coincide at  $x$  [KMS93]. If we have the curves  $x^i = a^i t$  with arbitrary  $a^i$ , then the coordinate condition for  $f \circ \gamma \sim_r g \circ \gamma$  reads  $(D_\alpha f^p(x))a^\alpha = (D_\alpha g^p(x))a^\alpha$ .

Now, the auxiliary relation  $\gamma \sim_r \delta$  can be expressed in terms of *r-jets*, namely two curves  $\gamma, \delta : \mathbb{R} \rightarrow M$  satisfy  $\gamma \sim_r \delta$  iff  $j_0^r \gamma = j_0^r \delta$ .

The elements of  $L_{m,n}^r = J_0^r(\mathbb{R}^m, \mathbb{R}^n)$  can be identified with the *rth* order Taylor expansions of the generating maps, i.e., with the  $n$ tuples of polynomials of degree  $r$  in  $m$  variables without absolute term. Such an expression  $a_\alpha^p x^\alpha$  is called the polynomial representative of an *rjet*. Hence  $L_{m,n}^r$  is a numerical space of the variables  $a_\alpha^p$ .  $\dim L_{m,n}^r = n \left[ \binom{m+r}{m} - 1 \right]$ .

The projection  $\pi_s^r : L_{m,n}^r \rightarrow L_{m,n}^s$  consists in suppressing all terms of degree  $> s$ . The jet composition  $L_{m,n}^r \times L_{n,q}^r \rightarrow L_{m,q}^r$ , also called truncated polynomial composition, is evaluated by taking the composition of the polynomial representatives and suppressing all terms of degree higher than  $r$ . The sets  $L_{m,n}^r$  represent the sets of morphisms of a category  $\mathcal{L}^r$  over non-negative integers, the composition in which is the jet composition. The set of all invertible elements of  $L_{m,m}^r$  with the jet composition is a Lie group  $G_m^r$  called the *rth* differential group or the *rth* jet group in dimension  $m$ . For  $r = 1$  the group  $G_m^1$  is identified with the general linear group  $GL(m, \mathbb{R})$  [KMS93].

The elements of the manifold  $T_k^r M = J_0^r(\mathbb{R}^k, M)$  are said to be the *k-dimensional velocities* of order  $r$  on  $M$ , in short *(k, r)-velocities*. The

inclusion  $T_k^r M \subset J^r(\mathbb{R}^m, M)$  defines the structure of a smooth fibre bundle on  $T_k^r M \rightarrow M$ . Every smooth map  $f : M \rightarrow N$  is extended into an  $\mathcal{FB}$ -morphism  $T_k^r f : T_k^r M \rightarrow T_k^r N$  defined by  $T_k^r f(j_0^r g) = j_0^r(f \circ g)$ . Hence  $T_k^r$  is a functor  $\mathcal{M} \rightarrow \mathcal{FB}$ . Since every map  $\mathbb{R}^k \rightarrow M_1 \times M_2$  coincides with a pair of maps  $\mathbb{R}^k \rightarrow M_1$  and  $\mathbb{R}^k \rightarrow M_2$ , functor  $T_k^r$  preserves products. For  $k = r = 1$  we get another definition of the *tangent functor*  $T = T_1^1$  [KMS93].

Analogously, the space  $T_k^{r*} M = J^r(M, \mathbb{R}^k)_0$  is called the space of all  $(k, r)$ -co-velocities on  $M$ . For  $k = 1$  we write in short  $T_k^{r*} = T^{r*}$ . Since  $\mathbb{R}^k$  is a vector space,  $T_k^{r*} M \rightarrow M$  is a vector bundle with  $j_x^r \varphi(u) + j_x^r \psi(u) = j_x^r(\varphi(u) + \psi(u))$ ,  $u \in M$ , and  $k j_x^r \varphi(u) = j_x^r k \varphi(u)$ ,  $k \in \mathbb{R}$ . Every local diffeomorphism  $f : M \rightarrow N$  is extended to a vector bundle morphism  $T_k^{r*} f : T_k^{r*} M \rightarrow T_k^{r*} N$ ,  $j_x^r \varphi \mapsto j_{f(x)}^r(\varphi \circ f^{-1})$ , where  $f^{-1}$  is constructed locally. In this sense  $T_k^{r*}$  is a functor on  $\mathcal{M}_n$ . For  $k = r = 1$  we get the construction of the cotangent bundles as a functor  $T_1^{1*} = T^*$  on  $\mathcal{M}_n$ .

The projection  $\pi_{r-1}^r : T^{r*} M \rightarrow T^{r-1*} M$  is a linear morphism of vector bundles. Its kernel is described by the following exact sequence of vector bundles over  $M$

$$0 \rightarrow S^r T^* M \rightarrow T^{r*} M \xrightarrow{\pi_{r-1}^r} T^{r-1*} M \rightarrow 0,$$

where  $S^r$  indicates the  $r$ th symmetric tensor power [KMS93].

Let  $\hat{y}$  denote the constant map of  $M$  into  $y \in N$ . The subspace  $(\pi_{r-1}^r)^{-1}(j_x^r \hat{y}) \subset J_x^r(M, N)_y$  is canonically identified with  $T_y N \otimes S^r T_x^* M$ . For  $r = 1$  we have a distinguished element  $j_x^1 \hat{y}$  in every fibre of  $J^1(M, N) \rightarrow M \times N$ . This identifies  $J^1(M, N)$  with  $TN \otimes T^*M$  [KMS93].

## 2.3 Sections of Biomechanical Bundles

In this section we introduce *sections of biomechanical bundles*, including vector (and tensor) fields and their flows, as well as exterior differential forms.

### 2.3.1 Biomechanical Evolution and Flow

As a motivational example, consider a biomechanical system that is capable of assuming various states described by points in a set  $U$ . For example,  $U$  might be  $\mathbb{R}^3 \times \mathbb{R}^3$  and a state might be the positions and momenta  $(x^i, p_i)$  of a particle moving under the influence of the central force field, with  $i = 1, 2, 3$ . As time passes, the state evolves. If the state is  $\gamma_0 \in U$  at time  $s$  and this changes to  $\gamma$  at a later time  $t$ , we set

$$F_{t,s}(\gamma_0) = \gamma,$$

and call  $F_{t,s}$  the *evolution operator*; it maps a state at time  $s$  to what the state would be at time  $t$ ; that is, after time  $t - s$  has elapsed. Determinism is expressed by the *Chapman-Kolmogorov law* [AMR88]:

$$F_{\tau,t} \circ F_{t,s} = F_{\tau,s}, \quad F_{t,t} = \text{identity}. \quad (2.2)$$

The evolution laws are called *time independent*, or *autonomous*, when  $F_{t,s}$  depends only on  $t - s$ . In this case the preceding law (2.2) becomes the *group property*:

$$F_t \circ F_s = F_{t+s}, \quad F_0 = \text{identity}. \quad (2.3)$$

We call such an  $F_t$  a *flow* and  $F_{t,s}$  a *time-dependent flow*, or an evolution operator. If the system is irreversible, that is, defined only for  $t \geq s$ , we speak of a *semi-flow* [AMR88].

Usually, instead of  $F_{t,s}$  the *laws of motion* are given in the form of ODEs that we must solve to find the flow. These equations of motion have the form:

$$\dot{\gamma} = X(\gamma), \quad \gamma(0) = \gamma_0,$$

where  $X$  is a (possibly time-dependent) vector-field on  $U$ .

As a continuation of the previous example, consider the motion of a particle of mass  $m$  under the influence of the central force field (like gravity, or Coulombic potential)  $F^i$  ( $i = 1, 2, 3$ ), described by the Newtonian equation of motion:

$$m\ddot{x}^i = F^i(x). \quad (2.4)$$

By introducing momenta  $p_i = m\dot{x}^i$ , equation (6.13) splits into two Hamiltonian equations:

$$\dot{x}^i = p_i/m, \quad \dot{p}_i = F_i(x). \quad (2.5)$$

Note that in Euclidean space we can freely interchange subscripts and superscripts. However, in general case of a Riemannian manifold,  $p_i = mg_{ij}\dot{x}^j$  and (2.5) properly reads

$$\dot{x}^i = g^{ij}p_j/m, \quad \dot{p}_i = F_i(x). \quad (2.6)$$

The phase-space here is the Riemannian manifold  $(\mathbb{R}^3 \setminus \{0\}) \times \mathbb{R}^3$ , that is, the cotangent bundle of  $\mathbb{R}^3 \setminus \{0\}$ , which is itself the manifold for the central force field. The r.h.s of equations (2.6) define a Hamiltonian vector-field on this 6D manifold by

$$X(x, p) = ((x^i, p_i), (p_i/m, F_i(x))). \quad (2.7)$$

Integration of equations (2.6) produces trajectories (in this particular case, planar conic sections). These trajectories comprise the flow  $F_t$  of the vector-field  $X(x, p)$  defined in (2.7).

### 2.3.2 Vector-Fields and Their Flows

#### Vector-Fields on $M$

A *vector-field*  $X$  on  $U$ , where  $U$  is an open chart in  $n$ -manifold  $M$ , is a *smooth function* from  $U$  to  $M$  assigning to each point  $m \in U$  a vector at that

point, i.e.,  $X(m) = (m, X(m))$ . If  $X(m)$  is tangent to  $M$  for each  $m \in M$ ,  $X$  is said to be a *tangent vector-field* on  $M$ . If  $X(m)$  is orthogonal to  $M$  (i.e.,  $X(p) \in M_m^\perp$ ) for each  $X(m) \in M$ ,  $X$  is said to be a *normal vector-field* on  $M$ .

In other words, let  $M$  be a  $C^k$ -manifold. A  $C^k$ -vector-field on  $M$  is a  $C^k$ -section of the tangent bundle  $TM$  of  $M$ . Thus a vector-field  $X$  on a manifold  $M$  is a  $C^k$ -map  $X : M \rightarrow TM$  such that  $X(m) \in T_m M$  for all points  $m \in M$ , and  $\pi_M \circ X = Id_M$ . Therefore, a vector-field assigns to each point  $m$  of  $M$  a vector based (i.e., bound) at that point. The set of all  $C^k$  vector-fields on  $M$  is denoted by  $\mathcal{X}^k(M)$ .

A vector-field  $X \in \mathcal{X}^k(M)$  represents a field of direction indicators [Thi79]: to every point  $m$  of  $M$  it assigns a vector in the tangent space  $T_m M$  at that point. If  $X$  is a vector-field on  $M$  and  $(U, \phi)$  is a chart on  $M$  and  $m \in U$ , then we have  $X(m) = X^i(m) \phi^i \frac{\partial}{\partial \phi^i}$ . Following [KMS93], we write  $X|_U = X^i \phi^i \frac{\partial}{\partial \phi^i}$ .

Let  $M$  be a connected  $n$ -manifold, and let  $f : U \rightarrow \mathbb{R}$  ( $U$  an open set in  $M$ ) and  $c \in \mathbb{R}$  be such that  $M = f^{-1}(c)$  (i.e.,  $M$  is the *level set* of the function  $f$  at *height*  $c$ ) and  $\nabla f(m) \neq 0$  for all  $m \in M$ . Then there exist on  $M$  exactly two smooth unit normal vector-fields  $N_{1,2}(m) = \pm \frac{\nabla f(m)}{|\nabla f(m)|}$  (here  $|X| = (X \cdot X)^{1/2}$  denotes the norm or length of a vector  $X$ , and  $(\cdot)$  denotes the scalar product on  $M$ ) for all  $m \in M$ , called *orientations* on  $M$ .

Let  $\varphi : M \rightarrow N$  be a smooth map. Recall that two vector-fields  $X \in \mathcal{X}^k(M)$  and  $Y \in \mathcal{X}(N)$  are called  $\varphi$ -related, if  $T\varphi \circ X = Y \circ \varphi$  holds, i.e., if the following diagram commutes:

$$\begin{array}{ccc} TM & \xrightarrow{T\varphi} & TN \\ X \uparrow & & \uparrow Y \\ M & \xrightarrow{\varphi} & N \end{array}$$

In particular, a diffeomorphism  $\varphi : M \rightarrow N$  induces a linear map between vector-fields on two manifolds,  $\varphi^* : \mathcal{X}^k(M) \rightarrow \mathcal{X}(N)$ , such that  $\varphi^* X = T\varphi \circ X \circ \varphi^{-1} : N \rightarrow TN$ , i.e., the following diagram commutes:

$$\begin{array}{ccc} TM & \xrightarrow{T\varphi} & TN \\ X \uparrow & & \uparrow \varphi^* X \\ M & \xrightarrow{\varphi} & N \end{array}$$

The correspondences  $M \rightarrow TM$  and  $\varphi \rightarrow T\varphi$  obviously define a functor  $T : \mathcal{M} \Rightarrow \mathcal{M}$  from the category of smooth manifolds to itself.  $T$  is another

special case of the vector bundle functor (2.2.3), and closely related to the tangent bundle functor (2.2.1).

A  $C^k$  time-dependent vector-field is a  $C^k$ -map  $X : \mathbb{R} \times M \rightarrow TM$  such that  $X(t, m) \in T_m M$  for all  $(t, m) \in \mathbb{R} \times M$ , i.e.,  $X_t(m) = X(t, m)$ .

### Integral Curves as Biomechanical Trajectories

Recall (2.2.1) that a curve  $\gamma$  at a point  $m$  of an  $n$ -manifold  $M$  is a  $C^0$ -map from an open interval  $I$  of  $\mathbb{R}$  into  $M$  such that  $0 \in I$  and  $\gamma(0) = m$ . For such a curve we may assign a tangent vector at each point  $\gamma(t)$ ,  $t \in I$ , by  $\dot{\gamma}(t) = T_t \gamma(1)$ .

Let  $X$  be a smooth tangent vector-field on the smooth  $n$ -manifold  $M$ , and let  $m \in M$ . Then there exists an open interval  $I \subset \mathbb{R}$  containing 0 and a parameterized curve  $\gamma : I \rightarrow M$  such that:

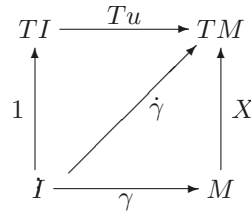
1.  $\gamma(0) = m$ ;
2.  $\dot{\gamma}(t) = X(\gamma(t))$  for all  $t \in I$ ; and
3. If  $\beta : \tilde{I} \rightarrow M$  is any other parameterized curve in  $M$  satisfying (1) and (2), then  $\tilde{I} \subset I$  and  $\beta(t) = \gamma(t)$  for all  $t \in \tilde{I}$ .

A parameterized curve  $\gamma : I \rightarrow M$  satisfying condition (2) is called an *integral curve* of the tangent vector-field  $X$ . The unique  $\gamma$  satisfying conditions (1)–(3) is the *maximal integral curve* of  $X$  through  $m \in M$ .

In other words, let  $\gamma : I \rightarrow M$ ,  $t \mapsto \gamma(t)$  be a smooth curve in a manifold  $M$  defined on an interval  $I \subseteq \mathbb{R}$ .  $\dot{\gamma}(t) = \frac{d}{dt} \gamma(t)$  defines a smooth vector-field along  $\gamma$  since we have  $\pi_M \circ \dot{\gamma} = \gamma$ . Curve  $\gamma$  is called an *integral curve* or *flow line* of a vector-field  $X \in \mathcal{X}^k(M)$  if the tangent vector determined by  $\gamma$  equals  $X$  at every point  $m \in M$ , i.e.,

$$\dot{\gamma} = X \circ \gamma,$$

or, if the following diagram commutes:



On a chart  $(U, \phi)$  with coordinates  $\phi(m) = (x^1(m), \dots, x^n(m))$ , for which  $\varphi \circ \gamma : t \mapsto \gamma_i(t)$  and  $T\varphi \circ X \circ \varphi^{-1} : x^i \mapsto (x^i, X_i(m))$ , this is written

$$\dot{\gamma}_i(t) = X_i(\gamma(t)), \text{ for all } t \in I \subseteq \mathbb{R}, \tag{2.8}$$

which is an ordinary differential equation of first order in  $n$  dimensions.

The *velocity*  $\dot{\gamma}$  of the parameterized curve  $\gamma(t)$  is a vector-field along  $\gamma$  defined by

$$\dot{\gamma}(t) = (\gamma(t), \dot{x}^1(t), \dots, \dot{x}^n(t)).$$

Its length  $|\dot{\gamma}| : I \rightarrow \mathbb{R}$ , defined by  $|\dot{\gamma}|(t) = |\dot{\gamma}(t)|$  for all  $t \in I$ , is a function along  $\alpha$ .  $|\dot{\gamma}|$  is called *speed* of  $\gamma$  [Arn89].

Each vector-field  $X$  along  $\gamma$  is of the form  $X(t) = (\gamma(t), X_1(t), \dots, X_n(t))$ , where each component  $X_i$  is a function along  $\gamma$ .  $X$  is *smooth* if each  $X_i : I \rightarrow M$  is smooth. The *derivative* of a smooth vector-field  $X$  along a curve  $\gamma(t)$  is the vector-field  $\dot{X}$  along  $\gamma$  defined by

$$\dot{X}(t) = (\gamma(t), \dot{X}_1(t), \dots, \dot{X}_n(t)).$$

$\dot{X}(t)$  measures the *rate of change of the vector part*  $(X_1(t), \dots, X_n(t))$  of  $X(t)$  along  $\gamma$ . Thus, the *acceleration*  $\ddot{\gamma}(t)$  of a parameterized curve  $\gamma(t)$  is the vector-field along  $\gamma$  obtained by differentiating the velocity field  $\dot{\gamma}(t)$ .

Differentiation of vector-fields along parameterized curves has the following properties. For  $X$  and  $Y$  smooth vector-fields on  $M$  along the parameterized curve  $\gamma : I \rightarrow M$  and  $f$  a smooth function along  $\gamma$ , we have:

1.  $\frac{d}{dt}(X + Y) = \dot{X} + \dot{Y}$ ;
2.  $\frac{d}{dt}(fX) = \dot{f}X + f\dot{X}$ ; and
3.  $\frac{d}{dt}(X \cdot Y) = \dot{X}Y + X\dot{Y}$ .

A *geodesic* in  $M$  is a parameterized curve  $\gamma : I \rightarrow M$  whose acceleration  $\ddot{\gamma}$  is everywhere orthogonal to  $M$ ; that is,  $\ddot{\gamma}(t) \in M_{\alpha(t)}^\perp$  for all  $t \in I \subset \mathbf{R}$ . Thus a geodesic is a curve in  $M$  which always goes ‘straight ahead’ in the surface. Its acceleration serves only to keep it in the surface. It has no component of acceleration tangent to the surface. Therefore, it also has a constant speed  $|\dot{\gamma}(t)|$ .

Let  $v \in M_m$  be a vector on  $M$ . Then there exists an open interval  $I \subset \mathbf{R}$  containing 0 and a geodesic  $\gamma : I \rightarrow M$  such that:

1.  $\gamma(0) = m$  and  $\dot{\gamma}(0) = v$ ; and
2. If  $\beta : \tilde{I} \rightarrow M$  is any other geodesic in  $M$  with  $\beta(0) = m$  and  $\dot{\beta}(0) = v$ , then  $\tilde{I} \subset I$  and  $\beta(t) = \gamma(t)$  for all  $t \in \tilde{I}$ .

The geodesic  $\gamma$  is now called the *maximal geodesic* in  $M$  passing through  $m$  with initial velocity  $v$ .

By definition, a parameterized curve  $\gamma : I \rightarrow M$  is a geodesic of  $M$  iff its acceleration is everywhere perpendicular to  $M$ , i.e., iff  $\ddot{\gamma}(t)$  is a multiple of the orientation  $N(\gamma(t))$  for all  $t \in I$ , i.e.,  $\ddot{\gamma}(t) = g(t)N(\gamma(t))$ , where  $g : I \rightarrow \mathbb{R}$ . Taking the scalar product of both sides of this equation with  $N(\gamma(t))$  we find  $g = -\dot{\gamma}\dot{N}(\gamma(t))$ . Thus  $\gamma : I \rightarrow M$  is geodesic iff it satisfies the differential equation

$$\ddot{\gamma}(t) + \dot{N}(\gamma(t))N(\gamma(t)) = 0.$$

This vector equation represents the system of second order component ODEs

$$\ddot{x}^i + N_i(x + 1, \dots, x^n) \frac{\partial N_j}{\partial x^k}(x + 1, \dots, x^n) \dot{x}^j \dot{x}^k = 0.$$

The substitution  $u^i = \dot{x}^i$  reduces this second order differential system (in  $n$  variables  $x^i$ ) to the first order differential system

$$\dot{x}^i = u^i, \quad \dot{u}^i = -N_i(x + 1, \dots, x^n) \frac{\partial N_j}{\partial x^k}(x + 1, \dots, x^n) \dot{x}^j \dot{x}^k$$

(in  $2n$  variables  $x^i$  and  $u^i$ ). This first order system is just the differential equation for the integral curves of the vector-field  $X$  in  $U \times \mathbb{R}$  ( $U$  open chart in  $M$ ), in which case  $X$  is called a *geodesic spray*.

Now, when an integral curve  $\gamma(t)$  is the path a biomechanical system  $\Xi$  follows, i.e., the solution of the equations of motion, it is called a *trajectory*. In this case the parameter  $t$  represents time, so that (2.8) describes motion of the system  $\Xi$  on its configuration manifold  $M$ .

If  $X_i(m)$  is  $C^0$  the existence of a local solution is guaranteed, and a *Lipschitz condition* would imply that it is unique. Therefore, exactly one integral curve passes through every point, and different integral curves can never cross. As  $X \in \mathcal{X}^k(M)$  is  $C^k$ , the following statement about the solution with arbitrary initial conditions holds [Thi79, Arn89]:

**Theorem.** Given a vector-field  $X \in \mathcal{X}(M)$ , for all points  $p \in M$ , there exist  $\eta > 0$ , a neighborhood  $V$  of  $p$ , and a function  $\gamma : (-\eta, \eta) \times V \rightarrow M$ ,  $(t, x^i(0)) \mapsto \gamma(t, x^i(0))$  such that

$$\dot{\gamma} = X \circ \gamma, \quad \gamma(0, x^i(0)) = x^i(0) \quad \text{for all } x^i(0) \in V \subseteq M.$$

For all  $|t| < \eta$ , the map  $x^i(0) \mapsto \gamma(t, x^i(0))$  is a diffeomorphism  $f_t^X$  between  $V$  and some open set of  $M$ . For proof, see [Die69], I, 10.7.4 and 10.8.

This theorem states that trajectories that are near neighbors cannot suddenly be separated. There is a well-known estimate (see [Die69], I, 10.5) according to which points cannot diverge faster than exponentially in time if the derivative of  $X$  is uniformly bounded.

An integral curve  $\gamma(t)$  is said to be *maximal* if it is not a restriction of an integral curve defined on a larger interval  $I \subseteq \mathbb{R}$ . It follows from the existence and uniqueness theorems for ODEs with smooth r.h.s and from elementary properties of Hausdorff spaces that for any point  $m \in M$  there exists a maximal integral curve  $\gamma_m$  of  $X$ , passing for  $t = 0$  through point  $m$ , i.e.,  $\gamma(0) = m$ .

**Theorem** (Local Existence, Uniqueness, and Smoothness) [AMR88]. Let  $E$  be a Banach space,  $U \subset E$  be open, and suppose  $X : U \subset E \rightarrow E$  is of class  $C^k$ ,  $k \geq 1$ . Then

1. For each  $x_0 \in U$ , there is a curve  $\gamma : I \rightarrow U$  at  $x_0$  such that  $\dot{\gamma}(t) = X(\gamma(t))$  for all  $t \in I$ .
2. Any two such curves are equal on the intersection of their domains.
3. There is a neighborhood  $U_0$  of the point  $x_0 \in U$ , a real number  $a > 0$ , and a  $C^k$  map  $F : U_0 \times I \rightarrow E$ , where  $I$  is the open interval  $] - a, a[$ , such

that the curve  $\gamma_u : I \rightarrow E$ , defined by  $\gamma_u(t) = F(u, t)$  is a curve at  $u \in E$  satisfying the ODEs  $\dot{\gamma}_u(t) = X(\gamma_u(t))$  for all  $t \in I$ .

**Proposition** (Global Uniqueness). Suppose  $\gamma_1$  and  $\gamma_2$  are two integral curves of a vector-field  $X$  at a point  $m \in M$ . Then  $\gamma_1 = \gamma_2$  on the intersection of their domains [AMR88].

If for every point  $m \in M$  the curve  $\gamma_m$  is defined on the entire real axis  $\mathbb{R}$ , then the vector-field  $X$  is said to be *complete*.

The *support* of a vector-field  $X$  defined on a manifold  $M$  is defined to be the closure of the set  $\{m \in M | X(m) = 0\}$ . A  $C^k$  vector-field with compact support on a manifold  $M$  is complete. In particular, a  $C^k$  vector-field on a compact manifold is complete. Completeness corresponds to well-defined dynamics persisting eternally.

Now, following [AMR88], for the *derivative* of a  $C^k$  function  $f : E \rightarrow \mathbb{R}$  in the direction  $X$  we use the notation  $X[f] = df \cdot X$ , where  $df$  stands for the *derivative map*. In standard coordinates on  $\mathbb{R}^n$  this is a standard *gradient*

$$df(x) = \nabla f = (\partial_{x^1} f, \dots, \partial_{x^n} f), \quad \text{and} \quad X[f] = X^i \partial_{x^i} f.$$

Let  $F_t$  be the flow of  $X$ . Then  $f(F_t(x)) = f(F_s(x))$  if  $t \geq s$ .

For example, Newtonian equations for a moving particle of mass  $m$  in a potential field  $V$  in  $\mathbb{R}^n$  are given by  $\ddot{q}^i(t) = -(1/m)\nabla V(q^i(t))$ , for a smooth function  $V : \mathbb{R}^n \rightarrow \mathbb{R}$ . If there are constants  $a, b \in \mathbb{R}$ ,  $b \geq 0$  such that  $(1/m)V(q^i) \geq a - b\|q^i\|^2$ , then *every solution exists for all time*. To show this, rewrite the second order equations as a first order system  $\dot{q}^i = (1/m)p_i$ ,  $\dot{p}_i = -V(q^i)$  and note that the energy  $E(q^i, p_i) = (1/2m)\|p_i\|^2 + V(q)$  is a *first integral* of the motion. Thus, for any solution  $(q^i(t), p_i(t))$  we have  $E(q^i(t), p_i(t)) = E(q^i(0), p_i(0)) = V(q(0))$ .

Let  $X_t$  be a  $C^k$  time-dependent vector-field on an  $n$ -manifold  $M$ ,  $k \geq 1$ , and let  $m_0$  be an *equilibrium* of  $X_t$ , that is,  $X_t(m_0) = 0$  for all  $t$ . Then for any  $T$  there exists a neighborhood  $V$  of  $m_0$  such that any  $m \in V$  has integral curve existing for time  $t \in [-T, T]$ .

### Biomechanical Flows on $M$

Recall (2.3.1) that the *flow*  $F_t$  of a  $C^k$  vector-field  $X \in \mathcal{X}^k(M)$  is the *one-parameter group of diffeomorphisms*  $F_t : M \rightarrow M$  such that  $t \mapsto F_t(m)$  is the integral curve of  $X$  with initial condition  $m$  for all  $m \in M$  and  $t \in I \subseteq \mathbb{R}$ . The flow  $F_t(m)$  is  $C^k$  by induction on  $k$ . It is defined as [AMR88]:

$$\frac{d}{dt} F_t(x) = X(F_t(x)).$$

Existence and uniqueness theorems for ODEs guarantee that  $F_t$  is smooth in  $m$  and  $t$ . From uniqueness, we get the *flow property*:

$$F_{t+s} = F_t \circ F_s$$

along with the initial conditions  $F_0 = \text{identity}$ . The flow property generalizes the situation where  $M = V$  is a linear space,  $X(x) = Ax$  for a (bounded) linear operator  $A$ , and where  $F_t(x) = e^{tA}x$  – to the nonlinear case. Therefore, the flow  $F_t(m)$  can be defined as a *formal exponential*

$$F_t(m) = \exp(tX) = (I + tX + \frac{t^2}{2}X^2 + \dots) = \sum_{k=0}^{\infty} \frac{X^k t^k}{k!}.$$

A *time-dependent vector-field* is a map  $X : M \times \mathbb{R} \rightarrow TM$  such that  $X(m, t) \in T_m M$  for each point  $m \in M$  and  $t \in \mathbb{R}$ . An *integral curve* of  $X$  is a curve  $\gamma(t)$  in  $M$  such that

$$\dot{\gamma}(t) = X(\gamma(t), t), \quad \text{for all } t \in I \subseteq \mathbb{R}.$$

In this case, the flow is the one-parameter group of diffeomorphisms  $F_{t,s} : M \rightarrow M$  such that  $t \mapsto F_{t,s}(m)$  is the integral curve  $\gamma(t)$  with initial condition  $\gamma(s) = m$  at  $t = s$ . Again, the existence and uniqueness theorem from ODE-theory applies here, and in particular, uniqueness gives the time-dependent flow property, i.e., the *Chapman-Kolmogorov law*

$$F_{t,r} = F_{t,s} \circ F_{s,r}.$$

If  $X$  happens to be time independent, the two notions of flows are related by  $F_{t,s} = F_{t-s}$  (see [MR99]).

### Categories of ODEs

Ordinary differential equations are naturally organized into their categories (see [Koc81]). First order ODEs are organized into a category  $ODE_1$ . A first order ODE on a manifold-like object  $M$  is a vector-field  $X : M \rightarrow TM$ , and a *morphism of vector-fields*  $(M_1, X_1) \rightarrow (M_2, X_2)$  is a map  $f : M_1 \rightarrow M_2$  such that the following diagram commutes

$$\begin{array}{ccc} TM_1 & \xrightarrow{Tf} & TM_2 \\ X_1 \uparrow & & \uparrow X_2 \\ M_1 & \xrightarrow{f} & M_2 \end{array}$$

A *global solution* of the differential equation  $(M, X)$ , or a *flow line* of a vector-field  $X$ , is a morphism from  $(\mathbb{R}, \frac{\partial}{\partial x})$  to  $(M, X)$ .

Similarly, second order ODEs are organized into a category  $ODE_2$ . A second order ODE on  $M$  is usually constructed as a vector-field on  $TM$ ,  $\xi : TM \rightarrow TTM$ , and a morphism of vector-fields  $(M_1, \xi_1) \rightarrow (M_2, \xi_2)$  is a map  $f : M_1 \rightarrow M_2$  such that the following diagram commutes

$$\begin{array}{ccc}
 TTM_1 & \xrightarrow{TTf} & TTM_2 \\
 \uparrow \xi_1 & & \uparrow \xi_2 \\
 TM_1 & \xrightarrow{Tf} & TM_2
 \end{array}$$

Unlike solutions for first order ODEs, solutions for second order ODEs are not in general homomorphisms from  $\mathbb{R}$ , unless the second order ODE is a *spray* [KR03].

### 2.3.3 Differential Forms on $M$

We are already familiar with the basic facts of exterior differential forms (see Introduction). To give a more precise exposition, here we start with 1-forms, which are dual to vector-fields, and after that introduce general  $k$ -forms.

#### 1-Forms on $M$

Dual to the notion of a  $C^k$  vector-field  $X$  on an  $n$ -manifold  $M$  is a  $C^k$  *covector-field*, or a  $C^k$  1-form  $\alpha$ , which is defined as a  $C^k$ -section of the cotangent bundle  $T^*M$ , i.e.,  $\alpha : M \rightarrow T^*M$  is smooth and  $\pi_M^* \circ \alpha = Id_M$ . We denote the set of all  $C^k$  1-forms by  $\Omega^1(M)$ . A basic example of a 1-form is the differential  $df$  of a real-valued function  $f \in C^k(M, \mathbb{R})$ . With point wise addition and scalar multiplication  $\Omega^1(M)$  becomes a vector space.

In other words, a  $C^k$  1-form  $\alpha$  on a  $C^k$  manifold  $M$  is a real-valued function on the set of all tangent vectors to  $M$ , i.e.,  $\alpha : TM \rightarrow \mathbb{R}$  with the following properties:

1.  $\alpha$  is linear on the tangent space  $T_m M$  for each  $m \in M$ ;
2. For any  $C^k$  vector-field  $X \in \mathcal{X}^k(M)$ , the function  $f : M \rightarrow \mathbb{R}$  is  $C^k$ .

Given a 1-form  $\alpha$ , for each point  $m \in M$  the map  $\alpha(m) : T_m M \rightarrow \mathbb{R}$  is an element of the dual space  $T_m^* M$ . Therefore, the space of 1-forms  $\Omega^1(M)$  is dual to the space of vector-fields  $\mathcal{X}^k(M)$ .

In particular, the *coordinate 1-forms*  $dx^1, \dots, dx^n$  are locally defined at any point  $m \in M$  by the property that for any vector-field  $X = (X^1, \dots, X^n) \in \mathcal{X}^k(M)$ ,

$$dx^i(X) = X^i.$$

The  $dx^i$ 's form a *basis* for the 1-forms at any point  $m \in M$ , with local coordinates  $(x^1, \dots, x^n)$ , so any other 1-form  $\alpha$  may be expressed in the form

$$\alpha = f_i(m) dx^i.$$

If a vector-field  $X$  on  $M$  has the form  $X(m) = (X^1(m), \dots, X^n(m))$ , then at any point  $m \in M$ ,

$$\alpha_m(X) = f_i(m) X^i(m),$$

where  $f \in C^k(M, \mathbb{R})$ .

The 1-forms on  $M$  are part of an algebra, called the *exterior algebra*, or *Grassmann algebra* on  $M$ . The multiplication  $\wedge$  in this algebra is called *wedge product* (see (2.9) below), and it is skew-symmetric,

$$dx^i \wedge dx^j = -dx^j \wedge dx^i.$$

One consequence of this is that  $dx^i \wedge dx^i = 0$ .

### **$k$ -Forms on $M$**

A differential form, or an exterior form  $\alpha$  of degree  $k$ , or a  $k$ -form for short, is a section of the vector bundle  $\Lambda^k T^*M$ , i.e.,  $\alpha : M \rightarrow \Lambda^k T^*M$ . In other words,  $\alpha(m) : T_m M \times \dots \times T_m M \rightarrow \mathbb{R}$  (with  $k$  factors  $T_m M$ ) is a function that assigns to each point  $m \in M$  a skew-symmetric  $k$ -multilinear map on the tangent space  $T_m M$  to  $M$  at  $m$ . Without the skew-symmetry assumption,  $\alpha$  would be called a  $(0, k)$ -tensor-field. The space of all  $k$ -forms is denoted by  $\Omega^k(M)$ . It may also be viewed as the space of all skew symmetric  $(0, k)$ -tensor-fields, the space of all maps

$$\Phi : \mathcal{X}^k(M) \times \dots \times \mathcal{X}^k(M) \rightarrow C^k(M, \mathbb{R}),$$

which are  $k$ -linear and skew-symmetric (see (2.9) below). We put  $\Omega^k(M) = C^k(M, \mathbb{R})$ .

In particular, a 2-form  $\omega$  on an  $n$ -manifold  $M$  is a section of the vector bundle  $\Lambda^2 T^*M$ . If  $(U, \phi)$  is a chart at a point  $m \in M$  with local coordinates  $(x^1, \dots, x^n)$  let  $\{e_1, \dots, e_n\} = \{\partial_{x^1}, \dots, \partial_{x^n}\}$  - be the corresponding basis for  $T_m M$ , and let  $\{e^1, \dots, e^n\} = \{dx^1, \dots, dx^n\}$  - be the dual basis for  $T_m^* M$ . Then at each point  $m \in M$ , we can write a 2-form  $\omega$  as

$$\omega_m(v, u) = \omega_{ij}(m) v^i u^j, \quad \text{where } \omega_{ij}(m) = \omega_m(\partial_{x^i}, \partial_{x^j}).$$

If each summand of a differential form  $\alpha \in \Omega^k(M)$  contains  $k$  basis 1-forms  $dx^{i_j}$ 's, the form is called a  $k$ -form. Functions  $f \in C^k(M, \mathbb{R})$  are considered to be 0-forms, and any form on an  $n$ -manifold  $M$  of degree  $k > n$  must be zero due to the skew-symmetry.

Any  $k$ -form  $\alpha \in \Omega^k(M)$  may be expressed in the form

$$\alpha = f_I dx^{i_1} \wedge \dots \wedge dx^{i_k} = f_I dx^I,$$

where  $I$  is a *multiindex*  $I = (i_1, \dots, i_k)$  of length  $k$ , and  $\wedge$  is the wedge product which is associative, bilinear and anticommutative.

Just as 1-forms act on vector-fields to give real-valued functions, so  $k$ -forms act on  $k$ -tuples of vector-fields to give real-valued functions.

The *wedge product* of two differential forms, a  $k$ -form  $\alpha \in \Omega^k(M)$  and an  $l$ -form  $\beta \in \Omega^l(M)$  is a  $(k+l)$ -form  $\alpha \wedge \beta$  defined as:

$$\alpha \wedge \beta = \frac{(k+l)!}{k!l!} \mathbf{A}(\alpha \otimes \beta), \quad (2.9)$$

where  $\mathbf{A} : \Omega^k(M) \times \Omega^l(M) \rightarrow \Omega^{k+l}(M)$ ,  $\mathbf{A}\tau(e_1, \dots, e_k) = \frac{1}{k!} \sum_{\sigma \in S_k} (\text{sign } \sigma) \tau(e_{\sigma(1)}, \dots, e_{\sigma(k)})$ , where  $S_k$  is the permutation group on  $k$  elements consisting of all bijections  $\sigma : \{1, \dots, k\} \rightarrow \{1, \dots, k\}$ .

For any  $k$ -form  $\alpha \in \Omega^k(M)$  and  $l$ -form  $\beta \in \Omega^l(M)$ , the wedge product is defined fiberwise, i.e.,  $(\alpha \wedge \beta)_m = \alpha_x \wedge \beta_m$  for each point  $m \in M$ . It is also associative, i.e.,  $(\alpha \wedge \beta) \wedge \gamma = \alpha \wedge (\beta \wedge \gamma)$ , and graded commutative, i.e.,  $\alpha \wedge \beta = (-1)^{kl} \beta \wedge \alpha$ . These properties are proved in multilinear algebra. So  $M \Rightarrow \Omega^k(M)$  is a contravariant functor from the category  $\mathcal{M}$  into the category of real graded commutative algebras [KMS93].

Let  $M$  be an  $n$ -manifold,  $X \in \mathcal{X}^k(M)$ , and  $\alpha \in \Omega^{k+1}(M)$ . The *interior product*, or *contraction*,  $i_X \alpha = X \lrcorner \alpha \in \Omega^k(M)$  of  $X$  and  $\alpha$  (with *insertion operator*  $i_X$ ) is defined as

$$i_X \alpha(X^1, \dots, X^k) = \alpha(X, X^1, \dots, X^k).$$

Insertion operator  $i_X$  of a vector-field  $X \in \mathcal{X}^k(M)$  is natural with respect to the pull-back  $F^*$  of a diffeomorphism  $F : M \rightarrow N$  between two manifolds, i.e., the following diagram commutes:

$$\begin{array}{ccc} \Omega^k(N) & \xrightarrow{F^*} & \Omega^k(M) \\ i_X \downarrow & & \downarrow i_{F^*X} \\ \Omega^{k-1}(N) & \xrightarrow{F^*} & \Omega^{k-1}(M) \end{array}$$

Similarly, insertion operator  $i_X$  of a vector-field  $X \in \mathcal{Y}^k(M)$  is natural with respect to the push-forward  $F_*$  of a diffeomorphism  $F : M \rightarrow N$ , i.e., the following diagram commutes:

$$\begin{array}{ccc} \Omega^k(M) & \xrightarrow{F_*} & \Omega^k(N) \\ i_Y \downarrow & & \downarrow i_{F_*Y} \\ \Omega^{k-1}(M) & \xrightarrow{F_*} & \Omega^{k-1}(N) \end{array}$$

In case of *Riemannian manifolds* there is another exterior operation. Let  $M$  be a smooth  $n$ -manifold with Riemannian metric  $g = \langle \cdot, \cdot \rangle$  and the corresponding volume element  $\mu$  (see section 2.5 below). The *Hodge star operator*  $*$  :  $\Omega^k(M) \rightarrow \Omega^{n-k}(M)$  on  $M$  is defined as (see Introduction)

$$\alpha \wedge * \beta = \langle \alpha, \beta \rangle \mu \quad \text{for } \alpha, \beta \in \Omega^k(M).$$

The Hodge star operator satisfies the following properties for  $\alpha, \beta \in \Omega^k(M)$  [AMR88]:

1.  $\alpha \wedge * \beta = \langle \alpha, \beta \rangle \mu = \beta \wedge * \alpha$ ;
2.  $*1 = \mu, \quad * \mu = (-1)^{Ind(g)}$ ;
3.  $** \alpha = (-1)^{Ind(g)} (-1)^{k(n-k)} \alpha$ ;
4.  $\langle \alpha, \beta \rangle = (-1)^{Ind(g)} \langle * \alpha, * \beta \rangle$ , where  $Ind(g)$  is the *index* of the metric  $g$ .

### Exterior Differential Systems

Here we give an informal introduction to *exterior differential systems* (EDS, for short), which are expressions involving differential forms related to any manifold  $M$ . Later, when we fully develop the necessary differential geometric as well as variational machinery (see (3.3.6) below), we will give a more precise definition of EDS.

Central in the language of EDS is the notion of *coframing*, which is a real finite-dimensional smooth manifold  $M$  with a given global *cobasis* and coordinates, but without requirement for a proper topological and differential structures. For example,  $M = \mathbb{R}^3$  is a coframing with cobasis  $\{dx, dy, dz\}$  and coordinates  $\{x, y, z\}$ . In addition to the cobasis and coordinates, a coframing can be given structure equations (2.5.2) and restrictions. For example,  $M = \mathbb{R}^2 \setminus \{0\}$  is a coframing with cobasis  $\{e^1, e^2\}$ , a single coordinate  $\{r\}$ , structure equations  $\{dr = e^1, de^1 = 0, de^2 = e^1 \wedge e^2 / r\}$  and restrictions  $\{r \neq 0\}$ .

A *system*  $S$  on  $M$  in EDS terminology is a list of expressions including differential forms (e.g.,  $S = \{dz - ydx\}$ ).

Now, a simple EDS is a triple  $(S, \Omega, M)$ , where  $S$  is a system on  $M$ , and  $\Omega$  is an *independence condition*: either a decomposable  $k$ -form or a system of  $k$ -forms on  $M$ . An EDS is a list of simple EDS objects where the various coframings are all disjoint.

An *integral element* of an exterior system  $(S, \Omega, M)$  is a subspace  $P \subset T_m M$  of the tangent space at some point  $m \in M$  such that all forms in  $S$  vanish when evaluated on vectors from  $P$ . Alternatively, an integral element  $P \subset T_m M$  can be represented by its annihilator  $P^\perp \subset T_m^* M$ , comprising those 1-forms at  $m$  which annihil every vector in  $P$ . For example, with  $M = \mathbb{R}^3 = \{(x, y, z)\}$ ,  $S = \{dx \wedge dz\}$  and  $\Omega = \{dx, dz\}$ , the integral element  $P = \{\partial_x + \partial_z, \partial_y\}$  is equally determined by its annihilator  $P^\perp = \{dz - dx\}$ . Again, for  $S = \{dz - ydx\}$  and  $\Omega = \{dx\}$ , the integral element  $P = \{\partial_x + y\partial_z\}$  can be specified simply as  $\{dy\}$ .

### Distributions and Nonholonomic Geometry

Let  $TM = \cup_{x \in M} T_x M$ , be the tangent bundle of a smooth  $n$ D biomechanical manifold  $M$ . A sub-bundle  $V = \cup_{x \in M} V_x$ , where  $V_x$  is a vector subspace of

$T_x M$ , smoothly dependent on points  $x \in M$ , is called the *distribution*. If the manifold  $M$  is connected,  $\dim V_x$  is called the dimension of the distribution. A vector-field  $X$  on  $M$  *belongs* to the distribution  $V$  if  $X(x) \subset V_x$ . A curve  $\gamma$  is *admissible relatively to*  $V$ , if the vector-field  $\dot{\gamma}$  belongs to  $V$ . A *differential system* is a linear space of vector-fields having a structure of  $C^\infty(M)$ -module. Vector-fields which belong to the distribution  $V$  form a differential system  $N(V)$ . A  $k$ D distribution  $V$  is *integrable* if the manifold  $M$  is foliated to  $k$ D sub-manifolds, having  $V_x$  as the tangent space at the point  $x$ . According to the Frobenius theorem,  $V$  is integrable iff the corresponding differential system  $N(V)$  is *involutive*, i.e., if it is a Lie sub-algebra of the Lie algebra of vector-fields on  $M$ . The *flag* of a differential system  $N$  is a sequence of differential systems:  $N_0 = N$ ,  $N_1 = [N, N], \dots$ ,  $N_l = [N_{l-1}, N], \dots$ .

The differential systems  $N_i$  are not always differential systems of some distributions  $V_i$ , but if for every  $i$ , there exists  $V_i$ , such that  $N_i = N(V_i)$ , then there exists a *flag* of the distribution  $V$ :  $V = V_0 \subset V_1 \dots$ . Such distributions, which have flags, will be called *regular*. It is clear that the sequence  $N(V_i)$  is going to stabilize, and there exists a number  $r$  such that  $N(V_{r-1}) \subset N(V_r) = N(V_{r+1})$ . If there exists a number  $r$  such that  $V_r = TM$ , the distribution  $V$  is called *completely nonholonomic*, and minimal such  $r$  is *the degree of nonholonomicity* of the distribution  $V$ .

Now, let us see the mechanical interpretation of these geometric objects. Consider a nonholonomic mechanical system corresponding to a Riemannian manifold  $(M, g)$ , where  $g$  is a metric defined by the system's kinetic energy [DG03]. Suppose that the distribution  $V$  is defined by  $(n - m)$  one-forms  $\omega_\alpha$ ; in local coordinates  $q = (q^1, \dots, q^n)$  on  $M$

$$\omega_\rho(q)(\dot{q}) = a_{\rho i}(q) \dot{q}^i = 0, \quad (\rho = m + 1, \dots, n; i = 1, \dots, n).$$

A *virtual displacement* is a vector-field  $X$  on  $M$ , such that  $\omega_\rho(X) = 0$ , i.e.,  $X$  belongs to the differential system  $N(V)$ .

Differential equations of motion of a given mechanical system follow from the *D'Alembert-Lagrange principle*: trajectory  $\gamma$  of the given system is a solution of the equation

$$\langle \nabla_{\dot{\gamma}} \dot{\gamma} - Q, X \rangle = 0, \quad (2.10)$$

where  $X$  is an arbitrary virtual displacement,  $Q$  a vector-field of internal forces, and  $\nabla$  is the affine Levi-Civita connection for the metric  $g$ .

The vector-field  $R(x)$  on  $M$ , such that  $R(x) \in V_x^\perp$ ,  $V_x^\perp \oplus V_x = T_x M$ , is called *reaction of ideal nonholonomic connections*. (2.10) can be rewritten as

$$\nabla_{\dot{\gamma}} \dot{\gamma} - Q = R, \quad \omega_\alpha(\dot{\gamma}) = 0. \quad (2.11)$$

If the system is potential, by introducing  $L = T - U$ , where  $U$  is the potential energy of the system ( $Q = -\text{grad} U$ ), then in local coordinates  $q$  on  $M$ , equations (2.11) becomes the *forced Lagrangian equation*:

$$\frac{d}{dt} L_{\dot{q}} - L_q = \tilde{R}, \quad \omega_\alpha(\dot{q}) = 0.$$

Now  $\tilde{R}$  is a one-form in  $(V^\perp)$ , and it can be represented as a linear combination of one-forms  $\omega^{m+1}, \dots, \omega^n$  which define the distribution,  $\tilde{R} = \lambda_\alpha \omega_\alpha$ .

Suppose  $e_1, \dots, e_n$  are the vector-fields on  $M$ , such that  $e_1(x), \dots, e_n(x)$  form a base of the vector space  $T_x M$  at every point  $x \in M$ , and  $e_1, \dots, e_m$  generate the differential system  $N(V)$ . Express them through the coordinate vector-fields:

$$e_i = A_i^j(q) \partial_{q^j}, \quad (i, j = 1, \dots, n).$$

Denote by  $p$  a projection  $p : TM \rightarrow V$  orthogonal according to the metric  $g$ . Corresponding homomorphism of  $C^\infty$ -modules of sections of  $TM$  and  $V$  is

$$p \partial_{q^i} = p_i^a e_a, \quad (a = 1, \dots, m, i = 1, \dots, n).$$

Projecting by  $p$  the equations (2.11), from  $R(x) \in V^\perp(x)$ , we get  $p(R) = 0$ , and denoting  $p(Q) = \tilde{Q}$  we get

$$\tilde{\nabla}_{\dot{\gamma}} \dot{\gamma} = \tilde{Q},$$

where  $\tilde{\nabla}$  is the *projected connection* [DG03]. A relationship between standard Christoffel symbols  $\Gamma_{ij}^k$  and coefficients  $\tilde{\Gamma}_{ab}^c$  of the connection  $\tilde{\nabla}$ , defined by

$$\begin{aligned} \tilde{\nabla}_{e_a} e_b &= \tilde{\Gamma}_{ab}^c e_c, \quad \text{is given by} \\ \tilde{\Gamma}_{ab}^c &= \Gamma_{ij}^k A_a^i A_b^j p_k^c + A_a^i \partial_{q^i} A_b^j p_j^c. \end{aligned}$$

If the motion takes place under the inertia ( $Q = \tilde{Q} = 0$ ), the trajectories of nonholonomic mechanical problem are the geodesics for  $\tilde{\nabla}$ .

Now, let  $V$  be a distribution on  $M$ . Denote a  $C^\infty(M)$ -module of sections on  $V$  by  $\Gamma(V)$ . A *nonholonomic connection* on the sub-bundle  $V$  of  $TM$  is a map  $\nabla : \Gamma(V) \times \Gamma(V) \rightarrow \Gamma(V)$  with the properties:

$$\begin{aligned} \nabla_X(Y + Z) &= \nabla_X Y + \nabla_X Z, & \nabla_X(f \cdot Y) &= X(f)Y + f \nabla_X Y, \\ \nabla_{fX + gY} Z &= f \nabla_X Z + g \nabla_Y Z, & (X, Y, Z \in \Gamma(V); f, g \in C^\infty(M)). \end{aligned}$$

Having a morphism of vector bundles  $p_0 : TM \rightarrow V$ , formed by the projection on  $V$ , denote by  $q_0 = 1_{TM} - p_0$  the projection on  $W$ ,  $V \oplus W = TM$ .

The tensor-field  $T_\nabla : \Gamma(V) \times \Gamma(V) \rightarrow \Gamma(V)$  defined by

$$T_\nabla(X, Y) = \nabla_X Y - \nabla_Y X - p_0[X, Y] \quad ; \quad X, Y \in \Gamma(V)$$

is called the *torsion tensor* for the connection  $\nabla$ .

Suppose there is a positively defined metric tensor  $g = g_{ij}$  on  $V$ . Given a distribution  $V$ , with  $p_0$  and  $g$ , there exists a unique nonholonomic connection  $\nabla$  with the properties [DG03]

$$\nabla_X g(Y, Z) = X(g(Y, Z)) - g(\nabla_X Y, Z) - g(Y, \nabla_X Z) = 0, \quad T_\nabla = 0.$$

These conditions can be rewritten in the form:

$$\nabla_X Y = \nabla_Y X + p_0[X, Y], \quad Z(g(X, Y)) = g(\nabla_Z X, Y) + g(X, \nabla_Z Y).$$

By cyclic permutation of  $X, Y, Z$  and summing we get:

$$\begin{aligned} g(\nabla_X Y, Z) &= \frac{1}{2} \{X(g(Y, Z)) + Y(g(Z, X)) - Z(g(X, Y))\} \\ &+ g(Z, p_0[X, Y]) + g(Y, p_0[Z, X]) - g(X, p_0[Y, Z]). \end{aligned} \quad (2.12)$$

Let  $q^i$ , ( $i = 1, \dots, n$ ) be local coordinates on  $M$ , such that the first  $m$  coordinate vector-fields  $\partial_{q^j}$  are projected by projection  $p_0$  into vector-fields  $e_a$ , ( $a = 1, \dots, m$ ), generating the distribution  $V$ :  $p_0 \partial_{q^j} = p_i^a(q) e_a$ . Vector-fields  $e_a$  can be expressed in the basis  $\partial_{q^j}$  as  $e_a = B_a^i \partial_{q^j}$ , with  $B_a^i p_i^b = \delta_a^b$ . Now we give coordinate expressions for the coefficients of the connection  $\Gamma_{ab}^c$ , defined as  $\nabla_{e_a} e_b = \Gamma_{ab}^c e_c$ . From (2.12) we get

$$\Gamma_{ab}^c = \{c_{ab}\} + g_{ae} g^{cd} \Omega_{bd}^e + g_{be} g^{cd} \Omega_{ad}^e - \Omega_{ab}^c,$$

where  $\Omega$  is obtained from  $p_0[e_a, e_b] = -2\Omega_{ab}^c e_c$  as

$$2\Omega_{ab}^c = p_i^c e_a(B_b^i) - p_i^c e_b(B_a^i),$$

and  $\{c_{ab}\} = \frac{1}{2} g^{ce} (e_a(g_{be}) + e_b(g_{ae}) - e_e(g_{ab}))$ .

### Exterior Derivative on $M$

The *exterior derivative* is an operation that takes  $k$ -forms to  $(k+1)$ -forms on a smooth manifold  $M$ . It defines a unique family of maps  $d : \Omega^k(U) \rightarrow \Omega^{k+1}(U)$ ,  $U$  open in  $M$ , such that (see [AMR88]):

1.  $d$  is a  $\wedge$ -antiderivation; that is,  $d$  is  $\mathbb{R}$ -linear and for two forms  $\alpha \in \Omega^k(U)$ ,  $\beta \in \Omega^l(U)$ ,

$$d(\alpha \wedge \beta) = d\alpha \wedge \beta + (-1)^k \alpha \wedge d\beta.$$

2. If  $f \in C^k(U, \mathbb{R})$  is a function on  $M$ , then  $df = \frac{\partial f}{\partial x^i} dx^i : M \rightarrow T^*M$  is the differential of  $f$ , such that  $df(X) = i_X df = \mathcal{L}_X f - di_X f = \mathcal{L}_X f = X[f]$  for any  $X \in \mathcal{X}^k(M)$ .
3.  $d^2 = d \circ d = 0$  (that is,  $d^{k+1}(U) \circ d^k(U) = 0$ ).
4.  $d$  is natural with respect to restrictions  $|U$ ; that is, if  $U \subset V \subset M$  are open and  $\alpha \in \Omega^k(V)$ , then  $d(\alpha|U) = (d\alpha)|U$ , or the following diagram commutes:

$$\begin{array}{ccc} \Omega^k(V) & \xrightarrow{|U} & \Omega^k(U) \\ d \downarrow & & \downarrow d \\ \Omega^{k+1}(V) & \xrightarrow{|U} & \Omega^{k+1}(U) \end{array}$$

5.  $d$  is natural with respect to the Lie derivative  $\mathcal{L}_X$  (2.2.3) along any vector-field  $X \in \mathcal{X}^k(M)$ ; that is, for  $\omega \in \Omega^k(M)$  we have  $\mathcal{L}_X \omega \in \Omega^k(M)$  and  $d\mathcal{L}_X \omega = \mathcal{L}_X d\omega$ , or the following diagram commutes:

$$\begin{array}{ccc} \Omega^k(M) & \xrightarrow{\mathcal{L}_X} & \Omega^k(M) \\ d \downarrow & & \downarrow d \\ \Omega^{k+1}(M) & \xrightarrow{\mathcal{L}_X} & \Omega^{k+1}(M) \end{array}$$

6. Let  $\varphi : M \rightarrow N$  be a  $C^k$  map of manifolds. Then  $\varphi^* : \Omega^k(N) \rightarrow \Omega^k(M)$  is a homomorphism of differential algebras (with  $\wedge$  and  $d$ ) and  $d$  is natural with respect to  $\varphi^* = F^*$ ; that is,  $\varphi^* d\omega = d\varphi^* \omega$ , or the following diagram commutes:

$$\begin{array}{ccc} \Omega^k(N) & \xrightarrow{\varphi^*} & \Omega^k(M) \\ d \downarrow & & \downarrow d \\ \Omega^{k+1}(N) & \xrightarrow{\varphi^*} & \Omega^{k+1}(M) \end{array}$$

7. Analogously,  $d$  is natural with respect to diffeomorphism  $\varphi_* = (F^*)^{-1}$ ; that is,  $\varphi_* d\omega = d\varphi_* \omega$ , or the following diagram commutes:

$$\begin{array}{ccc} \Omega^k(N) & \xrightarrow{\varphi_*} & \Omega^k(M) \\ d \downarrow & & \downarrow d \\ \Omega^{k+1}(N) & \xrightarrow{\varphi_*} & \Omega^{k+1}(M) \end{array}$$

8.  $\mathcal{L}_X = i_X \circ d + d \circ i_X$  for any  $X \in \mathcal{X}^k(M)$  (a ‘magic’ formula of Cartan).  
 9.  $\mathcal{L}_X \circ d = d \circ \mathcal{L}_X$ , i.e.,  $[\mathcal{L}_X, d] = 0$  for any  $X \in \mathcal{X}^k(M)$ .  
 10.  $[\mathcal{L}_X, i_Y] = i_{[X, Y]}$ ; in particular,  $i_X \circ \mathcal{L}_X = \mathcal{L}_X \circ i_X$  for all  $X, Y \in \mathcal{X}^k(M)$ .

Given a  $k$ -form  $\alpha = f_I dx^I \in \Omega^k(M)$ , the exterior derivative is defined in local coordinates  $(x^1, \dots, x^n)$  of a point  $m \in M$  as

$$d\alpha = d(f_I dx^I) = \frac{\partial f_I}{\partial x^{i_k}} dx^{i_k} \wedge dx^I = df_I \wedge dx^{i_1} \wedge \dots \wedge dx^{i_k}.$$

In particular, the exterior derivative of a function  $f \in C^k(M, \mathbb{R})$  is a 1-form  $df \in \Omega^1(M)$ , with the property that for any  $m \in M$ , and  $X \in \mathcal{X}^k(M)$ ,

$$df_m(X) = X(f),$$

i.e.,  $df_m(X)$  is a Lie derivative of  $f$  at  $m$  in the direction of  $X$ . Therefore, in local coordinates  $(x^1, \dots, x^n)$  of a point  $m \in M$  we have

$$df = \frac{\partial f}{\partial x^i} dx^i.$$

For any two functions  $f, g \in C^k(M, \mathbb{R})$ , exterior derivative obeys the *Leibniz rule*:

$$d(fg) = g df + f dg,$$

and the *chain rule*:

$$d(g(f)) = g'(f) df.$$

A  $k$ -form  $\alpha \in \Omega^k(M)$  is called *closed form* if  $d\alpha = 0$ , and it is called *exact form* if there exists a  $(k-1)$ -form  $\beta \in \Omega^{k-1}(M)$  such that  $\alpha = d\beta$ . Since  $d^2 = 0$ , every exact form is closed. The converse is only partially true (Poincaré Lemma): every closed form is *locally exact*. This means that given a closed  $k$ -form  $\alpha \in \Omega^k(M)$  on an open set  $U \subset M$ , any point  $m \in U$  has a neighborhood on which there exists a  $(k-1)$ -form  $\beta \in \Omega^{k-1}(U)$  such that  $d\beta = \alpha|_U$ .

The Poincaré lemma is a generalization and unification of two well-known facts in vector calculus:

1. If  $\text{curl } F = 0$ , then locally  $F = \text{grad } f$ ;
2. If  $\text{div } F = 0$ , then locally  $F = \text{curl } G$ .

*Poincaré lemma* for contractible manifolds: Any closed form on a smoothly contractible manifold is exact.

### De Rham Complex and Homotopy Operators on $M$

Given a biomechanical manifold  $M$ , let  $\Omega^p(M)$  denote the space of all smooth  $p$ -forms on  $M$ . The differential  $d$ , mapping  $p$ -forms to  $(p+1)$ -forms, serves to define the *De Rham complex* on  $M$ ,

$$0 \rightarrow \Omega^0(M) \xrightarrow{d^0} \Omega^1(M) \xrightarrow{d^1} \dots \xrightarrow{d^{n-1}} \Omega^n(M) \rightarrow 0. \quad (2.13)$$

In general, a *complex* (see subsection (1.2.8) above) is defined as a sequence of vector spaces, and linear maps between successive spaces, with the property that the composition of any pair of successive maps is identically 0. In the case of the de Rham complex (2.13), this requirement is a restatement of the closure property for the exterior differential:  $d \circ d = 0$ .

In particular, for  $n = 3$ , the De Rham complex on a biomechanical manifold  $M$  reads

$$0 \rightarrow \Omega^0(M) \xrightarrow{d^0} \Omega^1(M) \xrightarrow{d^1} \Omega^2(M) \xrightarrow{d^2} \Omega^3(M) \rightarrow 0. \quad (2.14)$$

If  $\omega \equiv f(x, y, z) \in \Omega^0(M)$ , then

$$d^0 \omega \equiv d^0 f = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz = \text{grad } \omega.$$

If  $\omega \equiv f dx + g dy + h dz \in \Omega^1(M)$ , then

$$d^1\omega \equiv \left(\frac{\partial g}{\partial x} - \frac{\partial f}{\partial y}\right) dx \wedge dy + \left(\frac{\partial h}{\partial y} - \frac{\partial g}{\partial z}\right) dy \wedge dz + \left(\frac{\partial f}{\partial z} - \frac{\partial h}{\partial x}\right) dz \wedge dx = \text{curl}\omega.$$

If  $\omega \equiv F dy \wedge dz + G dz \wedge dx + H dx \wedge dy \in \Omega^2(M)$ , then

$$d^2\omega \equiv \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} = \text{div}\omega.$$

Therefore, the De Rham complex (2.14) can be written as

$$0 \rightarrow \Omega^0(M) \xrightarrow{\text{grad}} \Omega^1(M) \xrightarrow{\text{curl}} \Omega^2(M) \xrightarrow{\text{div}} \Omega^3(M) \rightarrow 0.$$

Using the closure property for the exterior differential,  $d \circ d = 0$ , we get the standard identities from vector calculus

$$\text{curl} \cdot \text{grad} = 0 \quad \text{and} \quad \text{div} \cdot \text{curl} = 0.$$

The definition of the complex requires that the kernel of one of the linear maps contains the image of the preceding map. The complex is *exact* if this containment is *equality*. In the case of the De Rham complex (2.13), exactness means that a closed  $p$ -form  $\omega$ , meaning that  $d\omega = 0$ , is necessarily an exact  $p$ -form, meaning that there exists a  $(p-1)$ -form  $\theta$  such that  $\omega = d\theta$ . (For  $p = 0$ , it says that a smooth function  $f$  is closed,  $df = 0$ , iff it is constant). Clearly, any exact form is closed, but the converse need not hold. Thus the De Rham complex is *not* in general exact. The celebrated *De Rham theorem* states that the extent to which this complex fails to be exact measures purely topological information about the manifold  $M$ , its cohomology group.

On the local side, for special types of domains in Euclidean space  $\mathbb{R}^m$ , there is only trivial topology and we do have exactness of the De Rham complex (2.13). This result, known as the *Poincaré lemma*, holds for *star-shaped* domains  $M \subset \mathbb{R}^m$ : Let  $M \subset \mathbb{R}^m$  be a star-shaped domain. Then the De Rham complex over  $M$  is exact.

The key to the proof of exactness of the De Rham complex lies in the construction of suitable *homotopy operators*. By definition, these are linear operators  $h : \Omega^p \rightarrow \Omega^{p-1}$ , taking differential  $p$ -forms into  $(p-1)$ -forms, and satisfying the basic identity [Olv86]

$$\omega = dh(\omega) + h(d\omega), \tag{2.15}$$

for all  $p$ -forms  $\omega \in \Omega^p$ . The discovery of such a set of operators immediately implies exactness of the complex. For if  $\omega$  is closed,  $d\omega = 0$ , then (2.15) reduces to  $\omega = dh(\omega)$  where  $\theta = h(\omega)$ , so  $\omega$  is exact.

### Stokes Theorem and De Rham Cohomology of $M$

Stokes theorem states that if  $\alpha$  is an  $(n-1)$ -form on an orientable  $n$ -manifold  $M$ , then the integral of  $d\alpha$  over  $M$  equals the integral of  $\alpha$  over  $\partial M$ , the boundary of  $M$ . The classical theorems of Gauss, Green, and Stokes are special cases of this result.

A *manifold with boundary* is a set  $M$  together with an atlas of charts  $(U, \phi)$  with boundary on  $M$ . Define (see [AMR88]) the *interior* and *boundary* of  $M$  respectively as

$$\text{Int } M = \bigcup_U \phi^{-1}(\text{Int}(\phi(U))), \quad \text{and} \quad \partial M = \bigcup_U \phi^{-1}(\partial(\phi(U))).$$

If  $M$  is a manifold with boundary, then its interior  $\text{Int } M$  and its boundary  $\partial M$  are smooth manifolds without boundary. Moreover, if  $f : M \rightarrow N$  is a diffeomorphism,  $N$  being another manifold with boundary, then  $f$  induces, by restriction, two diffeomorphisms

$$\text{Int } f : \text{Int } M \rightarrow \text{Int } N, \quad \text{and} \quad \partial f : \partial M \rightarrow \partial N.$$

If  $n = \dim M$ , then  $\dim(\text{Int } M) = n$  and  $\dim(\partial M) = n - 1$ .

To integrate a differential  $n$ -form over an  $n$ -manifold  $M$ ,  $M$  must be oriented. If  $\text{Int } M$  is oriented, we want to choose an *orientation* on  $\partial M$  compatible with it. As for manifolds without boundary a volume form on an  $n$ -manifold with boundary  $M$  is a nowhere vanishing  $n$ -form on  $M$ . Fix an orientation on  $\mathbb{R}^n$ . Then a chart  $(U, \phi)$  is called *positively oriented* if the map  $T_m\phi : T_m M \rightarrow \mathbb{R}^n$  is orientation preserving for all  $m \in U$ .

Let  $M$  be a compact, oriented  $k$ D smooth manifold with boundary  $\partial M$ . Let  $\alpha$  be a smooth  $(k-1)$ -form on  $M$ . Then the classical *Stokes formula* holds

$$\int_M d\alpha = \int_{\partial M} \alpha.$$

If  $\partial M = \emptyset$  then  $\int_M d\alpha = 0$ .

The quotient space

$$H^k(M) = \frac{\text{Ker}(d : \Omega^k(M) \rightarrow \Omega^{k+1}(M))}{\text{Im}(d : \Omega^{k-1}(M) \rightarrow \Omega^k(M))}$$

is called the  $k$ th *De Rham cohomology group* of a manifold  $M$ . The *De Rham theorem* states that these Abelian groups are isomorphic to the so-called singular cohomology groups of  $M$  defined in algebraic topology in terms of simplices and that depend only on the topological structure of  $M$  and not on its differentiable structure. The isomorphism is provided by integration; the fact that the integration map drops to the preceding quotient is guaranteed by Stokes' theorem.

The exterior derivative commutes with the pull-back of differential forms. That means that the vector bundle  $A^k T^* M$  is in fact the value of a functor,

which associates a bundle over  $M$  to each manifold  $M$  and a vector bundle homomorphism over  $\varphi$  to each (local) diffeomorphism  $\varphi$  between manifolds of the same dimension. This is a simple example of the concept of a natural bundle. The fact that the exterior derivative  $d$  transforms sections of  $\Lambda^k T^*M$  into sections of  $\Lambda^{k+1} T^*M$  for every manifold  $M$  can be expressed by saying that  $d$  is an operator from  $\Lambda^k T^*M$  into  $\Lambda^{k+1} T^*M$ . That the exterior derivative  $d$  commutes with (local) diffeomorphisms now means, that  $d$  is a natural operator from the functor  $\Lambda^k T^*$  into functor  $\Lambda^{k+1} T^*$ . If  $k > 0$ , one can show that  $d$  is the unique natural operator between these two natural bundles up to a constant. So even linearity is a consequence of naturality [KMS93].

### Euler–Poincaré Characteristics of $M$

The *Euler–Poincaré characteristics* of a manifold  $M$  equals the sum of its *Betti numbers*

$$\chi(M) = \sum_{p=0}^n (-1)^p b_p.$$

In case of  $2n$ D oriented compact Riemannian manifold  $M$  (*Gauss–Bonnet theorem*) its Euler–Poincaré characteristics is equal

$$\chi(M) = \int_M \gamma,$$

where  $\gamma$  is a closed  $2n$  form on  $M$ , given by

$$\gamma = \frac{(-1)^n}{(4\pi)^n n!} \epsilon_{i_1 \dots i_{2n}}^{1 \dots 2n} \Omega_{i_2}^{i_1} \wedge \Omega_{i_{2n}}^{i_{2n-1}},$$

where  $\Omega_j^i$  is the curvature 2-form of a Riemannian connection on  $M$  (see Chapter 4 for more details).

*Poincaré–Hopf theorem*: The Euler–Poincaré characteristics  $\chi(M)$  of a compact manifold  $M$  equals the sum of indices of zeros of any vector-field on  $M$  which has only isolated zeros.

### Duality of Chains and Forms on $M$

In topology of finite-dimensional smooth (i.e.,  $C^{p+1}$  with  $p \geq 0$ ) manifolds, a fundamental notion is the *duality* between  $p$ -chains  $C$  and  $p$ -forms (i.e.,  $p$ -cochains)  $\omega$  on the smooth manifold  $M$ , or domains of integration and integrands – as an integral on  $M$  represents a bilinear functional (see [BM82, DP97])

$$\int_C \omega \equiv \langle C, \omega \rangle, \quad (2.16)$$

where the integral is called the *period* of  $\omega$ . Period depends only on the cohomology class of  $\omega$  and the homology class of  $C$ . A closed form (cocycle) is

exact (coboundary) if all its periods vanish, i.e.,  $d\omega = 0$  implies  $\omega = d\theta$ . The duality (2.16) is based on the classical Stokes formula

$$\int_C d\omega = \int_{\partial C} \omega.$$

This is written in terms of scalar products on  $M$  as

$$\langle C, d\omega \rangle = \langle \partial C, \omega \rangle,$$

where  $\partial C$  is the boundary of the  $p$ -chain  $C$  oriented coherently with  $C$ . While the boundary operator  $\partial$  is a global operator, the coboundary operator, that is, the exterior derivative  $d$ , is local, and thus more suitable for applications. The main property of the exterior differential,

$$d^2 = 0 \quad \text{implies} \quad \partial^2 = 0,$$

can be easily proved by the use of Stokes' formula

$$\langle \partial^2 C, \omega \rangle = \langle \partial C, d\omega \rangle = \langle C, d^2 \omega \rangle = 0.$$

The analysis of  $p$ -chains and  $p$ -forms on the finite-dimensional biomechanical manifold  $M$  is usually performed in (co)homology categories (see [DP97, Die88]) related to  $M$ .

Let  $\mathcal{M}^\bullet$  denote the category of cochains, (i.e.,  $p$ -forms) on the smooth manifold  $M$ . When  $\mathcal{C} = \mathcal{M}^\bullet$ , we have the category  $\mathcal{S}^\bullet(\mathcal{M}^\bullet)$  of generalized cochain complexes  $A^\bullet$  in  $\mathcal{M}^\bullet$ , and if  $A^n = 0$  for  $n < 0$  we have a subcategory  $\mathcal{S}_{DR}^\bullet(\mathcal{M}^\bullet)$  of the De Rham differential complexes in  $\mathcal{M}^\bullet$

$$\begin{aligned} A_{DR}^\bullet : 0 \rightarrow \Omega^0(M) \xrightarrow{d} \Omega^1(M) \xrightarrow{d} \Omega^2(M) \cdots \\ \cdots \xrightarrow{d} \Omega^n(M) \xrightarrow{d} \cdots \end{aligned} \quad (2.17)$$

Here  $A^n = \Omega^n(M)$  is the vector space over  $\mathbb{R}$  of all  $p$ -forms  $\omega$  on  $M$  (for  $p = 0$  the smooth functions on  $M$ ) and  $d_n = d : \Omega^{n-1}(M) \rightarrow \Omega^n(M)$  is the exterior differential. A form  $\omega \in \Omega^n(M)$  such that  $d\omega = 0$  is a closed form or  $n$ -cocycle. A form  $\omega \in \Omega^n(M)$  such that  $\omega = d\theta$ , where  $\theta \in \Omega^{n-1}(M)$ , is an exact form or  $n$ -coboundary. Let  $Z^n(M) = \text{Ker}(d)$  (resp.  $B^n(M) = \text{Im}(d)$ ) denote a real vector space of cocycles (resp. coboundaries) of degree  $n$ . Since  $d_{n+1} d_n = d^2 = 0$ , we have  $B^n(M) \subset Z^n(M)$ . The quotient vector space

$$H_{DR}^n(M) = \text{Ker}(d) / \text{Im}(d) = Z^n(M) / B^n(M)$$

is the De Rham cohomology group. The elements of  $H_{DR}^n(M)$  represent equivalence sets of cocycles. Two cocycles  $\omega_1, \omega_2$  belong to the same equivalence set, or are cohomologous (written  $\omega_1 \sim \omega_2$ ) iff they differ by a coboundary  $\omega_1 - \omega_2 = d\theta$ . The De Rham cohomology class of any form  $\omega \in \Omega^n(M)$  is

$[\omega] \in H_{DR}^n(M)$ . The De Rham differential complex (2.17) can be considered as a system of second-order ODEs  $d^2\theta = 0$ ,  $\theta \in \Omega^{n-1}(M)$  having a solution represented by  $Z^n(M) = \text{Ker}(d)$ .

Analogously let  $\mathcal{M}_\bullet$  denote the category of chains on the smooth manifold  $M$ . When  $\mathcal{C} = \mathcal{M}_\bullet$ , we have the category  $\mathcal{S}_\bullet(\mathcal{M}_\bullet)$  of generalized chain complexes  $A_\bullet$  in  $\mathcal{M}_\bullet$ , and if  $A_n = 0$  for  $n < 0$  we have a subcategory  $\mathcal{S}_\bullet^{\mathcal{C}}(\mathcal{M}_\bullet)$  of chain complexes in  $\mathcal{M}_\bullet$ .

$$A_\bullet : 0 \leftarrow C^0(M) \xleftarrow{\partial} C^1(M) \xleftarrow{\partial} C^2(M) \dots \xleftarrow{\partial} C^n(M) \xleftarrow{\partial} \dots$$

Here  $A_n = C^n(M)$  is the vector space over  $\mathbb{R}$  of all finite chains  $C$  on the manifold  $M$  and  $\partial_n = \partial : C^{n+1}(M) \rightarrow C^n(M)$ . A finite chain  $C$  such that  $\partial C = 0$  is an  $n$ -cycle. A finite chain  $C$  such that  $C = \partial B$  is an  $n$ -boundary. Let  $Z_n(M) = \text{Ker}(\partial)$  (resp.  $B_n(M) = \text{Im}(\partial)$ ) denote a real vector space of cycles (resp. boundaries) of degree  $n$ . Since  $\partial_{n+1}\partial_n = \partial^2 = 0$ , we have  $B_n(M) \subset Z_n(M)$ . The quotient vector space

$$H_n^{\mathcal{C}}(M) = \text{Ker}(\partial) / \text{Im}(\partial) = Z_n(M) / B_n(M)$$

is the  $n$ -homology group. The elements of  $H_n^{\mathcal{C}}(M)$  are equivalence sets of cycles. Two cycles  $C_1, C_2$  belong to the same equivalence set, or are homologous (written  $C_1 \sim C_2$ ), iff they differ by a boundary  $C_1 - C_2 = \partial B$ . The homology class of a finite chain  $C \in C^n(M)$  is  $[C] \in H_n^{\mathcal{C}}(M)$ .

The dimension of the  $n$ -cohomology (resp.  $n$ -homology) group equals the  $n$ th Betti number  $b^n$  (resp.  $b_n$ ) of the manifold  $M$ . *Poincaré lemma* says that on an open set  $U \in M$  diffeomorphic to  $\mathbb{R}^N$ , all closed forms (cycles) of degree  $p \geq 1$  are exact (boundaries). That is, the Betti numbers satisfy  $b^p = 0$  (resp.  $b_p = 0$ ) for  $p = 1, \dots, n$ .

The *De Rham theorem* states the following. The map  $\Phi: H_n \times H^n \rightarrow \mathbb{R}$  given by  $([C], [\omega]) \rightarrow \langle C, \omega \rangle$  for  $C \in Z_n, \omega \in Z^n$  is a bilinear nondegenerate map which establishes the duality of the groups (vector spaces)  $H_n$  and  $H^n$  and the equality  $b_n = b^n$ .

### Other Exterior Operators on $M$

As the configuration manifold  $M$  is an oriented ND Riemannian manifold, we may select an orientation on all tangent spaces  $T_m M$  and all cotangent spaces  $T_m^* M$ , with the local coordinates  $x^i = (q^i, p_i)$  at a point  $m \in M$ , in a consistent manner. The simplest way to do that is to choose the Euclidean orthonormal basis  $\partial_1, \dots, \partial_N$  of  $\mathbb{R}^N$  as being positive.

Since the manifold  $M$  carries a Riemannian structure  $g = \langle, \rangle$ , we have a scalar product on each  $T_m^* M$ . So, we can define (as above) the linear *Hodge star* operator

$$* : \Lambda^p(T_m^* M) \rightarrow \Lambda^{N-p}(T_m^* M),$$

which is a base point preserving operator

$$* : \Omega^p(M) \rightarrow \Omega^{N-p}(M), \quad (\Omega^p(M) = \Gamma(\Lambda^p(M)))$$

(here  $\Lambda^p(V)$  denotes the  $p$ -fold exterior product of any vector space  $V$ ,  $\Omega^p(M)$  is a space of all  $p$ -forms on  $M$ , and  $\Gamma(E)$  denotes the space of sections of the vector bundle  $E$ ). Also,

$$** = (-1)^{p(N-p)} : \Lambda^p(T_x^*M) \rightarrow \Lambda^p(T_m^*M).$$

As the metric on  $T_m^*M$  is given by  $g^{ij}(x) = (g_{ij}(x))^{-1}$ , we have the *volume form* defined in local coordinates as

$$*(1) = \sqrt{\det(g_{ij})} dx^1 \wedge \dots \wedge dx^n,$$

and

$$\text{vol}(M) = \int_M *(1).$$

For any two  $p$ -forms  $\alpha, \beta \in \Omega^p(M)$  with compact support, we define the (bilinear and positive definite)  $L^2$ -product as

$$(\alpha, \beta) = \int_M \langle \alpha, \beta \rangle *(1) = \int_M \alpha \wedge *\beta.$$

We can extend the product  $(\cdot, \cdot)$  to  $L^2(\Omega^p(M))$ ; it remains bilinear and positive definite, because as usual, in the definition of  $L^2$ , functions that differ only on a set of measure zero are identified.

Using the Hodge star operator  $*$ , we can introduce the *codifferential* operator  $\delta$ , which is formally adjoint to the exterior derivative  $d : \Omega^p(M) \rightarrow \Omega^{p+1}(M)$  on  $\oplus_{p=0}^N \Omega^p(M)$  w.r.t.  $(\cdot, \cdot)$ . This means that for  $\alpha \in \Omega^{p-1}(M), \beta \in \Omega^p(M)$

$$(d\alpha, \beta) = (\alpha, \delta\beta).$$

Therefore, we have  $\delta : \Omega^p(M) \rightarrow \Omega^{p-1}(M)$  and

$$\delta = (-1)^{N(p+1)+1} * d *.$$

Now, the Laplace–Beltrami operator (or, Hodge Laplacian, see subsection (4.3.1) below),  $\Delta$  on  $\Omega^p(M)$ , is defined by relation similar to (2.15) above

$$\Delta = d\delta + \delta d : \Omega^p(M) \rightarrow \Omega^p(M) \quad (2.18)$$

and  $\alpha \in \Omega^p(M)$  is called *harmonic* if  $\Delta\alpha = 0$ .

Let  $M$  be a compact, oriented Riemannian manifold,  $E$  a vector bundle with a bundle metric  $\langle \cdot, \cdot \rangle$  over  $M$ ,

$$D = d + A : \Omega^{p-1}(AdE) \rightarrow \Omega^p(AdE), \quad \text{with } A \in \Omega^1(AdE)$$

– a tensorial and  $\mathbb{R}$ -linear metric connection on  $E$  with curvature  $F_D \in \Omega^2(AdE)$  (Here by  $\Omega^p(AdE)$  we denote the space of those elements of  $\Omega^p(EndE)$  for which the endomorphism of each fibre is skew symmetric;  $EndE$  denotes the space of linear endomorphisms of the fibers of  $E$ ).

## 2.4 Lie Categories in Human-Like Biomechanics

In this section we introduce *Lie categories in biomechanics*, as a unique framework for the concepts of Lie derivative, Lie groups and their associated Lie algebras, as well as more general Lie symmetries.

### 2.4.1 Lie Derivative in Biomechanics

Lie derivative is popularly called ‘*fisherman’s derivative*’. In continuum mechanics it is called Liouville operator. This is a central differential operator in modern differential geometry and its physical and control applications.

#### Lie Derivative on Functions

To define how vector-fields operate on functions on an  $m$ -manifold  $M$ , we will use the *directional derivative* or *Lie derivative* (see (2.2.3)). Let  $f : M \rightarrow \mathbb{R}$  so  $Tf : TM \rightarrow T\mathbb{R} = \mathbb{R} \times \mathbb{R}$ . Following [AMR88] we write  $Tf$  acting on a vector  $v \in T_m M$  in the form

$$Tf \cdot v = (f(m), df(m) \cdot v).$$

This defines, for each point  $m \in M$ , the element  $df(m) \in T_m^* M$ . Thus  $df$  is a section of the cotangent bundle  $T^* M$ , i.e., a 1-form. The 1-form  $df : M \rightarrow T^* M$  defined this way is called the *differential* of  $f$ . If  $f$  is  $C^k$ , then  $df$  is  $C^{k-1}$ .

If  $\phi : U \subset M \rightarrow V \subset E$  is a local chart for  $M$ , then the local representative of  $f \in C^k(M, \mathbb{R})$  is the map  $f : V \rightarrow \mathbb{R}$  defined by  $f = f \circ \phi^{-1}$ . The local representative of  $Tf$  is the tangent map for local manifolds,

$$Tf(x, v) = (f(x), Df(x) \cdot v).$$

Thus the local representative of  $df$  is the derivative of the local representative of  $f$ . In particular, if  $(x^1, \dots, x^n)$  are local coordinates on  $M$ , then the local components of  $df$  are

$$(df)^i = \partial_{x^i} f.$$

The introduction of  $df$  leads to the following definition of the Lie derivative. The *directional* or *Lie derivative*  $\mathcal{L}_X : C^k(M, \mathbb{R}) \rightarrow C^{k-1}(M, \mathbb{R})$  of a function  $f \in C^k(M, \mathbb{R})$  along a vector-field  $X$  is defined by

$$\mathcal{L}_X f(m) = X[f](m) = df(m) \cdot X(m),$$

for any  $m \in M$ . Denote by  $X[f] = df(X)$  the map  $M \ni m \mapsto X[f](m) \in \mathbb{R}$ . If  $f$  is  $F$ -valued, the same definition is used, but now  $X[f]$  is  $F$ -valued.

If a local chart  $(U, \phi)$  on an  $n$ -manifold  $M$  has local coordinates  $(x^1, \dots, x^n)$ , the local representative of  $X[f]$  is given by the function

$$\mathcal{L}_X f = X[f] = X^i \partial_{x^i} f.$$

Evidently if  $f$  is  $C^k$  and  $X$  is  $C^{k-1}$  then  $X[f]$  is  $C^{k-1}$ .

Let  $\varphi : M \rightarrow N$  be a diffeomorphism. Then  $\mathcal{L}_X$  is natural with respect to push-forward by  $\varphi$ . That is, for each  $f \in C^k(M, \mathbb{R})$ ,

$$\mathcal{L}_{\varphi_* X}(\varphi_* f) = \varphi_* \mathcal{L}_X f,$$

i.e., the following diagram commutes:

$$\begin{array}{ccc} C^k(M, \mathbb{R}) & \xrightarrow{\varphi_*} & C^k(N, \mathbb{R}) \\ \mathcal{L}_X \downarrow & & \downarrow \mathcal{L}_{\varphi_* X} \\ C^k(M, \mathbb{R}) & \xrightarrow{\varphi_*} & C^k(N, \mathbb{R}) \end{array}$$

Also,  $\mathcal{L}_X$  is natural with respect to restrictions. That is, for  $U$  open in  $M$  and  $f \in C^k(M, \mathbb{R})$ ,

$$\mathcal{L}_{X|U}(f|U) = (\mathcal{L}_X f)|U,$$

where  $|U : C^k(M, \mathbb{R}) \rightarrow C^k(U, \mathbb{R})$  denotes restriction to  $U$ , i.e., the following diagram commutes:

$$\begin{array}{ccc} C^k(M, \mathbb{R}) & \xrightarrow{|U} & C^k(U, \mathbb{R}) \\ \mathcal{L}_X \downarrow & & \downarrow \mathcal{L}_{X|U} \\ C^k(M, \mathbb{R}) & \xrightarrow{|U} & C^k(U, \mathbb{R}) \end{array}$$

Since  $\varphi^* = (\varphi^{-1})_*$  the Lie derivative is also natural with respect to pull-back by  $\varphi$ . This has a generalization to  $\varphi$ -related vector-fields as follows: Let  $\varphi : M \rightarrow N$  be a  $C^k$ -map,  $X \in \mathcal{X}^{k-1}(M)$  and  $Y \in \mathcal{X}^{k-1}(N)$ ,  $k \geq 1$ . If  $X \sim_\varphi Y$ , then

$$\mathcal{L}_X(\varphi^* f) = \varphi^* \mathcal{L}_Y f$$

for all  $f \in C^k(N, \mathbb{R})$ , i.e., the following diagram commutes:

$$\begin{array}{ccc} C^k(N, \mathbb{R}) & \xrightarrow{\varphi^*} & C^k(M, \mathbb{R}) \\ \mathcal{L}_Y \downarrow & & \downarrow \mathcal{L}_X \\ C^k(N, \mathbb{R}) & \xrightarrow{\varphi^*} & C^k(M, \mathbb{R}) \end{array}$$

The Lie derivative map  $\mathcal{L}_X : C^k(M, \mathbb{R}) \rightarrow C^{k-1}(M, \mathbb{R})$  is a *derivation*, i.e., for two functions  $f, g \in C^k(M, \mathbb{R})$  the *Leibniz rule* is satisfied

$$\mathcal{L}_X(fg) = g\mathcal{L}_Xf + f\mathcal{L}_Xg;$$

Also, Lie derivative of a constant function is zero,  $\mathcal{L}_X(\text{const}) = 0$ .

The connection between the Lie derivative  $\mathcal{L}_Xf$  of a function  $f \in C^k(M, \mathbb{R})$  and the flow  $F_t$  of a vector-field  $X \in \mathcal{X}^{k-1}(M)$  is given as:

$$\frac{d}{dt}(F_t^*f) = F_t^*(\mathcal{L}_Xf).$$

### Lie Derivative of Vector Fields

If  $X, Y \in \mathcal{X}^k(M)$ ,  $k \geq 1$  are two vector-fields on  $M$ , then

$$[\mathcal{L}_X, \mathcal{L}_Y] = \mathcal{L}_X \circ \mathcal{L}_Y - \mathcal{L}_Y \circ \mathcal{L}_X$$

is a derivation map from  $C^{k+1}(M, \mathbb{R})$  to  $C^{k-1}(M, \mathbb{R})$ . Then there is a unique vector-field,  $[X, Y] \in \mathcal{X}^k(M)$  of  $X$  and  $Y$  such that  $\mathcal{L}_{[X, Y]} = [\mathcal{L}_X, \mathcal{L}_Y]$  and  $[X, Y](f) = X(Y(f)) - Y(X(f))$  holds for all functions  $f \in C^k(M, \mathbb{R})$ . This vector-field is also denoted  $\mathcal{L}_XY$  and is called the Lie derivative (2.2.3) of  $Y$  with respect to  $X$ , or the *Lie bracket* of  $X$  and  $Y$ . In a local chart  $(U, \phi)$  at a point  $m \in M$  with coordinates  $(x^1, \dots, x^n)$ , for  $X|_U = X^i\partial_{x^i}$  and  $Y|_U = Y^i\partial_{x^i}$  we have

$$[X^i\partial_{x^i}, Y^j\partial_{x^j}] = (X^i(\partial_{x^i}Y^j) - Y^i(\partial_{x^i}X^j))\partial_{x^j},$$

since second partials commute. If, also  $X$  has flow  $F_t$ , then [AMR88]

$$\frac{d}{dt}(F_t^*Y) = F_t^*(\mathcal{L}_XY).$$

In particular, if  $t = 0$ , this formula becomes

$$\frac{d}{dt}|_{t=0}(F_t^*Y) = \mathcal{L}_XY.$$

Then the unique  $C^{k-1}$  vector-field  $\mathcal{L}_XY = [X, Y]$  on  $M$  defined by

$$[X, Y] = \frac{d}{dt}|_{t=0}(F_t^*Y),$$

is called the Lie derivative of  $Y$  with respect to  $X$ , or the Lie bracket of  $X$  and  $Y$ , and can be interpreted as the leading order term that results from the sequence of flows

$$F_t^{-Y} \circ F_t^{-X} \circ F_t^Y \circ F_t^{-X}(m) = \epsilon^2[X, Y](m) + \mathcal{O}(\epsilon^3), \quad (2.19)$$

for some real  $\epsilon > 0$ . Therefore a Lie bracket can be interpreted as a ‘new direction’ in which the system can flow, by executing the sequence of flows (2.19).

Lie bracket satisfies the following property:

$$[X, Y][f] = X[Y[f]] - Y[X[f]],$$

for all  $f \in C^{k+1}(U, \mathbb{R})$ , where  $U$  is open in  $M$ .

An important relationship between flows of vector-fields is given by the *Campbell–Baker–Hausdorff* formula:

$$F_t^Y \circ F_t^X = F_t^{X+Y+\frac{1}{2}[X,Y]+\frac{1}{12}([X,[X,Y]]-[Y,[X,Y]])+\dots} \quad (2.20)$$

Essentially, if given the composition of multiple flows along multiple vector-fields, this formula gives the one flow along one vector-field which results in the same net flow. One way to prove the Campbell–Baker–Hausdorff formula (2.20) is to expand the product of two formal exponentials and equate terms in the resulting formal power series.

Lie bracket is the  $\mathbb{R}$ -bilinear map  $[\cdot, \cdot] : \mathcal{X}^k(M) \times \mathcal{X}^k(M) \rightarrow \mathcal{X}^k(M)$  with the following properties:

1.  $[X, Y] = -[Y, X]$ , i.e.,  $\mathcal{L}_X Y = -\mathcal{L}_Y X$  for all  $X, Y \in \mathcal{X}^k(M)$  – skew-symmetry;
2.  $[X, X] = 0$  for all  $X \in \mathcal{X}^k(M)$ ;
3.  $[X, [Y, Z]] + [Y, [Z, X]] + [Z, [X, Y]] = 0$  for all  $X, Y, Z \in \mathcal{X}^k(M)$  – the Jacobi identity;
4.  $[fX, Y] = f[X, Y] - (Yf)X$ , i.e.,  $\mathcal{L}_{fX}(Y) = f(\mathcal{L}_X Y) - (\mathcal{L}_Y f)X$  for all  $X, Y \in \mathcal{X}^k(M)$  and  $f \in C^k(M, \mathbb{R})$ ;
5.  $[X, fY] = f[X, Y] + (Xf)Y$ , i.e.,  $\mathcal{L}_X(fY) = f(\mathcal{L}_X Y) + (\mathcal{L}_X f)Y$  for all  $X, Y \in \mathcal{X}^k(M)$  and  $f \in C^k(M, \mathbb{R})$ ;
6.  $[\mathcal{L}_X, \mathcal{L}_Y] = \mathcal{L}_{[X, Y]}$  for all  $X, Y \in \mathcal{X}^k(M)$ .

The pair  $(\mathcal{X}^k(M), [\cdot, \cdot])$  is the prototype of a *Lie algebra* [KMS93]. In more general case of a *general linear Lie algebra*  $\mathfrak{gl}(n)$ , which is the Lie algebra associated to the Lie group  $GL(n)$ , Lie bracket is given by a *matrix commutator*

$$[A, B] = AB - BA,$$

for any two matrices  $A, B \in \mathfrak{gl}(n)$ .

Let  $\varphi : M \rightarrow N$  be a diffeomorphism. Then  $\mathcal{L}_X : \mathcal{X}^k(M) \rightarrow \mathcal{X}^k(M)$  is natural with respect to push-forward by  $\varphi$ . That is, for each  $f \in C^k(M, \mathbb{R})$ ,

$$\mathcal{L}_{\varphi_* X}(\varphi_* Y) = \varphi_* \mathcal{L}_X Y,$$

i.e., the following diagram commutes:

$$\begin{array}{ccc} \mathcal{X}^k(M) & \xrightarrow{\varphi_*} & \mathcal{X}^k(N) \\ \mathcal{L}_X \downarrow & & \downarrow \mathcal{L}_{\varphi_* X} \\ \mathcal{X}^k(M) & \xrightarrow{\varphi_*} & \mathcal{X}^k(N) \end{array}$$

Also,  $\mathcal{L}_X$  is natural with respect to restrictions. That is, for  $U$  open in  $M$  and  $f \in C^k(M, \mathbb{R})$ ,

$$[X|U, Y|U] = [X, Y]|U,$$

where  $|U : C^k(M, \mathbb{R}) \rightarrow C^k(U, \mathbb{R})$  denotes restriction to  $U$ , i.e., the following diagram commutes [AMR88]:

$$\begin{array}{ccc} \mathcal{X}^k(M) & \xrightarrow{|U} & \mathcal{X}^k(U) \\ \mathcal{L}_X \downarrow & & \downarrow \mathcal{L}_{X|U} \\ \mathcal{X}^k(M) & \xrightarrow{|U} & \mathcal{X}^k(U) \end{array}$$

If a local chart  $(U, \phi)$  on an  $n$ -manifold  $M$  has local coordinates  $(x^1, \dots, x^n)$ , then the local components of a Lie bracket are

$$[X, Y]^j = X^i \partial_{x^i} Y^j - Y^i \partial_{x^i} X^j,$$

that is,  $[X, Y] = (X \cdot \nabla)Y - (Y \cdot \nabla)X$ .

Let  $\varphi : M \rightarrow N$  be a  $C^k$ -map,  $X \in \mathcal{X}^{k-1}(M)$  and  $Y \in \mathcal{X}^{k-1}(N)$ ,  $k \geq 1$ . Then  $X \sim_\varphi Y$ , iff

$$(Y[f]) \circ \varphi = X[f \circ \varphi]$$

for all  $f \in C^k(V, \mathbb{R})$ , where  $V$  is open in  $N$ .

For every  $X \in \mathcal{X}^k(M)$ , the operator  $\mathcal{L}_X$  is a derivation on  $(C^k(M, \mathbb{R}), \mathcal{X}^k(M))$ , i.e.,  $\mathcal{L}_X$  is  $\mathbb{R}$ -linear.

For any two vector-fields  $X \in \mathcal{X}^k(M)$  and  $Y \in \mathcal{X}^k(N)$ ,  $k \geq 1$  with flows  $F_t$  and  $G_t$ , respectively, if  $[X, Y] = 0$  then  $F_t^* Y = Y$  and  $G_t^* X = X$ .

### Derivative of the Evolution Operator

Recall (2.3.1) that the time-dependent flow or evolution operator  $F_{t,s}$  of a vector-field  $X \in \mathcal{X}^k(M)$  is defined by the requirement that  $t \mapsto F_{t,s}(m)$  be the integral curve of  $X$  starting at a point  $m \in M$  at time  $t = s$ , i.e.,

$$\frac{d}{dt} F_{t,s}(m) = X(t, F_{t,s}(m)) \quad \text{and} \quad F_{t,t}(m) = m.$$

By uniqueness of integral curves we have  $F_{t,s} \circ F_{s,r} = F_{t,r}$  (replacing the flow property  $F_{t+s} = F_t + F_s$ ) and  $F_{t,t} = \text{identity}$ .

Let  $X_t \in \mathcal{X}^k(M)$ ,  $k \geq 1$  for each  $t$  and suppose  $X(t, m)$  is continuous in  $(t, m) \in \mathbb{R} \times M$ . Then  $F_{t,s}$  is of class  $C^k$  and for  $f \in C^{k+1}(M, \mathbb{R})$  [AMR88], and  $Y \in \mathcal{X}^k(M)$ , we have

1.  $\frac{d}{dt} F_{t,s}^* f = F_{t,s}^* (\mathcal{L}_{X_t} f)$ , and
2.  $\frac{d}{dt} F_{t,s}^* f = F_{t,s}^* ([X_t, Y]) = F_{t,s}^* (\mathcal{L}_{X_t} Y)$ .

From the above theorem, the following identity holds:

$$\frac{d}{dt} F_{t,s}^* f = -X_t [F_{t,s}^* f].$$

### Lie Derivative of Differential Forms

Since  $\mathcal{F} : M \implies \Lambda^k T^*M$  is a vector bundle functor on  $\mathcal{M}$ , the Lie derivative (2.2.3) of a  $k$ -form  $\alpha \in \Omega^k(M)$  along a vector-field  $X \in \mathcal{X}^k(M)$  is defined by

$$\mathcal{L}_X \alpha = \left. \frac{d}{dt} \right|_{t=0} F_t^* \alpha.$$

It has the following properties:

1.  $\mathcal{L}_X(\alpha \wedge \beta) = \mathcal{L}_X \alpha \wedge \beta + \alpha \wedge \mathcal{L}_X \beta$ , so  $\mathcal{L}_X$  is a derivation.
2.  $[\mathcal{L}_X, \mathcal{L}_Y] \alpha = \mathcal{L}_{[X, Y]} \alpha$ .
3.  $\frac{d}{dt} F_t^* \alpha = F_t^* \mathcal{L}_X \alpha = \mathcal{L}_X (F_t^* \alpha)$ .

Formula (3) holds also for time-dependent vector-fields in the sense that  $\frac{d}{dt} F_{t,s}^* \alpha = F_{t,s}^* \mathcal{L}_X \alpha = \mathcal{L}_X (F_{t,s}^* \alpha)$  and in the expression  $\mathcal{L}_X \alpha$  the vector-field  $X$  is evaluated at time  $t$ .

*Cartan magic formula* (see [MR99]) states: the Lie derivative of a  $k$ -form  $\alpha \in \Omega^k(M)$  along a vector-field  $X \in \mathcal{X}^k(M)$  on a smooth manifold  $M$  is defined as

$$\mathcal{L}_X \alpha = di_X \alpha + i_X d\alpha = d(X \lrcorner \alpha) + X \lrcorner d\alpha.$$

Also, the following identities hold [MR99, KMS93]:

1.  $\mathcal{L}_{fX} \alpha = f \mathcal{L}_X \alpha + df \wedge i_X \alpha$ .
2.  $\mathcal{L}_{[X, Y]} \alpha = \mathcal{L}_X \mathcal{L}_Y \alpha - \mathcal{L}_Y \mathcal{L}_X \alpha$ .
3.  $i_{[X, Y]} \alpha = \mathcal{L}_X i_Y \alpha - i_Y \mathcal{L}_X \alpha$ .
4.  $\mathcal{L}_X d\alpha = d\mathcal{L}_X \alpha$ , i.e.,  $[\mathcal{L}_X, d] = 0$ .
5.  $\mathcal{L}_X i_X \alpha = i_X \mathcal{L}_X \alpha$ , i.e.,  $[\mathcal{L}_X, i_X] = 0$ .
6.  $\mathcal{L}_X(\alpha \wedge \beta) = \mathcal{L}_X \alpha \wedge \beta + \alpha \wedge \mathcal{L}_X \beta$ .

### Lie Derivative of Various Tensor Fields

In this subsection, we use local coordinates  $x^i$  ( $i = 1, \dots, n$ ) on a biomechanical  $n$ -manifold  $M$ , to calculate the Lie derivative  $\mathcal{L}_{X^i}$  with respect to a generic vector-field  $X^i$ . (As always,  $\partial_{x^i} \equiv \frac{\partial}{\partial x^i}$ ).

#### *Lie Derivative of a Scalar Field*

Given the scalar field  $\phi$ , its Lie derivative  $\mathcal{L}_{X^i} \phi$  is given as

$$\mathcal{L}_{X^i} \phi = X^i \partial_{x^i} \phi = X^1 \partial_{x^1} \phi + X^2 \partial_{x^2} \phi + \dots + X^n \partial_{x^n} \phi.$$

#### *Lie Derivative of Vector and Covector-Fields*

Given a contravariant vector-field  $V^i$ , its Lie derivative  $\mathcal{L}_{X^i} V^i$  is given as

$$\mathcal{L}_{X^i} V^i = X^k \partial_{x^k} V^i - V^k \partial_{x^k} X^i \equiv [X^i, V^i] - \text{the Lie bracket.}$$

Given a covariant vector-field (i.e., a one-form)  $\omega_i$ , its Lie derivative  $\mathcal{L}_{X^i} \omega_i$  is given as

$$\mathcal{L}_{X^i} \omega_i = X^k \partial_{x^k} \omega_i + \omega_k \partial_{x^i} X^k.$$

*Lie Derivative of a Second-Order Tensor-Field*

Given a (2, 0) tensor-field  $S^{ij}$ , its Lie derivative  $\mathcal{L}_{X^i} S^{ij}$  is given as

$$\mathcal{L}_{X^i} S^{ij} = X^i \partial_{x^i} S^{ij} - S^{ij} \partial_{x^i} X^i - S^{ii} \partial_{x^i} X^j.$$

Given a (1, 1) tensor-field  $S_j^i$ , its Lie derivative  $\mathcal{L}_{X^i} S_j^i$  is given as

$$\mathcal{L}_{X^i} S_j^i = X^i \partial_{x^i} S_j^i - S_j^i \partial_{x^i} X^i + S_i^i \partial_{x^j} X^i.$$

Given a (0, 2) tensor-field  $S_{ij}$ , its Lie derivative  $\mathcal{L}_{X^i} S_{ij}$  is given as

$$\mathcal{L}_{X^i} S_{ij} = X^i \partial_{x^i} S_{ij} + S_{ij} \partial_{x^i} X^i + S_{ii} \partial_{x^j} X^i.$$

*Lie Derivative of a Third-Order Tensor-Field*

Given a (3, 0) tensor-field  $T^{ijk}$ , its Lie derivative  $\mathcal{L}_{X^i} T^{ijk}$  is given as

$$\mathcal{L}_{X^i} T^{ijk} = X^i \partial_{x^i} T^{ijk} - T^{ijk} \partial_{x^i} X^i - T^{iik} \partial_{x^i} X^j - T^{ijj} \partial_{x^i} X^k.$$

Given a (2, 1) tensor-field  $T_k^{ij}$ , its Lie derivative  $\mathcal{L}_{X^i} T_k^{ij}$  is given as

$$\mathcal{L}_{X^i} T_k^{ij} = X^i \partial_{x^i} T_k^{ij} - T_k^{ij} \partial_{x^i} X^i + T_i^{ij} \partial_{x^k} X^i - T_k^{ii} \partial_{x^j} X^j.$$

Given a (1, 2) tensor-field  $T_{jk}^i$ , its Lie derivative  $\mathcal{L}_{X^i} T_{jk}^i$  is given as

$$\mathcal{L}_{X^i} T_{jk}^i = X^i \partial_{x^i} T_{jk}^i - T_{jk}^i \partial_{x^i} X^i + T_{ik}^i \partial_{x^j} X^i + T_{ji}^i \partial_{x^k} X^i.$$

Given a (0, 3) tensor-field  $T_{ijk}$ , its Lie derivative  $\mathcal{L}_{X^i} T_{ijk}$  is given as

$$\mathcal{L}_{X^i} T_{ijk} = X^i \partial_{x^i} T_{ijk} + T_{ijk} \partial_{x^i} X^i + T_{iik} \partial_{x^j} X^i + T_{ijj} \partial_{x^k} X^i.$$

*Lie Derivative of a Fourth-Order Tensor-Field*

Given a (4, 0) tensor-field  $R^{ijkl}$ , its Lie derivative  $\mathcal{L}_{X^i} R^{ijkl}$  is given as

$$\mathcal{L}_{X^i} R^{ijkl} = X^i \partial_{x^i} R^{ijkl} - R^{ijkl} \partial_{x^i} X^i - R^{iikl} \partial_{x^i} X^j - R^{ijil} \partial_{x^i} X^k - R^{ijki} \partial_{x^i} X^l.$$

Given a (3, 1) tensor-field  $R_l^{ijk}$ , its Lie derivative  $\mathcal{L}_{X^i} R_l^{ijk}$  is given as

$$\mathcal{L}_{X^i} R_l^{ijk} = X^i \partial_{x^i} R_l^{ijk} - R_l^{ijk} \partial_{x^i} X^i + R_i^{ijk} \partial_{x^l} X^i - R_l^{iik} \partial_{x^i} X^j - R_l^{ijj} \partial_{x^i} X^k.$$

Given a (2, 2) tensor-field  $R_{kl}^{ij}$ , its Lie derivative  $\mathcal{L}_{X^i} R_{kl}^{ij}$  is given as

$$\mathcal{L}_{X^i} R_{kl}^{ij} = X^i \partial_{x^i} R_{kl}^{ij} - R_{kl}^{ij} \partial_{x^i} X^i + R_{il}^{ij} \partial_{x^k} X^i + R_{ki}^{ij} \partial_{x^l} X^i - R_{kl}^{ii} \partial_{x^j} X^j.$$

Given a (1, 3) tensor-field  $R_{jkl}^i$ , its Lie derivative  $\mathcal{L}_{X^i} R_{jkl}^i$  is given as

$$\mathcal{L}_{X^i} R_{jkl}^i = X^i \partial_{x^i} R_{jkl}^i - R_{jkl}^i \partial_{x^i} X^i + R_{ikl}^i \partial_{x^j} X^i + R_{jil}^i \partial_{x^k} X^i + R_{jki}^i \partial_{x^l} X^i.$$

Given a  $(0, 4)$  tensor-field  $R_{ijkl}$ , its Lie derivative  $\mathcal{L}_{X^i} R_{ijkl}$  is given as

$$\mathcal{L}_{X^i} R_{ijkl} = X^i \partial_{x^i} R_{ijkl} + R_{ijkl} \partial_{x^i} X^i + R_{iikl} \partial_{x^j} X^i + R_{ijil} \partial_{x^k} X^i + R_{ijki} \partial_{x^l} X^i.$$

Finally, recall that a *spinor* is a two-component complex column vector. Physically, spinors can describe both bosons and fermions, while tensors can describe only bosons. The Lie derivative of a spinor  $\phi$  is defined by

$$\mathcal{L}_X \phi(x) = \lim_{t \rightarrow 0} \frac{\bar{\phi}_t(x) - \phi(x)}{t},$$

where  $\bar{\phi}_t$  is the image of  $\phi$  by a one-parameter group of isometries with  $X$  its generator. For a vector field  $X^a$  and a covariant derivative  $\nabla_a$ , the Lie derivative of  $\phi$  is given explicitly by

$$\mathcal{L}_X \phi = X^a \nabla_a \phi - \frac{1}{8} (\nabla_a X_b - \nabla_b X_a) \gamma^a \gamma^b \phi,$$

where  $\gamma^a$  and  $\gamma^b$  are *Dirac matrices* (see, e.g., [BM00]).

## Lie Algebras

Recall from Introduction that an *algebra*  $A$  is a vector space with a product. The product must have the property that

$$a(uv) = (au)v = u(av),$$

for every  $a \in \mathbb{R}$  and  $u, v \in A$ . A map  $\phi : A \rightarrow A'$  between algebras is called an *algebra homomorphism* if  $\phi(u \cdot v) = \phi(u) \cdot \phi(v)$ . A vector subspace  $\mathfrak{I}$  of an algebra  $A$  is called a *left ideal* (resp. *right ideal*) if it is closed under algebra multiplication and if  $u \in A$  and  $i \in \mathfrak{I}$  implies that  $ui \in \mathfrak{I}$  (resp.  $iu \in \mathfrak{I}$ ). A subspace  $\mathfrak{I}$  is said to be a *two-sided ideal* if it is both a left and right ideal. An ideal may not be an algebra itself, but the quotient of an algebra by a two-sided ideal inherits an algebra structure from  $A$ .

A *Lie algebra* is an algebra  $A$  where the multiplication, i.e., the *Lie bracket*  $(u, v) \mapsto [u, v]$ , has the following properties:

LA 1.  $[u, u] = 0$  for every  $u \in A$ , and

LA 2.  $[u, [v, w]] + [w, [u, v]] + [v, w, u] = 0$  for all  $u, v, w \in A$ .

The condition LA 2 is usually called *Jacobi identity*. A subspace  $E \subset A$  of a Lie algebra is called a *Lie subalgebra* if  $[u, v] \in E$  for every  $u, v \in E$ . A map  $\phi : A \rightarrow A'$  between Lie algebras is called a *Lie algebra homomorphism* if  $\phi([u, v]) = [\phi(u), \phi(v)]$  for each  $u, v \in A$ .

All Lie algebras (over a given field  $\mathbb{K}$ ) and all smooth homomorphisms between them form the category  $\mathcal{LAL}$ , which is itself a complete subcategory of the category  $\mathcal{AL}$  of all algebras and their homomorphisms.

### 2.4.2 Lie Groups in Human–Like Biomechanics

In the middle of the 19th century S. Lie made a far reaching discovery that techniques designed to solve particular unrelated types of ODEs, such as separable, homogeneous and exact equations, were in fact all special cases of a general form of integration procedure based on the invariance of the differential equation under a continuous group of symmetries. Roughly speaking a symmetry group of a system of differential equations is a group that transforms solutions of the system to other solutions. Once the symmetry group has been identified a number of techniques to solve and classify these differential equations becomes possible. In the classical framework of Lie, these groups were local groups and arose locally as groups of transformations on some Euclidean space. The passage from the local Lie group to the present day definition using manifolds was accomplished by E. Cartan at the end of the 19th century, whose work is a striking synthesis of Lie theory, classical geometry, differential geometry and topology.

These continuous groups, which originally appeared as symmetry groups of differential equations, have over the years had a profound impact on diverse areas such as algebraic topology, differential geometry, numerical analysis, control theory, classical mechanics, quantum mechanics etc. They are now universally known as Lie groups.

#### Lie Groups and Their Associated Lie Algebras

Recall that a *Lie group* is a smooth (Banach) manifold  $M$  that has at the same time a group  $G$ –structure consistent with its manifold  $M$ –structure in the sense that group multiplication

$$\mu : G \times G \rightarrow G, \quad (g, h) \mapsto gh \quad (2.21)$$

and the inversion

$$\nu : G \rightarrow G, \quad g \mapsto g^{-1} \quad (2.22)$$

are  $C^k$ –maps [Che55, AMR88, MR99, Put93]. A point  $e \in G$  is called the group *identity* element.

For example, any finite–dimensional Banach vector space  $V$  is an Abelian Lie group with group operations  $\mu : V \times V \rightarrow V$ ,  $\mu(x, y) = x + y$ , and  $\nu : V \rightarrow V$ ,  $\nu(x) = -x$ . The identity is just the zero vector. We call such a Lie group a *vector group*.

Let  $G$  and  $H$  be two Lie groups. A map  $G \rightarrow H$  is said to be a *morphism* of Lie groups (or their *smooth homomorphism*) if it is their homomorphism as abstract groups and their smooth map as manifolds [Pos86].

All Lie groups and all their morphisms form the category  $\mathcal{LG}$  (more precisely, there is a countable family of categories  $\mathcal{LG}$  depending on  $C^k$ –smoothness of the corresponding manifolds).

Similarly, a group  $G$  which is at the same time a topological space is said to be a *topological group* if maps (2.21–2.22) are continuous, i.e.,  $C^0$ -maps for it. The homomorphism  $G \rightarrow H$  of topological groups is said to be continuous if it is a continuous map. Topological groups and their continuous homomorphisms form the category  $\mathcal{TG}$ .

A topological group (as well as a smooth manifold) is not necessarily Hausdorff. A topological group  $G$  is Hausdorff iff its identity is closed. As a corollary we have that every Lie group is a Hausdorff topological group (see [Pos86]).

For every  $g$  in a Lie group  $G$ , the two maps,

$$\begin{aligned} L_g : G &\rightarrow G, & h &\mapsto gh, & \text{and} \\ R_h : G &\rightarrow G, & g &\mapsto gh, \end{aligned}$$

are called *left* and *right translation* maps. Since  $L_g \circ L_h = L_{gh}$ , and  $R_g \circ R_h = R_{gh}$ , it follows that  $(L_g)^{-1} = L_{g^{-1}}$  and  $(R_g)^{-1} = R_{g^{-1}}$ , so both  $L_g$  and  $R_g$  are diffeomorphisms. Moreover  $L_g \circ R_h = R_h \circ L_g$ , i.e., left and right translation commute.

A vector-field  $X$  on  $G$  is called *left invariant vector-field* if for every  $g \in G$ ,  $L_g^*X = X$ , that is, if  $(T_h L_g)X(h) = X(gh)$  for all  $h \in G$ , i.e., the following diagram commutes:

$$\begin{array}{ccc} TG & \xrightarrow{TL_g} & TG \\ \uparrow X & & \uparrow X \\ G & \xrightarrow{L_g} & G \end{array}$$

The correspondences  $G \rightarrow TG$  and  $L_g \rightarrow TL_g$  obviously define a functor  $\mathcal{F} : \mathcal{LG} \Rightarrow \mathcal{LG}$  from the category  $\mathcal{G}$  of Lie groups to itself.  $\mathcal{F}$  is another special case of the vector bundle functor (2.2.3).

Let  $\mathcal{X}_L(G)$  denote the set of left invariant vector-fields on  $G$ ; it is a Lie subalgebra of  $\mathcal{X}(G)$ , the set of all vector-fields on  $G$ , since  $L_g^*[X, Y] = [L_g^*X, L_g^*Y] = [X, Y]$ , so the Lie bracket  $[X, Y] \in \mathcal{X}_L(G)$ .

Let  $e$  be the identity element of  $G$ . Then for each  $\xi$  on the tangent space  $T_e G$  we define a vector-field  $X_\xi$  on  $G$  by

$$X_\xi(g) = T_e L_g(\xi).$$

$\mathcal{X}_L(G)$  and  $T_e G$  are isomorphic as vector spaces. Define the Lie bracket on  $T_e G$  by

$$[\xi, \eta] = [X_\xi, X_\eta](e),$$

for all  $\xi, \eta \in T_e G$ . This makes  $T_e G$  into a Lie algebra. Also, by construction, we have

$$[X_\xi, X_\eta] = X_{[\xi, \eta]},$$

this defines a bracket in  $T_eG$  via *left extension*. The vector space  $T_eG$  with the above algebra structure is called the Lie algebra of the Lie group  $G$  and is denoted  $\mathfrak{g}$ .

For example, let  $V$  be a finite-dimensional vector space. Then  $T_eV \simeq V$  and the left invariant vector-field defined by  $\xi \in T_eV$  is the constant vector-field  $X_\xi(\eta) = \xi$ , for all  $\eta \in V$ . The Lie algebra of  $V$  is  $V$  itself.

Since any two elements of an Abelian Lie group  $G$  commute, it follows that all adjoint operators  $Ad_g$ ,  $g \in G$ , equal the identity. Therefore, the Lie algebra  $\mathfrak{g}$  is Abelian; that is,  $[\xi, \eta] = 0$  for all  $\xi, \eta \in \mathfrak{g}$  [MR99].

Recall (2.4.1) that Lie algebras and their smooth homomorphisms form the category  $\mathcal{LAL}$ . We can now introduce the fundamental *Lie functor*,  $\mathcal{F} : \mathcal{LG} \Rightarrow \mathcal{LAL}$ , from the category of Lie groups to the category of Lie algebras [Pos86].

Let  $X_\xi$  be a left invariant vector-field on  $G$  corresponding to  $\xi$  in  $\mathfrak{g}$ . Then there is a unique integral curve  $\gamma_\xi : \mathbb{R} \rightarrow G$  of  $X_\xi$  starting at  $e$ , i.e.,

$$\dot{\gamma}_\xi(t) = X_\xi(\gamma_\xi(t)), \quad \gamma_\xi(0) = e.$$

$\gamma_\xi(t)$  is a smooth *one parameter subgroup* of  $G$ , i.e.,

$$\gamma_\xi(t+s) = \gamma_\xi(t) \cdot \gamma_\xi(s),$$

since, as functions of  $t$  both sides equal  $\gamma_\xi(s)$  at  $t = 0$  and both satisfy differential equation

$$\dot{\gamma}(t) = X_\xi(\gamma_\xi(t))$$

by left invariance of  $X_\xi$ , so they are equal. Left invariance can be also used to show that  $\gamma_\xi(t)$  is defined for all  $t \in \mathbb{R}$ . Moreover, if  $\phi : \mathbb{R} \rightarrow G$  is a one parameter subgroup of  $G$ , i.e., a *smooth homomorphism* of the additive group  $\mathbb{R}$  into  $G$ , then  $\phi = \gamma_\xi$  with  $\xi = \dot{\phi}(0)$ , since taking derivative at  $s = 0$  in the relation

$$\phi(t+s) = \phi(t) \cdot \phi(s) \quad \text{gives} \quad \dot{\phi}(t) = X_{\dot{\phi}(0)}(\phi(t)),$$

so  $\phi = \gamma_\xi$  since both equal  $e$  at  $t = 0$ . Therefore, all one parameter subgroups of  $G$  are of the form  $\gamma_\xi(t)$  for some  $\xi \in \mathfrak{g}$ .

The map  $\exp : \mathfrak{g} \rightarrow G$ , given by

$$\exp(\xi) = \gamma_\xi(1), \quad \exp(0) = e, \quad (2.23)$$

is called the *exponential map* of the Lie algebra  $\mathfrak{g}$  of  $G$  into  $G$ .  $\exp$  is a  $C^k$ -map, similar to the projection  $\pi$  of tangent and cotangent bundles;  $\exp$  is locally a diffeomorphism from a neighborhood of zero in  $\mathfrak{g}$  onto a neighborhood of  $e$  in  $G$ ; if  $f : G \rightarrow H$  is a smooth homomorphism of Lie groups, then

$$f \circ \exp_G = \exp_H \circ T_e f.$$

Also, in this case (see [Che55, MR99, Pos86])

$$\exp(s\xi) = \gamma_\xi(s).$$

Indeed, for fixed  $s \in \mathbb{R}$ , the curve  $t \mapsto \gamma_\xi(ts)$ , which at  $t = 0$  passes through  $e$ , satisfies the differential equation

$$\frac{d}{dt}\gamma_\xi(ts) = sX_\xi(\gamma_\xi(ts)) = X_{s\xi}(\gamma_\xi(ts)).$$

Since  $\gamma_{s\xi}(t)$  satisfies the same differential equation and passes through  $e$  at  $t = 0$ , it follows that  $\gamma_{s\xi}(t) = \gamma_\xi(st)$ . Putting  $t = 1$  yields  $\exp(s\xi) = \gamma_\xi(s)$  [MR99].

Hence  $\exp$  maps the line  $s\xi$  in  $\mathfrak{g}$  onto the one–parameter subgroup  $\gamma_\xi(s)$  of  $G$ , which is tangent to  $\xi$  at  $e$ . It follows from left invariance that the flow  $F_t^\xi$  of  $X$  satisfies  $F_t^\xi(g) = g \exp(s\xi)$ .

Globally, the exponential map  $\exp$ , as given by (2.23), is a natural operation, i.e., for any morphism  $\varphi : G \rightarrow H$  of Lie groups  $G$  and  $H$  and a Lie functor  $\mathcal{F}$ , the following diagram commutes [Pos86]:

$$\begin{array}{ccc} \mathcal{F}(G) & \xrightarrow{\mathcal{F}(\varphi)} & \mathcal{F}(H) \\ \exp \downarrow & & \downarrow \exp \\ G & \xrightarrow{\varphi} & H \end{array}$$

Let  $G_1$  and  $G_2$  be Lie groups with Lie algebras  $\mathfrak{g}_1$  and  $\mathfrak{g}_2$ . Then  $G_1 \times G_2$  is a Lie group with Lie algebra  $\mathfrak{g}_1 \times \mathfrak{g}_2$ , and the exponential map is given by [MR99].

$$\exp : \mathfrak{g}_1 \times \mathfrak{g}_2 \rightarrow G_1 \times G_2, \quad (\xi_1, \xi_2) \mapsto (\exp_1(\xi_1), \exp_2(\xi_2)).$$

For example, in case of a finite–dimensional vector space, or infinite–dimensional Banach space, the exponential map is the identity.

The unit circle in the complex plane  $S^1 = \{z \in \mathbb{C} : |z| = 1\}$  is an Abelian Lie group under multiplication. The tangent space  $T_e S^1$  is the imaginary axis, and we identify  $\mathbb{R}$  with  $T_e S^1$  by  $t \mapsto 2\pi it$ . With this identification, the exponential map  $\exp : \mathbb{R} \rightarrow S^1$  is given by  $\exp(t) = e^{2\pi it}$ .

The  $n$ D torus  $T^n = S^1 \times \dots \times S^1$  ( $n$  times) is an Abelian Lie group. The exponential map  $\exp : \mathbb{R}^n \rightarrow T^n$  is given by

$$\exp(t_1, \dots, t_n) = (e^{2\pi it_1}, \dots, e^{2\pi it_n}).$$

Since  $S^1 = \mathbb{R}/\mathbb{Z}$ , it follows that

$$T^n = \mathbb{R}^n / \mathbb{Z}^n,$$

the projection  $\mathbb{R}^n \rightarrow T^n$  being given by the  $\exp$  map (see [MR99, Pos86]).

For every  $g \in G$ , the map

$$Ad_g = T_e (R_{g^{-1}} \circ L_g) : \mathfrak{g} \rightarrow \mathfrak{g}$$

is called the *adjoint map* (or *operator*) associated with  $g$ .

For each  $\xi \in \mathfrak{g}$  and  $g \in G$  we have

$$\exp(Ad_g \xi) = g (\exp \xi) g^{-1}.$$

The relation between the adjoint map and the Lie bracket is the following: For all  $\xi, \eta \in \mathfrak{g}$  we have

$$\left. \frac{d}{dt} \right|_{t=0} Ad_{\exp(t\xi)} \eta = [\xi, \eta].$$

A Lie subgroup  $H$  of  $G$  is a subgroup  $H$  of  $G$  which is also a submanifold of  $G$ . Then  $\mathfrak{h}$  is a Lie subalgebra of  $\mathfrak{g}$  and moreover  $\mathfrak{h} = \{\xi \in \mathfrak{g} | \exp(t\xi) \in H, \text{ for all } t \in \mathbb{R}\}$ .

One can characterize Lebesgue measure up to a multiplicative constant on  $\mathbb{R}^n$  by its invariance under translations. Similarly, on a locally compact group there is a unique (up to a nonzero multiplicative constant) left-invariant measure, called *Haar measure*. For Lie groups the existence of such measures is especially simple [MR99]: Let  $G$  be a Lie group. Then there is a volume form *Ub5*, unique up to nonzero multiplicative constants, that is left invariant. If  $G$  is compact, *Ub5* is right invariant as well.

### Actions of Lie Groups on $M$

Let  $M$  be a smooth manifold. An action of a Lie group  $G$  (with the unit element  $e$ ) on  $M$  is a smooth map  $\phi : G \times M \rightarrow M$ , such that for all  $x \in M$  and  $g, h \in G$ , (i)  $\phi(e, x) = x$  and (ii)  $\phi(g, \phi(h, x)) = \phi(gh, x)$ . In other words, letting  $\phi_g : x \in M \mapsto \phi_g(x) = \phi(g, x) \in M$ , we have (i')  $\phi_e = id_M$  and (ii')  $\phi_g \circ \phi_h = \phi_{gh}$ .  $\phi_g$  is a diffeomorphism, since  $(\phi_g)^{-1} = \phi_{g^{-1}}$ . We say that the map  $g \in G \mapsto \phi_g \in Diff(M)$  is a homomorphism of  $G$  into the group of diffeomorphisms of  $M$ . In case that  $M$  is a vector space and each  $\phi_g$  is a linear operator, the function of  $G$  on  $M$  is called a representation of  $G$  on  $M$  [Put93]

An action  $\phi$  of  $G$  on  $M$  is said to be *transitive action*, if for every  $x, y \in M$ , there is  $g \in G$  such that  $\phi(g, x) = y$ ; *effective action*, if  $\phi_g = id_M$  implies  $g = e$ , that is  $g \mapsto \phi_g$  is one-to-one; and *free action*, if for each  $x \in M$ ,  $g \mapsto \phi_g(x)$  is one-to-one.

For example,

1.  $G = \mathbb{R}$  acts on  $M = \mathbb{R}$  by translations; explicitly,

$$\phi : G \times M \rightarrow M, \quad \phi(s, x) = x + s.$$

Then for  $x \in \mathbb{R}$ ,  $O_x = \mathbb{R}$ . Hence  $M/G$  is a single point, and the action is transitive and free.

2. A complete flow  $\phi_t$  of a vector-field  $X$  on  $M$  gives an action of  $\mathbb{R}$  on  $M$ , namely

$$(t, x) \in \mathbb{R} \times M \mapsto \phi_t(x) \in M.$$

3. Left translation  $L_g : G \rightarrow G$  defines an effective action of  $G$  on itself. It is also transitive.  
 4. The coadjoint action of  $G$  on  $\mathfrak{g}^*$  is given by

$$Ad^* : (g, \alpha) \in G \times \mathfrak{g}^* \mapsto Ad_{g^{-1}}^*(\alpha) = (T_e(R_{g^{-1}} \circ L_g))^* \alpha \in \mathfrak{g}^*.$$

Let  $\phi$  be an action of  $G$  on  $M$ . For  $x \in M$  the *orbit* of  $x$  is defined by

$$O_x = \{\phi_g(x) | g \in G\} \subset M$$

and the *isotropy group* of  $\phi$  at  $x$  is given by

$$G_x = \{g \in G | \phi(g, x) = x\} \subset G.$$

An action  $\phi$  of  $G$  on a manifold  $M$  defines an equivalence relation on  $M$  by the relation belonging to the same orbit; explicitly, for  $x, y \in M$ , we write  $x \sim y$  if there exists a  $g \in G$  such that  $\phi(g, x) = y$ , that is, if  $y \in O_x$ . The set of all orbits  $M/G$  is called the *orbit space*.

For example, let  $M = \mathbb{R}^2 \setminus \{0\}$ ,  $G = SO(2)$ , the group of rotations in plane, and the action of  $G$  on  $M$  given by

$$\left( \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}, (x, y) \right) \mapsto (x \cos \theta - y \sin \theta, x \sin \theta + y \cos \theta).$$

The action is always free and effective, and the orbits are concentric circles, thus the orbit space is  $M/G \simeq \mathbb{R}_+^*$ .

A crucial concept in mechanics is the infinitesimal description of an action. Let  $\phi : G \times M \rightarrow M$  be an action of a Lie group  $G$  on a smooth manifold  $M$ . For each  $\xi \in \mathfrak{g}$ ,

$$\phi_\xi : \mathbb{R} \times M \rightarrow M, \quad \phi_\xi(t, x) = \phi(\exp(t\xi), x)$$

is an  $\mathbb{R}$ -action on  $M$ . Therefore,  $\phi_{\exp(t\xi)} : M \rightarrow M$  is a flow on  $M$ ; the corresponding vector-field on  $M$ , given by

$$\xi_M(x) = \left. \frac{d}{dt} \right|_{t=0} \phi_{\exp(t\xi)}(x)$$

is called the infinitesimal generator of the action, corresponding to  $\xi$  in  $\mathfrak{g}$ .

The tangent space at  $x$  to an orbit  $O_x$  is given by

$$T_x O_x = \{\xi_M(x) | \xi \in \mathfrak{g}\}.$$

Let  $\phi : G \times M \rightarrow M$  be a smooth  $G$ -action. For all  $g \in G$ , all  $\xi, \eta \in \mathfrak{g}$  and all  $\alpha, \beta \in \mathbb{R}$ , we have:

$$(Ad_g \xi)_M = \phi_{g^{-1}}^* \xi_M, [\xi_M, \eta_M] = -[\xi, \eta]_M, \text{ and } (\alpha\xi + \beta\eta)_M = \alpha\xi_M + \beta\eta_M.$$

Let  $M$  be a smooth manifold,  $G$  a Lie group and  $\phi : G \times M \rightarrow M$  a  $G$ -action on  $M$ . We say that a smooth map  $f : M \rightarrow M$  is with respect to this action if for all  $g \in G$ ,

$$f \circ \phi_g = \phi_g \circ f.$$

Let  $f : M \rightarrow M$  be an equivariant smooth map. Then for any  $\xi \in \mathfrak{g}$  we have

$$Tf \circ \xi_M = \xi_M \circ f.$$

### Cohomology of Lie Groups

E. Cartan only studied real cohomology, using the De Rham theorems (see Chapter 4). Let  $G$  be a compact Lie group, operating on the right on a  $C^k$  manifold  $M$  by a  $C^k$ -operation  $(s, x) \mapsto x \cdot s$ . Since there exists a measure  $ds$  on  $G$ , invariant by left and right translations and of total mass 1, Hurewicz's idea of taking *mean values* on  $G$  of an arbitrary exterior  $p$ -form  $\alpha$  on  $M$  may be applied: for any point  $x \in M$ , the mean value  $m(\alpha)$  of a  $p$ -form  $\alpha$  takes the value

$$m(\alpha)(x) = \int_G \alpha(x \cdot s) ds.$$

Now  $m(\alpha)$  is *invariant* under the action of  $G$  on  $M$ , and if  $\alpha$  is closed (resp. exact), then  $m(\alpha)$  is also closed (resp. exact). Furthermore,  $\alpha$  and  $m(\alpha)$  are *cohomologous* on  $M$ ; if  $H_G^\bullet(M)$  is the graded subspace of the real cohomology space  $H^\bullet(M)$ , consisting of the classes of the differential forms invariant under the action of  $G$ , this defines an *isomorphism*

$$m^* : H^\bullet(M) \xrightarrow{\sim} H_G^\bullet(M).$$

Cartan's interpretation of the real cohomology  $H^\bullet(G)$  of a compact Lie group  $G$  is obtained as a corollary by consideration of the action  $((s, t), x) \mapsto s^{-1}xt$  of  $G \times G$  on  $G$ . A  $p$ -form is invariant under the action if it is *bi-invariant*, that is, invariant under both left and right translations in  $G$ . The Lie-Cartan theory implies that for such a form  $\alpha$ ,  $d\alpha = 0$ , so that when one computes  $H_{G \times G}^\bullet(G)$ , all cochains are cocycles and all coboundaries are 0. Hence the fundamental result that  $H^\bullet(G)$  is *isomorphic to the graded algebra  $b^*(G)$  of all bi-invariant differential forms*.

The explicit determination of  $H^\bullet(G)$  is thus reduced to an algebraic problem. The group  $G$  operates on the dual  $\mathfrak{g}^*$  of the Lie algebra  $\mathfrak{g}$  by the coadjoint representation  $s \mapsto {}^tAd(s)$ ;  $b^*(G)$  is the sum of the 1D subspaces of  $\mathfrak{g}^*$  stable for that representation; for a compact group, they can in principle be determined by Cartan's method of *highest weights*.

## Basic Biomechanical Groups

### *Galilei Group*

The *Galilei group* is the group of transformations in space and time that connect those Cartesian systems that are termed ‘inertial frames’ in Newtonian mechanics. The most general relationship between two such frames is the following. The origin of the time scale in the inertial frame  $S'$  may be shifted compared with that in  $S$ ; the orientation of the Cartesian axes in  $S'$  may be different from that in  $S$ ; the origin  $O$  of the Cartesian frame in  $S'$  may be moving relative to the origin  $O$  in  $S$  at a uniform velocity. The transition from  $S$  to  $S'$  involves ten parameters; thus the Galilei group is a ten parameter group. The basic assumption inherent in Galilei–Newtonian relativity is that there is an absolute time scale, so that the only way in which the time variables used by two different ‘inertial observers’ could possibly differ is that the zero of time for one of them may be shifted relative to the zero of time for the other.

Galilei space–time structure involves the following three elements:

1. *World*, as a 4D affine space  $A^4$ . The points of  $A^4$  are called *world points* or *events*. The parallel transitions of the world  $A^4$  form a linear (i.e., Euclidean) space  $\mathbb{R}^4$ .
2. *Time*, as a linear map  $t : \mathbb{R}^4 \rightarrow \mathbb{R}$  of the linear space of the world parallel transitions onto the real ‘time axes’. Time interval from the event  $a \in A^4$  to  $b \in A^4$  is called the number  $t(b-a)$ ; if  $t(b-a) = 0$  then the events  $a$  and  $b$  are called synchronous. The set of all mutually synchronous events consists a 3D affine space  $A^3$ , being a subspace of the world  $A^4$ . The kernel of the mapping  $t$  consists of the parallel transitions of  $A^4$  translating arbitrary (and every) event to the synchronous one; it is a linear 3D subspace  $\mathbb{R}^3$  of the space  $\mathbb{R}^4$ .
3. *Distance (metric)* between the synchronous events,

$$\rho(a, b) = \| a - b \|, \quad \text{for all } a, b \in A^3,$$

given by the scalar product in  $\mathbb{R}^3$ . The distance transforms arbitrary space of synchronous events into the well known 3D Euclidean space  $E^3$ .

The space  $A^4$ , with the Galilei space–time structure on it, is called Galilei space. Galilei group is the group of all possible transformations of the Galilei space, preserving its structure. The elements of the Galilei group are called Galilei transformations. Therefore, Galilei transformations are affine transformations of the world  $A^4$  preserving the time intervals and distances between the synchronous events.

The direct product  $\mathbb{R} \times \mathbb{R}^3$ , of the time axes with the 3D linear space  $\mathbb{R}^3$  with a fixed Euclidean structure, has a natural Galilei structure. It is called Galilei coordinate system.

*General Linear Group*

The group of linear isomorphisms of  $\mathbb{R}^n$  to  $\mathbb{R}^n$  is a Lie group of dimension  $n^2$ , called the general linear group and denoted  $Gl(n, \mathbb{R})$ . It is a smooth manifold, since it is a subset of the vector space  $L(\mathbb{R}^n, \mathbb{R}^n)$  of all linear maps of  $\mathbb{R}^n$  to  $\mathbb{R}^n$ , as  $Gl(n, \mathbb{R})$  is the inverse image of  $\mathbb{R} \setminus \{0\}$  under the continuous map  $A \mapsto \det A$  of  $L(\mathbb{R}^n, \mathbb{R}^n)$  to  $\mathbb{R}$ . The group operation is composition

$$(A, B) \in Gl(n, \mathbb{R}) \times Gl(n, \mathbb{R}) \mapsto A \circ B \in Gl(n, \mathbb{R})$$

and the inverse map is

$$A \in Gl(n, \mathbb{R}) \mapsto A^{-1} \in Gl(n, \mathbb{R}).$$

If we choose a basis in  $\mathbb{R}^n$ , we can represent each element  $A \in Gl(n, \mathbb{R})$  by an invertible  $(n \times n)$ -matrix. The group operation is then matrix multiplication and the inversion is matrix inversion. The identity is the identity matrix  $I_n$ . The group operations are smooth since the formulas for the product and inverse of matrices are smooth in the matrix components.

The Lie algebra of  $Gl(n, \mathbb{R})$  is  $\mathfrak{gl}(n)$ , the vector space  $L(\mathbb{R}^n, \mathbb{R}^n)$  of all linear transformations of  $\mathbb{R}^n$ , with the commutator bracket

$$[A, B] = AB - BA.$$

For every  $A \in L(\mathbb{R}^n, \mathbb{R}^n)$ ,

$$\gamma_A : t \in \mathbb{R} \mapsto \gamma_A(t) = \sum_{i=0}^{\infty} \frac{t^i}{i!} A^i \in Gl(n, \mathbb{R})$$

is a one parameter subgroup of  $Gl(n, \mathbb{R})$ , because

$$\gamma_A(0) = I, \quad \text{and} \quad \dot{\gamma}_A(t) = \sum_{i=0}^{\infty} \frac{t^{i-1}}{(i-1)!} A^i = \gamma_A(t) A.$$

Hence  $\gamma_A$  is an integral curve of the left invariant vector-field  $X_A$ . Therefore, the exponential map is given by

$$\exp : A \in L(\mathbb{R}^n, \mathbb{R}^n) \mapsto \exp(A) \equiv e^A = \gamma_A(1) = \sum_{i=0}^{\infty} \frac{A^i}{i!} \in Gl(n, \mathbb{R}).$$

For each  $A \in Gl(n, \mathbb{R})$  the corresponding adjoint map

$$Ad_A : L(\mathbb{R}^n, \mathbb{R}^n) \rightarrow L(\mathbb{R}^n, \mathbb{R}^n)$$

is given by

$$Ad_A B = A \cdot B \cdot A^{-1}.$$

### Groups of Joint Rotations

Local kinematics at each rotational robot or (synovial) human joint, is defined as a *group action* of an  $n$ D constrained rotational Lie group  $SO(n)$  on the Euclidean space  $\mathbb{R}^n$ . In particular, there is an action of  $SO(2)$ -group in uniaxial human joints (cylindrical, or *hinge joints*, like knee and elbow) and an action of  $SO(3)$ -group in three-axial human joints (spherical, or *ball-and-socket joints*, like hip, shoulder, neck, wrist and ankle). In both cases,  $SO(n)$  acts, with its operators of rotation, on the vector  $x = \{x^\mu\}$ , ( $i = 1, 2, 3$ ) of external, Cartesian coordinates of the parent body-segment, depending, at the same time, on the vector  $q = \{q^s\}$ , ( $s = 1, \dots, n$ ) on  $n$  group-parameters, i.e., joint angles.

Each joint rotation  $R \in SO(n)$  defines a map

$$R : x^\mu \mapsto \hat{x}^\mu, \quad R(x^\mu, q^s) = R_{q^s} x^\mu,$$

where  $R_{q^s} \in SO(n)$  are joint group operators. The vector  $v = \{v_s\}$ , ( $s = 1, \dots, n$ ) of  $n$  infinitesimal generators of these rotations, i.e., joint angular velocities, given by

$$v_s = -\left[\frac{\partial R(x^\mu, q^s)}{\partial q^s}\right]_{q=0} \frac{\partial}{\partial x^\mu},$$

constitute an  $n$ D Lie algebra  $\mathfrak{so}(n)$  corresponding to the joint rotation group  $SO(n)$ . Conversely, each joint group operator  $R_{q^s}$ , representing a one-parameter subgroup of  $SO(n)$ , is defined as the exponential map of the corresponding joint group generator  $v_s$

$$R_{q^s} = \exp(q^s v_s). \quad (2.24)$$

The exponential map (2.24) represents a solution of the joint operator differential equation in the joint group-parameter space  $\{q^s\}$

$$\frac{dR_{q^s}}{dq^s} = v_s R_{q^s}.$$

#### *Uniaxial Group of Joint Rotations*

The uniaxial joint rotation in a single Cartesian plane around a perpendicular axis, e.g.,  $xy$ -plane about the  $z$  axis, by an internal joint angle  $\theta$ , leads to the following transformation of the joint coordinates

$$\hat{x} = x \cos \theta - y \sin \theta, \quad \hat{y} = x \sin \theta + y \cos \theta.$$

In this way, the joint  $SO(2)$ -group, given by

$$SO(2) = \left\{ R_\theta = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \mid \theta \in [0, 2\pi] \right\},$$

acts in a canonical way on the Euclidean plane  $\mathbb{R}^2$  by

$$SO(2) = \left( \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}, \begin{pmatrix} x \\ w \end{pmatrix} \right) \mapsto \begin{pmatrix} x \cos \theta - y \sin \theta \\ x \sin \theta + y \cos \theta \end{pmatrix}.$$

Its associated Lie algebra  $\mathfrak{so}(2)$  is given by

$$\mathfrak{so}(2) = \left\{ \begin{pmatrix} 0 & -t \\ t & 0 \end{pmatrix} \mid t \in \mathbb{R} \right\},$$

since the curve  $\gamma_\theta \in SO(2)$  given by

$$\gamma_\theta : t \in \mathbb{R} \mapsto \gamma_\theta(t) = \begin{pmatrix} \cos t\theta & -\sin t\theta \\ \sin t\theta & \cos t\theta \end{pmatrix} \in SO(2),$$

passes through the identity  $I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$  and then

$$\left. \frac{d}{dt} \right|_{t=0} \gamma_\theta(t) = \begin{pmatrix} 0 & -\theta \\ \theta & 0 \end{pmatrix},$$

so that  $I_2$  is a basis of  $\mathfrak{so}(2)$ , since  $\dim(SO(2)) = 1$ .

The *exponential map*  $\exp : \mathfrak{so}(2) \rightarrow SO(2)$  is given by

$$\exp \begin{pmatrix} 0 & -\theta \\ \theta & 0 \end{pmatrix} = \gamma_\theta(1) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}.$$

The *infinitesimal generator* of the action of  $SO(2)$  on  $\mathbb{R}^2$ , i.e., joint angular velocity  $v$ , is given by

$$v = -y \frac{\partial}{\partial x} + x \frac{\partial}{\partial y},$$

since

$$v_{\mathbb{R}^2}(x, y) = \left. \frac{d}{dt} \right|_{t=0} \exp(tv)(x, y) = \left. \frac{d}{dt} \right|_{t=0} \begin{pmatrix} \cos tv & -\sin tv \\ \sin tv & \cos tv \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}.$$

The *momentum map* (see subsection 2.6.3 below)  $J : T^*\mathbb{R}^2 \rightarrow \mathbb{R}$  associated to the lifted action of  $SO(2)$  on  $T^*\mathbb{R}^2 \simeq \mathbb{R}^4$  is given by

$$\begin{aligned} J(x, y, p_1, p_2) &= xp_2 - yp_1, & \text{since} \\ J(x, y, p_x, p_y)(\xi) &= (p_x dx + p_y dy)(v_{\mathbb{R}^2}) = -vp_x y + -vp_y x. \end{aligned}$$

The Lie group  $SO(2)$  acts on the symplectic manifold  $(\mathbb{R}^4, \omega = dp_x \wedge dx + dp_y \wedge dy)$  by

$$\begin{aligned} &\phi \left( \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}, (x, y, p_x, p_y) \right) \\ &= (x \cos \theta - y \sin \theta, x \sin \theta + y \cos \theta, p_x \cos \theta - p_y \sin \theta, p_x \sin \theta + p_y \cos \theta). \end{aligned}$$

*Three-Axial Group of Joint Rotations*

The three-axial  $SO(3)$ -group of human-like joint rotations depends on three parameters, Euler joint angles  $q^i = (\varphi, \psi, \theta)$ , defining the rotations about the Cartesian coordinate triedar  $(x, y, z)$  placed at the joint pivot point. Each of the Euler angles are defined in the constrained range  $(-\pi, \pi)$ , so the joint group space is a constrained sphere of radius  $\pi$ .

Let  $G = SO(3) = \{A \in \mathcal{M}_{3 \times 3}(\mathbb{R}) : A^t A = I_3, \det(A) = 1\}$  be the group of rotations in  $\mathbb{R}^3$ . It is a Lie group and  $\dim(G) = 3$ . Let us isolate its one-parameter joint subgroups, i.e., consider the three operators of the finite joint rotations  $R_\varphi, R_\psi, R_\theta \in SO(3)$ , given by

$$R_\varphi = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \varphi & -\sin \varphi \\ 0 & \sin \varphi & \cos \varphi \end{bmatrix}, \quad R_\psi = \begin{bmatrix} \cos \psi & 0 & \sin \psi \\ 0 & 1 & 0 \\ -\sin \psi & 0 & \cos \psi \end{bmatrix}, \quad R_\theta = \begin{bmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

corresponding respectively to rotations about  $x$ -axis by an angle  $\varphi$ , about  $y$ -axis by an angle  $\psi$ , and about  $z$ -axis by an angle  $\theta$ .

The total three-axial joint rotation  $A$  is defined as the product of above one-parameter rotations  $R_\varphi, R_\psi, R_\theta$ , i.e.,  $A = R_\varphi R_\psi R_\theta$  is equal

$$A = \begin{bmatrix} \cos \psi \cos \varphi - \cos \theta \sin \varphi \sin \psi & \cos \psi \cos \varphi + \cos \theta \cos \varphi \sin \psi & \sin \theta \sin \psi \\ -\sin \psi \cos \varphi - \cos \theta \sin \varphi \sin \psi & -\sin \psi \sin \varphi + \cos \theta \cos \varphi \cos \psi & \sin \theta \cos \psi \\ \sin \theta \sin \varphi & -\sin \theta \cos \varphi & \cos \theta \end{bmatrix}.$$

$R_\varphi, R_\psi$  and  $R_\theta$  are curves in  $SO(3)$  starting from  $I_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ . Their

derivatives in  $\varphi = 0, \psi = 0$  and  $\theta = 0$  belong to the associated *tangent Lie algebra*  $\mathfrak{so}(3)$ . That is the corresponding infinitesimal generators of joint rotations – joint angular velocities  $v_\varphi, v_\psi, v_\theta \in \mathfrak{so}(3)$  – are respectively given by

$$v_\varphi = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} = -y \frac{\partial}{\partial z} + z \frac{\partial}{\partial y}, \quad v_\psi = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix} = -z \frac{\partial}{\partial x} + x \frac{\partial}{\partial z},$$

$$v_\theta = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} = -x \frac{\partial}{\partial y} + y \frac{\partial}{\partial x}.$$

Moreover, the elements are linearly independent and so

$$\mathfrak{so}(3) = \left\{ \begin{bmatrix} 0 & -a & b \\ a & 0 & -\gamma \\ -b & \gamma & 0 \end{bmatrix} \mid a, b, \gamma \in \mathbb{R} \right\}.$$

the Lie algebra  $\mathfrak{so}(3)$  is identified with  $\mathbb{R}^3$  by associating to each  $v =$

$(v_\varphi, v_\psi, v_\theta) \in \mathbb{R}^3$  the matrix  $v \in \mathfrak{so}(3)$  given by  $v = \begin{bmatrix} 0 & -a & b \\ a & 0 & -\gamma \\ -b & \gamma & 0 \end{bmatrix}$ . Then

we have the following identities:

1.  $\widehat{u \times v} = [\hat{u}, v]$ ; and
2.  $u \cdot v = -\frac{1}{2} \text{Tr}(\hat{u} \cdot v)$ .

The exponential map  $\exp : \mathfrak{so}(3) \rightarrow SO(3)$  is given by *Rodrigues relation*

$$\exp(v) = I + \frac{\sin \|v\|}{\|v\|} v + \frac{1}{2} \left( \frac{\sin \frac{\|v\|}{2}}{\frac{\|v\|}{2}} \right)^2 v^2,$$

where the norm  $\|v\|$  is given by

$$\|v\| = \sqrt{(v^1)^2 + (v^2)^2 + (v^3)^2}.$$

The dual, *cotangent Lie algebra*  $\mathfrak{so}(3)^*$ , includes the three joint angular momenta  $p_\varphi, p_\psi, p_\theta \in \mathfrak{so}(3)^*$ , derived from the joint velocities  $v$  by multiplying them with corresponding moments of inertia.

### Special Euclidean Groups of Total Joint Motions

Biomechanically realistic joint movement is predominantly rotational, plus restricted translational (translational motion in human joints is observed after reaching the limit of rotational amplitude). Gross translation in any human joint means joint dislocation, which is a severe injury. Obvious models for uniaxial and triaxial joint motions are *special Euclidean groups of rigid body motions*,  $SE(2)$  and  $SE(3)$ , respectively.

#### *Special Euclidean Group in the Plane*

The motion in uniaxial human joints is naturally modelled by the *special Euclidean group in the plane*,  $SE(2)$ . It consists of all transformations of  $\mathbb{R}^2$  of the form  $Az + a$ , where  $z, a \in \mathbb{R}^2$ , and

$$A \in SO(2) = \left\{ \text{matrices of the form } \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \right\}.$$

In other words [MR99], group  $SE(2)$  consists of matrices of the form:

$$(R_\theta, a) = \begin{pmatrix} R_\theta & a \\ 0 & I \end{pmatrix}, \text{ where } a \in \mathbb{R}^2 \text{ and } R_\theta \text{ is the rotation matrix:}$$

$R_\theta = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$ , while  $I$  is the  $3 \times 3$  identity matrix. The inverse  $(R_\theta, a)^{-1}$  is given by

$$(R_\theta, a)^{-1} = \begin{pmatrix} R_\theta & a \\ 0 & I \end{pmatrix}^{-1} = \begin{pmatrix} R_{-\theta} & -R_{-\theta}a \\ 0 & I \end{pmatrix}.$$

The Lie algebra  $\mathfrak{se}(2)$  of  $SE(2)$  consists of  $3 \times 3$  block matrices of the form

$$\begin{pmatrix} -\xi J & v \\ 0 & 0 \end{pmatrix}, \quad \text{where} \quad J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad (J^T = J^{-1} = -J),$$

with the usual commutator bracket. If we identify  $\mathfrak{se}(2)$  with  $\mathbb{R}^3$  by the isomorphism

$$\begin{pmatrix} -\xi J & v \\ 0 & 0 \end{pmatrix} \in \mathfrak{se}(2) \longmapsto (\xi, v) \in \mathbb{R}^3,$$

then the expression for the Lie algebra bracket becomes

$$[(\xi, v_1, v_2), (\zeta, w_1, w_2)] = (0, \zeta v_2 - \xi w_2, \xi w_1 - \zeta v_1) = (0, \xi J^T w - \zeta J^T v),$$

where  $v = (v_1, v_2)$  and  $w = (w_1, w_2)$ .

The *adjoint group action* of

$$(R_\theta, a) \begin{pmatrix} R_\theta & a \\ 0 & I \end{pmatrix} \quad \text{on} \quad (\xi, v) = \begin{pmatrix} -\xi J & v \\ 0 & 0 \end{pmatrix}$$

is given by the *group conjugation*,

$$\begin{pmatrix} R_\theta & a \\ 0 & I \end{pmatrix} \begin{pmatrix} -\xi J & v \\ 0 & 0 \end{pmatrix} \begin{pmatrix} R_{-\theta} & -R_{-\theta}a \\ 0 & I \end{pmatrix} = \begin{pmatrix} -\xi J \xi Ja + R_\theta v \\ 0 & 0 \end{pmatrix},$$

or, in coordinates [MR99],

$$Ad_{(R_\theta, a)}(\xi, v) = (\xi, \xi Ja + R_\theta v). \quad (2.25)$$

In proving (2.25) we used the identity  $R_\theta J = J R_\theta$ . Identify the dual algebra,  $\mathfrak{se}(2)^*$ , with matrices of the form  $\begin{pmatrix} \frac{\mu}{2} J & 0 \\ \alpha & 0 \end{pmatrix}$ , via the nondegenerate pairing given by the trace of the product. Thus,  $\mathfrak{se}(2)^*$  is isomorphic to  $\mathbb{R}^3$  via

$$\begin{pmatrix} \frac{\mu}{2} J & 0 \\ \alpha & 0 \end{pmatrix} \in \mathfrak{se}(2)^* \longmapsto (\mu, \alpha) \in \mathbb{R}^3,$$

so that in these coordinates, the pairing between  $\mathfrak{se}(2)^*$  and  $\mathfrak{se}(2)$  becomes

$$\langle (\mu, \alpha), (\xi, v) \rangle = \mu \xi + \alpha \cdot v,$$

that is, the usual dot product in  $\mathbb{R}^3$ . The *coadjoint group action* is thus given by

$$Ad_{(R_\theta, a)}^*(\mu, \alpha) = (\mu - R_\theta \alpha \cdot Ja + R_\theta \alpha). \quad (2.26)$$

Formula (2.26) shows that the coadjoint orbits are the cylinders  $T^*S_\alpha^1 = \{(\mu, \alpha) \mid \|\alpha\| = \text{const}\}$  if  $\alpha \neq 0$  together with the points are on the  $\mu$ -axis. The canonical cotangent bundle projection  $\pi : T^*S_\alpha^1 \rightarrow S_\alpha^1$  is defined as  $\pi(\mu, \alpha) = \alpha$ .

### Special Euclidean Group in the 3D Space

The most common group structure in human-like biomechanics is the *special Euclidean group in 3D space*,  $SE(3)$ . It is defined as a semidirect (noncommutative) product of 3D rotations and 3D translations,  $SO(3) \triangleright \mathbb{R}^3$ .

*The Heavy Top*

As a starting point consider a rigid body (see (3.2.1) below) moving with a fixed point but under the influence of gravity. This problem still has a configuration space  $SO(3)$ , but the symmetry group is only the circle group  $S^1$ , consisting of rotations about the direction of gravity. One says that gravity has broken the symmetry from  $SO(3)$  to  $S^1$ . This time, eliminating the  $S^1$  symmetry mysteriously leads one to the larger Euclidean group  $SE(3)$  of rigid motion of  $\mathbb{R}^3$ . Conversely, we can start with  $SE(3)$  as the configuration space for the rigid-body and ‘reduce out’ translations to arrive at  $SO(3)$  as the configuration space (see [MR99]).

The equations of motion for a rigid body with a fixed point in a gravitational field provide an interesting example of a system that is Hamiltonian (see (3.2.1)) relative to a *Lie–Poisson bracket* (see (3.2.3)). The underlying Lie algebra consists of the algebra of infinitesimal Euclidean motions in  $\mathbb{R}^3$ .

The basic phase-space we start with is again  $T^*SO(3)$ , parameterized by Euler angles and their conjugate momenta. In these variables, the equations are in canonical Hamiltonian form; however, the presence of gravity breaks the symmetry, and the system is no longer  $SO(3)$  invariant, so it cannot be written entirely in terms of the body angular momentum  $p$ . One also needs to keep track of  $\Gamma$ , the ‘direction of gravity’ as seen from the body. This is defined by  $\Gamma = A^{-1}k$ , where  $k$  points upward and  $A$  is the element of  $SO(3)$  describing the current configuration of the body. The equations of motion are

$$\begin{aligned}\dot{p}_1 &= \frac{I_2 - I_3}{I_2 I_3} p_2 p_3 + Mgl(\Gamma^2 \chi^3 - \Gamma^3 \chi^2), \\ \dot{p}_2 &= \frac{I_3 - I_1}{I_3 I_1} p_3 p_1 + Mgl(\Gamma^3 \chi^1 - \Gamma^1 \chi^3), \\ \dot{p}_3 &= \frac{I_1 - I_2}{I_1 I_2} p_1 p_2 + Mgl(\Gamma^1 \chi^2 - \Gamma^2 \chi^1),\end{aligned}$$

and

$$\dot{\Gamma} = \Gamma \times \Omega,$$

where  $\Omega$  is the body angular velocity vector,  $I_1, I_2, I_3$  are the body’s principal moments of inertia,  $M$  is the body’s mass,  $g$  is the acceleration of gravity,  $\chi$  is the body fixed unit vector on the line segment connecting the fixed point with the body’s center of mass, and  $l$  is the length of this segment.

*The Euclidean Group and Its Lie Algebra*

An element of  $SE(3)$  is a pair  $(A, a)$  where  $A \in SO(3)$  and  $a \in \mathbb{R}^3$ . The action of  $SE(3)$  on  $\mathbb{R}^3$  is the rotation  $A$  followed by translation by the vector  $a$  and has the expression

$$(A, a) \cdot x = Ax + a.$$

Using this formula, one sees that multiplication and inversion in  $SE(3)$  are given by

$$(A, a)(B, b) = (AB, Ab + a) \quad \text{and} \quad (A, a)^{-1} = (A^{-1}, -A^{-1}a),$$

for  $A, B \in SO(3)$  and  $a, b \in \mathbb{R}^3$ . The identity element is  $(I, 0)$ .

The Lie algebra of the Euclidean group  $SE(3)$  is  $\mathfrak{se}(3) = \mathbb{R}^3 \times \mathbb{R}^3$  with the Lie bracket

$$[(\xi, u), (\eta, v)] = (\xi \times \eta, \xi \times v - \eta \times u). \quad (2.27)$$

The Lie algebra of the Euclidean group has a structure that is a special case of what is called a *semidirect product*. Here it is the *product of the group of rotations with the corresponding group of translations*. It turns out that semidirect products occur under rather general circumstances when the symmetry in  $T^*G$  is broken.

The dual Lie algebra of the Euclidean group  $SE(3)$  is  $\mathfrak{se}(3)^* = \mathbb{R}^3 \times \mathbb{R}^3$  with the same Lie bracket (2.27). For the further details on adjoint orbits in  $\mathfrak{se}(3)$  as well as coadjoint orbits in  $\mathfrak{se}(3)^*$  see [MR99].

#### *Symplectic Group in Hamiltonian Mechanics*

Let  $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$ , with  $I$  the  $n \times n$  identity matrix. Now,  $A \in L(\mathbb{R}^{2n}, \mathbb{R}^{2n})$  is called a *symplectic matrix* if  $A^T J A = J$ . Let  $Sp(2n, \mathbb{R})$  be the set of  $2n \times 2n$  symplectic matrices. Taking determinants of the condition  $A^T J A = J$  gives  $\det A = \pm 1$ , and so  $A \in GL(2n, \mathbb{R})$ . Furthermore, if  $A, B \in Sp(2n, \mathbb{R})$ , then  $(AB)^T J (AB) = B^T A^T J AB = J$ . Hence,  $AB \in Sp(2n, \mathbb{R})$ , and if  $A^T J A = J$ , then  $JA = (A^T)^{-1} J = (A^{-1})^T J$ , so  $J = (A^{-1})^T J A^{-1}$ , or  $A^{-1} \in Sp(2n, \mathbb{R})$ . Thus,  $Sp(2n, \mathbb{R})$  is a group [MR99].

The *symplectic Lie group*

$$Sp(2n, \mathbb{R}) = \{A \in GL(2n, \mathbb{R}) : A^T J A = J\}$$

is a noncompact, connected Lie group of dimension  $2n^2 + n$ . Its Lie algebra

$$\mathfrak{sp}(2n, \mathbb{R}) = \{A \in L(\mathbb{R}^{2n}, \mathbb{R}^{2n}) : A^T J A = J = 0\},$$

called the *symplectic Lie algebra*, consists of the  $2n \times 2n$  matrices  $A$  satisfying  $A^T J A = 0$  [MR99].

Consider a particle of mass  $m$  moving in a potential  $V(q)$ , where  $q^i = (q^1, q^2, q^3) \in \mathbb{R}^3$ . Newtonian second law states that the particle moves along a curve  $q(t)$  in  $\mathbb{R}^3$  in such a way that  $m\ddot{q}^i = -\text{grad } V(q^i)$ . Introduce the momentum  $p_i = m\dot{q}^i$ , and the energy

$$H(q, p) = \frac{1}{2m} \sum_{i=1}^3 p_i^2 + V(q).$$

Then

$$\begin{aligned}\frac{\partial H}{\partial q^i} &= \frac{\partial V}{\partial q^i} = -m\dot{q}^i = -\dot{p}_i, \quad \text{and} \\ \frac{\partial H}{\partial p_i} &= \frac{1}{m}p_i = \dot{q}^i, \quad (i = 1, 2, 3),\end{aligned}$$

and hence Newtonian law  $F = m\ddot{q}^i$  is equivalent to Hamilton's equations

$$\dot{q}^i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q^i}.$$

Now, writing  $z = (q^i, p_i)$  [MR99],

$$J \operatorname{grad} H(z) = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial H}{\partial q^i} \\ \frac{\partial H}{\partial p_i} \end{pmatrix} = (\dot{q}^i, \dot{p}_i) = \dot{z},$$

so Hamilton's equations read

$$\dot{z} = J \operatorname{grad} H(z). \quad (2.28)$$

Now let  $f : \mathbb{R}^3 \times \mathbb{R}^3 \rightarrow \mathbb{R}^3 \times \mathbb{R}^3$  and write  $w = f(z)$ . If  $z(t)$  satisfies Hamilton's equations (2.28) then  $w(t) = f(z(t))$  satisfies  $\dot{w} = A^T \dot{z}$ , where  $A^T = [\partial w^i / \partial z^j]$  is the Jacobian matrix of  $f$ . By the chain rule,

$$\dot{w} = A^T \underset{z}{J} \operatorname{grad} H(z) = A^T \underset{w}{J} \operatorname{grad} H(z(w)).$$

Thus, the equations for  $w(t)$  have the form of Hamilton's equations with energy  $K(w) = H(z(w))$  iff  $A^T J A = J$ , that is, iff  $A$  is symplectic. A nonlinear transformation  $f$  is canonical iff its Jacobian matrix is symplectic.  $Sp(2n, \mathbb{R})$  is the linear invariance group of classical mechanics [MR99].

Now, before giving our main biomechanical applications of Lie groups, we give an interesting application in the realm of dynamical games.

### 2.4.3 Dynamical Games on Lie Groups

In this section we propose a general approach to modelling *conflict resolution manoeuvres* for land, sea and airborne *vehicles*, using dynamical games on Lie groups. We use the generic name 'vehicle' to represent all planar vehicles, namely land and sea vehicles, as well as fixed altitude motion of aircrafts (see, e.g., [LGS, TPS98]). First, we elaborate on the two-vehicle conflict resolution manoeuvres, and after that discuss the multi-vehicle manoeuvres.

We explore special features of the dynamical games solution when the underlying dynamics correspond to left-invariant control systems on Lie groups. We show that the 2D (i.e., planar) motion of a vehicle may be modelled as a control system on the Lie group  $SE(2)$ . The proposed algorithm surrounds each vehicle with a circular protected zone, while the simplification in the

derivation of *saddle* and *Nash strategies* follows from the use of symplectic reduction techniques [MR99]. To model the two-vehicle conflict resolution, we construct the safe subset of the state space for one of the vehicles using zero-sum non-cooperative dynamic game theory [BO95] which we specialize to the  $SE(2)$  group. If the underlying continuous dynamics are left-invariant control systems, reduction techniques can be used in the computation of safe sets.

### Configuration Models for Planar Vehicles

The configuration of each individual vehicle is described by an element of the *Lie group*  $SE(2)$  of rigid-body motions in  $\mathbb{R}^2$ . Let  $g_i \in SE(2)$  denote the configurations of vehicles labelled  $i$ , with  $i = 1, 2$ . The motion of each vehicle may be modelled as a left-invariant vector-field on  $SE(2)$ :

$$\dot{g}_i = g_i X_i, \quad (2.29)$$

where the vector-fields  $X_i$  belong to the vector space  $\mathfrak{se}(2)$ , the *Lie algebra* associated with the group  $SE(2)$ .

Each  $g_i \in SE(2)$  can be represented in standard local coordinates  $(x_i, y_i, \theta_i)$  as

$$g_i = \begin{bmatrix} \cos \theta_i & -\sin \theta_i & x_i \\ \sin \theta_i & \cos \theta_i & y_i \\ 0 & 0 & 1 \end{bmatrix},$$

where  $x_i, y_i$  is the position of vehicle  $i$  and  $\theta_i$  is its orientation, or heading. The associated Lie algebra is  $\mathfrak{se}(2)$ , with  $X_i \in \mathfrak{se}(2)$  represented as

$$X_i = \begin{bmatrix} 0 & -\omega_i & v_i \\ \omega_i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

where  $v_i$  and  $\omega_i$  represent the *translational* (linear) and *rotational* (angular) *velocities*, respectively.

Now, to determine *dynamics of the relative configuration* of two vehicles, we perform a change (transformation) of coordinates, to place the identity element of the group  $SE(2)$  on vehicle 1. If  $g^{rel} \in SE(2)$  denotes the relative configuration of vehicle 2 with respect to vehicle 1, then

$$g_2 = g_1 g^{rel} \implies g^{rel} = g_1^{-1} g_2.$$

Differentiation with respect to time yields the dynamics of the relative configuration:

$$\dot{g}^{rel} = g^{rel} X_2 - X_1 g^{rel},$$

which expands into:

$$\begin{aligned} \dot{x}^{rel} &= -v_1 + v_2 \cos \theta^{rel} + \omega_1 y^{rel}, \\ \dot{y}^{rel} &= v_2 \sin \theta^{rel} - \omega_1 x^{rel}, \\ \dot{\theta}^{rel} &= \omega_2 - \omega_1. \end{aligned}$$

### Two-Vehicles Conflict Resolution Manoeuvres

Next, we seek *control strategies* for each vehicle, which are *safe* under (possible) *uncertainty* in the actions of neighbouring vehicle. For this, we expand the dynamics of two vehicles (2.29),

$$\dot{g}_1 = g_1 X_1, \quad \dot{g}_2 = g_2 X_2,$$

and write it in the matrix form as

$$\dot{g} = gX, \quad (2.30)$$

with

$$g = \begin{bmatrix} g_1 & 0 \\ 0 & g_2 \end{bmatrix}, \quad X = \begin{bmatrix} X_1 & 0 \\ 0 & X_2 \end{bmatrix},$$

in which  $g$  is an element in the configuration manifold  $M = SE(2) \times SE(2)$ , while the vector-fields  $X_i \in \mathfrak{se}(2) \times \mathfrak{se}(2)$  are linearly parameterised by velocity inputs  $(\omega_1, v_1) \in \mathbb{R}^2$  and  $(\omega_2, v_2) \in \mathbb{R}^2$ .

The goal of each vehicle is to maintain *safe operation*, meaning that

(i) the vehicles remain outside of a specified *target set*  $T$  with boundary  $\partial T$ , defined by

$$T = \{g \in M | l(g) < 0\},$$

where  $l(g)$  is a differentiable circular function,

$$l(g) = (x_2 - x_1)^2 + (y_2 - y_1)^2 - \rho^2$$

(with  $\rho$  denoting the *radius of a circular protected zone*) defines the minimum allowable lateral separation between vehicles; and

(ii)

$$dl(g) \neq 0 \quad \text{on} \quad \partial T = \{g \in M | l(g) = 0\},$$

where  $d$  represents the *exterior derivative* (a unique generalization of the gradient, divergence and curl).

Now, due to possible uncertainty in the actions of vehicle 2, the safest possible strategy of vehicle 1 is to drive along a *trajectory* which guarantees that the minimum allowable separation with vehicle 2 is maintained regardless of the actions of vehicle 2. We therefore formulate this problem as a *zero-sum dynamical game* with two players: control vs. disturbance. The *control* is the action of vehicle 1,

$$u = (\omega_1, v_1) \in U,$$

and the *disturbance* is the action of vehicle 2,

$$d = (\omega_2, v_2) \in D.$$

Here the control and disturbance sets,  $U$  and  $D$ , are defined as

$$U = ([\omega_1^{\min}, \omega_1^{\max}], [v_1^{\min}, v_1^{\max}]),$$

$$D = ([\omega_2^{\min}, \omega_2^{\max}], [v_2^{\min}, v_2^{\max}])$$

and the corresponding control and disturbance functional spaces,  $\mathcal{U}$  and  $\mathcal{D}$  are defined as:

$$\mathcal{U} = \{u(\cdot) \in PC^0(\mathbb{R}^2) | u(t) \in U, t \in \mathbb{R}\},$$

$$\mathcal{D} = \{d(\cdot) \in PC^0(\mathbb{R}^2) | d(t) \in U, t \in \mathbb{R}\},$$

where  $PC^0(\mathbb{R}^2)$  is the space of piecewise continuous functions over  $\mathbb{R}^2$ .

We define the *cost of a trajectory*  $g(t)$  which starts at state  $g$  at initial time  $t \leq 0$ , evolves according to (2.30) with input  $(u(\cdot), d(\cdot))$ , and ends at the final state  $g(0)$  as:

$$J(g, u(\cdot), d(\cdot), t) : SE(2) \times SE(2) \times \mathcal{U} \times \mathcal{D} \times \mathbb{R}_- \rightarrow \mathbb{R},$$

such that  $J(g, u(\cdot), d(\cdot), t) = l(g(0)),$  (2.31)

where 0 is the final time (without loss of generality). Thus the cost depends only on the final state  $g(0)$  (the Lagrangian, or running cost, is identically zero). The game is won by vehicle 1 if the terminal state  $g(0)$  is either outside  $T$  or on  $\partial T$  (i.e.,  $J(g, 0) \geq 0$ ), and is won by vehicle 2 otherwise.

This two-player zero-sum dynamical game on  $SE(2)$  is defined as follows. Consider the matrix system (2.30),  $\dot{g} = gX$ , over the time interval  $[t, 0]$  where  $t < 0$  with the cost function  $J(g, u(\cdot), d(\cdot), t)$  defined by (2.31) As vehicle 1 attempts to maximize this cost assuming that vehicle 2 is acting blindly, the optimal control action and worst disturbance actions are calculated as

$$u^* = \arg \max_{u \in \mathcal{U}} \min_{d \in \mathcal{D}} J(g, u(\cdot), d(\cdot), t), \quad d^* = \arg \min_{d \in \mathcal{D}} \max_{u \in \mathcal{U}} J(g, u(\cdot), d(\cdot), t).$$

The game is said to have a *saddle solution*  $(u^*, d^*)$  if the resulting optimal cost  $J^*(g, t)$  does not depend on the order of play, i.e., on the order in which the maximization and minimization is performed:

$$J^*(g, t) = \max_{u \in \mathcal{U}} \min_{d \in \mathcal{D}} J(g, u(\cdot), d(\cdot), t) = \min_{d \in \mathcal{D}} \max_{u \in \mathcal{U}} J(g, u(\cdot), d(\cdot), t).$$

Using this saddle solution we calculate the ‘losing states’ for vehicle 1, called the *predecessor*  $Pre_t(T)$  of the target set  $T$ ,

$$Pre_t(T) = \{g \in M | J(g, u^*(\cdot), d(\cdot), t) < 0\}.$$

### Symplectic Reduction and Dynamical Games on $SE(2)$

Since vehicles 1 and 2 have dynamics given by left-invariant control systems on the Lie group  $SE(2)$ , we have

$$X_1 = \xi^1 \omega_1 + \xi^2 v_1, \quad X_2 = \xi^1 \omega_2 + \xi^2 v_2,$$

with  $\xi^1, \xi^2$  being two of the three basis elements for the tangent Lie algebra  $\mathfrak{se}(2)$  given by

$$\xi^1 = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \xi^2 = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \xi^3 = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}.$$

If  $p_1$  (resp.  $p_2$ ) is a cotangent vector-field to  $SE(2)$  at  $g_1$  (resp.  $g_2$ ), belonging to the cotangent (dual) Lie algebra  $\mathfrak{se}(2)^*$ , we can define the *momentum functions* for both vehicles:

$$\begin{aligned} P_1^1 &= \langle p_1, g_1 \xi^1 \rangle, & P_1^2 &= \langle p_1, g_1 \xi^2 \rangle, & P_1^3 &= \langle p_1, g_1 \xi^3 \rangle, \\ P_2^1 &= \langle p_2, g_2 \xi^1 \rangle, & P_2^2 &= \langle p_2, g_2 \xi^2 \rangle, & P_2^3 &= \langle p_2, g_2 \xi^3 \rangle, \end{aligned}$$

which can be compactly written as

$$P_i^j = \langle p_i, g_i \xi^j \rangle.$$

Defining  $p = (p_1, p_2) \in \mathfrak{se}(2)^* \times \mathfrak{se}(2)^*$ , the *optimal cost* for the two-player, zero-sum dynamical game is given by

$$J^*(g, t) = \max_{u \in \mathcal{U}} \min_{d \in \mathcal{D}} J(g, u(\cdot), d(\cdot), t) = \max_{u \in \mathcal{U}} \min_{d \in \mathcal{D}} l(g(0)).$$

The *Hamiltonian*  $H(g, p, u, d)$  is given by

$$H(g, p, u, d) = P_1^1 \omega_1 + P_1^2 v_1 + P_2^1 \omega_1 + P_2^2 v_1$$

for control and disturbance inputs  $(\omega_1, v_1) \in U$  and  $(\omega_2, v_2) \in D$  as defined above. It follows that the *optimal Hamiltonian*  $H^*(g, p)$ , defined on the cotangent bundle  $T^*SE(2)$ , is given by

$$\begin{aligned} H^*(g, p) &= P_1^1 \frac{\omega_1^{\max} + \omega_1^{\min}}{2} + P_2^1 \frac{\omega_2^{\max} + \omega_2^{\min}}{2} + |P_1^1| \frac{\omega_1^{\max} - \omega_1^{\min}}{2} \\ &\quad - |P_1^1| \frac{\omega_2^{\max} - \omega_2^{\min}}{2} + P_1^2 \frac{v_1^{\max} + v_1^{\min}}{2} + P_2^2 \frac{v_2^{\max} + v_2^{\min}}{2} \\ &\quad + |P_1^2| \frac{v_1^{\max} - v_1^{\min}}{2} - |P_2^2| \frac{v_2^{\max} - v_2^{\min}}{2} \end{aligned}$$

and the *saddle solution*  $(u^*, d^*)$  is given by

$$u^* = \arg \max_{u \in \mathcal{U}} \min_{d \in \mathcal{D}} H(g, p, u, d), \quad d^* = \arg \min_{d \in \mathcal{D}} \max_{u \in \mathcal{U}} H(g, p, u, d). \quad (2.32)$$

Note that  $H(g, p, u, d)$  and  $H^*(g, p)$  do not depend on the state  $g$  and costate  $p$  directly, rather through the momentum functions  $P_1^j, P_2^j$ . This is because the dynamics are determined by left-invariant vector fields on the Lie group and the Lagrangian is state independent [MR99].

The optimal Hamiltonian  $H^*(g, p)$  determines a 12D Hamiltonian vector-field  $X_{H^*}$  on the symplectic manifold  $T^*M = SE(2) \times SE(2) \times \mathfrak{se}(2)^* \times \mathfrak{se}(2)^*$  (which is the cotangent bundle of the configuration manifold  $M$ ), defined by Hamilton's equations

$$X_{H^*} : \dot{g} = \frac{\partial H^*(g, p)}{\partial p}, \quad \dot{p} = -\frac{\partial H^*(g, p)}{\partial g},$$

with initial condition at time  $t$  being  $g(t) = g$  and final condition at time 0 being  $p(0) = dl(g(0))$ . In general, to solve for the saddle solution (2.32), one needs to solve the ODE system for all states. However since the original system on  $M = SE(2) \times SE(2)$  is left-invariant, it induces generic symmetries in the Hamiltonian dynamics on  $T^*M$ , referred to as Marsden-Weinstein reduction of Hamiltonian systems on symplectic manifolds, see [MR99]. In general for such systems one only needs to solve an ODE system with half of the dimensions of the underlying symplectic manifold.

For the two-vehicle case we only need to solve an ODE system with 6 states. That is exactly given by the dynamics of the 6 momentum functions

$$\dot{P}_i^j = L_{X_{H^*}} P_i^j = \{P_i^j, H^*(g, p)\}, \quad (2.33)$$

for  $i, j = 1, 2$ , which is the *Lie derivative* of  $P_i^j$  with respect to the Hamiltonian vector-field  $X_{H^*}$ . In the equation (2.33), the bracket  $\{\cdot, \cdot\}$  is the *Poisson bracket* [IP01a], giving the commutation relations:

$$\begin{aligned} \{P_1^1, P_1^2\} &= P_1^3, & \{P_1^2, P_1^3\} &= 0, & \{P_1^3, P_1^1\} &= P_1^2, \\ \{P_2^1, P_2^2\} &= P_2^3, & \{P_2^2, P_2^3\} &= 0, & \{P_2^3, P_2^1\} &= P_2^2. \end{aligned}$$

Using these commutation relations, equation (2.33) can be written explicitly:

$$\begin{aligned} \dot{P}_1^1 &= P_1^3 \left( \frac{v_1^{\max} + v_1^{\min}}{2} + \text{sign}(P_1^2) \frac{v_1^{\max} - v_1^{\min}}{2} \right), \\ \dot{P}_1^2 &= P_1^3 \left( -\frac{\omega_1^{\max} + \omega_1^{\min}}{2} - \text{sign}(P_1^1) \frac{\omega_1^{\max} - \omega_1^{\min}}{2} \right), \\ \dot{P}_1^3 &= P_1^2 \left( \frac{\omega_1^{\max} + \omega_1^{\min}}{2} + \text{sign}(P_1^1) \frac{\omega_1^{\max} - \omega_1^{\min}}{2} \right), \\ \dot{P}_2^1 &= P_2^3 \left( \frac{v_2^{\max} + v_2^{\min}}{2} + \text{sign}(P_2^2) \frac{v_2^{\max} - v_2^{\min}}{2} \right), \\ \dot{P}_2^2 &= P_2^3 \left( -\frac{\omega_2^{\max} + \omega_2^{\min}}{2} - \text{sign}(P_2^1) \frac{\omega_2^{\max} - \omega_2^{\min}}{2} \right), \\ \dot{P}_2^3 &= P_2^2 \left( \frac{\omega_2^{\max} + \omega_2^{\min}}{2} + \text{sign}(P_2^1) \frac{\omega_2^{\max} - \omega_2^{\min}}{2} \right). \end{aligned}$$

The final conditions for the variables  $P_1^j(t)$  and  $P_2^j(t)$  are obtained from the boundary of the safe set as

$$P_1^j(0) = \langle d_1 l(g), g_1 \xi^j \rangle, \quad P_2^j(0) = \langle d_2 l(g), g_2 \xi^j \rangle,$$

where  $d_1$  is the derivative of  $l$  taken with respect to its first argument  $g_1$  only (and similarly for  $d_2$ ). In this way,  $P_1^j(t)$  and  $P_2^j(t)$  are obtained for  $t \leq 0$ . Once this has been calculated, the optimal input  $u^*(t)$  and the worst disturbance  $d^*(t)$  are given respectively as

$$u^*(t) = \begin{cases} \omega_1^*(t) = \begin{cases} \omega_1^{\max} & \text{if } P_1^1(t) > 0 \\ \omega_1^{\min} & \text{if } P_1^1(t) < 0 \end{cases} \\ v_1^*(t) = \begin{cases} v_1^{\max} & \text{if } P_1^2(t) > 0 \\ v_1^{\min} & \text{if } P_1^2(t) < 0 \end{cases} \end{cases} \\ d^*(t) = \begin{cases} \omega_2^*(t) = \begin{cases} \omega_2^{\max} & \text{if } P_2^1(t) > 0 \\ \omega_2^{\min} & \text{if } P_2^1(t) < 0 \end{cases} \\ v_2^*(t) = \begin{cases} v_2^{\max} & \text{if } P_2^2(t) > 0 \\ v_2^{\min} & \text{if } P_2^2(t) < 0 \end{cases} \end{cases} .$$

### Nash Solutions for Multi-Vehicle Manoeuvres

The methodology introduced in the previous sections can be generalized to find conflict-resolutions for multi-vehicle manoeuvres. Consider the three-vehicle dynamics:

$$\dot{g} = gX, \quad (2.34)$$

with

$$g = \begin{bmatrix} g_1 & 0 & 0 \\ 0 & g_2 & 0 \\ 0 & 0 & g_3 \end{bmatrix}, \quad X = \begin{bmatrix} X_1 & 0 & 0 \\ 0 & X_2 & 0 \\ 0 & 0 & X_3 \end{bmatrix},$$

where  $g$  is an element in the configuration space  $M = SE(2) \times SE(2) \times SE(2)$  and  $X \in \mathfrak{se}(2) \times \mathfrak{se}(2) \times \mathfrak{se}(2)$  is linearly parameterised by inputs  $(\omega_1, v_1)$ ,  $(\omega_2, v_2)$  and  $(\omega_3, v_3)$ .

Now, the target set  $T$  is defined as

$$T = \{g \in M \mid l_1(g) < 0 \vee l_2(g) < 0 \vee l_3(g) < 0\},$$

where

$$l_1(g) = \min\{(x_2 - x_1)^2 + (y_2 - y_1)^2 - \rho^2, (x_3 - x_1)^2 + (y_3 - y_1)^2 - \rho^2\}, \\ l_2(g) = \min\{(x_3 - x_2)^2 + (y_3 - y_2)^2 - \rho^2, (x_1 - x_2)^2 + (y_1 - y_2)^2 - \rho^2\}, \\ l_3(g) = \min\{(x_2 - x_3)^2 + (y_2 - y_3)^2 - \rho^2, (x_1 - x_3)^2 + (y_1 - y_3)^2 - \rho^2\}.$$

The control inputs  $u = (u_1, u_2, u_3)$  are the actions of vehicle 1, 2 and 3:

$$u_i = (\omega_i, v_i) \in U_i,$$

where  $U_i$  are defined as

$$U_i = ([\omega_i^{\min}, \omega_i^{\max}], [v_i^{\min}, v_i^{\max}]).$$

Clearly, this can be generalized to  $N$  vehicles.

The cost functions  $J_i(g, \{u_i(\cdot)\}, t)$  are defined as

$$J_i(g, \{u_i(\cdot)\}, t) : \prod_{i=1}^N SE_i(2) \times \prod_{i=1}^N \mathcal{U}_i \times \mathbb{R}_- \rightarrow \mathbb{R},$$

such that  $J_i(g, \{u_i(\cdot)\}, t) = l_i(g(0))$ .

The simplest non-cooperative solution strategy is also called *non-cooperative Nash equilibrium* (see e.g., [BO95]). A set of controls  $u_i^*$ , ( $i = 1, \dots, N$ ) is said to be a *Nash strategy*, if for each player modification of that strategy under the assumption that the others play their Nash strategies results in a decrease in his payoff, that is for  $i = 1, \dots, N$ , and  $\forall u_i(\cdot)$ ,

$$J_i(u_1, \dots, u_i, \dots, u_N) \leq J_i(u_1^*, \dots, u_i^*, \dots, u_N^*), \quad (u \neq u^*).$$

(Note that Nash equilibria may not be unique. It is also easy to see that for the two-player zero-sum game, a Nash equilibrium is a saddle solution with  $J = J_1 = -J_2$ .)

For  $N$  vehicles, the momentum functions are defined as in the two-vehicle case:

$$P_i^j = \langle p_i, g_i \xi^j \rangle,$$

with  $p_i \in \mathfrak{se}(2)^*$  for  $i = 1, \dots, N$  and  $\xi^j$  defined as above.

Then the Hamiltonian  $H(g, p, u_1, \dots, u_N)$  is given by

$$H(g, p, u_1, \dots, u_N) = P_i^1 \omega_i + P_i^2 v_i.$$

The first case we consider is one in which all the vehicles are *cooperating*, meaning that each tries to avoid conflict assuming the others are doing the same. In this case, the optimal Hamiltonian  $H^*(g, p)$  is

$$H^*(g, p) = \max_{u_i \in U_i} H(g, p, u_1, \dots, u_N).$$

For example, if  $N = 3$ , one may solve for  $(u_1^*, u_2^*, u_3^*)$ , on the 9D quotient space  $T^*M/M$ , so that the optimal control inputs are given as

$$u_i^*(t) = \begin{cases} \omega_i^*(t) = \begin{cases} \omega_i^{\max} & \text{if } P_i^1(t) > 0 \\ \omega_i^{\min} & \text{if } P_i^1(t) < 0 \end{cases} \\ v_i^*(t) = \begin{cases} v_i^{\max} & \text{if } P_i^2(t) > 0 \\ v_i^{\min} & \text{if } P_i^2(t) < 0 \end{cases} \end{cases}.$$

One possibility for the optimal Hamiltonian corresponding to the *non-cooperative case* is

$$H^*(g, p) = \max_{u_1 \in U_1} \max_{u_2 \in U_2} \max_{u_3 \in U_3} H(g, p, u_1, u_2, u_3).$$

### 2.4.4 Group Structure of the Biomechanical Manifold $M$

#### Purely Rotational Biomechanical Manifold

Kinematics of an  $n$ -segment human-body chain (like arm, leg or spine) is usually defined as a map between *external coordinates* (usually, end-effector coordinates)  $x^r$  ( $r = 1, \dots, n$ ) and *internal joint coordinates*  $q^i$  ( $i = 1, \dots, N$ ) (see [IS01, Iva02, IP01b, IP01b, Iva05]). The *forward kinematics* are defined as a nonlinear map  $x^r = x^r(q^i)$  with a corresponding linear vector functions  $dx^r = \partial x^r / \partial q^i dq^i$  of differentials: and  $\dot{x}^r = \partial x^r / \partial q^i \dot{q}^i$  of velocities. When the rank of the configuration-dependent Jacobian matrix  $J \equiv \partial x^r / \partial q^i$  is less than  $n$  the *kinematic singularities* occur; the onset of this condition could be detected by the *manipulability measure*. The *inverse kinematics* are defined conversely by a nonlinear map  $q^i = q^i(x^r)$  with a corresponding linear vector functions  $dq^i = \partial q^i / \partial x^r dx^r$  of differentials and  $\dot{q}^i = \partial q^i / \partial x^r \dot{x}^r$  of velocities. Again, in the case of *redundancy* ( $n < N$ ), the inverse kinematic problem admits infinite solutions; often the *pseudo-inverse* configuration-control is used instead:  $\dot{q}^i = J^* \dot{x}^r$ , where  $J^* = J^T (J J^T)^{-1}$  denotes the Moore-Penrose pseudo-inverse of the Jacobian matrix  $J$ .

Humanoid joints, that is, internal coordinates  $q^i$  ( $i = 1, \dots, N$ ), constitute a smooth configuration manifold  $M$ , described as follows. Uniaxial, ‘hinge’ joints represent constrained, rotational Lie groups  $SO(2)_{cnstr}^i$ , parameterized by constrained angles  $q_{cnstr}^i \equiv q^i \in [q_{min}^i, q_{max}^i]$ . Three-axial, ‘ball-and-socket’ joints represent constrained rotational Lie groups  $SO(3)_{cnstr}^i$ , parameterized by constrained Euler angles  $q^i = q_{cnstr}^{\phi_i}$  (in the following text, the subscript ‘cnstr’ will be omitted, for the sake of simplicity, and always assumed in relation to internal coordinates  $q^i$ ).

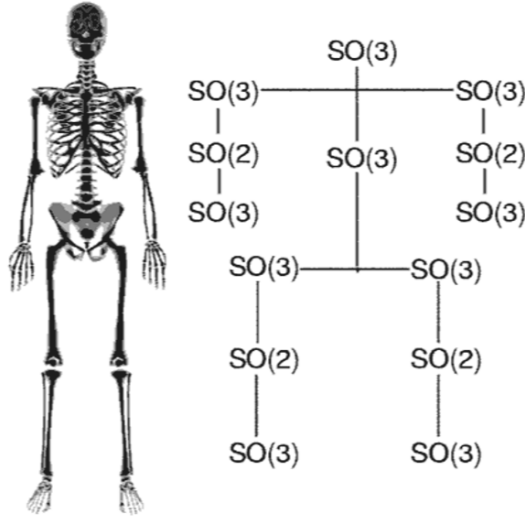
All  $SO(n)$ -joints are Hausdorff  $C^k$ -manifolds with atlases  $(U_\alpha, u_\alpha)$ ; in other words, they are paracompact and metrizable smooth manifolds, admitting Riemannian metric.

Let  $A$  and  $B$  be two smooth manifolds described by smooth atlases  $(U_\alpha, u_\alpha)$  and  $(V_\beta, v_\beta)$ , respectively. Then the family  $(U_\alpha \times V_\beta, u_\alpha \times v_\beta : U_\alpha \times V_\beta \rightarrow \mathbb{R}^m \times \mathbb{R}^n)_{(\alpha, \beta) \in A \times B}$  is a smooth atlas for the direct product  $A \times B$ . Now, if  $A$  and  $B$  are two Lie groups (say,  $SO(n)$ ), then their *direct product*  $G = A \times B$  is at the same time their direct product as smooth manifolds and their direct product as algebraic groups, with the product law

$$(a_1, b_1)(a_2, b_2) = (a_1 a_2, b_1 b_2), \quad (a_{1,2} \in A, b_{1,2} \in B).$$

Generalizing the direct product to  $N$  rotational joint groups, we can draw an *anthropomorphic product-tree* (see Figure 2.1) using a line segment ‘-’ to represent direct products of human  $SO(n)$ -joints. This is our basic model of the biomechanical configuration manifold  $M$  (see (3.2.1) below).

Let  $T_q M$  be a tangent space to  $M$  at the point  $q$ . The *tangent bundle*  $TM$  represents a union  $\cup_{q \in M} T_q M$ , together with the standard topology on  $TM$  and a natural smooth manifold structure, the dimension of which is twice the



**Fig. 2.1.** Purely rotational, whole-body biomechanical manifold, with a single  $SO(3)$ -joint representing the whole spinal movability.

dimension of  $M$ . A vector-field  $X$  on  $M$  represents a section  $X : M \rightarrow TM$  of the tangent bundle  $TM$ .

Analogously let  $T_q^*M$  be a cotangent space to  $M$  at  $q$ , the dual to its tangent space  $T_qM$ . The *cotangent bundle*  $T^*M$  represents a union  $\cup_{q \in M} T_q^*M$ , together with the standard topology on  $T^*M$  and a natural smooth manifold structure, the dimension of which is twice the dimension of  $M$ . A 1-form  $\theta$  on  $M$  represents a section  $\theta : M \rightarrow T^*M$  of the cotangent bundle  $T^*M$ .

We refer to the tangent bundle  $TM$  of biomechanical configuration manifold  $M$  as the *velocity phase-space* manifold, and to its cotangent bundle  $T^*M$  as the *momentum phase-space* manifold.

**Reduction of the Rotational Biomechanical Manifold**

The biomechanical configuration manifold  $M$  (Figure 2.1) can be (for the sake of the brain-like motor control) reduced to  $N$ -torus  $T^N$ , in three steps, as follows.

First, a single three-axial  $SO(3)$ -joint can be reduced to the direct product of three uniaxial  $SO(2)$ -joints, in the sense that three hinge joints can produce any orientation in space, just as a ball-joint can. Algebraically, this means reduction (using symbol ‘ $\gtrsim$ ’) of each of the three  $SO(3)$  rotation matrices to the corresponding  $SO(2)$  rotation matrices

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \phi & -\sin \phi \\ 0 & \sin \phi & \cos \phi \end{pmatrix} \gtrsim \begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix}$$

$$\begin{pmatrix} \cos \psi & 0 & \sin \psi \\ 0 & 1 & 0 \\ -\sin \psi & 0 & \cos \psi \end{pmatrix} \gtrsim \begin{pmatrix} \cos \psi & \sin \psi \\ -\sin \psi & \cos \psi \end{pmatrix}$$

$$\begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \gtrsim \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$

In this way we can set the *reduction equivalence relation*  $SO(3) \gtrsim SO(2) \triangleright SO(2) \triangleright SO(2)$ , where ‘ $\triangleright$ ’ denotes the noncommutative *semidirect product* (see (2.4.2) above).

Second, we have a homeomorphism:  $SO(2) \sim S^1$ , where  $S^1$  denotes the constrained unit circle in the complex plane, which is an Abelian Lie group.

Third, let  $I^N$  be the unit cube  $[0, 1]^N$  in  $\mathbb{R}^N$  and ‘ $\sim$ ’ an equivalence relation on  $\mathbb{R}^N$  obtained by ‘gluing’ together the opposite sides of  $I^N$ , preserving their orientation. The manifold of human-body configurations (Figure 2.1) can be represented as the *quotient space* of  $\mathbb{R}^N$  by the space of the integral lattice points in  $\mathbb{R}^N$ , that is a constrained  $ND$  torus  $T^N$  (4.2),

$$\mathbb{R}^N / \mathbb{Z}^N = I^N / \sim \cong \prod_{i=1}^N S_i^1 \equiv \{(q^i, i = 1, \dots, N) : \text{mod } 2\pi\} = T^N. \quad (2.35)$$

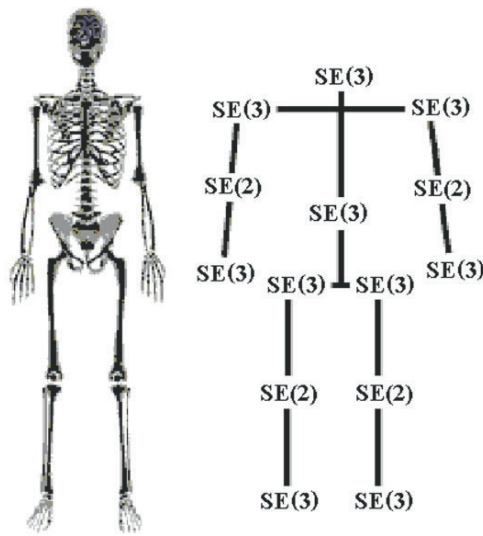
Since  $S^1$  is an Abelian Lie group, its  $N$ -fold tensor product  $T^N$  is also an Abelian Lie group, the toral group, of all nondegenerate diagonal  $N \times N$  matrices. As a Lie group, the biomechanical configuration space  $M \equiv T^N$  has a natural Banach manifold structure with local internal coordinates  $q^i \in U$ ,  $U$  being an open set (chart) in  $T^N$ .

Conversely by ‘ungluing’ the configuration space we get the primary unit cube. Let ‘ $\sim^*$ ’ denote an equivalent decomposition or ‘ungluing’ relation. By the Tychonoff product-topology theorem, for every such quotient space there exists a ‘selector’ such that their quotient models are homeomorphic, that is,  $T^N / \sim^* \approx A^N / \sim^*$ . Therefore  $I^N$  represents a ‘selector’ for the configuration torus  $T^N$  and can be used as an  $N$ -directional ‘command-space’ for the topological control of human motion. Any subset of DOF on the configuration torus  $T^N$  representing the joints included in human motion has its simple, rectangular image in the command space – selector  $I^N$ . Operationally, this resembles what the *brain-motor-controller*, the *cerebellum*, actually performs on the highest level of human motor control (see Chapter 5).

### The Complete Biomechanical Manifold

The full kinematics of a whole human-like body can be split down into *five kinematic chains*: one for each leg and arm, plus one for spine with the head. In all five chains internal joint coordinates, namely  $n_1$  constrained rotations

$x_{rt}^k$  together with  $n_2$  of even more constrained translations  $x_{tr}^j$  (see Figure 2.2), constitute a smooth  $nD$  anthropomorphic configuration manifold  $M$ , with local coordinates  $x^i$ , ( $i = 1, \dots, n$ ). That is, the motion space in each joint is defined as a semidirect (noncommutative) product of the Lie group  $SO(n)$  of constrained rotations and a corresponding Lie group  $\mathbb{R}^n$  of even more restricted translations. More precisely, in each movable human-like joint we have an action of the constrained special Euclidean  $SE(3)$  group (see (2.4.2) above). The joints themselves are linked by direct (commutative) products.

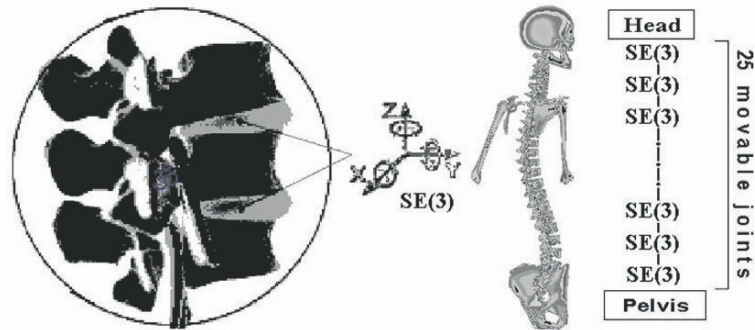


**Fig. 2.2.** A medium-resolution, whole-body biomechanical manifold, with just a single  $SE(3)$ -joint representing the spinal movability.

### Realistic Human Spine Manifold

The high-resolution human spine manifold is a dynamical chain consisting of 25 constrained  $SE(3)$ -joints. Each movable spinal joint has 6 DOF: 3 dominant rotations, (performed first in any free spinal movement), restricted to about 7 angular degrees and 3 secondary translations (performed after reaching the limit of rotational amplitude), restricted to about 5 mm (see Figure 2.3).

Now,  $SE(3) = SO(3) \triangleright \mathbb{R}^3$  is a non-compact group, so there is no natural metric given by the kinetic energy on  $SE(3)$ , and consequently, no natural controls in the sense of geodesics on  $SE(3)$ . However, both of its subgroups,  $SO(3)$  and  $\mathbb{R}^3$ , are compact with quadratic metric forms defined by standard line element  $g_{ij}dq^i dq^j$ , and therefore admit optimal muscular-like controls in the sense of geodesics (see section 2.5.1 below).



**Fig. 2.3.** The high-resolution human spine manifold is a dynamical chain consisting of 25 constrained  $SE(3)$ -joints.

### 2.4.5 Lie Symmetries in Biomechanics

#### Lie Symmetry Groups

##### Exponentiation of Vector Fields on $M$

Let  $x = (x^1, \dots, x^r)$  be local coordinates at a point  $m$  on a smooth  $n$ -manifold  $M$ . Recall that the flow generated by the vector-field

$$v = \xi^i(x) \partial_{x^i} \in M,$$

is a solution of the system of ODEs

$$\frac{dx^i}{d\varepsilon} = \xi^i(x^1, \dots, x^m), \quad (i = 1, \dots, r).$$

The computation of the flow, or one-parameter group of diffeomorphisms, generated by a given vector-field  $v$  (i.e., solving the system of ODEs) is often referred to as *exponentiation* of the vector-field, denoted by  $\exp(\varepsilon v)x$  (see [Olv86]).

If  $v, w \in M$  are two vectors defined by

$$v = \xi^i(x) \partial_{x^i} \quad \text{and} \quad w = \eta^i(x) \partial_{x^i},$$

then

$$\exp(\varepsilon v) \exp(\theta w) x = \exp(\theta w) \exp(\varepsilon v) x,$$

for all  $\varepsilon, \theta \in \mathbb{R}, x \in M$ , such that both sides are defined, iff they commute, i.e.,  $[v, w] = 0$  everywhere [Olv86].

A system of vector-fields  $\{v_1, \dots, v_r\}$  on a smooth manifold  $M$  is in *involution* if there exist smooth real-valued functions  $h_{ij}^k(x), x \in M, i, j, k = 1, \dots, r$ , such that for each  $i, j$ ,

$$[v_i, v_j] = h_{ij}^k \cdot v_k.$$

Let  $v \neq 0$  be a right-invariant vector-field on a Lie group  $G$ . Then the flow generated by  $v$  through the identity  $e$ , namely

$$g_\varepsilon = \exp(\varepsilon v) e \equiv \exp(\varepsilon v),$$

is defined for all  $\varepsilon \in \mathbb{R}$  and forms a one-parameter subgroup of  $G$ , with

$$g_{\varepsilon+\delta} = g_\varepsilon \cdot g_\delta, \quad g_0 = e, \quad g_\varepsilon^{-1} = g_{-\varepsilon},$$

isomorphic to either  $\mathbb{R}$  itself or the circle group  $SO(2)$ . Conversely, any connected 1D subgroup of  $G$  is generated by such a right-invariant vector-field in the above manner [Olv86].

For example, let  $G = GL(n)$  with Lie algebra  $\mathfrak{gl}(n)$ , the space of all  $n \times n$  matrices with commutator as the Lie bracket. If  $A \in \mathfrak{gl}(n)$ , then the corresponding right-invariant vector-field  $v_A$  on  $GL(n)$  has the expression [Olv86]

$$v_A = a_k^i x_j^k \partial_{x_j^i}.$$

The one-parameter subgroup  $\exp(\varepsilon v_A) e$  is found by integrating the system of  $n^2$  ordinary differential equations

$$\frac{dx_j^i}{d\varepsilon} = a_k^i x_j^k, \quad x_j^i(0) = \delta_j^i, \quad (i, j = 1, \dots, n),$$

involving matrix entries of  $A$ . The solution is just the matrix exponential  $X(\varepsilon) = e^{\varepsilon A}$ , which is the one-parameter subgroup of  $GL(n)$  generated by a matrix  $A$  in  $\mathfrak{gl}(n)$ .

Recall that the *exponential map*  $\exp : \mathfrak{g} \rightarrow G$  is obtained by setting  $\varepsilon = 1$  in the one-parameter subgroup generated by vector-field  $v$  :

$$\exp(v) \equiv \exp(v) e.$$

Its differential at 0,

$$d\exp : T\mathfrak{g}|_0 \simeq \mathfrak{g} \rightarrow TG|_e \simeq \mathfrak{g}$$

is the identity map.

#### *Lie Symmetry Groups and General Differential Equations*

Consider a system  $\mathcal{S}$  of general differential equations (DEs, to be distinguished from ODEs) involving  $p$  independent variables  $x = (x^1, \dots, x^p)$ , and  $q$  dependent variables  $u = (u^1, \dots, u^q)$ . The solution of the system will be of the form  $u = f(x)$ , or, in components,  $u^\alpha = f^\alpha(x^1, \dots, x^p)$ ,  $\alpha = 1, \dots, q$  (so that Latin indices refer to independent variables while Greek indices refer to dependent variables). Let  $X = \mathbb{R}^p$ , with coordinates  $x = (x^1, \dots, x^p)$ , be the space representing the independent variables, and let  $U = \mathbb{R}^q$ , with coordinates  $u = (u^1, \dots, u^q)$ , represent dependent variables. A Lie symmetry group  $G$  of the system  $\mathcal{S}$  will be a local group of transformations acting on some

open subset  $M \subset X \times U$  in such way that  $G$  transforms solutions of  $\mathcal{S}$  to other solutions of  $\mathcal{S}$  [Olv86].

More precisely, we need to explain exactly how a given transformation  $g \in G$ , where  $G$  is a Lie group, transforms a function  $u = f(x)$ . We firstly identify the function  $u = f(x)$  with its graph

$$\Gamma_f \equiv \{(x, f(x)) : x \in \text{dom } f \equiv \Omega\} \subset X \times U,$$

where  $\Gamma_f$  is a submanifold of  $X \times U$ . If  $\Gamma_f \subset M_g \equiv \text{dom } g$ , then the transform of  $\Gamma_f$  by  $g$  is defined as

$$g \cdot \Gamma_f = \{(\tilde{x}, \tilde{u}) = g \cdot (x, u) : (x, u) \in \Gamma_f\}.$$

We write  $\tilde{f} = g \cdot f$  and call the function  $\tilde{f}$  the *transform* of  $f$  by  $g$ .

For example, let  $p = 1$  and  $q = 1$ , so  $X = \mathbb{R}$  with a single independent variable  $x$ , and  $U = \mathbb{R}$  with a single dependent variable  $u$ , so we have a single ODE involving a single function  $u = f(x)$ . Let  $G = SO(2)$  be the rotation group acting on  $X \times U \simeq \mathbb{R}^2$ . The transformations in  $G$  are given by

$$(\tilde{x}, \tilde{u}) = \theta \cdot (x, u) = (x \cos \theta - u \sin \theta, x \sin \theta + u \cos \theta).$$

Let  $u = f(x)$  be a function whose graph is a subset  $\Gamma_f \subset X \times U$ . The group  $SO(2)$  acts on  $f$  by rotating its graph.

In general, the procedure for finding the transformed function  $\tilde{f} = g \cdot f$  is given by [Olv86]:

$$g \cdot f = [\Phi_g \circ (1 \times f)] \circ [\Xi_g \circ (1 \times f)]^{-1}, \quad (2.36)$$

where  $\Xi_g = \Xi_g(x, u)$ ,  $\Phi_g = \Phi_g(x, u)$  are smooth functions such that

$$(\tilde{x}, \tilde{u}) = g \cdot (x, u) = (\Xi_g(x, u), \Phi_g(x, u)),$$

while  $1$  denotes the identity function of  $X$ , so  $1(x) = x$ . Formula (2.36) holds whenever the second factor is invertible.

Let  $\mathcal{S}$  be a system of DEs. A *symmetry group* of the system  $\mathcal{S}$  is a local Lie group of transformations  $G$  acting on an open subset  $M \subset X \times U$  of the space  $X \times U$  of independent and dependent variables of the system with the property that whenever  $u = f(x)$  is a solution of  $\mathcal{S}$ , and whenever  $g \cdot f$  is defined for  $g \in G$ , then  $u = g \cdot f(x)$  is also a solution of the system.

For example, in the case of the ODE  $u_{xx} = 0$ , the rotation group  $SO(2)$  is obviously a symmetry group, since the solutions are all linear functions and  $SO(2)$  takes any linear function to another linear function. Another easy example is given by the classical *heat equation*  $u_t = u_{xx}$ . Here the group of translations

$$(x, t, u) \mapsto (x + \varepsilon a, t + \varepsilon b, u), \quad \varepsilon \in \mathbb{R},$$

is a symmetry group since  $u = f(x - \varepsilon a, t - \varepsilon b)$  is a solution to the heat equation whenever  $u = f(x, t)$  is.

### Prolongations

#### *Prolongations of Functions*

Given a smooth real-valued function  $u = f(x) = f(x^1, \dots, x^p)$  of  $p$  independent variables, there is an induced function  $u^{(n)} = \mathbf{pr}^{(n)}f(x)$ , called the  $n$ th *prolongation* of  $f$  [Olv86], which is defined by the equations

$$u_J = \partial_J f(x) = \frac{\partial^k f(x)}{\partial x^{j_1} \partial x^{j_2} \dots \partial x^{j_k}},$$

where the multi-index  $J = (j_1, \dots, j_k)$  is an unordered  $k$ -tuple of integers, with entries  $1 \leq j_k \leq p$  indicating which derivatives are being taken. More generally, if  $f : X \rightarrow U$  is a smooth function from  $X \simeq \mathbb{R}^p$  to  $U \simeq \mathbb{R}^q$ , so  $u = f(x) = f(f^1(x), \dots, f^q(x))$ , there are  $q \cdot p_k$  numbers

$$u_J^\alpha = \partial_J f^\alpha(x) = \frac{\partial^k f^\alpha(x)}{\partial x^{j_1} \partial x^{j_2} \dots \partial x^{j_k}},$$

needed to represent all the different  $k$ th order derivatives of the components of  $f$  at a point  $x$ . Thus  $\mathbf{pr}^{(n)}f : X \rightarrow U^{(n)}$  is a function from  $X$  to the space  $U^{(n)}$ , and for each  $x \in X$ ,  $\mathbf{pr}^{(n)}f(x)$  is a vector whose  $q \cdot p^{(n)}$  entries represent the values of  $f$  and all its derivatives up to order  $n$  at the point  $x$ .

For example, in the case  $p = 2$ ,  $q = 1$  we have  $X \simeq \mathbb{R}^2$  with coordinates  $(x^1, x^2) = (x, y)$ , and  $U \simeq \mathbb{R}$  with the single coordinate  $u = f(x, y)$ . The second prolongation  $u^{(2)} = \mathbf{pr}^{(2)}f(x, y)$  is given by [Olv86]

$$(u; u_x, u_y; u_{xx}, u_{xy}, u_{yy}) = \left( f; \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}; \frac{\partial^2 f}{\partial x^2}, \frac{\partial^2 f}{\partial x \partial y}, \frac{\partial^2 f}{\partial y^2} \right), \quad (2.37)$$

all evaluated at  $(x, y)$ .

The  $n$ th prolongation  $\mathbf{pr}^{(n)}f(x)$  is also known as the  $n$ -jet of  $f$ . In other words, the  $n$ th prolongation  $\mathbf{pr}^{(n)}f(x)$  represents the Taylor polynomial of degree  $n$  for  $f$  at the point  $x$ , since the derivatives of order  $\leq n$  determine the Taylor polynomial and vice versa.

#### *Prolongations of Differential Equations*

A system  $\mathcal{S}$  of  $n$ th order DEs in  $p$  independent and  $q$  dependent variables is given as a system of equations [Olv86]

$$\Delta_r(x, u^{(n)}) = 0, \quad (r = 1, \dots, l), \quad (2.38)$$

involving  $x = (x^1, \dots, x^p)$ ,  $u = (u^1, \dots, u^q)$  and the derivatives of  $u$  with respect to  $x$  up to order  $n$ . The functions  $\Delta(x, u^{(n)}) = (\Delta_1(x, u^{(n)}), \dots, \Delta_l(x, u^{(n)}))$  are assumed to be smooth in their arguments, so  $\Delta : X \times U^{(n)} \rightarrow \mathbb{R}^l$  represents a smooth map from the *jet space*  $X \times U^{(n)}$  to some  $l$ D Euclidean space. The DEs

themselves tell where the given map  $\Delta$  vanishes on the jet space  $X \times U^{(n)}$ , and thus determine a submanifold

$$\mathcal{S}_\Delta = \left\{ (x, u^{(n)}) : \Delta(x, u^{(n)}) = 0 \right\} \subset X \times U^{(n)} \quad (2.39)$$

of the total the jet space  $X \times U^{(n)}$ .

We can identify the system of DEs (2.38) with its corresponding submanifold  $\mathcal{S}_\Delta$  (2.39). From this point of view, a smooth *solution* of the given system of DEs is a smooth function  $u = f(x)$  such that [Olv86]

$$\Delta_r(x, \mathbf{pr}^{(n)} f(x)) = 0, \quad (r = 1, \dots, l),$$

whenever  $x$  lies in the domain of  $f$ . This is just a restatement of the fact that the derivatives  $\partial_j f^\alpha(x)$  of  $f$  must satisfy the algebraic constraints imposed by the system of DEs. This condition is equivalent to the statement that the graph of the prolongation  $\mathbf{pr}^{(n)} f(x)$  must lie entirely within the submanifold  $\mathcal{S}_\Delta$  determined by the system:

$$\Gamma_f^{(n)} \equiv \left\{ (x, \mathbf{pr}^{(n)} f(x)) \right\} \subset \mathcal{S}_\Delta = \left\{ \Delta(x, u^{(n)}) = 0 \right\}.$$

We can thus take an  $n$ th order system of DEs to be a submanifold  $\mathcal{S}_\Delta$  in the  $n$ -jet space  $X \times U^{(n)}$  and a solution to be a function  $u = f(x)$  such that the graph of the  $n$ th prolongation  $\mathbf{pr}^{(n)} f(x)$  is contained in the submanifold  $\mathcal{S}_\Delta$ .

For example, consider the case of *Laplace equation* in the plane

$$u_{xx} + u_{yy} = 0 \quad (\text{remember, } u_x \equiv \partial_x u).$$

Here  $p = 2$  since there are two independent variables  $x$  and  $y$ , and  $q = 1$  since there is one dependent variable  $u$ . Also  $n = 2$  since the equation is second order, so  $\mathcal{S}_\Delta \subset X \times U^{(2)}$  is given by (2.37). A solution  $u = f(x, y)$  must satisfy

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 0$$

for all  $(x, y)$ . This is the same as requiring that the graph of the second prolongation  $\mathbf{pr}^{(2)} f$  lie in  $\mathcal{S}_\Delta$ .

#### *Prolongations of Group Actions*

Let  $G$  be a local group of transformations acting on an open subset  $M \subset X \times U$  of the space of independent and dependent variables. There is an induced local action of  $G$  on the  $n$ -jet space  $M^{(n)}$ , called the  $n$ th prolongation  $\mathbf{pr}^{(n)} G$  of the action of  $G$  on  $M$ . This prolongation is defined so that it transforms the derivatives of functions  $u = f(x)$  into the corresponding derivatives of the transformed function  $\tilde{u} = \tilde{f}(\tilde{x})$  [Olv86].

More precisely, suppose  $(x_0, u_0^{(n)})$  is a given point in  $M^{(n)}$ . Choose any smooth function  $u = f(x)$  defined in a neighborhood of  $x_0$ , whose graph  $\Gamma_f$  lies in  $M$ , and has the given derivatives at  $x_0$  :

$$u_0^{(n)} = \mathbf{pr}^{(n)} f(x_0), \quad \text{i.e.,} \quad u_{J0}^\alpha = \partial_J f^\alpha(x_0).$$

If  $g$  is an element of  $G$  sufficiently near the identity, the transformed function  $g \cdot f$  as given by (2.36) is defined in a neighborhood of the corresponding point  $(\tilde{x}_0, \tilde{u}_0) = g \cdot (x_0, u_0)$ , with  $u_0 = f(x_0)$  being the zeroth order components of  $u_0^{(n)}$ . We then determine the action of the prolonged group of transformations  $\mathbf{pr}^{(n)}g$  on the point  $(x_0, u_0^{(n)})$  by evaluating the derivatives of the transformed function  $g \cdot f$  at  $\tilde{x}_0$ ; explicitly [Olv86]

$$\mathbf{pr}^{(n)}g \cdot (x_0, u_0^{(n)}) = (\tilde{x}_0, \tilde{u}_0^{(n)}),$$

where

$$\tilde{u}_0^{(n)} \equiv \mathbf{pr}^{(n)}(g \cdot f)(\tilde{x}_0).$$

For example, let  $p = q = 1$ , so  $X \times U \simeq \mathbb{R}^2$ , and consider the action of the rotation group  $SO(2)$ . To calculate its first prolongation  $\mathbf{pr}^{(1)}SO(2)$ , first note that  $X \times U^{(1)} \simeq \mathbb{R}^3$ , with coordinates  $(x, u, u_x)$ . Given a function  $u = f(x)$ , the first prolongation is [Olv86]

$$\mathbf{pr}^{(1)}f(x) = (f(x), f'(x)).$$

Now, given a point  $(x^0, u^0, u_x^0) \in X \times U^{(1)}$ , and a rotation in  $SO(2)$  characterized by the angle  $\theta$  as given above, the corresponding transformed point

$$\mathbf{pr}^{(1)}\theta \cdot (x^0, u^0, u_x^0) = (\tilde{x}^0, \tilde{u}^0, \tilde{u}_x^0)$$

(provided it exists). As for the first order derivative, we find

$$\tilde{u}_x^0 = \frac{\sin \theta + u_x \cos \theta}{\cos \theta - u_x \sin \theta}.$$

Now, applying the group transformations given above, and dropping the 0-indices, we find that the prolonged action  $\mathbf{pr}^{(1)}SO(2)$  on  $X \times U^{(1)}$  is given by

$$\mathbf{pr}^{(1)}\theta \cdot (x, u, u_x) = \left( x \cos \theta - u \sin \theta, x \sin \theta + u \cos \theta, \frac{\sin \theta + u_x \cos \theta}{\cos \theta - u_x \sin \theta} \right),$$

which is defined for  $|\theta| < |\operatorname{arccot} u_x|$ . Note that even though  $SO(2)$  is a linear, globally defined group of transformations, its first prolongation  $\mathbf{pr}^{(1)}SO(2)$  is both nonlinear and only locally defined. This fact demonstrates the complexity of the operation of prolonging a group of transformations.

In general, for any Lie group  $G$ , the first prolongation  $\mathbf{pr}^{(1)}G$  acts on the original variables  $(x, u)$  exactly the same way that  $G$  itself does; only the action on the derivative  $u_x$  provides an new information. Therefore,  $\mathbf{pr}^{(0)}G$  agrees with  $G$  itself, acting on  $M^{(0)} = M$ .

*Prolongations of Vector Fields*

Prolongation of the infinitesimal generators of the group action turn out to be the *infinitesimal generators* of the *prolonged group action* [Olv86]. Let  $M \subset X \times U$  be open and suppose  $v$  is a vector-field on  $M$ , with corresponding local one-parameter group  $\exp(\varepsilon v)$ . The  $n$ th prolongation of  $v$ , denoted  $\mathbf{pr}^{(n)}v$ , will be a vector-field on the  $n$ -jet space  $M^{(n)}$ , and is defined to be the infinitesimal generator of the corresponding prolonged one-parameter group  $\mathbf{pr}^{(n)}[\exp(\varepsilon v)]$ . In other words,

$$\mathbf{pr}^{(n)}v|_{(x,u^{(n)})} = \left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} \mathbf{pr}^{(n)}[\exp(\varepsilon v)](x, u^{(n)}) \quad (2.40)$$

for any  $(x, u^{(n)}) \in M^{(n)}$ .

For a vector-field  $v$  on  $M$ , given by

$$v = \xi^i(x, u) \frac{\partial}{\partial x^i} + \phi^\alpha(x, u) \frac{\partial}{\partial u^\alpha}, \quad (i = 1, \dots, p, \alpha = 1, \dots, q),$$

the  $n$ th prolongation  $\mathbf{pr}^{(n)}v$  is given by [Olv86]

$$\mathbf{pr}^{(n)}v = \xi^i(x, u) \frac{\partial}{\partial x^i} + \phi_J^\alpha(x, u^{(n)}) \frac{\partial}{\partial u_J^\alpha},$$

with  $\phi_0^\alpha = \phi^\alpha$ , and  $J$  a multiindex defined above.

For example, in the case of  $SO(2)$  group, the corresponding infinitesimal generator is

$$v = -u \frac{\partial}{\partial x} + x \frac{\partial}{\partial u},$$

with

$$\exp(\varepsilon v)(x, u) = (x \cos \varepsilon - u \sin \varepsilon, x \sin \varepsilon + u \cos \varepsilon),$$

being the rotation through angle  $\varepsilon$ . The first prolongation takes the form

$$\mathbf{pr}^{(1)}[\exp(\varepsilon v)](x, u, u_x) = \left( x \cos \varepsilon - u \sin \varepsilon, x \sin \varepsilon + u \cos \varepsilon, \frac{\sin \varepsilon + u_x \cos \varepsilon}{\cos \varepsilon - u_x \sin \varepsilon} \right).$$

According to (2.40), the first prolongation of  $v$  is obtained by differentiating these expressions with respect to  $\varepsilon$  and setting  $\varepsilon = 0$ , which gives

$$\mathbf{pr}^{(1)}v = -u \frac{\partial}{\partial x} + x \frac{\partial}{\partial u} + (1 + u_x^2) \frac{\partial}{\partial u_x}.$$

*General Prolongation Formula*

Let

$$v = \xi^i(x, u) \frac{\partial}{\partial x^i} + \phi^\alpha(x, u) \frac{\partial}{\partial u^\alpha}, \quad (i = 1, \dots, p, \alpha = 1, \dots, q), \quad (2.41)$$

be a vector-field defined on an open subset  $M \subset X \times U$ . The  $n$ th prolongation of  $v$  is the vector-field [Olv86]

$$\mathbf{pr}^{(n)}v = v + \phi_J^\alpha(x, u^{(n)}) \frac{\partial}{\partial u_J^\alpha}, \quad (2.42)$$

defined on the corresponding jet space  $M^{(n)} \subset X \times U^{(n)}$ . The coefficient functions  $\phi_J^\alpha$  are given by the following formula:

$$\phi_J^\alpha = D_J(\phi^\alpha - \xi^i u_i^\alpha) + \xi^i u_{J,i}^\alpha, \quad (2.43)$$

where  $u_i^\alpha = \partial u^\alpha / \partial x^i$ , and  $u_{J,i}^\alpha = \partial u_J^\alpha / \partial x^i$ .  $D_J$  is the *total derivative* with respect to the multiindex  $J$ , i.e.,

$$D_J = D_{j_1} D_{j_2} \dots D_{j_k},$$

while the total derivative with respect to the ordinary index,  $D_i$ , is defined as follows. Let  $P(x, u^{(n)})$  be a smooth function of  $x, u$  and derivatives of  $u$  up to order  $n$ , defined on an open subset  $M^{(n)} \subset X \times U^{(n)}$ . The total derivative of  $P$  with respect to  $x^i$  is the unique smooth function  $D_i P(x, u^{(n)})$  defined on  $M^{(n+1)}$  and depending on derivatives of  $u$  up to order  $n+1$ , with the *recursive property* that if  $u = f(x)$  is any smooth function then

$$D_i P(x, \mathbf{pr}^{(n+1)}f(x)) = \partial_{x^i} \{P(x, \mathbf{pr}^{(n)}f(x))\}.$$

For example, in the case of  $SO(2)$  group, with the infinitesimal generator

$$v = -u \frac{\partial}{\partial x} + x \frac{\partial}{\partial u},$$

the first prolongation is (as calculated above)

$$\mathbf{pr}^{(1)}v = -u \frac{\partial}{\partial x} + x \frac{\partial}{\partial u} + \phi^x \frac{\partial}{\partial u_x},$$

where

$$\phi^x = D_x(\phi - \xi u_x) + \xi u_{xx} = 1 + u_x^2.$$

Also,

$$\phi^{xx} = D_x \phi^x - u_{xx} D_x \xi = 3u_x u_{xx},$$

thus the infinitesimal generator of the second prolongation  $\mathbf{pr}^{(2)}SO(2)$  acting on  $X \times U^{(2)}$  is

$$\mathbf{pr}^{(2)}v = -u \frac{\partial}{\partial x} + x \frac{\partial}{\partial u} + (1 + u_x^2) \frac{\partial}{\partial u_x} + 3u_x u_{xx} \frac{\partial}{\partial u_{xx}}.$$

Let  $v$  and  $w$  be two smooth vector-fields on  $M \subset X \times U$ . Then their  $n$ th prolongations,  $\mathbf{pr}^{(n)}v$  and  $\mathbf{pr}^{(n)}w$  respectively, have the *linearity property*

$$\mathbf{pr}^{(n)}(c_1 v + c_2 w) = c_1 \mathbf{pr}^{(n)}v + c_2 \mathbf{pr}^{(n)}w, \quad (c_1, c_2 - \text{constant}),$$

and the *Lie bracket property*

$$\mathbf{pr}^{(n)}[v, w] = [\mathbf{pr}^{(n)}v, \mathbf{pr}^{(n)}w].$$

### Lie Symmetries of Special Biomechanical Equations

Here we consider two most important equations for human-like biomechanics:

1. The heat equation, which has been analyzed in muscular mechanics since the early works of A.V. Hill ([Hil38]); and
2. The Korteweg–De Vries equation, the basic equation for solitary models of muscular excitation–contraction dynamics (see subsection (3.2.3) below).

Suppose

$$\mathcal{S} : \Delta_r(x, u^{(n)}) = 0, \quad (r = 1, \dots, l),$$

is a system of DEs of maximal rank defined over  $M \subset X \times U$ . If  $G$  is a local group of transformations acting on  $M$ , and

$$\mathbf{pr}^{(n)}v[\Delta_r(x, u^{(n)})] = 0, \quad \text{whenever} \quad \Delta(x, u^{(n)}) = 0, \quad (2.44)$$

(with  $r = 1, \dots, l$ ) for every infinitesimal generator  $v$  of  $G$ , then  $G$  is a symmetry group of the system  $\mathcal{S}$  [Olv86].

#### The Heat Equation

The (1 + 1)D *heat equation* (with the thermal diffusivity normalized to unity)

$$u_t = u_{xx} \quad (2.45)$$

has two independent variables  $x$  and  $t$ , and one dependent variable  $u$ , so  $p = 2$  and  $q = 1$ . Equation (A.30) has the second order,  $n = 2$ , and can be identified with the linear submanifold  $M^{(2)} \subset X \times U^{(2)}$  determined by the vanishing of  $\Delta(x, t, u^{(2)}) = u_t - u_{xx}$ .

Let

$$v = \xi(x, t, u) \frac{\partial}{\partial x} + \tau(x, t, u) \frac{\partial}{\partial t} + \phi(x, t, u) \frac{\partial}{\partial u}$$

be a vector-field on  $X \times U$ . According to (2.44) we need to now the second prolongation

$$\mathbf{pr}^{(2)}v = v + \phi^x \frac{\partial}{\partial u_x} + \phi^t \frac{\partial}{\partial u_t} + \phi^{xx} \frac{\partial}{\partial u_{xx}} + \phi^{xt} \frac{\partial}{\partial u_{xt}} + \phi^{tt} \frac{\partial}{\partial u_{tt}}$$

of  $v$ . Applying  $\mathbf{pr}^{(2)}v$  to (A.30) we find the infinitesimal criterion (2.44) to be

$$\phi^t = \phi^{xx},$$

which must be satisfied whenever  $u_t = u_{xx}$ .

*The Korteweg–De Vries Equation*

The Korteweg–De Vries equation

$$u_t + u_{xxx} + uu_x = 0 \quad (2.46)$$

arises in physical systems in which both nonlinear and dispersive effects are relevant. A vector–field

$$v = \xi(x, t, u) \frac{\partial}{\partial x} + \tau(x, t, u) \frac{\partial}{\partial t} + \phi(x, t, u) \frac{\partial}{\partial u}$$

generates a one–parameter symmetry group iff

$$\phi^t + \phi^{xxx} + u\phi^x + u_x\phi = 0,$$

whenever  $u$  satisfies (2.46), etc.

**Generalized Lie Symmetries**

Consider a vector–field (2.41) defined on an open subset  $M \subset X \times U$ . Provided the coefficient functions  $\xi^i$  and  $\phi^\alpha$  depend only on  $x$  and  $u$ ,  $v$  will generate a (local) one–parameter group of transformations  $\exp(\varepsilon v)$  acting pointwise on the underlying space  $M$ . A significant generalization of the notion of symmetry group is obtained by relaxing this geometric assumption, and allowing the coefficient functions  $\xi^i$  and  $\phi^\alpha$  to also depend on derivatives of  $u$  [Olv86].

A *generalized vector–field* is a (formal) expression

$$v = \xi^i[u] \frac{\partial}{\partial x^i} + \phi^\alpha[u] \frac{\partial}{\partial u^\alpha}, \quad (i = 1, \dots, p, \alpha = 1, \dots, q), \quad (2.47)$$

in which  $\xi^i$  and  $\phi^\alpha$  are smooth functions. For example,

$$v = xu_x \frac{\partial}{\partial x} + u_{xx} \frac{\partial}{\partial u}$$

is a generalized vector in the case  $p = q = 1$ .

According to the general prolongation formula (2.42), we can define the *prolonged generalized vector–field*

$$\mathbf{pr}^{(n)}v = v + \phi_{,J}^\alpha[u] \frac{\partial}{\partial u_J^\alpha},$$

whose coefficients are as before determined by the formula (2.43). Thus, in our previous example [Olv86],

$$\mathbf{pr}^{(n)}v = xu_x \frac{\partial}{\partial x} + u_{xx} \frac{\partial}{\partial u} + [u_{xxx} - (xu_{xx} + u_x)u_x] \frac{\partial}{\partial u_x}.$$

Given a generalized vector-field  $v$ , its *infinite prolongation* (including all the derivatives) is the formal expression

$$\mathbf{pr} v = \xi^i \frac{\partial}{\partial x^i} + \phi_J^\alpha \frac{\partial}{\partial u_J^\alpha}.$$

Now, a generalized vector-field  $v$  is a *generalized infinitesimal symmetry* of a system  $\mathcal{S}$  of differential equations

$$\Delta_r[u] = \Delta_r(x, u^{(n)}) = 0, \quad (r = 1, \dots, l),$$

iff

$$\mathbf{pr} v[\Delta_r] = 0$$

for every smooth solution  $u = f(x)$  [Olv86].

For example, consider the heat equation

$$\Delta[u] = u_t - u_{xx} = 0.$$

The generalized vector-field  $v = u_x \frac{\partial}{\partial u}$  has prolongation

$$\mathbf{pr} v = u_x \frac{\partial}{\partial u} + u_{xx} \frac{\partial}{\partial u_x} + u_{xt} \frac{\partial}{\partial u_t} + u_{xxx} \frac{\partial}{\partial u_{xx}} + \dots$$

Thus

$$\mathbf{pr} v(\Delta) = u_{xt} - u_{xxx} = D_x(u_t - u_{xx}) = D_x \Delta,$$

and hence  $v$  is a generalized symmetry of the heat equation.

### Noether Symmetries

Here we present some results about *Noether symmetries*, in particular for the first order Lagrangians  $L(q, \dot{q})$  (see [BGG89, PSS96]). We start with a *Noether Lagrangian symmetry*,

$$\delta L = \dot{F},$$

and we will investigate the conversion of this symmetry to the Hamiltonian formalism. Defining

$$G = (\partial L / \partial \dot{q}^i) \delta q^i - F,$$

we can write

$$\delta_i L \delta q^i + \dot{G} = 0, \quad (2.48)$$

where  $\delta_i L$  is the *Euler-Lagrange functional derivative* of  $L$ ,

$$\delta_i L = \alpha_i - W_{ik} \ddot{q}^k,$$

where

$$W_{ik} \equiv \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^k} \quad \text{and} \quad \alpha_i \equiv -\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^k} \dot{q}^k + \frac{\partial L}{\partial q^i}.$$

We consider the general case where the mass matrix, or *Hessian* ( $W_{ij}$ ), may be a singular matrix. In this case there exists a kernel for the pull-back  $\mathbb{F}L^*$  of the *Legendre map*, i.e., *fiber-derivative*  $\mathbb{F}L$ , from the velocity phase-space  $TM$  (tangent bundle of the biomechanical manifold  $M$ ) to the momentum phase-space  $T^*M$  (cotangent bundle of  $M$ ). This kernel is spanned by the vector-fields

$$\Gamma_\mu = \gamma_\mu^i \frac{\partial}{\partial \dot{q}^i},$$

where  $\gamma_\mu^i$  are a basis for the null vectors of  $W_{ij}$ . The Lagrangian time-evolution differential operator can therefore be expressed as:

$$X = \partial_t + \dot{q}^k \frac{\partial}{\partial q^k} + a^k(q, \dot{q}) \frac{\partial}{\partial \dot{q}^k} + \lambda^\mu \Gamma_\mu \equiv X_o + \lambda^\mu \Gamma_\mu,$$

where  $a^k$  are functions which are determined by the formalism, and  $\lambda^\mu$  are arbitrary functions. It is not necessary to use the Hamiltonian technique to find the  $\Gamma_\mu$ , but it does facilitate the calculation:

$$\gamma_\mu^i = \mathbb{F}L^* \left( \frac{\partial \phi_\mu}{\partial p_i} \right), \quad (2.49)$$

where the  $\phi_\mu$  are the Hamiltonian primary first class constraints.

Notice that the highest derivative in (2.48),  $\ddot{q}^i$ , appears linearly. Because  $\delta L$  is a symmetry, (2.48) is identically satisfied, and therefore the coefficient of  $\ddot{q}^i$  vanishes:

$$W_{ik} \delta q^k - \frac{\partial G}{\partial \dot{q}^i} = 0. \quad (2.50)$$

We contract with a null vector  $\gamma_\mu^i$  to find that

$$\Gamma_\mu G = 0.$$

It follows that  $G$  is projectable to a function  $G_H$  in  $T^*Q$ ; that is, it is the pull-back of a function (not necessarily unique) in  $T^*Q$ :

$$G = \mathbb{F}L^*(G_H).$$

This important property is valid for any conserved quantity associated with a Noether symmetry. Observe that  $G_H$  is determined up to the addition of linear combinations of the primary constraints. Substitution of this result in (2.50) gives

$$W_{ik} \left[ \delta q^k - \mathbb{F}L^* \left( \frac{\partial G_H}{\partial p_k} \right) \right] = 0,$$

and so the brackets enclose a null vector of  $W_{ik}$ :

$$\delta q^i - \mathbb{F}L^* \left( \frac{\partial G_H}{\partial p_i} \right) = r^\mu \gamma_\mu^i, \quad (2.51)$$

for some  $r^\mu(t, q, \dot{q})$ .

We shall investigate the projectability of variations generated by diffeomorphisms in the following section. Assume that an infinitesimal transformation  $\delta q^i$  is projectable:

$$\Gamma_\mu \delta q^i = 0.$$

If  $\delta q^i$  is projectable, so must be  $r^\mu$ , so that  $r^\mu = \mathbb{F}L^*(r_H^\mu)$ . Then, using (2.49) and (2.51), we see that

$$\delta q^i = \mathbb{F}L^* \left( \frac{\partial(G_H + r_H^\mu \phi_\mu)}{\partial p_i} \right).$$

We now redefine  $G_H$  to absorb the piece  $r_H^\mu \phi_\mu$ , and from now on we will have

$$\delta q^i = \mathbb{F}L^* \left( \frac{\partial G_H}{\partial p_i} \right).$$

Define

$$\hat{p}_i = \frac{\partial L}{\partial \dot{q}^i};$$

after eliminating (2.50) times  $\ddot{q}^i$  from (2.48), we get

$$\left( \frac{\partial L}{\partial q^i} - \dot{q}^k \frac{\partial \hat{p}_i}{\partial q^k} \right) \mathbb{F}L^* \left( \frac{\partial G_H}{\partial p_i} \right) + \dot{q}^i \frac{\partial}{\partial q^i} \mathbb{F}L^*(G_H) + \mathbb{F}L^* \partial_t G_H = 0,$$

which simplifies to

$$\frac{\partial L}{\partial q^i} \mathbb{F}L^* \left( \frac{\partial G_H}{\partial p_i} \right) + \dot{q}^i \mathbb{F}L^* \left( \frac{\partial G_H}{\partial q^i} \right) + \mathbb{F}L^* \partial_t G_H = 0. \quad (2.52)$$

Now let us invoke two identities [BGG89] that are at the core of the connection between the Lagrangian and the Hamiltonian equations of motion. They are

$$\dot{q}^i = \mathbb{F}L^* \left( \frac{\partial H}{\partial p_i} \right) + v^\mu(q, \dot{q}) \mathbb{F}L^* \left( \frac{\partial \phi_\mu}{\partial p_i} \right),$$

and

$$\frac{\partial L}{\partial q^i} = -\mathbb{F}L^* \left( \frac{\partial H}{\partial q^i} \right) - v^\mu(q, \dot{q}) \mathbb{F}L^* \left( \frac{\partial \phi_\mu}{\partial q^i} \right);$$

where  $H$  is any canonical Hamiltonian, so that  $\mathbb{F}L^*(H) = \dot{q}^i (\partial L / \partial \dot{q}^i) - L = \hat{E}$ , the Lagrangian energy, and the functions  $v^\mu$  are determined so as to render the first relation an identity. Notice the important relation

$$\Gamma_\mu v^\nu = \delta_\mu^\nu,$$

which stems from applying  $\Gamma_\mu$  to the first identity and taking into account that

$$\Gamma_\mu \circ \mathbb{F}L^* = 0.$$

Substitution of these two identities into (2.52) yields (where  $\{ , \}$  denotes the *Poisson bracket*)

$$\mathbb{F}L^*\{G_H, H\} + v^\mu \mathbb{F}L^*\{G_H, \phi_\mu\} + \mathbb{F}L^*\partial_t G_H = 0.$$

This result can be split through the action of  $\Gamma_\mu$  into

$$\mathbb{F}L^*\{G_H, H\} + \mathbb{F}L^*\partial_t G_H = 0,$$

and

$$\mathbb{F}L^*\{G_H, \phi_\mu\} = 0;$$

or equivalently,

$$\{G_H, H\} + \partial_t G_H = pc,$$

and

$$\{G_H, \phi_\mu\} = pc,$$

where  $pc$  stands for any linear combination of primary constraints. In this way, we have arrived at a neat characterization for a generator  $G_H$  of Noether transformations in the canonical formalism.

## Lie–Invariant Differential Forms

### *Robot Kinematics*

Recall that a typical *motion planning* problem in robotics consists in a collection of objects moving around obstacles from an initial to a final configuration (see [BL92, Pry96]). This may include in particular, solving the *collision detection* problem.

When a solid object undergoes a rigid motion, the totality of points through which it passed constitutes a region in space called the *swept volume*. To describe the geometric structure of the swept volume we pose this problem as one of geometric study of some manifold swept by surface points using powerful tools from both modern differential geometry and nonlinear dynamical systems theory [Ric93, LP94, Pry96, GJ94] on manifolds. For some special cases of the Euclidean motion in the space  $\mathbb{R}^3$  one can construct a very rich hydrodynamic system [BL92] modelling a sweep flow, which appears to be a *completely integrable Hamiltonian system* having a special *Lax type representation*. To describe in detail these and other properties of swept volume dynamical systems, we develop *Cartan’s theory of Lie–invariant geometric objects* generated by closed ideals in the Grassmann algebra, following [BPS98].

Let a Lie group  $G$  act on an analytical manifold  $Y$  in the transitive way, that is the action  $G \times Y \xrightarrow{\rho} Y$  generates some nonlinear exact representation of the Lie group  $G$  on the manifold  $Y$ . In the frame of the Cartan’s theory, the representation  $G \times Y \xrightarrow{\rho} Y$  can be described by means of a system of differential 1–forms (see section 3.3.6 below)

$$\bar{\beta}^j = dy^j + \xi_i^j \bar{\omega}^i(a, da) \quad (2.53)$$

in the Grassmann algebra  $\Lambda(Y \times G)$  on the product  $Y \times G$ , where  $\bar{\omega}^i(a, da) \in T_a^*(G)$ ,  $i = 1, \dots, r = \dim G$  is a basis of left invariant Cartan's forms of the Lie group  $G$  at a point  $a \in G$ ,  $y = \{y^j : j = 1, \dots, n = \dim Y\} \in Y$  and  $\xi_i^j : Y \times G \rightarrow \mathbb{R}$  are some smooth real valued functions.

The following *Cartan theorem* is basic in describing a geometric object invariant with respect to the mentioned above group action  $G \times Y \xrightarrow{L} Y$ : The system of differential forms (2.53) is a system of an invariant geometric object iff the following conditions are fulfilled:

1. The coefficients  $\xi_i^j \in C^k(Y; \mathbb{R})$  for all  $i = 1, \dots, r, j = 1, \dots, n$ , are some *analytical functions* on  $Y$ ; and
2. The differential system (2.53) is completely integrable within the *Frobenius-Cartan criterion*.

The Cartan's theorem actually says that the differential system (2.53) can be written down as

$$\bar{\beta}^j = dy^j + \xi_i^j(y) \bar{\omega}^i(a, da), \quad (2.54)$$

where 1-forms  $\{\bar{\omega}^i(a, da) : i = 1, \dots, r\}$  satisfy the standard *Maurer-Cartan equations*

$$\bar{\Omega}^j = d\bar{\omega}^j + \frac{1}{2} c_{ik}^j \bar{\omega}^i \wedge \bar{\omega}^k = 0, \quad (2.55)$$

for all  $j = 1, \dots, r$  on  $G$ , coefficients  $c_{ik}^j \in \mathbb{R}$ ,  $i, j, k = 1, \dots, r$ , being the corresponding structure constants of the Lie algebra  $\mathfrak{g}$  of the Lie group  $G$ .

#### *Maurer-Cartan 1-Forms*

Consider a Lie group  $G$  with the Lie algebra  $\mathfrak{g} \simeq T_e(G)$ , whose basis is a set  $\{A_i \in \mathfrak{g} : i = 1, \dots, r\}$ , where  $r = \dim G \equiv \dim \mathfrak{g}$ . Let also a set  $U_0 \subset \{a^i \in \mathbb{R} : i = 1, \dots, r\}$  be some open neighborhood of the zero point in  $\mathbb{R}^r$ . The exponential mapping  $\exp : U_0 \rightarrow G_0$ , where by definition [BPS98]

$$\mathbb{R}^r \supset U_0 \ni (a^1, \dots, a^r) : \xrightarrow{\exp} \exp(a^i A_i) = a \in G_0 \subset G, \quad (2.56)$$

is an analytical mapping of the whole  $U_0$  on some open neighborhood  $G_0$  of the unity element  $e \in G$ . From (2.56) it is easy to find that  $T_e(G) = T_e(G_0) \simeq \mathfrak{g}$ , where  $e = \exp(0) \in G$ . Define now the following left invariant  $\mathfrak{g}$ -valued differential 1-form on  $G_0 \subset G$ :

$$\bar{\omega}(a, da) = a^{-1} da = \bar{\omega}^j(a, da) A_j, \quad (2.57)$$

where  $A_j \in \mathfrak{g}$ ,  $\bar{\omega}^j(a, da) \in T_a^*(G)$ ,  $a \in G_0$ ,  $j = 1, \dots, r$ . To build effectively the unknown forms  $\{\bar{\omega}^j(a, da) : j = 1, \dots, r\}$ , let us consider the following analytical one-parameter 1-form  $\bar{\omega}_t(a, da) = \bar{\omega}(a_t; da_t)$  on  $G_0$ , where

$a_t = \exp(ta^i A_i)$ ,  $t \in [0, 1]$ , and differentiate this form with respect to the parameter  $t \in [0, 1]$ . We will get [BPS98]

$$d\bar{\omega}_t/dt = -a^j A_j a_t^{-1} da_t + a_t^{-1} a_t da^j A_j + a_t^{-1} da_t a^j A_j = -a^j [A_j, \bar{\omega}_t] + A_j da_j. \quad (2.58)$$

Having used the Lie identity,  $[A_j, A_k] = c_{jk}^i A_i$ ,  $j, k = 1, \dots, r$ , and the r.h.s of (2.57) in form

$$\bar{\omega}^j(a, da) = \bar{\omega}_k^j(a) da^k, \quad (2.59)$$

we finally get

$$\frac{d}{dt}(t\bar{\omega}_i^j(ta)) = \mathcal{A}_i^j t\bar{\omega}_i^k(ta) + \delta_i^j, \quad (2.60)$$

with

$$\mathcal{A}_i^k = c_{ij}^k a^j. \quad (2.61)$$

The series solution of (2.60) is [BPS98]

$$\bar{\omega}_k^j(a) = W_k^j(t) \Big|_{t=1} = \sum_{n=1}^{\infty} \frac{1}{n!} \mathcal{A}^{n-1}. \quad (2.62)$$

#### General Structure of Integrable One-Forms

Given 2-forms generating a closed ideal  $\mathfrak{I}(\alpha)$  in the Grassmann algebra  $\Lambda(M)$ , we will denote by  $\mathfrak{I}(\alpha, \beta)$  an augmented ideal in  $\Lambda(M; Y)$ , where the manifold  $Y$  will be called in further the *representation space* of some adjoint Lie group  $G$  action:  $G \times Y \xrightarrow{\rho} Y$ . In this way, we can define the set of 1-forms  $\{\beta\}$  and 2-forms  $\{\alpha\}$

$$\begin{aligned} \{\alpha\} &= \{\alpha^i \in \Lambda^2(M) : i = 1, \dots, m_\alpha\}, \\ \{\beta\} &= \{\beta^j \in \Lambda^1(M \times Y) : j = 1, \dots, n = \dim Y\}, \end{aligned} \quad (2.63)$$

satisfying [BPS98]:

$$d\alpha^i = a_k^i(\alpha) \wedge \alpha^k, \quad d\beta^j = f_k^j \alpha^k + \omega_s^j \wedge \beta^s, \quad (2.64)$$

where  $a_k^i(\alpha) \in \Lambda^1(M)$ ,  $f_k^j \in \Lambda^0(M \times Y)$  and  $\omega_s^j \in \Lambda^1(M \times Y)$  for all  $i, k = 1, \dots, m_\alpha$ ,  $j, s = 1, \dots, n$ . Since the identity  $d^2\beta^j \equiv 0$  takes place for all  $j = 1, \dots, n$ , from (2.64) it follows that

$$\left(d\omega_k^j + \omega_s^j \wedge \omega_k^s\right) \wedge \beta^k + \left(df_s^j + \omega_k^j f_s^k + f_i^j a_s^i(\alpha)\right) \wedge \alpha^s \equiv 0. \quad (2.65)$$

From (2.65) we get [BPS98]

$$d\omega_k^j + \omega_s^j \wedge \omega_k^s \in \mathfrak{I}(\alpha, \beta), \quad df_s^j + \omega_k^j f_s^k + f_i^j a_s^i(\alpha) \in \mathfrak{I}(\alpha, \beta) \quad (2.66)$$

for all  $j, k = 1, \dots, n$ ,  $s = 1, \dots, m_\alpha$ . The second inclusion in (2.66) gives a possibility to define the 1-forms  $\theta_s^j = f_i^j a_s^i(\alpha)$  satisfying the inclusion

$$d\theta_s^j + \omega_k^j \wedge \theta_s^k \in \mathfrak{J}(\alpha, \beta) \oplus f_l^j c_s^l(\alpha), \quad (2.67)$$

which we got using the identities  $d^2\alpha^j \equiv 0$ ,  $j = 1, \dots, m_\alpha$ , in the form  $c_s^j(\alpha) \wedge \alpha^s \equiv 0$ ,

$$c_s^j(\alpha) = da_s^j(\alpha) + a_l^j(\alpha) \wedge a_s^l(\alpha), \quad (2.68)$$

following from (2.64). Further, if  $s = s_0$  the 2-forms  $c_{s_0}^j(\alpha) \equiv 0$  for all  $j = 1, \dots, m_\alpha$ , then as  $s = s_0$ , we can define a set of 1-forms  $\theta^j = \theta_{s_0}^j \in \Lambda^1(M \times Y)$ ,  $j = 1, \dots, n$ , satisfying the exact inclusions

$$d\theta^j + \omega_k^j \wedge \theta^k = \Theta^j \in \mathfrak{J}(\alpha, \beta), \quad (2.69)$$

together with a set of inclusions for 1-forms  $\omega_k^j \in \Lambda^1(M \times Y)$

$$d\omega_k^j + \omega_s^j \wedge \omega_k^s = \Omega_k^j \in \mathfrak{J}(\alpha, \beta). \quad (2.70)$$

Using the *general theory of connections on the fibered frame space*  $P(M; GL(n))$  over a base manifold  $M$  (see [SW72]), we can interpret the equations (2.70) as defining the curvature 2-forms  $\Omega_k^j \in \Lambda^2(P)$ , and (2.69) as defining the torsion 2-forms  $\Theta^j \in \Lambda^2(P)$ . Since  $\mathfrak{J}(\alpha) = 0 = \mathfrak{J}(\alpha, \beta)$  upon the integral submanifold  $\bar{M} \subset M$ , the reduced fibered frame space  $P(\bar{M}; GL(n))$  will have the flat curvature and be torsion free, being as a result, completely trivialized on  $\bar{M} \subset M$ .

### *Lax Integrable Dynamical Systems*

Consider some set  $\{\beta\}$  defining a Cartan's Lie group  $G$  invariant object on a manifold  $M \times Y$ :

$$\beta^j = dy^j + \xi_k^j(y)b^k(z), \quad (2.71)$$

where  $i = 1, \dots, n = \dim Y$ ,  $r = \dim G$ . (2.71) defines a set  $\{\xi\}$  of vector-fields on  $Y$ , giving a representation  $\rho : \mathfrak{g} \rightarrow \{\xi\}$  of a given Lie algebra  $\mathfrak{g}$ . In other words, for the vector-fields  $\xi_s = \xi_s^j(y) \frac{\partial}{\partial y^j} \in \{\xi\}$ ,  $s = 1, \dots, r$  the following Lie algebra  $\mathfrak{g}$  relationships are valid

$$[\xi_s, \xi_l] = c_{sl}^k \xi_k, \quad (s, l, k = 1, \dots, r). \quad (2.72)$$

Now, we can compute the differentials  $d\beta^j \in \Lambda^2(M \times Y)$ ,  $j = 1, \dots, n$ , using (2.71) and (2.72) as [BPS98]:

$$d\beta^j = \frac{\partial \xi_k^j(y)}{\partial y^l} (\beta^l - \xi_s^l(y)b^s(z)) \wedge b^k(z) + \xi_k^j(y) db^k(z), \quad (2.73)$$

which is equal to

$$\frac{\partial \xi_k^j(y)}{\partial y^l} \beta^l \wedge b_k(z) + \xi_l^j(db^l(z) + \frac{1}{2}c_{ks}^l db^k(z) \wedge db^s(z)),$$

where  $\{\alpha\} \subset \Lambda^2(M)$  is some *a priori* given integrable system of 2-forms on  $M$ , vanishing upon the integral submanifold  $\bar{M} \subset M$ .

*Example: Burgers Dynamical System*

Consider the *Burgers dynamical system* on a *functional manifold*  $M \subset C^k(\mathbb{R}; \mathbb{R})$ :

$$u_t = uu_x + u_{xx}, \quad (2.74)$$

where  $u \in M$  and  $t \in \mathbb{R}$  is an evolution (time) parameter. The flow of (2.74) on  $M$  can be recast into a set of 2-forms  $\{\alpha\} \subset \Lambda^2(J(\mathbb{R}^2; \mathbb{R}))$  upon the adjoint jet-manifold  $J(\mathbb{R}^2; \mathbb{R})$  (see section 3.3.6 below) as follows [BPS98]:

$$\begin{aligned} \{\alpha\} = \{ & du^{(0)} \wedge dt - u^{(1)} dx \wedge dt = \alpha^1, \quad du^{(0)} \wedge dx + u^{(0)} du^{(0)} \wedge dt \\ & + du^{(1)} \wedge dt = \alpha^2 : (x, t; u^{(0)}, u^{(1)})^\tau \in M^4 \subset J^1(\mathbb{R}^2; \mathbb{R}) \}, \end{aligned} \quad (2.75)$$

where  $M^4$  is some finite-dimensional submanifold in  $J^1(\mathbb{R}^2; \mathbb{R})$  with coordinates  $(x, t, u^{(0)} = u, u^{(1)} = u_x)$ . The set of 2-forms (2.75) generates the closed ideal  $\mathfrak{I}(\alpha)$ , since

$$d\alpha^1 = dx \wedge \alpha^2 - u^{(0)} dx \wedge \alpha^1, \quad d\alpha^2 = 0, \quad (2.76)$$

the integral submanifold  $\bar{M} = \{x, t \in \mathbb{R}\} \subset M^4$  being defined by the condition  $\mathfrak{I}(\alpha) = 0$ . We now look for a reduced ‘curvature’ 1-form  $\Gamma \in \Lambda^1(M^4) \otimes \mathfrak{g}$ , belonging to some (not yet determined) Lie algebra  $\mathfrak{g}$ . This 1-form can be represented using (2.75), as follows:

$$\Gamma = b^{(x)}(u^{(0)}, u^{(1)})dx + b^{(t)}(u^{(0)}, u^{(1)})dt, \quad (2.77)$$

where elements  $b^{(x)}, b^{(t)} \in \mathfrak{g}$  satisfy [BPS98]

$$\begin{aligned} \frac{\partial b^{(x)}}{\partial u^{(0)}} = g_2, \quad \frac{\partial b^{(x)}}{\partial u^{(1)}} = 0, \quad \frac{\partial b^{(t)}}{\partial u^{(0)}} = g_1 + g_2 u^{(0)}, \\ \frac{\partial b^{(t)}}{\partial u^{(1)}} = g_2, \quad [b^{(x)}, b^{(t)}] = -u^{(1)} g_1. \end{aligned} \quad (2.78)$$

The set (2.78) has the following unique solution

$$b^{(x)} = A_0 + A_1 u^{(0)}, \quad b^{(t)} = u^{(1)} A_1 + \frac{u^{(0)^2}{2}}{2} A_1 + [A_1, A_0] u^{(0)} + A_2, \quad (2.79)$$

where  $A_j \in \mathfrak{g}$ ,  $j = \overline{0, 2}$ , are some constant elements on  $M$  of a Lie algebra  $\mathfrak{g}$  under search, satisfying the next Lie structure equations:

$$\begin{aligned} [A_0, A_2] &= 0, \\ [A_0, [A_1, A_0]] + [A_1, A_2] &= 0, \\ [A_1, [A_1, A_0]] + \frac{1}{2}[A_0, A_1] &= 0. \end{aligned} \quad (2.80)$$

From (2.78) one can see that the curvature 2-form  $\Omega \in \text{span}_{\mathbb{R}}\{A_1, [A_0, A_1] : A_j \in \mathfrak{g}, j = \overline{0, 1}\}$ . Therefore, reducing via the *Ambrose–Singer theorem* the associated principal fibered frame space  $P(M; G = GL(n))$  to the principal

fibre bundle  $P(M; G(h))$ , where  $G(h) \subset G$  is the corresponding holonomy Lie group of the connection  $\Gamma$  on  $P$ , we need to satisfy the following conditions for the set  $\mathfrak{g}(h) \subset \mathfrak{g}$  to be a Lie subalgebra in  $\mathfrak{g} : \nabla_x^m \nabla_t^n \Omega \in \mathfrak{g}(h)$  for all  $m, n \in \mathbb{Z}_+$ .

Let us try now to close the above procedure requiring that [BPS98]

$$\mathfrak{g}(h) = \mathfrak{g}(h)_0 = \text{span}_{\mathbb{R}}\{\nabla_x^m \nabla_t^n \Omega \in \mathfrak{g} : m + n = 0\} \quad (2.81)$$

This means that

$$\mathfrak{g}(h)_0 = \text{span}_{\mathbb{R}}\{A_1, A_3 = [A_0, A_1]\}. \quad (2.82)$$

To satisfy the set of relations (2.80) we need to use expansions over the basis (2.82) of the external elements  $A_0, A_2 \in \mathfrak{g}(h)$ :

$$A_0 = q_{01}A_1 + q_{13}A_3, \quad A_2 = q_{21}A_1 + q_{23}A_3. \quad (2.83)$$

Substituting expansions (2.83) into (2.80), we get that  $q_{01} = q_{23} = \lambda$ ,  $q_{21} = -\lambda^2/2$  and  $q_{03} = -2$  for some arbitrary real parameter  $\lambda \in \mathbb{R}$ , that is  $\mathfrak{g}(h) = \text{span}_{\mathbb{R}}\{A_1, A_3\}$ , where

$$[A_1, A_3] = A_3/2; \quad A_0 = \lambda A_1 - 2A_3, \quad A_2 = -\lambda^2 A_1/2 + \lambda A_3. \quad (2.84)$$

As a result of (2.84) we can state that the holonomy Lie algebra  $\mathfrak{g}(h)$  is a real 2D one, assuming the following  $(2 \times 2)$ -matrix representation [BPS98]:

$$\begin{aligned} A_1 &= \begin{pmatrix} 1/4 & 0 \\ 0 & -1/4 \end{pmatrix}, & A_3 &= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \\ A_0 &= \begin{pmatrix} \lambda/4 & -2 \\ 0 & -\lambda/4 \end{pmatrix}, & A_2 &= \begin{pmatrix} -\lambda^2/8 & \lambda \\ 0 & \lambda^2/8 \end{pmatrix}. \end{aligned} \quad (2.85)$$

Thereby from (2.77), (2.79) and (2.85) we get the *reduced curvature 1-form*  $\Gamma \in \Lambda^1(M) \otimes \mathfrak{g}$ ,

$$\Gamma = (A_0 + uA_1)dx + ((u_x + u^2/2)A_1 - uA_3 + A_2)dt, \quad (2.86)$$

generating *parallel transport* of vectors from the representation space  $Y$  of the holonomy Lie algebra  $\mathfrak{g}(h)$ :

$$dy + \Gamma y = 0, \quad (2.87)$$

upon the integral submanifold  $\bar{M} \subset M^4$  of the ideal  $\mathcal{I}(\alpha)$ , generated by the set of 2-forms (2.75). The result (2.87) means also that the Burgers dynamical system (2.74) is endowed with the standard Lax type representation, having the spectral parameter  $\lambda \in \mathbb{R}$  necessary for its integrability in quadratures.

## 2.5 Riemannian Geometry in Human-Like Biomechanics

In this section we develop the basic techniques of Riemannian geometry on the biomechanical manifold  $M$ , from both local and global perspective. We

start with the local Riemannian notions of metric, geodesics and curvature on  $M$ , including the first variation formula and parallel transport along the vector-fields on  $M$ . After that we move to the global Riemannian notions on  $M$ , including the second variation and Gauss–Bonnet formulae, as well as the global Ricci flow on  $M$ . The last part of the section presents the structure equations on  $M$ , the basics of Morse theory (as a preparation for the next Chapter), and the basics of (co)bordism theory.

### 2.5.1 Local Riemannian Geometry on $M$

An important class of problems in Riemannian geometry is to understand the interaction between the curvature and topology on a differentiable manifold [CC99]. A prime example of this interaction is the *Gauss–Bonnet formula* on a closed surface  $M^2$ , which says

$$\int_M K dA = 2\pi \chi(M), \quad (2.88)$$

where  $dA$  is the area element of a metric  $g$  on  $M$ ,  $K$  is the Gaussian curvature of  $g$ , and  $\chi(M)$  is the Euler characteristic of  $M$ .

To study the geometry of a differentiable manifold we need an additional structure: the *Riemannian metric*. The metric is an inner product on each of the tangent spaces and tells us how to measure angles and distances infinitesimally. In local coordinates  $(x^1, x^2, \dots, x^n)$ , the metric  $g$  is given by  $g_{ij}(x) dx^i \otimes dx^j$ , where  $(g_{ij}(x))$  is a positive definite symmetric matrix at each point  $x$ . For a differentiable manifold one can differentiate functions. A Riemannian metric defines a natural way of differentiating vector-fields: *covariant differentiation*. In Euclidean space, one can change the order of differentiation. On a Riemannian manifold the commutator of twice covariant differentiating vector-fields is in general nonzero and is called the *Riemann curvature tensor*, which is a 4-tensor-field on the manifold.

For surfaces, the Riemann curvature tensor is equivalent to the *Gaussian curvature*  $K$ , a scalar function. In dimensions 3 or more, the Riemann curvature tensor is inherently a tensor-field. In local coordinates, it is denoted by  $R_{ijkl}$ , which is anti-symmetric in  $i$  and  $k$  and in  $j$  and  $l$ , and symmetric in the pairs  $\{ij\}$  and  $\{kl\}$ . Thus, it can be considered as a bilinear form on 2-forms which is called the *curvature operator*. We now describe heuristically the various curvatures associated to the *Riemann curvature tensor*. Given a point  $x \in M^n$  and 2-plane  $\Pi$  in the tangent space of  $M$  at  $x$ , we can define a surface  $S$  in  $M$  to be the union of all geodesics passing through  $x$  and tangent to  $\Pi$ . In a neighborhood of  $x$ ,  $S$  is a smooth 2D submanifold of  $M$ . We define the *sectional curvature*  $K(\Pi)$  of the 2-plane to be the Gauss curvature of  $S$  at  $x$ :

$$K(\Pi) = K_S(x).$$

Thus the sectional curvature  $K$  of a Riemannian manifold associates to each 2-plane in a tangent space a real number. Given a line  $L$  in a tangent space, we

can average the sectional curvatures of all planes through  $L$  to get the *Ricci curvature*  $Rc(L)$ . Likewise, given a point  $x \in M$ , we can average the Ricci curvatures of all lines in the tangent space of  $x$  to get the *scalar curvature*  $R(x)$ . In local coordinates, the *Ricci tensor* is given by  $R_{ik} = g^{jl} R_{ijkl}$  and the scalar curvature is given by  $R = g^{ik} R_{ik}$ , where  $(g^{ij}) = (g_{ij})^{-1}$  is the inverse of the metric tensor  $(g_{ij})$ .

### Riemannian Metric on $M$

In this subsection we mainly follow [Pet99, Pet98].

Riemann in 1854 observed that around each point  $m \in M$  one can pick a *special* coordinate system  $(x^1, \dots, x^n)$  such that there is a symmetric  $(0, 2)$ -tensor-field  $g_{ij}(m)$  called the *metric tensor* defined as

$$g_{ij}(m) = g(\partial_{x^i}, \partial_{x^j}) = \delta_{ij}, \quad \partial_{x^k} g_{ij}(m) = 0.$$

Thus the metric, at the specified point  $m \in M$ , in the coordinates  $(x^1, \dots, x^n)$  looks like the Euclidean metric on  $\mathbb{R}^n$ . We emphasize that these conditions only hold at the specified point  $m \in M$ . When passing to different points it is necessary to pick different coordinates. If a curve  $\gamma$  passes through  $m$ , say,  $\gamma(0) = m$ , then the acceleration at 0 is simply defined by firstly, writing the curve out in our special coordinates

$$\gamma(t) = (\gamma^1(t), \dots, \gamma^n(t)),$$

secondly, defining the tangent, *velocity* vector-field, as

$$\dot{\gamma} = \dot{\gamma}^i(t) \cdot \partial_{x^i},$$

and finally, the *acceleration* vector-field as

$$\ddot{\gamma}(0) = \ddot{\gamma}^i(0) \cdot \partial_{x^i}.$$

Here, the background idea is that we have a *connection*.

A vector-field  $X$  along a parameterized curve  $\alpha : I \rightarrow M$  in  $M$  is *tangent to  $M$  along  $\alpha$*  if  $X(t) \in M_{\alpha(t)}$  for all for  $t \in I \subset \mathbb{R}$ . The derivative  $\dot{X}$  of such a vector-field is, however, generally not tangent to  $M$ . We can, nevertheless, get a vector-field tangent to  $M$  by projecting  $\dot{X}(t)$  orthogonally onto  $M_{\alpha(t)}$  for each  $t \in I$ . This process of differentiating and then projecting onto the tangent space to  $M$  defines an operation with the same properties as differentiation, except that now differentiation of vector-fields tangent to  $M$  yields vector-fields tangent to  $M$ . This operation is called *covariant differentiation*.

Let  $\gamma : I \rightarrow M$  be a parameterized curve in  $M$ , and let  $X$  be a smooth vector-field tangent to  $M$  along  $\alpha$ . The *absolute covariant derivative* of  $X$  is the vector-field  $\dot{X}$  tangent to  $M$  along  $\alpha$ , defined by  $\dot{X} = \dot{X}(t) - [\dot{X}(t) \cdot N(\alpha(t))] N(\alpha(t))$ , where  $N$  is an orientation on  $M$ . Note that  $\dot{X}$  is independent of the choice of  $N$  since replacing  $N$  by  $-N$  has no effect on the above formula.

Lie bracket (2.4.1) defines a *symmetric affine connection*  $\nabla$  on any manifold  $M$ :

$$[X, Y] = \nabla_X Y - \nabla_Y X.$$

In case of a Riemannian manifold  $M$ , the connection  $\nabla$  is also compatible with the Riemannian metrics  $g$  on  $M$  and is called the *Levi-Civita connection* on  $TM$ .

For a function  $f \in C^k(M, \mathbb{R})$  and a vector field  $X \in \mathcal{X}^k(M)$  we always have the Lie derivative (2.4.1)

$$\mathcal{L}_X f = \nabla_X f = df(X).$$

But there is no natural definition for  $\nabla_X Y$ , where  $Y \in \mathcal{X}^k(M)$ , unless one also has a Riemannian metric. Given the tangent field  $\dot{\gamma}$ , the acceleration can then be computed by using a Leibniz rule on the r.h.s, if we can make sense of the derivative of  $\partial_{x^i}$  in the direction of  $\dot{\gamma}$ . This is exactly what the *covariant derivative*  $\nabla_X Y$  does. If  $Y \in T_m M$  then we can simply write  $Y = a^i \partial_{x^i}$ , and therefore

$$\nabla_X Y = \mathcal{L}_X a^i \partial_{x^i}. \quad (2.89)$$

Since there are several ways of choosing these coordinates, one must check that the definition does not depend on the choice. Note that for two vector-fields we define  $(\nabla_Y X)(m) = \nabla_{Y(m)} X$ . In the end we get a *connection*

$$\nabla : \mathcal{X}^k(M) \times \mathcal{X}^k(M) \rightarrow \mathcal{X}^k(M),$$

which satisfies (for all  $f \in C^k(M, \mathbb{R})$  and  $X, Y, Z \in \mathcal{X}^k(M)$ ):

1.  $Y \rightarrow \nabla_Y X$  is tensorial, i.e., linear and  $\nabla_{fY} X = f \nabla_Y X$ .
2.  $X \rightarrow \nabla_Y X$  is linear.
3.  $\nabla_X (fY) = (\nabla_X f)Y(m) + f(m) \nabla_X Y$ .
4.  $\nabla_X Y - \nabla_Y X = [X, Y]$ .
5.  $\mathcal{L}_X g(Z, Y) = g(\nabla_X Z, Y) + g(Z, \nabla_X Y)$ .

A semicolon is commonly used to denote covariant differentiation with respect to a natural basis vector. If  $X = \partial_{x^i}$ , then the components of  $\nabla_X Y$  in (2.89) are denoted

$$Y^k_{;i} = \partial_{x^i} Y^k + \Gamma^k_{ij} Y^j, \quad (2.90)$$

where  $\Gamma^k_{ij}$  are *Christoffel symbols* defined in (2.91) below. Similar relations hold for higher-order tensor-fields (with as many terms with Christoffel symbols as is the tensor valence).

Therefore, no matter which coordinates we use, we can now define the acceleration of a curve in the following way:

$$\begin{aligned} \gamma(t) &= (\gamma^1(t), \dots, \gamma^n(t)), \\ \dot{\gamma}(t) &= \dot{\gamma}^i(t) \partial_{x^i}, \\ \ddot{\gamma}(t) &= \ddot{\gamma}^i(t) \partial_{x^i} + \dot{\gamma}^i(t) \nabla_{\dot{\gamma}(t)} \partial_{x^i}. \end{aligned}$$

We call  $\gamma$  a *geodesic* if  $\gamma(t) = 0$ . This is a second order nonlinear ODE in a fixed coordinate system  $(x^1, \dots, x^n)$  at the specified point  $m \in M$ . Thus we see that given any tangent vector  $X \in T_m M$ , there is a unique geodesic  $\gamma_X(t)$  with  $\dot{\gamma}_X(0) = X$ . If the manifold  $M$  is closed, the geodesic must exist for all time, but in case the manifold  $M$  is open this might not be so. To see this, simply take as  $M$  any open subset of Euclidean space with the induced metric.

Given an arbitrary vector-field  $Y(t)$  along  $\gamma$ , i.e.,  $Y(t) \in T_{\gamma(t)} M$  for all  $t$ , we can also define the derivative  $\dot{Y} \equiv \frac{dY}{dt}$  in the direction of  $\dot{\gamma}$  by writing

$$\begin{aligned} Y(t) &= a^i(t) \partial_{x^i}, \\ \dot{Y}(t) &= \dot{a}^i(t) \partial_{x^i} + a^i(t) \nabla_{\dot{\gamma}(t)} \partial_{x^i}. \end{aligned}$$

Here the derivative of the tangent field  $\dot{\gamma}$  is simply the acceleration  $\gamma$ . The field  $Y$  is said to be *parallel* iff  $\dot{Y} = 0$ . The equation for a field to be parallel is a first order linear ODE, so we see that for any  $X \in T_{\gamma(t_0)} M$  there is a unique parallel field  $Y(t)$  defined on the entire domain of  $\gamma$  with the property that  $Y(t_0) = X$ . Given two such parallel fields  $Y, Z \in \mathcal{X}^k(M)$ , we have that

$$\dot{g}(Y, Z) = D_{\dot{\gamma}} g(Y, Z) = g(\dot{Y}, Z) + g(Y, \dot{Z}) = 0.$$

Thus  $X$  and  $Y$  are both of constant length and form constant angles along  $\gamma$ . Hence, ‘parallel translation’ along a curve defines an orthogonal transformation between the tangent spaces to the manifold along the curve. However, in contrast to Euclidean space, this parallel translation will depend on the choice of curve.

An infinitesimal distance between the two nearby local points  $m$  and  $n$  on  $M$  is defined by an *arc-element*

$$ds^2 = g_{ij} dx^i dx^j,$$

and realized by the curves  $x^i(s)$  of shortest distance, called *geodesics*, addressed by the *Hilbert 4th problem*. In local coordinates  $(x^1(s), \dots, x^n(s))$  at a point  $m \in M$ , the geodesic defining equation is a second order ODE,

$$\ddot{x}^i + \Gamma_{jk}^i \dot{x}^j \dot{x}^k = 0,$$

where the overdot denotes the derivative with respect to the affine parameter  $s$ ,  $\dot{x}^i(s) = \frac{d}{ds} x^i(s)$  is the tangent vector to the base geodesic, while the *Christoffel symbols*  $\Gamma_{jk}^i = \Gamma_{jk}^i(m)$  (see Appendix) of the *affine connection* (Levi-Civita)  $\nabla$  at the point  $m \in M$  are defined as

$$\begin{aligned} \Gamma_{ij}^k &= g^{kl} \Gamma_{ijl}, \quad \text{with} \quad g^{ij} = (g_{ij})^{-1} \quad \text{and} \quad (2.91) \\ \Gamma_{ijk} &= \frac{1}{2} (\partial_{x^i} g_{jk} - \partial_{x^j} g_{ki} + \partial_{x^k} g_{ij}). \end{aligned}$$

The *torsion* tensor-field  $T$  of the connection  $\nabla$  is the function  $T : \mathcal{X}^k(M) \times \mathcal{X}^k(M) \rightarrow \mathcal{X}^k(M)$  given by

$$T(X, Y) = \nabla_X Y - \nabla_Y X - [X, Y].$$

From the skew symmetry ( $[X, Y] = -[Y, X]$ ) of the Lie bracket, follows the skew symmetry ( $T(X, Y) = -T(Y, X)$ ) of the torsion tensor. The mapping  $T$  is said to be  $f$ -bilinear since it is linear in both arguments and also satisfies  $T(fX, Y) = fT(X, Y)$  for smooth functions  $f$ . Since  $[\partial_{x^i}, \partial_{x^j}] = 0$  for all  $1 \leq i, j \leq n$ , it follows that

$$T(\partial_{x^i}, \partial_{x^j}) = (\Gamma_{ij}^k - \Gamma_{ji}^k) \partial_{x^k}. \quad (2.92)$$

Consequently, torsion  $T$  is a  $(1, 2)$  tensor-field, locally given by

$$T = T_{ij}^k dx^i \otimes \partial_{x^k} \otimes dx^j, \quad (2.93)$$

where the torsion components  $T_{ij}^k$  are given by

$$T_{ij}^k = \Gamma_{ij}^k - \Gamma_{ji}^k. \quad (2.94)$$

Therefore, the torsion tensor provides a measure of the nonsymmetry of the connection coefficients. Hence,  $T = 0$  if and only if these coefficients are symmetric in their subscripts. A connection  $\nabla$  with  $T = 0$  is said to be *torsion free* or *symmetric*.

The connection also enables us to define many other classical concepts from calculus in the setting of Riemannian manifolds. Suppose we have a function  $f \in C^k(M, \mathbb{R})$ . If the manifold is not equipped with a Riemannian metric, then we have the differential of  $f$  defined by  $df(X) = \mathcal{L}_X f$ , which is a 1-form. The dual concept, the *gradient* of  $f$ , is supposed to be a vector-field. But we need a metric  $g$  to define it. Namely,  $\nabla f$  is defined by the relationship

$$g(\nabla f, X) = df(X).$$

Having defined the gradient of a function on a Riemannian manifold, we can then use the connection to define the *Hessian* as the linear map

$$\nabla^2 f : TM \rightarrow TM, \quad \nabla^2 f(X) = \nabla_X \nabla f.$$

The corresponding bilinear map is then defined as

$$\nabla^2 f(X, Y) = g(\nabla^2 f(X), Y).$$

One easily checks that this is a symmetric bilinear form. The *Laplacian* of  $f$ ,  $\Delta f$ , is now defined as the trace of the Hessian

$$\Delta f = \text{Tr}(\nabla^2 f(X)) = \text{Tr}(\nabla_X \nabla f),$$

which is a linear map. It is also called the *Laplace-Beltrami operator*, since Beltrami first considered this operator on Riemannian manifolds.

Riemannian metric has the following mechanical interpretation. Let  $M$  be a closed Riemannian manifold with the *mechanical metric*  $g = g_{ij}v^i v^j \equiv \langle v, v \rangle$ , with  $v^i = \dot{x}^i$ . Consider the *Lagrangian function*

$$L : TM \rightarrow \mathbb{R}, \quad (x, v) \mapsto \frac{1}{2} \langle v, v \rangle - U(x) \quad (2.95)$$

where  $U(x)$  is a smooth function on  $M$  called the *potential*. On a fixed level of energy  $E$ , bigger than the maximum of  $U$ , the Lagrangian flow generated by (2.95) is conjugate to the geodesic flow with metric  $\bar{g} = 2(e - U(x))\langle v, v \rangle$ . Moreover, the reduced action of the Lagrangian is the distance for  $g = \langle v, v \rangle$  [Arn89, AMR88]. Both of these statements are known as the *Maupertius action principle* (see subsection 3.3.5 below).

### Geodesics on $M$

For a  $C^k$ ,  $k \geq 2$  curve  $\gamma : I \rightarrow M$ , we define its *length* on  $I$  as

$$L(\gamma, I) = \int_I |\dot{\gamma}| dt = \int_I \sqrt{g(\dot{\gamma}, \dot{\gamma})} dt.$$

This length is independent of our parametrization of the curve  $\gamma$ . Thus the curve  $\gamma$  can be reparameterized, in such a way that it has unit velocity. The *distance between two points*  $m_1$  and  $m_2$  on  $M$ ,  $d(m_1, m_2)$ , can now be defined as the infimum of the lengths of all curves from  $m_1$  to  $m_2$ , i.e.,

$$L(\gamma, I) \rightarrow \min.$$

This means that the distance measures the shortest way one can travel from  $m_1$  to  $m_2$ .

If we take a variation  $V(s, t) : (-\varepsilon, \varepsilon) \times [0, \ell] \rightarrow M$  of a smooth curve  $\gamma(t) = V(0, t)$  parameterized by arc-length  $L$  and of length  $\ell$ , then the first derivative of the arc-length function

$$L(s) = \int_0^\ell |\dot{V}| dt, \quad \text{is given by}$$

$$\frac{dL(0)}{ds} \equiv \dot{L}(0) = g(\dot{\gamma}, X)|_0^\ell - \int_0^\ell g(\gamma, X) dt, \quad (2.96)$$

where  $X(t) = \frac{\partial V}{\partial s}(0, t)$  is the so-called *variation vector-field*. Equation (2.96) is called the *first variation formula*. Given any vector-field  $X$  along  $\gamma$ , one can produce a variation whose variational field is  $X$ . If the variation fixes the endpoints,  $X(a) = X(b) = 0$ , then the second term in the formula drops out, and we note that the length of  $\gamma$  can always be decreased as long as the acceleration of  $\gamma$  is not everywhere zero. Thus the *Euler-Lagrange equation* for the arc-length functional is simply the equation for a curve to be a *geodesic*.

In local coordinates  $x^i \in U$ , where  $U$  is an open subset in the Riemannian manifold  $M$ , the geodesics are defined by the *geodesic equation* (see Appendix)

$$\ddot{x}^i + \Gamma_{jk}^i \dot{x}^j \dot{x}^k = 0, \quad (2.97)$$

where overdot means derivative upon the line parameter  $s$ , while  $\Gamma_{jk}^i$  are Christoffel symbols of the affine Levi-Civita connection  $\nabla$  on  $M$ . From (6.18) it follows that the linear *connection homotopy*,

$$\bar{\Gamma}_{jk}^i = s\Gamma_{jk}^i + (1-s)\Gamma_{jk}^i, \quad (0 \leq s \leq 1),$$

determines the same geodesics as the original  $\Gamma_{jk}^i$ .

### Riemannian Curvature on $M$

The *Riemann curvature tensor* is a rather ominous tensor of type  $(1, 3)$ ; i.e., it has three vector variables and its value is a vector as well. It is defined through the Lie bracket (2.4.1) as

$$R(X, Y)Z = (\nabla_{[X, Y]} - [\nabla_X, \nabla_Y])Z = \nabla_{[X, Y]}Z - \nabla_X\nabla_YZ + \nabla_Y\nabla_XZ.$$

This turns out to be a vector valued  $(1, 3)$ -tensor-field in the three variables  $X, Y, Z \in \mathcal{X}^k(M)$ . We can then create a  $(0, 4)$ -tensor,

$$R(X, Y, Z, W) = g(\nabla_{[X, Y]}Z - \nabla_X\nabla_YZ + \nabla_Y\nabla_XZ, W).$$

Clearly this tensor is skew-symmetric in  $X$  and  $Y$ , and also in  $Z$  and  $W \in \mathcal{X}^k(M)$ . This was already known to Riemann, but there are some further, more subtle properties that were discovered a little later by Bianchi. The *Bianchi symmetry condition* reads

$$R(X, Y, Z, W) = R(Z, W, X, Y).$$

Thus the Riemannian curvature tensor is a symmetric *curvature operator*

$$\mathfrak{R} : \Lambda^2 TM \rightarrow \Lambda^2 TM.$$

The *Ricci tensor* is the  $(1, 1)$ - or  $(0, 2)$ -tensor defined by

$$\text{Ric}(X) = R(\partial_{x^i}, X)\partial_{x^i}, \quad \text{Ric}(X, Y) = g(R(\partial_{x^i}, X)\partial_{x^i}, Y),$$

for any orthonormal basis  $(\partial_{x^i})$ . In other words, the Ricci curvature is simply a trace of the curvature tensor. Similarly one can define the *scalar curvature* as the trace

$$\text{scal}(m) = \text{Tr}(\text{Ric}) = \text{Ric}(\partial_{x^i}, \partial_{x^i}).$$

When the Riemannian manifold has dimension 2, all of these curvatures are essentially the same. Since  $\dim \Lambda^2 TM = 1$  and is spanned by  $X \wedge Y$  where

$X, Y \in \mathcal{X}^k(M)$  form an orthonormal basis for  $T_m M$ , we see that the curvature tensor depends only on the scalar value

$$K(m) = R(X, Y, X, Y),$$

which also turns out to be the *Gaussian curvature*. The Ricci tensor is a *homothety*

$$\text{Ric}(X) = K(m)X, \quad \text{Ric}(Y) = K(m)Y,$$

and the scalar curvature is twice the Gauss curvature. In dimension 3 there are also some redundancies as  $\dim TM = \dim \Lambda^2 TM = 3$ . In particular, the Ricci tensor and the curvature tensor contain the same amount of information.

The *sectional curvature* is a kind of generalization of the Gauss curvature whose importance Riemann was already aware of. Given a 2-plane  $\pi \subset T_m M$  spanned by an orthonormal basis  $X, Y \in \mathcal{X}^k(M)$  it is defined as

$$\text{sec}(\pi) = R(X, Y, X, Y).$$

The remarkable observation by Riemann was that the *curvature operator is a homothety*, i.e., looks like  $\mathfrak{R} = kI$  on  $\Lambda^2 T_m M$  iff all sectional curvatures of planes in  $T_m M$  are equal to  $k$ . This result is not completely trivial, as the sectional curvature is not the entire quadratic form associated to the symmetric operator  $\mathfrak{R}$ . In fact, it is not true that  $\text{sec} \geq 0$  implies that the curvature operator is nonnegative in the sense that all its eigenvalues are nonnegative. What Riemann did was to show that our special coordinates  $(x^1, \dots, x^n)$  at  $m$  can be chosen to be *normal* at  $m$ , i.e., satisfy the condition

$$x^i = \delta_j^i x^j, \quad (\delta_j^i x^j = g_{ij})$$

on a neighborhood of  $m$ . One can easily show that such coordinates are actually exponential coordinates together with a choice of an orthonormal basis for  $T_m M$  so as to identify  $T_m M$  with  $\mathbb{R}^n$ . In these coordinates one can then expand the metric as follows:

$$g_{ij} = \delta_{ij} - \frac{1}{3} R_{ikjl} x^k x^l + O(r^3).$$

Now the equations  $x^i = g_{ij} x^j$  evidently give conditions on the curvatures  $R_{ijkl}$  at  $m$ .

If  $\Gamma_{jk}^i(m) = 0$ , the manifold  $M$  is flat at the point  $m$ . This means that the (1, 3) curvature tensor, defined locally at  $m \in M$  as

$$R_{ijk}^l = \partial_{x^j} \Gamma_{ik}^l - \partial_{x^k} \Gamma_{ij}^l + \Gamma_{rj}^l \Gamma_{ik}^r - \Gamma_{rk}^l \Gamma_{ij}^r,$$

also vanishes at that point, i.e.,  $R_{ijk}^l(m) = 0$ .

Now, the rate of change of a vector-field  $A^k$  on the manifold  $M$  along the curve  $x^i(s)$  is properly defined by the *absolute covariant derivative*

$$\frac{D}{ds}A^k = \dot{x}^i \nabla_i A^k = \dot{x}^i (\partial_{x^i} A^k + \Gamma_{ij}^k A^j) = \dot{A}^k + \Gamma_{ij}^k \dot{x}^i A^j.$$

By applying this result to itself, we can get an expression for the second covariant derivative of the vector-field  $A^k$  along the curve  $x^i(s)$ :

$$\frac{D^2}{ds^2}A^k = \frac{d}{ds} \left( \dot{A}^k + \Gamma_{ij}^k \dot{x}^i A^j \right) + \Gamma_{ij}^k \dot{x}^i (\dot{A}^j + \Gamma_{mn}^j \dot{x}^m A^n).$$

In the local coordinates  $(x^1(s), \dots, x^n(s))$  at a point  $m \in M$ , if  $\delta x^i = \delta x^i(s)$  denotes the *geodesic deviation*, i.e., the infinitesimal vector describing perpendicular separation between the two neighboring geodesics, passing through two neighboring points  $m, n \in M$ , then the *Jacobi equation of geodesic deviation* on the manifold  $M$  holds:

$$\frac{D^2 \delta x^i}{ds^2} + R_{jkl}^i \dot{x}^j \delta x^k \dot{x}^l = 0. \quad (2.98)$$

This equation describes the *relative acceleration* between two infinitesimally close facial geodesics, which is proportional to the facial curvature (measured by the Riemann tensor  $R_{jkl}^i$  at a point  $m \in M$ ), and to the geodesic deviation  $\delta x^i$ . Solutions of equation (6.19) are called *Jacobi fields*.

In particular, if the manifold  $M$  is a 2D-surface in  $\mathbb{R}^3$ , the Riemann curvature tensor simplifies into

$$R_{jmn}^i = \frac{1}{2} R g^{ik} (g_{km} g_{jn} - g_{kn} g_{jm}),$$

where  $R$  denotes the *scalar curvature*. Consequently the equation of geodesic deviation (6.19) also simplifies into

$$\frac{D^2}{ds^2} \delta x^i + \frac{R}{2} \delta x^i - \frac{R}{2} \dot{x}^i (g_{jk} \dot{x}^j \delta x^k) = 0. \quad (2.99)$$

This simplifies even more if we work in a locally Cartesian coordinate system; in this case the covariant derivative  $\frac{D^2}{ds^2}$  reduces to an ordinary derivative  $\frac{d^2}{ds^2}$  and the metric tensor  $g_{ij}$  reduces to identity matrix  $I_{ij}$ , so our 2D equation of geodesic deviation (6.20) reduces into a simple second order ODE in just two coordinates  $x^i$  ( $i = 1, 2$ )

$$\ddot{x}^i + \frac{R}{2} \delta x^i - \frac{R}{2} \dot{x}^i (I_{jk} \dot{x}^j \delta x^k) = 0.$$

## 2.5.2 Global Riemannian Geometry on $M$

### The Second Variation Formula

Cartan also establishes another important property of manifolds with nonpositive curvature. First he observes that all spaces of constant zero curvature

have torsion-free fundamental groups. This is because any isometry of finite order on Euclidean space must have a fixed point (the center of mass of any orbit is necessarily a fixed point). Then he notices that one can geometrically describe the  $L^\infty$  center of mass of finitely many points  $\{m_1, \dots, m_k\}$  in Euclidean space as the unique minimum for the strictly convex function

$$x \rightarrow \max_{i=1, \dots, k} \frac{1}{2} \left\{ (d(m_i, x))^2 \right\}.$$

In other words, the center of mass is the center of the ball of smallest radius containing  $\{m_1, \dots, m_k\}$ . Now Cartan's observation from above was that the exponential map is expanding and globally distance nondecreasing as a map:

$$(T_m M, \text{Euclidean metric}) \rightarrow (T_m M, \text{with pull-back metric}).$$

Thus distance functions are convex in nonpositive curvature as well as in Euclidean space. Hence the above argument can in fact be used to conclude that any Riemannian manifold of nonpositive curvature must also have torsion free fundamental group.

Now, let us set up the *second variation formula* and explain how it is used. We have already seen the first variation formula and how it can be used to characterize geodesics. Now suppose that we have a unit speed geodesic  $\gamma(t)$  parameterized on  $[0, \ell]$  and consider a variation  $V(s, t)$ , where  $V(0, t) = \gamma(t)$ . Synge then shows that ( $\ddot{L} \equiv \frac{d^2 L}{ds^2}$ )

$$\ddot{L}(0) = \int_0^\ell \{g(\dot{X}, \dot{X}) - (g(\dot{X}, \dot{\gamma}))^2 - g(R(X, \dot{\gamma})X, \dot{\gamma})\} dt + g(\dot{\gamma}, A)|_0^\ell,$$

where  $X(t) = \frac{\partial V}{\partial s}(0, t)$  is the variational vector-field,  $\dot{X} = \nabla_{\dot{\gamma}} X$ , and  $A(t) = \nabla_{\frac{\partial V}{\partial s}} X$ . In the special case where the variation fixes the endpoints, i.e.,  $s \rightarrow V(s, a)$  and  $s \rightarrow V(s, b)$  are constant, the term with  $A$  in it falls out. We can also assume that the variation is perpendicular to the geodesic and then drop the term  $g(\dot{X}, \dot{\gamma})$ . Thus, we arrive at the following simple form:

$$\ddot{L}(0) = \int_0^\ell \{g(\dot{X}, \dot{X}) - g(R(X, \dot{\gamma})X, \dot{\gamma})\} dt = \int_0^\ell \{|\dot{X}|^2 - \sec(\dot{\gamma}, X) |X|^2\} dt.$$

Therefore, if the sectional curvature is nonpositive, we immediately observe that any geodesic locally minimizes length (that is, among close-by curves), even if it does not minimize globally (for instance  $\gamma$  could be a closed geodesic). On the other hand, in positive curvature we can see that if a geodesic is too long, then it cannot minimize even locally. The motivation for this result comes from the unit sphere, where we can consider geodesics of length  $> \pi$ . Globally, we of course know that it would be shorter to go in the opposite direction. However, if we consider a variation of  $\gamma$  where the variational field

looks like  $X = \sin\left(t \cdot \frac{\pi}{\ell}\right) E$  and  $E$  is a unit length parallel field along  $\gamma$  which is also perpendicular to  $\gamma$ , then we get

$$\begin{aligned} \ddot{L}(0) &= \int_0^\ell \left\{ |\dot{X}|^2 - \sec(\dot{\gamma}, X) |X|^2 \right\} dt \\ &= \int_0^\ell \left\{ \left(\frac{\pi}{\ell}\right)^2 \cdot \cos^2\left(t \cdot \frac{\pi}{\ell}\right) - \sec(\dot{\gamma}, X) \sin^2\left(t \cdot \frac{\pi}{\ell}\right) \right\} dt \\ &= \int_0^\ell \left( \left(\frac{\pi}{\ell}\right)^2 \cdot \cos^2\left(t \cdot \frac{\pi}{\ell}\right) - \sin^2\left(t \cdot \frac{\pi}{\ell}\right) \right) dt = -\frac{1}{2\ell} (\ell^2 - \pi^2), \end{aligned}$$

which is negative if the length  $\ell$  of the geodesic is greater than  $\pi$ . Therefore, the variation gives a family of curves that are both close to and shorter than  $\gamma$ . In the general case, we can then observe that if  $\sec \geq 1$ , then for the same type of variation we get

$$\ddot{L}(0) \leq -\frac{1}{2\ell} (\ell^2 - \pi^2).$$

Thus we can conclude that, if the space is complete, then the diameter must be  $\leq \pi$  because in this case any two points are joined by a segment, which cannot minimize if it has length  $> \pi$ . With some minor modifications one can now conclude that any complete Riemannian manifold  $(M, g)$  with  $\sec \geq k^2 > 0$  must satisfy  $\text{diam}(M, g) \leq \pi \cdot k^{-1}$ . In particular,  $M$  must be compact. Since the universal covering of  $M$  satisfies the same curvature hypothesis, the conclusion must also hold for this space; hence  $M$  must have compact universal covering space and finite fundamental group.

In odd dimensions all spaces of constant positive curvature must be orientable, as orientation reversing orthogonal transformation on odd-dimensional spheres have fixed points. This can now be generalized to manifolds of varying positive curvature. Synge did it in the following way: Suppose  $M$  is not simply connected (or not orientable), and use this to find a shortest closed geodesic in a free homotopy class of curves (that reverses orientation). Now consider parallel translation around this geodesic. As the tangent field to the geodesic is itself a parallel field, we see that parallel translation preserves the orthogonal complement to the geodesic. This complement is now odd dimensional (even dimensional), and by assumption parallel translation preserves (reverses) the orientation; thus it must have a fixed point. In other words, there must exist a closed parallel field  $X$  perpendicular to the closed geodesic  $\gamma$ . We can now use the above second variation formula

$$\ddot{L}(0) = \int_0^\ell \{ |\dot{X}|^2 - |X|^2 \sec(\dot{\gamma}, X) \} dt + g(\dot{\gamma}, A)|_0^\ell = - \int_0^\ell |X|^2 \sec(\dot{\gamma}, X) dt.$$

Here the boundary term drops out because the variation closes up at the endpoints, and  $\dot{X} = 0$  since we used a parallel field. In case the sectional curvature is always positive we then see that the above quantity is negative.

But this means that the closed geodesic has nearby closed curves which are shorter. This is, however, in contradiction with the fact that the geodesic was constructed as a length minimizing curve in a free homotopy class.

In 1941 Myers generalized the diameter bound to the situation where one only has a lower bound for the Ricci curvature. The idea is simply that  $\text{Ric}(\dot{\gamma}, \dot{\gamma}) = \sum_{i=1}^{n-1} \sec(E_i, \dot{\gamma})$  for any set of vector-fields  $E_i$  along  $\gamma$  such that  $\dot{\gamma}, E_1, \dots, E_{n-1}$  forms an orthonormal frame. Now assume that the fields are parallel and consider the  $n - 1$  variations coming from the variational vector-fields  $\sin(t \cdot \frac{\pi}{\ell}) E_i$ . Adding up the contributions from the variational formula applied to these fields then yields

$$\begin{aligned} \sum_{i=1}^{n-1} \ddot{L}(0) &= \sum_{i=1}^{n-1} \int_0^\ell \left\{ \left(\frac{\pi}{\ell}\right)^2 \cdot \cos^2\left(t \cdot \frac{\pi}{\ell}\right) - \sec(\dot{\gamma}, E_i) \sin^2\left(t \cdot \frac{\pi}{\ell}\right) \right\} dt \\ &= \int_0^\ell \left\{ (n-1) \left(\frac{\pi}{\ell}\right)^2 \cdot \cos^2\left(t \cdot \frac{\pi}{\ell}\right) - \text{Ric}(\dot{\gamma}, \dot{\gamma}) \sin^2\left(t \cdot \frac{\pi}{\ell}\right) \right\} dt. \end{aligned}$$

Therefore, if  $\text{Ric}(\dot{\gamma}, \dot{\gamma}) \geq (n - 1) k^2$  (this is the Ricci curvature of  $S_k^n$ ), then

$$\begin{aligned} \sum_{i=1}^{n-1} \ddot{L}(0) &\leq (n-1) \int_0^\ell \left\{ \left(\frac{\pi}{\ell}\right)^2 \cdot \cos^2\left(t \cdot \frac{\pi}{\ell}\right) - k^2 \sin^2\left(t \cdot \frac{\pi}{\ell}\right) \right\} dt \\ &= -(n-1) \frac{1}{2\ell} (\ell^2 k^2 - \pi^2), \end{aligned}$$

which is negative when  $\ell > \pi \cdot k^{-1}$  (the diameter of  $S_k^n$ ). Thus at least one of the contributions  $\frac{d^2 L_i}{ds^2}(0)$  must be negative as well, implying that the geodesic cannot be a segment in this situation.

### Gauss-Bonnet Formula

In 1926 Hopf proved that in fact there is a Gauss-Bonnet formula for all even-dimensional hypersurfaces  $H^{2n} \subset \mathbb{R}^{2n+1}$ . The idea is simply that the determinant of the differential of the Gauss map  $G : H^{2n} \rightarrow S^{2n}$  is the Gaussian curvature of the hypersurface. Moreover, this is an intrinsically computable quantity. If we integrate this over the hypersurface, we get,

$$\frac{1}{\text{vol } S^{2n}} \int_H \det(DG) = \text{deg}(G),$$

where  $\text{deg}(G)$  is the *Brouwer degree* of the *Gauss map*. Note that this can also be done for odd-dimensional surfaces, in particular curves, but in this case the degree of the Gauss map will depend on the embedding or immersion of the hypersurface. Instead one gets the so-called winding number. Hopf then showed, as Dyck had earlier done for surfaces, that  $\text{deg}(G)$  is always half the *Euler characteristic* of  $H$ , thus yielding

$$\frac{2}{\text{vol } S^{2n}} \int_H \det(DG) = \chi(H). \quad (2.100)$$

Since the l.h.s of this formula is in fact intrinsic, it is natural to conjecture that such a formula should hold for all manifolds.

### Ricci Flow on $M$

*Ricci flow*, or the *parabolic Einstein equation*, was introduced by R. Hamilton in 1982 [Ham82] in the form

$$\partial_t g_{ij} = -2R_{ij}. \quad (2.101)$$

Now, because of the minus sign in the front of the Ricci tensor  $R_{ij}$  in this equation, the solution metric  $g_{ij}$  to the Ricci flow shrinks in positive Ricci curvature direction while it expands in the negative Ricci curvature direction. For example, on the 2-sphere  $S^2$ , any metric of positive Gaussian curvature will shrink to a point in finite time. Since the Ricci flow (2.101) does not preserve volume in general, one often considers the *normalized* Ricci flow defined by

$$\partial_t g_{ij} = -2R_{ij} + \frac{2}{n} r g_{ij}, \quad (2.102)$$

where  $r = \int R dV / \int dV$  is the average scalar curvature. Under this normalized flow, which is equivalent to the (unnormalized) Ricci flow (2.101) by reparameterizing in time  $t$  and scaling the metric in space by a function of  $t$ , the volume of the solution metric is constant in time. Also that Einstein metrics (i.e.,  $R_{ij} = c g_{ij}$ ) are fixed points of (2.102).

Hamilton [Ham82] showed that on a closed Riemannian 3-manifold  $M^3$  with initial metric of positive Ricci curvature, the solution  $g(t)$  to the normalized Ricci flow (2.102) exists for all time and the metrics  $g(t)$  converge exponentially fast, as time  $t$  tends to the infinity, to a constant positive sectional curvature metric  $g_\infty$  on  $M^3$ .

Since the Ricci flow lies in the realm of parabolic partial differential equations, where the prototype is the heat equation, here is a brief review of the *heat equation* [CC99].

Let  $(M^n, g)$  be a Riemannian manifold. Given a  $C^2$  function  $u : M \rightarrow \mathbb{R}$ , its Laplacian is defined in local coordinates  $\{x^i\}$  to be

$$\Delta u = \text{Tr}(\nabla^2 u) = g^{ij} \nabla_i \nabla_j u,$$

where  $\nabla_i = \nabla_{\partial_{x^i}}$  is its associated covariant derivative (Levi-Civita connection). We say that a  $C^2$  function  $u : M^n \times [0, T] \rightarrow \mathbb{R}$ , where  $T \in (0, \infty]$ , is a solution to the heat equation if

$$\partial_t u = \Delta u.$$

One of the most important properties satisfied by the heat equation is the maximum principle, which says that for any smooth solution to the heat equation, whatever pointwise bounds hold at  $t = 0$  also hold for  $t > 0$ . Let  $u : M^n \times [0, T) \rightarrow \mathbb{R}$  be a  $C^2$  solution to the heat equation on a complete Riemannian manifold. If  $C_1 \leq u(x, 0) \leq C_2$  for all  $x \in M$ , for some constants  $C_1, C_2 \in \mathbb{R}$ , then  $C_1 \leq u(x, t) \leq C_2$  for all  $x \in M$  and  $t \in [0, T)$  [CC99].

Now, given a differentiable manifold  $M$ , a one-parameter family of metrics  $g(t)$ , where  $t \in [0, T)$  for some  $T > 0$ , is a solution to the Ricci flow if (2.101) is valid at all  $x \in M$  and  $t \in [0, T)$ . The minus sign in the equation (2.101) makes the Ricci flow a *forward* heat equation [CC99] (with the normalization factor 2).

In local geodesic coordinates  $\{x^i\}$ , we have [CC99]

$$g_{ij}(x) = \delta_{ij} - \frac{1}{3}R_{ipjq}x^p x^q + O(|x|^3), \quad \text{therefore,} \quad \Delta g_{ij}(0) = -\frac{1}{3}R_{ij},$$

where  $\Delta$  is the standard Euclidean Laplacian. Hence the Ricci flow is like the heat equation for a Riemannian metric

$$\partial_t g_{ij} = 6\Delta g_{ij}.$$

The practical study of the Ricci flow is made possible by the following short-time existence result: Given any smooth compact Riemannian manifold  $(M, g_o)$ , there exists a unique smooth solution  $g(t)$  to the Ricci flow defined on some time interval  $t \in [0, \epsilon)$  such that  $g(0) = g_o$  [CC99].

Now, given that short-time existence holds for any smooth initial metric, one of the main problems concerning the Ricci flow is to determine under what conditions the solution to the normalized equation exists for all time and converges to a constant curvature metric. Results in this direction have been established under various curvature assumptions, most of them being some sort of positive curvature. Since the Ricci flow (2.101) does not preserve volume in general, one often considers, as we mentioned in the Introduction, the normalized Ricci flow (2.102). Under this flow, the volume of the solution  $g(t)$  is independent of time.

To study the long-time existence of the normalized Ricci flow, it is important to know what kind of curvature conditions are preserved under the equation. In general, the Ricci flow tends to preserve some kind of positivity of curvatures. For example, positive scalar curvature is preserved in all dimensions. This follows from applying the maximum principle to the evolution equation for scalar curvature  $R$ , which is

$$\partial_t R = \Delta R + 2|R_{ij}|^2.$$

In dimension 3, positive Ricci curvature is preserved under the Ricci flow. This is a special feature of dimension 3 and is related to the fact that the Riemann curvature tensor may be recovered algebraically from the Ricci tensor and the metric in dimension 3. Positivity of sectional curvature is not preserved

in general. However, the stronger condition of positive curvature operator is preserved under the Ricci flow. Recall that the Riemann curvature tensor may be considered as a self-adjoint map  $Rm : \wedge^2 M \rightarrow \wedge^2 M$ . We say that a metric  $g$  has positive (non-negative) curvature operator if the eigenvalues of  $Rm$  are positive (non-negative). We remark that positivity of curvature operator implies the positivity of the sectional curvature (and in dimension 3, the two conditions are equivalent).

Although the condition of positive scalar curvature is preserved in all dimensions, no convergence results are known for metrics satisfying this condition except in dimension 2.

### Structure Equations on $M$

Let  $\{X_a\}_{a=1}^m$ ,  $\{Y_i\}_{i=1}^n$  be local orthonormal framings on  $M$ ,  $N$  respectively and  $\{e_i\}_{i=1}^n$  be the induced framing on  $E$  defined by  $e_i = Y_i \circ \phi$ , then there exist smooth local coframings  $\{\omega_a\}_{a=1}^m$ ,  $\{\eta_i\}_{i=1}^n$  and  $\{\phi^* \eta_i\}_{i=1}^n$  on  $TM$ ,  $TN$  and  $E$  respectively such that (locally)

$$g = \sum_{a=1}^m \omega_a^2 \quad \text{and} \quad h = \sum_{i=1}^n \eta_i^2.$$

The corresponding first *structure equations* are [Mus99]:

$$\begin{aligned} d\omega_a &= \omega_b \wedge \omega_{ba}, & \omega_{ab} &= -\omega_{ba}, \\ d\eta_i &= \eta_j \wedge \eta_{ji}, & \eta_{ij} &= -\eta_{ji}, \\ d(\phi^* \eta_i) &= \phi^* \eta_j \wedge \phi^* \eta_{ji}, & \phi^* \eta_{ij} &= -\phi^* \eta_{ji}, \end{aligned}$$

where the unique 1-forms  $\omega_{ab}$ ,  $\eta_{ij}$ ,  $\phi^* \eta_{ij}$  are the respective connection forms. The second structure equations are

$$\begin{aligned} d\omega_{ab} &= \omega_{ac} \wedge \omega_{cb} + \Omega_{ab}^M, & d\eta_{ij} &= \eta_{ik} \wedge \eta_{kj} + \Omega_{ij}^N, \\ d(\phi^* \eta_{ij}) &= \phi^* \eta_{ik} \wedge \phi^* \eta_{kj} + \phi^* \Omega_{ij}^N, \end{aligned}$$

where the curvature 2-forms are given by

$$\Omega_{ab}^M = -\frac{1}{2} R_{abcd}^M \omega_c \wedge \omega_d \quad \text{and} \quad \Omega_{ij}^N = -\frac{1}{2} R_{ijkl}^N \eta_k \wedge \eta_l.$$

The pull back map  $\phi^*$  and the push forward map  $\phi_*$  can be written as [Mus99]

$$\phi^* \eta_i = f_{ia} \omega_a$$

for unique functions  $f_{ia}$  on  $U \subset M$ , so that

$$\phi_* = e_i \otimes \phi^* \eta_i = f_{ia} e_i \otimes \omega_a.$$

Note that  $\phi_*$  is a section of the vector bundle  $\phi^{-1}TN \otimes T^*M$ .

The covariant differential operators are represented as

$$\nabla^M X_a = \omega_{ab} \otimes X_b, \quad \nabla^N Y_i = \eta_{ij} \otimes Y_j, \quad \nabla^* \omega_a = -\omega_{ca} \otimes \omega_c,$$

where  $\nabla^*$  is the dual connection on the cotangent bundle  $T^*M$ .

Furthermore, the induced connection  $\nabla^\phi$  on  $E$  is

$$\nabla^\phi e_i = (\eta_{ij}(Y_k) \circ \phi) e_j \otimes f_{ka} \omega_a.$$

The components of the Ricci tensor and scalar curvature are defined respectively by

$$R_{ab}^M = R_{abc}^M \quad \text{and} \quad R^M = R_{aa}^M.$$

Given a function  $f : M \rightarrow \mathbb{R}$ , there exist unique functions  $f_{cb} = f_{bc}$  such that

$$df_c - f_b \omega_{cb} = f_{cb} \omega_b, \quad (2.103)$$

where  $f_c = df(X_c)$  for a local orthonormal frame  $\{X_c\}_{c=1}^m$ . To prove this we take the exterior derivative of  $df = \sum_{c=1}^m f_c \omega_c$  and using structure equations, we have

$$0 = [df_c \wedge \omega_c + f_{bc} \omega_b \wedge \omega_{bc}] = [(df_c - f_b \omega_{cb}) \wedge \omega_c].$$

Hence by *Cartan's lemma* (cf. [Wil93]), there exist unique functions  $f_{cb} = f_{bc}$  such that

$$df_c - f_b \omega_{cb} = f_{cb} \omega_b.$$

The Laplacian of a function  $f$  on  $M$  is given by

$$\Delta f = -\text{Tr}(\nabla df),$$

that is, negative of the usual Laplacian on functions.

### Basics of Morse Theory

At the same time the variational formulae were discovered, a related technique, called *Morse theory*, was introduced into Riemannian geometry. This theory was developed by Morse, first for functions on manifolds in 1925, and then in 1934, for the loop space. The latter theory, as we shall see, sets up a very nice connection between the first and second variation formulae from the previous section and the topology of  $M$ . It is this relationship that we shall explore at a general level here. In section 5 we shall then see how this theory was applied in various specific settings.

If we have a *proper function*  $f : M \rightarrow \mathbb{R}$ , then its Hessian (as a quadratic form) is in fact well defined at its *critical points* without specifying an underlying Riemannian metric. The *nullity* of  $f$  at a *critical point* is defined as the dimension of the *kernel* of  $\nabla^2 f$ , while the *index* is the number of negative eigenvalues counted with multiplicity. A function is said to be a *Morse function* if the nullity at any of its critical points is zero. Note that this guarantees

in particular that all critical points are isolated. The first fundamental theorem of Morse theory is that one can determine the topological structure of a manifold from a Morse function. More specifically, if one can order the critical points  $x_1, \dots, x_k$  so that  $f(x_1) < \dots < f(x_k)$  and the index of  $x_i$  is denoted  $\lambda_i$ , then  $M$  has the structure of a CW complex with a cell of dimension  $\lambda_i$  for each  $i$ . Note that in case  $M$  is closed then  $x_1$  must be a minimum and so  $\lambda_1 = 0$ , while  $x_k$  is a maximum and  $\lambda_k = n$ . The classical example of Milnor of this theorem in action is a torus in 3-space and  $f$  the height function.

We are now left with the problem of trying to find appropriate Morse functions. While there are always plenty of such functions, there does not seem to be a natural way of finding one. However, there are natural choices for Morse functions on the loop space to a Riemannian manifold. This is, somewhat inconveniently, infinite-dimensional. Still, one can develop Morse theory as above for suitable functions, and moreover *the loop space of a manifold determines the topology of the underlying manifold*.

If  $m, p \in M$ , then we denote by  $\Omega_{mp}$  the space of all  $C^k$  paths from  $m$  to  $p$ . The first observation about this space is that

$$\pi_{i+1}(M) = \pi_i(\Omega_{mp}).$$

To see this, just fix a path from  $m$  to  $p$  and then join this path to every curve in  $\Omega_{mp}$ . In this way  $\Omega_{mp}$  is identified with  $\Omega_m$ , *the space of loops fixed at  $m$* . For this space the above relationship between the homotopy groups is almost self-evident.

On the space  $\Omega_{mp}$  we have two naturally defined functions, the *arc-length* and *energy functionals*:

$$L(\gamma, I) = \int_I |\dot{\gamma}| dt, \quad \text{and} \quad E(\gamma, I) = \frac{1}{2} \int_I |\dot{\gamma}|^2 dt.$$

While the energy functional is easier to work with, it is of course the arc-length functional that we are really interested in. In order to make things work out nicely for the arc-length functional, it is convenient to parameterize all curves on  $[0, 1]$  and proportionally to arc-length. We shall think of  $\Omega_{mp}$  as an *infinite-dimensional manifold*. For each curve  $\gamma \in \Omega_{mp}$  the natural choice for the tangent space consists of the vector-fields along  $\gamma$  which vanish at the endpoints of  $\gamma$ . This is because these vector-fields are exactly the variational fields for curves through  $\gamma$  in  $\Omega_{mp}$ , i.e., fixed endpoint variations of  $\gamma$ . An inner product on the tangent space is then naturally defined by

$$(X, Y) = \int_0^1 g(X, Y) dt.$$

Now the first variation formula for arc-length tells us that the gradient for  $L$  at  $\gamma$  is  $-\nabla_{\dot{\gamma}} \dot{\gamma}$ . Actually this cannot be quite right, as  $-\nabla_{\dot{\gamma}} \dot{\gamma}$  does not vanish at the endpoints. The real gradient is gotten in the same way we find the gradient for a function on a surface in space, namely, by projecting it down

into the correct tangent space. In any case we note that the critical points for  $L$  are exactly the geodesics from  $m$  to  $p$ . The second variation formula tells us that the Hessian of  $L$  at these critical points is given by

$$\nabla^2 L(X) = \ddot{X} + R(X, \dot{\gamma}) \dot{\gamma},$$

at least for vector-fields  $X$  which are perpendicular to  $\gamma$ . Again we ignore the fact that we have the same trouble with endpoint conditions as above. We now need to impose the Morse condition that this Hessian is not allowed to have any kernel. The vector-fields  $J$  for which  $\ddot{J} + R(J, \dot{\gamma}) \dot{\gamma} = 0$  are called *Jacobi fields*. Thus we have to figure out whether there are any Jacobi fields which vanish at the endpoints of  $\gamma$ . The first observation is that Jacobi fields must always come from geodesic variations. The Jacobi fields which vanish at  $m$  can therefore be found using the exponential map  $\exp_m$ . If the Jacobi field also has to vanish at  $p$ , then  $p$  must be a critical value for  $\exp_m$ . Now Sard's theorem asserts that the set of critical values has measure zero. For given  $m \in M$  it will therefore be true that the arc-length functional on  $\Omega_{mp}$  is a Morse function for almost all  $p \in M$ . Note that it may not be possible to choose  $p = m$ , the simplest example being the standard sphere. We are now left with trying to decide what the *index* should be. This is of course the dimension of the largest subspace on which the Hessian is negative definite. It turns out that this index can also be computed using Jacobi fields and is in fact always finite. Thus one can compute the topology of  $\Omega_{mp}$ , and hence  $M$ , by finding all the geodesics from  $m$  to  $p$  and then computing their index.

In geometric situations it is often unrealistic to suppose that one can compute the index precisely, but as we shall see it is often possible to give lower bounds for the index. As an example, note that if  $M$  is not simply connected, then  $\Omega_{mp}$  is not connected. Each curve of minimal length in the path components is a geodesic from  $m$  to  $p$  which is a local minimum for the arc-length functional. Such geodesics evidently have index zero. In particular, if one can show that all geodesics, except for the minimal ones from  $m$  to  $p$ , have index  $> 0$ , then the manifold must be simply connected. We continue the exposition of Morse theory on  $M$  in section (4.2.1) below.

### Basics of (Co)Bordism Theory

(Co)bordism appeared as a revival of Poincaré's unsuccessful 1895 attempts to define homology using only manifolds. Smooth manifolds (without boundary) are again considered as 'negligible' when they are *boundaries* of smooth manifolds-with-boundary. But there is a big difference, which keeps definition of 'addition' of manifolds from running into the difficulties encountered by Poincaré; it is now the disjoint union. The (unoriented) *(co)bordism relation* between two compact smooth manifolds  $M_1, M_2$  of same dimension  $n$  simply means that their disjoint union  $\partial W = M_1 \cup M_2$  is the boundary  $\partial W$  of an  $(n + 1)$ D smooth manifold-with-boundary  $W$ . This is an *equivalence*

relation, and the classes for that relation of  $n$ D manifolds form a commutative group  $\mathfrak{N}_n$  in which every element has order 2. The direct sum  $\mathfrak{N}_\bullet = \bigoplus_{n \geq 0} \mathfrak{N}_n$  is a ring for the multiplication of classes deduced from the Cartesian product of manifolds.

More precisely, a manifold  $M$  is said to be a (co)bordism from  $A$  to  $B$  if exists a diffeomorphism from a disjoint sum,  $\varphi \in \text{diff}(A^* \cup B, \partial M)$ . Two (co)bordisms  $M(\varphi)$  and  $M'(\varphi')$  are equivalent if there is a  $\Phi \in \text{diff}(M, M')$  such that  $\varphi' = \Phi \circ \varphi$ . The equivalence class of (co)bordisms is denoted by  $M(A, B) \in \text{Cob}(A, B)$  [Sto68].

Composition  $c_{\text{Cob}}$  of (co)bordisms comes from gluing of manifolds [BD95]. Let  $\varphi' \in \text{diff}(C^* \cup D, \partial N)$ . One can glue (co)bordism  $M$  with  $N$  by identifying  $B$  with  $C^*$ ,  $(\varphi')^{-1} \circ \varphi \in \text{diff}(B, C^*)$ . We obtain the glued (co)bordism  $(M \circ N)(A, D)$  and a semigroup operation,

$$c(A, B, D) : \text{Cob}(A, B) \times \text{Cob}(B, D) \longrightarrow \text{Cob}(A, D).$$

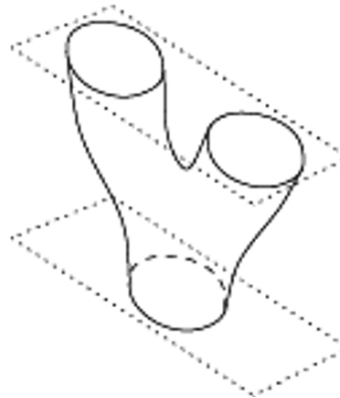
A surgery is an operation of cutting a manifold  $M$  and gluing to cylinders. A surgery gives new (co)bordism: from  $M(A, B)$  into  $N(A, B)$ . The disjoint sum of  $M(A, B)$  with  $N(C, D)$  is a (co)bordism  $(M \cup N)(A \cup C, B \cup D)$ . We got a 2-graph of (co)bordism  $\text{Cob}$  with  $\text{Cob}_0 = \text{Man}_d$ ,  $\text{Cob}_1 = \text{Man}_{d+1}$ , whose 2-cells from  $\text{Cob}_2$  are surgery operations.

There is an  $n$ -category of (co)bordisms  $\mathcal{BO}$  [Lei03] with:

- 0-cells: 0-manifolds, where ‘manifold’ means ‘compact, smooth, oriented manifold’. A typical 0-cell is . . . . .
- 1-cells: 1-manifolds with corners, i.e., (co)bordisms between 0-manifolds,



such as (this being a 1-cell from the 4-point manifold to the 2-point 0-manifold).



- 2-cells: 2-manifolds with corners, such as
- 3-cells, 4-cells, ... are defined similarly;

- Composition is gluing of manifolds.

The (co)bordisms theme was taken a step further by Baez and Dolan in [BD95], when they started a programme to understand the subtle relations between certain TMFT models for manifolds of different dimensions, frequently referred to as the dimensional ladder. This programme is based on higher-dimensional algebra, a generalization of the theory of categories and functors to  $n$ -categories and  $n$ -functors. In this framework a topological quantum field theory (TMFT) becomes an  $n$ -functor from the  $n$ -category  $\mathcal{BO}$  of  $n$ -cobordisms to the  $n$ -category of  $n$ -Hilbert spaces.

### 2.5.3 Complex and Kähler Manifolds

Just as a smooth manifold has enough structure to define the notion of differentiable functions, a *complex manifold* is one with enough structure to define the notion of holomorphic (or, analytic) functions  $f : X \rightarrow \mathbb{C}$ . Namely, if we demand that the transition functions  $\phi_j \circ \phi_i^{-1}$  in the charts  $U_i$  on  $M$  (see Figure 2.4) satisfy the *Cauchy–Riemann equations*

$$\partial_x u = \partial_y v, \quad \partial_y u = -\partial_x v,$$

then the analytic properties of  $f$  can be studied using its coordinate representative  $f \circ \phi_i^{-1}$  with assurance that the conclusions drawn are patch independent. Introducing local complex coordinates in the charts  $U_i$  on  $M$ , the  $\phi_i$  can be expressed as maps from  $U_i$  to an open set in  $\mathbb{C}^{\frac{n}{2}}$ , with  $\phi_j \circ \phi_i^{-1}$  being a holomorphic map from  $\mathbb{C}^{\frac{n}{2}}$  to  $\mathbb{C}^{\frac{n}{2}}$ . Clearly,  $n$  must be even for this to make sense. In local complex coordinates, we recall that a function  $h : \mathbb{C}^{\frac{n}{2}} \rightarrow \mathbb{C}^{\frac{n}{2}}$  is *holomorphic* if  $h(z^1, \bar{z}^1, \dots, z^{\frac{n}{2}}, \bar{z}^{\frac{n}{2}})$  is actually independent of all the  $\bar{z}^j$ .

In a given patch on any even-dimensional manifold, we can always introduce local complex coordinates by, for instance, forming the combinations  $z^j = x^j + ix^{\frac{n}{2}+j}$ , where the  $x^j$  are local real coordinates on  $M$ . The real test is whether the transition functions from one patch to another — when expressed in terms of the local complex coordinates — are holomorphic maps. If they are, we say that  $M$  is a complex manifold of complex dimension  $d = n/2$ . The local complex coordinates with holomorphic transition functions provide  $M$  with a *complex structure* [Gre96].

Given a smooth manifold with even real dimension  $n$ , it can be a difficult question to determine whether or not a complex structure exists. On the other hand, if some differentiable manifold  $M$  does admit a complex structure, we are not able to decide whether it is unique, i.e., there may be numerous inequivalent ways of defining complex coordinates on  $M$  [Gre96].

Now, in the same way as a *homeomorphism* defines an equivalence between topological manifolds, and a *diffeomorphism* defines an equivalence between smooth manifolds, a *biholomorphism* defines an equivalence between complex manifolds. If  $M$  and  $N$  are complex manifolds, we consider them to be equivalent if there is a map  $\phi : M \rightarrow N$  which in addition to being a diffeomorphism,

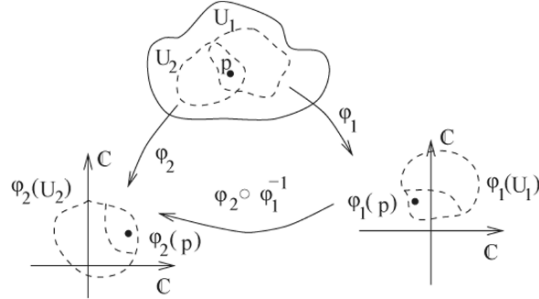


Fig. 2.4. The charts for a complex manifold  $M$  have the complex coordinates.

is also a holomorphic map. That is, when expressed in terms of the complex structures on  $M$  and  $N$  respectively,  $\phi$  is holomorphic. It is not hard to show that this necessarily implies that  $\phi^{-1}$  is holomorphic as well and hence  $\phi$  is known as a biholomorphism. Such a map allows us to identify the complex structures on  $M$  and  $N$  and hence they are isomorphic as complex manifolds.

These definitions are important because there are pairs of smooth manifolds  $M$  and  $N$  which are homeomorphic but not diffeomorphic, as well as, there are complex manifolds  $M$  and  $N$  which are diffeomorphic but not biholomorphic. This means that if one simply ignored the fact that  $M$  and  $N$  admit local complex coordinates (with holomorphic transition functions), and one only worked in real coordinates, there would be no distinction between  $M$  and  $N$ . The difference between them only arises from the way in which complex coordinates have been laid down upon them.

Again, recall that a *tangent space* to a manifold  $M$  at a point  $p$  is the closest flat approximation to  $M$  at that point. A convenient basis for the tangent space of  $M$  at  $p$  consists of the  $n$  linearly independent partial derivatives,

$$T_p M : \{ \partial_{x^1}|_p, \dots, \partial_{x^n}|_p \}. \tag{2.104}$$

A vector  $v \in T_p M$  can then be expressed as  $v = v^\alpha \partial_{x^\alpha}|_p$ .

Also, a convenient basis for the dual, *cotangent space*  $T_p^* M$ , is the basis of one-forms, which is dual to (2.104) and usually denoted by

$$T_p^* M : \{ dx^1|_p, \dots, dx^n|_p \}, \tag{2.105}$$

where, by definition,  $dx^i : T_p M \rightarrow \mathbb{R}$  is a linear map with  $dx^i_p(\partial_{x^j}|_p) = \delta^i_j$ .

Now, if  $M$  is a complex manifold of complex dimension  $d = n/2$ , there is a notion of the *complexified tangent space* of  $M$ , denoted by  $T_p M^{\mathbb{C}}$ , which is the same as the real tangent space  $T_p M$  except that we allow complex coefficients to be used in the vector space manipulations. This is often denoted by writing  $T_p M^{\mathbb{C}} = T_p M \otimes \mathbb{C}$ . We can still take our basis to be as in (2.104) with an arbitrary vector  $v \in T_p M^{\mathbb{C}}$  being expressed as  $v = v^\alpha \frac{\partial}{\partial x^\alpha}|_p$ , where the  $v^\alpha$  can now be complex numbers. In fact, it is convenient to rearrange the basis vectors in

(2.104) to more directly reflect the underlying complex structure. Specifically, we take the following linear combinations of basis vectors in (2.104) to be our new basis vectors:

$$T_p M^{\mathbb{C}} : \{(\partial_{x^1} + i\partial_{x^{d+1}})|_p, \dots, (\partial_{x^d} + i\partial_{x^{2d}})|_p, (\partial_{x^1} - i\partial_{x^{d+1}})|_p, \dots, (\partial_{x^d} - i\partial_{x^{2d}})|_p\}. \quad (2.106)$$

In terms of complex coordinates we can write the basis (2.106) as

$$T_p M^{\mathbb{C}} : \{\partial_{z^1}|_p, \dots, \partial_{z^d}|_p, \partial_{\bar{z}^1}|_p, \dots, \partial_{\bar{z}^d}|_p\}.$$

From the point of view of real vector spaces,  $\partial_{x^j}|_p$  and  $i\partial_{x^j}|_p$  would be considered linearly independent and hence  $T_p M^{\mathbb{C}}$  has real dimension  $4d$ .

In exact analogy with the real case, we can define the dual to  $T_p M^{\mathbb{C}}$ , which we denote by  $T_p^* M^{\mathbb{C}} = T_p^* M \otimes \mathbb{C}$ , with the one-forms basis

$$T_p^* M^{\mathbb{C}} : \{dz^1|_p, \dots, dz^d|_p, d\bar{z}^1|_p, \dots, d\bar{z}^d|_p\}.$$

For certain types of complex manifolds  $M$ , it is worthwhile to refine the definition of the complexified tangent and cotangent spaces, which pulls apart the holomorphic and anti-holomorphic directions in each of these two vector spaces. That is, we can write

$$T_p M^{\mathbb{C}} = T_p M^{(1,0)} \oplus T_p M^{(0,1)},$$

where  $T_p M^{(1,0)}$  is the vector space spanned by  $\{\partial_{z^1}|_p, \dots, \partial_{z^d}|_p\}$  and  $T_p M^{(0,1)}$  is the vector space spanned by  $\{\partial_{\bar{z}^1}|_p, \dots, \partial_{\bar{z}^d}|_p\}$ . Similarly, we can write

$$T_p^* M^{\mathbb{C}} = T_p^* M^{(1,0)} \oplus T_p^* M^{(0,1)},$$

where  $T_p^* M^{(1,0)}$  is the vector space spanned by  $\{dz^1|_p, \dots, dz^d|_p\}$  and  $T_p^* M^{(0,1)}$  is the vector space spanned by  $\{d\bar{z}^1|_p, \dots, d\bar{z}^d|_p\}$ . We call  $T_p M^{(1,0)}$  the *holomorphic tangent space*; it has complex dimension  $d$  and we call  $T_p^* M^{(1,0)}$  the *holomorphic cotangent space*. It also has complex dimension  $d$ . Their complements are known as the *anti-holomorphic tangent* and *cotangent spaces* respectively [Gre96].

Now, a *complex vector bundle* is a vector bundle  $\pi : E \rightarrow M$  whose fiber bundle  $\pi^{-1}(x)$  is a complex vector space. It is not necessarily a complex manifold, even if its base manifold  $M$  is a complex manifold. If a complex vector bundle also has the structure of a complex manifold, and is holomorphic, then it is called a *holomorphic vector bundle*.

A *Hermitian metric* on a complex vector bundle assigns a *Hermitian inner product* to every fiber bundle. The basic example is the trivial bundle  $\pi : U \times \mathbb{C}^2 \rightarrow U$ , where  $U$  is an open set in  $\mathbb{R}^n$ . Then a positive definite Hermitian matrix  $H$  defines a Hermitian metric by

$$\langle v, w \rangle = v^T H \bar{w},$$

where  $\bar{w}$  is the complex conjugate of  $w$ . By a partition of unity, any complex vector bundle has a Hermitian metric.

In the special case of a complex manifold, the complexified tangent bundle  $TM \otimes \mathbb{C}$  may have a Hermitian metric, in which case its real part is a Riemannian metric and its imaginary part is a nondegenerate alternating multilinear form  $\omega$ . When  $\omega$  is closed, i.e., in this case a symplectic form, then  $\omega$  is a *Kähler form*.

On a holomorphic vector bundle with a Hermitian metric  $h$ , there is a unique connection compatible with  $h$  and the complex structure. Namely, it must be  $\nabla = \partial + \bar{\partial}$ .

A *Kähler structure* on a complex manifold  $M$  combines a Riemannian metric on the underlying real manifold with the complex structure. Such a structure brings together geometry and complex analysis, and the main examples come from algebraic geometry. When  $M$  has  $n$  complex dimensions, then it has  $2n$  real dimensions. A Kähler structure is related to the unitary group  $U(n)$ , which embeds in  $SO(2n)$  as the orthogonal matrices that preserve the *almost complex structure* (multiplication by  $i$ ). In a coordinate chart, the complex structure of  $M$  defines a multiplication by  $i$  and the metric defines orthogonality for tangent vectors. On a Kähler manifold, these two notions (and their derivatives) are related.

A Kähler manifold is a complex manifold for which the exterior derivative of the fundamental form  $\omega$  associated with the given *Hermitian metric* vanishes, so  $d\omega = 0$ . In other words, it is a complex manifold with a *Kähler structure*. It has a *Kähler form*, so it is also a symplectic manifold. It has a *Kähler metric*, so it is also a Riemannian manifold.

The simplest example of a Kähler manifold is a Riemann surface, which is a complex manifold of dimension 1. In this case, the imaginary part of any Hermitian metric must be a closed form since all 2-forms are closed on a real two-dimensional manifold.

A *Kähler form* is a closed two-form  $\omega$  on a complex manifold  $M$  which is also the negative imaginary part of a Hermitian metric  $h = g - iw$  is called a Kähler form. In this case,  $M$  is called a Kähler manifold and  $g$ , the real part of the Hermitian metric, is called a Kähler metric. The Kähler form combines the metric and the complex structure,  $g(X, Y) = \omega(X, JY)$ , where  $J$  is the *almost complex structure* induced by multiplication by  $i$ . Since the Kähler form comes from a Hermitian metric, it is preserved by  $J$ , since  $h(X, Y) = h(JX, JY)$ . The equation  $d\omega = 0$  implies that the metric and the complex structure are related. It gives  $M$  a Kähler structure, and has many implications.

On  $\mathbb{C}^2$ , the Kähler form can be written as

$$\omega = -\frac{1}{2}i (dz_1 \wedge \bar{dz}_1 + dz_2 \wedge \bar{dz}_2) = dx_1 \wedge dy_1 + dx_2 \wedge dy_2,$$

where  $z_n = x_n + iy_n$ . In general, the Kähler form can be written in coordinates

$$\omega = g_{ij} dz_i \wedge \bar{dz}_j,$$

where  $g_{ij}$  is a Hermitian metric, the real part of which is the Kähler metric. Locally, a Kähler form can be written as  $\partial\bar{\partial}f$ , where  $f$  is a function called a *Kähler potential*. The Kähler form is a real  $(1, 1)$ -complex form. The Kähler potential is a real-valued function  $f$  on a Kähler manifold for which the Kähler form  $\omega$  can be written as  $\omega = i\partial\bar{\partial}f$ , where,

$$\partial = \partial_{z_k} dz_k \quad \text{and} \quad \bar{\partial} = \partial_{\bar{z}_k} d\bar{z}_k.$$

Since the Kähler form  $\omega$  is closed, it represents a cohomology class in the De Rham cohomology. On a compact manifold, it cannot be exact because  $\omega^n/n! \neq 0$  is the volume form determined by the metric. In the special case of a projective variety, the Kähler form represents an integral cohomology class. That is, it integrates to an integer on any one-dimensional submanifold, i.e., an algebraic curve. The Kodaira embedding theorem says that if the Kähler form represents an integral cohomology class on a compact manifold, then it must be a projective variety. There exist Kähler forms which are not projective algebraic, but it is an open question whether or not any Kähler manifold can be deformed to a projective variety (in the compact case).

A Kähler form satisfies *Wirtinger's inequality*,

$$|\omega(X, Y)| \leq |X \wedge Y|,$$

where the r.h.s is the volume of the parallelogram formed by the tangent vectors  $X$  and  $Y$ . Corresponding inequalities hold for the *exterior powers* of  $\omega$ . Equality holds iff  $X$  and  $Y$  form a complex subspace. Therefore, there is a *calibration form*, and the complex submanifolds of a Kähler manifold are *calibrated submanifolds*. In particular, the complex submanifolds are locally volume minimizing in a Kähler manifold. For example, the graph of a holomorphic function is a locally area-minimizing surface in  $\mathbb{C}^2 = \mathbb{R}^4$ .

*Kähler identities* is a collection of identities which hold on a Kähler manifold, also called the *Hodge identities*. Let  $\omega$  be a Kähler form,  $d = \partial + \bar{\partial}$  be the exterior derivative,  $[A, B] = AB - BA$  be the commutator of two differential operators, and  $A^*$  denote the formal adjoint of  $A$ . The following operators also act on differential forms  $\alpha$  on a Kähler manifold:

$$L(\alpha) = \alpha \wedge \omega, \quad \Lambda(\alpha) = L^*(\alpha) = \alpha \lrcorner \omega, \quad d_c = -JdJ,$$

where  $J$  is the almost complex structure,  $J = -I$ , and  $\lrcorner$  denotes the interior product. Then

$$\begin{aligned} [L, \bar{\partial}] &= [L, \partial] = 0, & [A, \bar{\partial}^*] &= [A, \partial^*] = 0, \\ [L, \bar{\partial}^*] &= -i\partial, & [L, \partial^*] &= i\bar{\partial}, & [A, \bar{\partial}] &= -i\partial^*, & [A, \partial] &= -i\bar{\partial}. \end{aligned}$$

These identities have many implications. For instance, the two operators

$$\Delta_d = dd^* + d^*d \quad \text{and} \quad \Delta_{\bar{\partial}} = \bar{\partial}\bar{\partial}^* + \bar{\partial}^*\bar{\partial}$$

(called Laplacians because they are elliptic operators) satisfy

$$\Delta_d = 2\Delta_{\bar{d}}.$$

At this point, assume that  $M$  is also a compact manifold. Along with Hodge’s theorem, this equality of Laplacians proves the *Hodge decomposition*. The operators  $L$  and  $\Lambda$  commute with these Laplacians. By *Hodge’s theorem* (see Chapter 4 below), they act on cohomology, which is represented by *harmonic forms*. Moreover, defining

$$H = [L, \Lambda] = \sum (p + q - n) \Pi^{p,q},$$

where  $\Pi^{p,q}$  is projection onto the  $(p, q)$ –Dolbeault cohomology, they satisfy

$$[L, \Lambda] = H, \quad [H, L] = -2L, \quad [H, \Lambda] = 2L.$$

In other words, these operators provide a group representation of the special linear Lie algebra  $\mathfrak{sl}_2(\mathbb{C})$  on the complex cohomology of a compact Kähler manifold (*Lefschetz theorem*).

#### 2.5.4 Conformal Killing–Riemannian Geometry

In this subsection we present some basic facts from *conformal Killing–Riemannian geometry*. In mechanics (see Chapter 3) it is well–known that *symmetries of Lagrangian* or *Hamiltonian* result in *conservation laws*, that are used to deduce constants of motion for the trajectories (geodesics) on the configuration manifold  $M$ . The same constants of motion are obtained using geometric language, where a *Killing vector–field* is the standard tool for the description of symmetry [MTW73]. A Killing vector–field  $\xi^i$  is a vector–field on a Riemannian manifold  $M$  with metrics  $g$ , which in coordinates  $x^j \in M$  satisfies the *Killing equation*

$$\xi^{i;j} + \xi^{j;i} = \xi^{(i;j)} = 0, \quad \text{or} \quad \mathcal{L}_{\xi^i} g_{ij} = 0, \quad (2.107)$$

where semicolon denotes the covariant derivative on  $M$  (as in (2.90) above), the indexed bracket denotes the tensor symmetry, and  $\mathcal{L}$  is the Lie derivative.

The *conformal Killing vector–fields* are, by definition, infinitesimal conformal symmetries i.e., the flow of such vector–fields preserves the conformal class of the metric. The number of linearly–independent conformal Killing fields measures the degree of *conformal symmetry of the manifold*. This number is bounded by  $\frac{1}{2}(n+1)(n+2)$ , where  $n$  is the dimension of the manifold. It is the maximal one if the manifold is conformally flat [Bau00].

Now, to properly initialize our conformal geometry, recall that *conformal twistor spinor–fields*  $\varphi$  were introduced by R. Penrose into physics (see [Pen67, PR86]) as solutions of the *conformally covariant twistor equation*

$$\nabla_X^S \varphi + \frac{1}{n} X \cdot D\varphi = 0,$$

for each vector-fields  $X$  on a Riemannian manifold  $(M, g)$ , where  $D$  is the *Dirac operator*. Each twistor spinor-field  $\varphi$  on  $(M, g)$  defines a *conformal vector-field*  $V_\varphi$  on  $M$  by

$$g(V_\varphi, X) = i^{k+1} \langle X \cdot \varphi, \varphi \rangle.$$

Also, each twistor spinor-field  $\varphi$  that satisfies the *Dirac equation* on  $(M, g)$ ,

$$D\varphi = \mu\varphi,$$

is called a *Killing spinor-field*. Each twistor spinor-field without zeros on  $(M, g)$  can be transformed by a conformal change of the metric  $g$  into a Killing spinor-field [Bau00].

### Conformal Killing Vector-Fields and Forms on $M$

The space of all conformal Killing vector-fields forms the Lie algebra of the *isometry group* of a Riemannian manifold  $(M, g)$  and the number of linearly independent Killing vector-fields measures the *degree of symmetry* of  $M$ . It is known that this number is bounded from above by the dimension of the isometry group of the standard sphere and, on compact manifolds, equality is attained if and only if the manifold  $M$  is isometric to the standard sphere or the real projective space. Slightly more generally one can consider *conformal vector-fields*, i.e., vector-fields with a flow preserving a given conformal class of metrics. There are several geometric conditions which force a conformal vector-field to be Killing [Sem02].

A natural generalization of conformal vector-fields are the *conformal Killing forms* [Yan52], also called *twistor forms* [MS03]. These are  $p$ -forms  $\alpha$  satisfying for any vector-field  $X$  on the manifold  $M$  the *Killing-Yano equation*

$$\nabla_X \alpha - \frac{1}{p+1} X \lrcorner d\alpha + \frac{1}{n-p+1} X^* \wedge d^* \alpha = 0, \quad (2.108)$$

where  $n$  is the dimension of the manifold  $(M, g)$ ,  $\nabla$  denotes the covariant derivative of the Levi-Civita connection on  $M$ ,  $X^*$  is 1-form dual to  $X$  and  $\lrcorner$  is the operation dual to the wedge product on  $M$ . It is easy to see that a conformal Killing 1-form is dual to a conformal vector-field. *Coclosed* conformal Killing  $p$ -forms are called *Killing forms*. For  $p = 1$  they are dual to Killing vector-fields.

Let  $\alpha$  be a Killing  $p$ -form and let  $\gamma$  be a geodesic on  $(M, g)$ , i.e.,  $\nabla_{\dot{\gamma}} \dot{\gamma} = 0$ . Then

$$\nabla_{\dot{\gamma}} (\dot{\gamma} \lrcorner \alpha) = (\nabla_{\dot{\gamma}} \dot{\gamma}) \lrcorner \alpha + \dot{\gamma} \lrcorner \nabla_{\dot{\gamma}} \alpha = 0,$$

i.e.,  $\dot{\gamma} \lrcorner \alpha$  is a  $(p-1)$ -form parallel along the geodesic  $\gamma$  and in particular its length is constant along  $\gamma$ .

The l.h.s of equation (2.108) defines a first order elliptic differential operator  $T$ , the so-called *twistor operator*. Equivalently one can describe a conformal

Killing form as a form in the kernel of twistor operator  $T$ . From this point of view conformal Killing forms are similar to Penrose's *twistor spinors* in *Lorentzian spin geometry*. One shared property is the conformal invariance of the defining equation. In particular, any form which is parallel for some metric  $g$ , and thus a Killing form for trivial reasons, induces non-parallel conformal Killing forms for metrics conformally equivalent to  $g$  (by a non-trivial change of the metric) [Sem02].

### Conformal Killing Tensors and Laplacian Symmetry on $M$

In an  $n$ D Riemannian manifold  $(M, g)$ , a *Killing tensor-field* (of order 2) is a symmetric tensor  $K^{ab}$  satisfying (generalizing (2.107))

$$K^{(ab;c)} = 0. \quad (2.109)$$

A *conformal Killing tensor-field* (of order 2) is a symmetric tensor  $Q^{ab}$  satisfying

$$Q^{(ab;c)} = q^{(a} g^{bc)}, \quad \text{with} \quad q^a = (Q^{,a} + 2Q_d^{a;d})/(n+2), \quad (2.110)$$

where comma denotes partial derivative and  $Q = Q_d^d$ . When the associated *conformal vector*  $q^a$  is nonzero, the conformal Killing tensor will be called *proper* and otherwise it is a (ordinary) Killing tensor. If  $q^a$  is a Killing vector,  $Q^{ab}$  is referred to as a *homothetic Killing tensor*. If the associated conformal vector  $q^a = q^{,a}$  is the gradient of some scalar field  $q$ , then  $Q^{ab}$  is called a *gradient conformal Killing tensor*. For each gradient conformal Killing tensor  $Q^{ab}$  there is an associated Killing tensor  $K^{ab}$  given by

$$K^{ab} = Q^{ab} - qg^{ab}, \quad (2.111)$$

which is defined only up to the addition of a constant multiple of the inverse metric tensor  $g^{ab}$ .

Some authors define a conformal Killing tensor as a *trace-free* tensor  $P^{ab}$  satisfying  $P^{(ab;c)} = p^{(a} g^{bc)}$ . Note that there is no contradiction between the two definitions: if  $P^{ab}$  is a trace-free conformal Killing tensor then for any scalar field  $\lambda$ ,  $P^{ab} + \lambda g^{ab}$  is a conformal Killing tensor and conversely if  $Q^{ab}$  is a conformal Killing tensor, its trace-free part  $Q^{ab} - \frac{1}{n}Qg^{ab}$  is a trace-free Killing tensor [REB03].

Killing tensor-fields are of importance owing to their connection with quadratic first integrals of the geodesic equations: if  $p^a$  is tangent to an affinely parameterized geodesic (i.e.,  $p^a_{;b}p^b = 0$ ) it is easy to see that  $K_{ab}p^ap^b$  is constant along the geodesic. For conformal Killing tensors  $Q_{ab}p^ap^b$  is constant along *null* geodesics and here, only the trace-free part of  $Q_{ab}$  contributes to the constants of motion. Both Killing tensors and conformal Killing tensors are also of importance in connection with the separability of the Hamilton-Jacobi equations [CH64] (as well as other PDEs).

A Killing tensor is said to be *reducible* if it can be written as a constant linear combination of the metric and symmetrised products of Killing vectors,

$$K_{ab} = a^0 g_{ab} + a^{IJ} \xi_{I(a} \xi_{J|b)}, \quad (2.112)$$

where  $\xi_I$  for  $I = 1 \dots N$  are the Killing vectors admitted by the manifold  $(M, g)$  and  $a^0$  and  $a^{IJ}$  for  $1 \leq I \leq J \leq N$  are constants. Generally one is interested only in Killing tensors which are not reducible since the quadratic constant of motion associated with a reducible Killing tensor is simply a constant linear combination of  $p^a p_a$  and of pairwise products of the linear constants of motion  $\xi_{Ia} p^a$  [REB03].

More generally, any linear differential operator on a Riemannian manifold  $(M, g)$  may be written in the form [EG91, Eas02]

$$\mathcal{D} = V^{bc\dots d} \nabla_b \nabla_c \dots \nabla_d + \text{lower order terms},$$

where  $V^{bc\dots d}$  is symmetric in its indices, and  $\nabla_a = \partial/\partial x^a$  (differentiation in coordinates). This tensor is called the symbol of  $\mathcal{D}$ . We shall write  $\phi^{(ab\dots c)}$  for the symmetric part of  $\phi^{ab\dots c}$ .

Now, a *conformal Killing tensor* on  $(M, g)$  is a symmetric trace-free tensor field, with  $s$  indices, satisfying

$$\text{the trace-free part of } \nabla^{(a} V^{bc\dots d)} = 0, \quad (2.113)$$

or, equivalently,

$$\nabla^{(a} V^{bc\dots d)} = g^{(ab} T^{c\dots d)}, \quad (2.114)$$

for some tensor field  $T^{c\dots d}$  or, equivalently,

$$\nabla^{(a} V^{bc\dots d)} = \frac{s}{n+2s-2} g^{(ab} \nabla_e V^{c\dots d)e}, \quad (2.115)$$

where  $\nabla^a = g^{ab} \nabla_b$  (the standard convention of raising and lowering indices with the metric tensor  $g_{ab}$ ). When  $s = 1$ , these equations define a *conformal Killing vector*.

M. Eastwood proved the following theorem: *Any symmetry  $\mathcal{D}$  of the Laplacian  $\Delta = \nabla^a \nabla_a$  on a Riemannian manifold  $(M, g)$  is canonically equivalent to one whose symbol is a conformal Killing tensor* [EG91, Eas02].

## 2.6 Symplectic Geometry in Human–Like Biomechanics

In this section we develop the basic techniques of symplectic geometry on the biomechanical manifold  $M$  [Iva04].

### 2.6.1 Symplectic Algebra

Symplectic algebra works in the category of symplectic vector spaces  $V_i$  and linear symplectic mappings  $t \in L(V_i, V_j)$  [Put93].

Let  $V$  be a  $n$ D real vector space and  $L^2(V, \mathbb{R})$  the space of all bilinear maps from  $V \times V$  to  $\mathbb{R}$ . We say that a bilinear map  $\omega \in L^2(V, \mathbb{R})$  is *nondegenerate*, i.e., if  $\omega(v_1, v_2) = 0$  for all  $v_2 \in V$  implies  $v_1 = 0$ .

If  $\{e_1, \dots, e_n\}$  is a basis of  $V$  and  $\{e^1, \dots, e^n\}$  is the dual basis,  $\omega_{ij} = \omega(e_i, e_j)$  is the matrix of  $\omega$ . A bilinear map  $\omega \in L^2(V, \mathbb{R})$  is nondegenerate iff its matrix  $\omega_{ij}$  is nonsingular. The transpose  $\omega^t$  of  $\omega$  is defined by  $\omega^t(e_i, e_j) = \omega(e_j, e_i)$ .  $\omega$  is *symmetric* if  $\omega^t = \omega$ , and *skew-symmetric* if  $\omega^t = -\omega$ .

Let  $A^2(V)$  denote the space of skew-symmetric bilinear maps on  $V$ . An element  $\omega \in A^2(V)$  is called a 2-form on  $V$ . If  $\omega \in A^2(V)$  is nondegenerate then in the basis  $\{e_1, \dots, e_n\}$  its matrix  $\omega(e_i, e_j)$  has the form  $J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}$ .

A *symplectic form* on a real vector space  $V$  of dimension  $2n$  is a nondegenerate 2-form  $\omega \in A^2(V)$ . The pair  $(V, \omega)$  is called a symplectic vector space. If  $(V_1, \omega_1)$  and  $(V_2, \omega_2)$  are symplectic vector spaces, a linear map  $t \in L(V_1, V_2)$  is a *symplectomorphism* (i.e., a symplectic mapping) iff  $t^*\omega_2 = \omega_1$ . If  $(V, \omega)$  is a symplectic vector space, we have an orientation  $\Omega_\omega$  on  $V$  given by

$$\Omega_\omega = \frac{(-1)^{\frac{n(n-1)}{2}}}{n!} \omega^n.$$

Let  $(V, \omega)$  be a  $2n$ D symplectic vector space and  $t \in L(V, V)$  a symplectomorphism. Then  $t$  is volume preserving, i.e.,  $t^*(\Omega_\omega) = \Omega_\omega$ , and  $\det_{\Omega_\omega}(t) = 1$ .

The set of all symplectomorphisms  $t : V \rightarrow V$  of a  $2n$ D symplectic vector space  $(V, \omega)$  forms a group under composition, called the *symplectic group*, denoted by  $Sp(V, \omega)$ .

In matrix notation, there is a basis of  $V$  in which the matrix of  $\omega$  is  $J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}$ , such that  $J^{-1} = J^t = -J$ , and  $J^2 = -I$ . For  $t \in L(V, V)$  with matrix  $T = [T_j^i]$  relative to this basis, the condition  $t \in Sp(V, \omega)$ , i.e.,  $t^*\omega = \omega$ , becomes

$$T^t J T = J.$$

In general, by definition a matrix  $A \in M_{2n \times 2n}(\mathbb{R})$  is symplectic iff  $A^t J A = J$ .

Let  $(V, \omega)$  be a symplectic vector space,  $t \in Sp(V, \omega)$  and  $\lambda \in \mathbb{C}$  an eigenvalue of  $t$ . Then  $\lambda^{-1}$ ,  $\bar{\lambda}$  and  $\bar{\lambda}^{-1}$  are eigenvalues of  $t$ .

### 2.6.2 Symplectic Geometry on $M$

Symplectic geometry is a globalization of symplectic algebra [Put93]; it works in the category **Symplec** of symplectic manifolds  $M$  and symplectic diffeomorphisms  $f$ . The phase-space of a conservative dynamical system is a symplectic manifold, and its time evolution is a one-parameter family of symplectic diffeomorphisms.

A *symplectic form* or a symplectic structure on a smooth (i.e.,  $C^k$ ) manifold  $M$  is a nondegenerate closed 2-form  $\omega$  on  $M$ , i.e., for each  $x \in M$   $\omega(x)$  is nondegenerate, and  $d\omega = 0$ . A *symplectic manifold* is a pair  $(M, \omega)$  where  $M$  is a smooth  $2n$ D manifold and  $\omega$  is a symplectic form on it. If  $(M_1, \omega_1)$  and  $(M_2, \omega_2)$  are symplectic manifolds then a smooth map  $f : M_1 \rightarrow M_2$  is called *symplectic map* or *canonical transformation* if  $f^*\omega_2 = \omega_1$ .

For example, any symplectic vector space  $(V, \omega)$  is also a symplectic manifold; the requirement  $d\omega = 0$  is automatically satisfied since  $\omega$  is a constant map. Also, any orientable, compact surface  $\Sigma$  is a symplectic manifold; any nonvanishing 2-form (volume element)  $\omega$  on  $\Sigma$  is a symplectic form on  $\Sigma$ .

If  $(M, \omega)$  is a symplectic manifold then it is orientable with the standard volume form

$$\Omega_\omega = \frac{(-1)^{\frac{n(n-1)}{2}}}{n!} \omega^n,$$

If  $f : M \rightarrow M$  is a symplectic map, then  $f$  is volume preserving,  $\det_{\Omega_\omega}(f) = 1$  and  $f$  is a local diffeomorphism.

In general, if  $(M, \omega)$  is a  $2n$ D compact symplectic manifold then  $\omega^n$  is a volume element on  $M$ , so the De Rham cohomology class  $[\omega^n] \in H^{2n}(M, \mathbb{R})$  is nonzero. Since  $[\omega^n] = [\omega]^n$ ,  $[\omega] \in H^2(M, \mathbb{R})$  and all of its powers through the  $n$ th must be nonzero as well. The existence of such an element of  $H^2(M, \mathbb{R})$  is a *necessary condition* for the compact manifold to admit a symplectic structure.

However, if  $M$  is a  $2n$ D compact manifold without boundary, then there does not exist any exact symplectic structure,  $\omega = d\theta$  on  $M$ , as its total volume is zero (by Stokes' theorem),

$$\int_M \Omega_\omega = \frac{(-1)^{\frac{n(n-1)}{2}}}{n!} \int_M \omega^n = \frac{(-1)^{\frac{n(n-1)}{2}}}{n!} \int_M d(\theta \wedge \omega^{n-1}) = 0.$$

For example, spheres  $S^{2n}$  do not admit a symplectic structure for  $n \geq 2$ , since the second De Rham group vanishes, i.e.,  $H^2(S^{2n}, \mathbb{R}) = 0$ . This argument applies to any compact manifold without boundary and having  $H^2(M, \mathbb{R}) = 0$ .

In mechanics, the phase-space is the cotangent bundle  $T^*M$  of a configuration space  $M$ . There is a natural symplectic structure on  $T^*M$  that is usually defined as follows. Let  $M$  be a smooth  $n$ D manifold and pick local coordinates  $\{dq^1, \dots, dq^n\}$ . Then  $\{dq^1, \dots, dq^n\}$  defines a basis of the tangent space  $T_q^*M$ , and by writing  $\theta \in T_q^*M$  as  $\theta = p_i dq^i$  we get local coordinates  $\{q^1, \dots, q^n, p_1, \dots, p_n\}$  on  $T^*M$ . Define the canonical symplectic form  $\omega$  on  $T^*M$  by

$$\omega = dp_i \wedge dq^i.$$

This 2-form  $\omega$  is obviously independent of the choice of coordinates  $\{q^1, \dots, q^n\}$  and independent of the base point  $\{q^1, \dots, q^n, p_1, \dots, p_n\} \in T_q^*M$ ; therefore, it is locally constant, and so  $d\omega = 0$ .

The canonical 1-form  $\theta$  on  $T^*M$  is the unique 1-form with the property that, for any 1-form  $\beta$  which is a section of  $T^*M$  we have  $\beta^*\theta = \theta$ .

Let  $f : M \rightarrow M$  be a diffeomorphism. Then  $T^*f$  preserves the canonical 1-form  $\theta$  on  $T^*M$ , i.e.,  $(T^*f)^*\theta = \theta$ . Thus  $T^*f$  is symplectic diffeomorphism.

If  $(M, \omega)$  is a  $2n$ D symplectic manifold then about each point  $x \in M$  there are local coordinates  $\{q^1, \dots, q^n, p_1, \dots, p_n\}$  such that  $\omega = dp_i \wedge dq^i$ . These coordinates are called canonical or symplectic. By the Darboux theorem,  $\omega$  is constant in this local chart, i.e.,  $d\omega = 0$ .

### 2.6.3 Momentum Map and Symplectic Reduction of $M$

Let  $(M, \omega)$  be a connected symplectic manifold and  $\phi : G \times M \rightarrow M$  a symplectic action of the Lie group  $G$  on  $M$ , that is, for each  $g \in G$  the map  $\phi_g : M \rightarrow M$  is a symplectic diffeomorphism. If for each  $\xi \in \mathfrak{g}$  there exists a globally defined function  $\hat{J}(\xi) : M \rightarrow \mathbb{R}$  such that  $\xi_M = X_{\hat{J}(\xi)}$ , then the map  $J : M \rightarrow \mathfrak{g}^*$ , given by

$$J : x \in M \mapsto J(x) \in \mathfrak{g}^*, \quad J(x)(\xi) = \hat{J}(\xi)(x)$$

is called the *momentum map* for  $\phi$  [MR99, Put93].

Since  $\phi$  is symplectic,  $\phi_{\exp(t\xi)}$  is a one parameter family of canonical transformations, i.e.,  $\phi_{\exp(t\xi)}^*\omega = \omega$ , hence  $\xi_M$  is locally Hamiltonian and not generally Hamiltonian. That is why not every symplectic action has a momentum map.  $\phi : G \times M \rightarrow M$  is Hamiltonian iff  $J : \mathfrak{g} \rightarrow C^k(M, \mathbb{R})$  is a Lie algebra homomorphism.

Let  $H : M \rightarrow \mathbb{R}$  be  $G$ -invariant, that is  $H(\phi_g(x)) = H(x)$  for all  $x \in M$  and  $g \in G$ . Then  $\hat{J}(\xi)$  is a constant of motion for dynamics generated by  $H$ .

Let  $\phi$  be a symplectic action of  $G$  on  $(M, \omega)$  with the momentum map  $J$ . Suppose  $H : M \rightarrow \mathbb{R}$  is  $G$ -invariant under this action. Then the Noether's theorem states that  $J$  is a constant of motion of  $H$ , i.e.,  $J \circ \phi_t = J$ , where  $\phi_t$  is the flow of  $X_H$ .

A *Hamiltonian action* is a symplectic action with an  $Ad^*$ -equivariant momentum map  $J$ , i.e.,

$$J(\phi_g(x)) = Ad_{g^{-1}}^*(J(x)),$$

for all  $x \in M$  and  $g \in G$ .

Let  $\phi$  be a symplectic action of a Lie group  $G$  on  $(M, \omega)$ . Assume that the symplectic form  $\omega$  on  $M$  is exact, i.e.,  $\omega = d\theta$ , and that the action  $\phi$  of  $G$  on  $M$  leaves the one form  $\theta \in M$  invariant. Then  $J : M \rightarrow \mathfrak{g}^*$  given by  $(J(x))(\xi) = (i_{\xi_M}\theta)(x)$  is an  $Ad^*$ -equivariant momentum map of the action.

In particular, in the case of the cotangent bundle  $(M = T^*M, \omega = d\theta)$  of a mechanical configuration manifold  $M$ , we can *lift* up an action  $\phi$  of a Lie group  $G$  on  $M$  to obtain an action of  $G$  on  $T^*M$ . To perform this lift, let  $G$  act on  $M$  by transformations  $\phi_g : M \rightarrow M$  and define the *lifted action* to the cotangent bundle by  $(\phi_g)_* : T^*M \rightarrow T^*M$  by pushing forward one forms,  $(\phi_g)_*(\alpha) \cdot v = \alpha(T\phi_g^{-1}v)$ , where  $\alpha \in T_q^*M$  and  $v \in T_{\phi_g(q)}M$ . The lifted action  $(\phi_g)_*$  preserves the canonical one form  $\theta$  on  $T^*M$  and the momentum map for  $(\phi_g)_*$  is given by

$$J : T^*M \rightarrow \mathfrak{g}^*, \quad J(\alpha_q)(\xi) = \alpha_q(\xi_M(q)).$$

For example, let  $M = \mathbb{R}^n$ ,  $G = \mathbb{R}^n$  and let  $G$  act on  $\mathbb{R}^n$  by translations:

$$\phi : (t, q) \in \mathbb{R}^n \times \mathbb{R}^n \mapsto t + q \in \mathbb{R}^n.$$

Then  $\mathfrak{g} = \mathbb{R}^n$  and for each  $\xi \in \mathfrak{g}$  we have  $\xi_{\mathbb{R}^n}(q) = \xi$ .

In case of the group of rotations in  $\mathbb{R}^3$ ,  $M = \mathbb{R}^3$ ,  $G = SO(3)$  and let  $G$  act on  $\mathbb{R}^3$  by  $\phi(A, q) = A \cdot q$ . Then  $\mathfrak{g} \simeq \mathbb{R}^3$  and for each  $\xi \in \mathfrak{g}$  we have  $\xi_{\mathbb{R}^3}(q) = \xi \times q$ .

Let  $G$  act transitively on  $(M, \omega)$  by a Hamiltonian action. Then  $J(M) = \{Ad_{g^{-1}}^*(J(x)) \mid g \in G\}$  is a coadjoint orbit.

Now, let  $(M, \omega)$  be a symplectic manifold,  $G$  a Lie group and  $\phi : G \times M \rightarrow M$  a Hamiltonian action of  $G$  on  $M$  with  $Ad^*$ -equivariant momentum map  $J : M \rightarrow \mathfrak{g}^*$ . Let  $\mu \in \mathfrak{g}^*$  be a regular value of  $J$ ; then  $J^{-1}(\mu)$  is a submanifold of  $M$  such that  $\dim(J^{-1}(\mu)) = \dim(M) - \dim(G)$ . Let  $G_\mu = \{g \in G \mid Ad_g^*\mu = \mu\}$  be the isotropy subgroup of  $\mu$  for the coadjoint action. By  $Ad^*$ -equivariance, if  $x \in J^{-1}(\mu)$  then  $\phi_g(x) = J^{-1}(\mu)$  for all  $g \in G$ , i.e.,  $J^{-1}(\mu)$  is invariant under the induced  $G_\mu$ -action and we can form the quotient space  $M_\mu = J^{-1}(\mu)/G_\mu$ , called the *reduced phase-space* at  $\mu \in \mathfrak{g}^*$ .

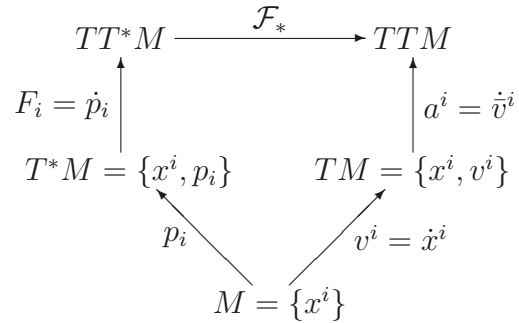
Let  $(M, \omega)$  be a symplectic  $2n$ D manifold and let  $f_1, \dots, f_k$  be  $k$  functions in involution, i.e.,  $\{f_i, f_j\}_\omega = 0$ ,  $i, j = 1, \dots, k$ . Because the flow of  $X_{f_i}$  and  $X_{f_j}$  commute, we can use them to define a symplectic action of  $G = \mathbb{R}^k$  on  $M$ . Here  $\mu \in \mathbb{R}^k$  is in the range space of  $f_1 \times \dots \times f_k$  and  $J = f_1 \times \dots \times f_k$  is the momentum map of this action. Assume that  $\{df_1, \dots, df_k\}$  are independent at each point, so  $\mu$  is a regular value for  $J$ . Since  $G$  is Abelian,  $G_\mu = G$  so we get a symplectic manifold  $J^{-1}(\mu)/G$  of dimension  $2n - 2k$ . If  $k = n$  we have *integrable systems*.

For example, let  $G = SO(3)$  and  $(M, \omega) = (\mathbb{R}^6, \sum_{i=1}^3 dp_i \wedge dq^i)$ , and the action of  $G$  on  $\mathbb{R}^6$  is given by  $\phi : (R, (q, p)) \mapsto (Rq, Rp)$ . Then the momentum map is the well known angular momentum and for each  $\mu \in \mathfrak{g}^* \simeq \mathbb{R}^3$ ,  $\mu \neq 0$ ,  $G_\mu \simeq S^1$  and the reduced phase-space  $(M_\mu, \omega_\mu)$  is  $(T^*\mathbb{R}, \omega = dp_i \wedge dq^i)$ , so that  $\dim(M_\mu) = \dim(M) - \dim(G) - \dim(G_\mu)$ . This reduction is in celestial mechanics called by Jacobi 'the elimination of the nodes'.

The equations of motion:  $\dot{f} = \{f, H\}_\omega$  on  $M$  reduce to the equations of motion:  $\dot{f}_\mu = \{f_\mu, H_\mu\}_{\omega_\mu}$  on  $M_\mu$  (see [MR99]).

## 2.7 The Covariant Force Functor

We summarize this geometrical Chapter by stating that our central construct, the *covariant force law*,  $F_i = mg_{ij}a^j$  (see subsection A.1.4 in Appendix), in categorical language represents the *covariant force functor*  $\mathcal{F}_*$  defined by the following commutative diagram:



saying that the force 1-form-field  $F_i = \dot{p}_i$ , defined on the mixed tangent-cotangent bundle  $TT^*M$ , causes the acceleration vector-field  $a^i = \dot{v}^i$ , defined on the second tangent bundle  $TTM$  of the configuration manifold  $M$ .

The Lie biomechanical functors (defined in the section 3.5 below) represent special versions of the fundamental force functor  $\mathcal{F}_* : TT^*M \rightarrow TTM$ .

The corresponding *contravariant acceleration functor* is defined as its inverse map  $\mathcal{F}^* : TTM \rightarrow TT^*M$ .

## Mechanical Basis of Human–Like Biomechanics

This Chapter studies various aspects of modern mechanics as is currently used in biomechanics. It includes both Lagrangian and Hamiltonian variations on the central theme of our *covariant force law*,  $F_i = mg_{ij}a^j$ . We start with the basics of Lagrangian and Hamiltonian formalisms. After that we move on to the general variational principles of holonomic mechanics. Next we depart to nonholonomic. At the end, we present the current research in biomechanics given in the framework of Lie–Lagrangian and Lie–Hamiltonian functors.

### 3.1 Lagrangian Formalism in Human–Like Biomechanics

In this section we present classical Lagrangian formalism, as has been used in human and humanoid biomechanics for over fifty years now. It describes the motion of mechanical systems by the use of the *configuration space*. Recall that the configuration space of the mechanical system has the structure of the *Riemannian manifold*. On each smooth manifold there acts a group of diffeomorphisms. Essential terms and theorems of Lagrangian mechanics (even if formulated in local coordinates) are invariant with respect to this group, as well as to the extended Riemannian space–time group.

Lagrangian mechanical system is given by its configuration manifold and the ‘Lagrange’s energetic function’ on its tangent bundle.

Each one–parameter group of diffeomorphisms of the configuration space, preserving the Lagrange’s function, determines the conservation law (i.e., the first integral of the equation of motion).

Newtonian potential system is the particular case of the Lagrangian one (here, the configuration space is Euclidean, and Lagrange’s function equals the difference between kinetic and potential energy).

Lagrangian mechanics enables us to analyze up to the end a series of important mechanical problems, e.g., in the theory of small oscillations and rigid body dynamics.

Consider our  $n$ D configuration manifold  $M$  and its tangent bundle  $TM$ . We denote coordinates on  $M$  by  $q^i$  and those on  $TM$  by  $(q^i, \dot{q}^i)$ . Consider a Lagrangian  $L : TM \rightarrow \mathbb{R}$ . Construct the corresponding action functional  $S$  on  $C^2$  curves  $q(t)$  in  $M$  by integration of  $L$  along the tangent to the curve. In coordinate notation, this reads [MR99]

$$S(q(t)) \equiv \int_a^b L\left(q^i(t), \frac{dq^i}{dt}(t)\right) dt. \quad (3.1)$$

The action functional (3.1) depends on  $a$  and  $b$ , but this is not explicit in the notation. *Hamilton's principle* seeks the curves  $q(t)$  for which the functional  $S$  is stationary under variations of  $q(t)$  with fixed endpoints; namely, we seek curves  $q(t)$  which satisfy

$$dS(q(t)) \cdot \delta q(t) \equiv \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} S(q_\epsilon(t)) = 0 \quad (3.2)$$

for all  $\delta q(t)$  with  $\delta q(a) = \delta q(b) = 0$ , where  $q_\epsilon$  is a smooth family of curves with  $q_0 = q$  and  $(d/d\epsilon)|_{\epsilon=0} q_\epsilon = \delta q$ . Using integration by parts, the calculation for this is simply

$$\begin{aligned} dS(q(t)) \cdot \delta q(t) &= \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \int_a^b L\left(q_\epsilon^i(t), \frac{dq_\epsilon^i}{dt}(t)\right) dt \\ &= \int_a^b \delta q^i \left( \frac{\partial L}{\partial q^i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} \right) dt + \left. \frac{\partial L}{\partial \dot{q}^i} \delta q^i \right|_a^b. \end{aligned} \quad (3.3)$$

The last term in (3.3) vanishes since  $\delta q(a) = \delta q(b) = 0$ , so that the requirement (3.2) for  $S$  to be stationary yields the *Euler-Lagrange equation*

$$\frac{\partial L}{\partial q^i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} = 0. \quad (3.4)$$

Recall that  $L$  is called *regular* when the symmetric matrix  $[\partial^2 L / \partial \dot{q}^i \partial \dot{q}^j]$  is everywhere nonsingular. If  $L$  is regular, the Euler-Lagrange equations (3.4) are second order ODEs for the required curves. The action principle is further developed in the section (3.3) below.

In particular, for a system of  $N$  particles moving in Euclidean 3-space, we choose the configuration space to be  $M = \mathbb{R}^{3N} = \mathbb{R}^3 \times \dots \times \mathbb{R}^3$  ( $N$  times), and in the case of *simple mechanical systems*  $L$  has the form of kinetic minus potential energy (see [AM78, Arn89, MR99])

$$L(y^i, \dot{y}^i, t) = \frac{1}{2} m_i \|\dot{y}^i\|^2 - V(y).$$

where we write points in  $M$  as  $y^1, \dots, y^N$ , where  $y^i \in \mathbb{R}^3$ . In this case the Euler-Lagrange equations (3.4) reduce to Newtonian second law

$$\frac{d}{dt}(m_i \dot{y}^i) = -\frac{\partial V}{\partial y^i}, \quad (i = 1, \dots, N),$$

that is,  $\mathbf{F} = m\mathbf{a}$ , for the motion of particles in the potential field  $V = V(y)$ .

In general, one identifies the  $2n$ D *velocity phase-space* with the tangent bundle  $TM$ , using local coordinates  $(q^i, \dot{q}^i, i = 1, \dots, n)$  in an open chart  $U \subset TM$ .

Recall that the biomechanical manifold  $M$  is Riemannian, with the metric tensor  $g_{ij}(q)$  (see (2.5.1)) which is now material, also called the *inertia matrix*. If we consider the kinetic energy Lagrangian

$$L(q^i, \dot{q}^i) = \frac{1}{2} g_{ij}(q) \dot{q}^i \dot{q}^j,$$

then the Euler-Lagrange equations are equivalent to the equations of geodesic motion (2.96).

### 3.1.1 Basis of Lagrangian Mechanics

Riemannian metric  $g = \langle, \rangle$  on the configuration manifold  $M$  is a positive-definite quadratic form  $g : TM \rightarrow \mathbb{R}$ , given in local coordinates  $q^i \in U$  ( $U$  open in  $M$ ) as

$$g_{ij} \mapsto g_{ij}(q, m) dq^i dq^j. \quad (3.5)$$

Here

$$g_{ij}(q, m) = m_\mu \delta_{rs} \frac{\partial x^r}{\partial q^i} \frac{\partial x^s}{\partial q^j} \quad (3.6)$$

is the covariant material metric tensor defining a relation between internal and external coordinates and including  $n$  segmental masses  $m_\mu$ . The quantities  $x^r$  are external coordinates ( $r, s = 1, \dots, 6n$ ) and  $i, j = 1, \dots, N \equiv 6n - h$ , where  $h$  denotes the number of holonomic constraints.

The *Lagrangian* of the system is a quadratic form  $L : TM \rightarrow \mathbb{R}$  dependent on velocity  $v$  and such that  $L(v) = \frac{1}{2} \langle v, v \rangle$ . It is given by

$$L(v) = \frac{1}{2} g_{ij}(q, m) v^i v^j,$$

in local coordinates  $q^i, v^i = \dot{q}^i \in U_v$  ( $U_v$  open in  $TM$ ).

On the velocity phase-space manifold  $TM$  exists:

1. A unique 1-form  $\theta_L$ , defined in local coordinates  $q^i, v^i = \dot{q}^i \in U_v$  ( $U_v$  open in  $TM$ ) by  $\theta_L = L_{v^i} dq^i$ , where  $L_{v^i} \equiv \partial L / \partial v^i$ .
2. A unique nondegenerate Lagrangian symplectic 2-form  $\omega_L$ , which is closed ( $d\omega_L = 0$ ) and exact ( $\omega_L = d\theta_L = dL_{v^i} \wedge dq^i$ ).

$TM$  is an orientable manifold, admitting the standard volume given by

$$\Omega_{\omega_L} = \frac{(-1)^{\frac{N(N+1)}{2}}}{N!} \omega_L^N,$$

in local coordinates  $q^i$ ,  $v^i = \dot{q}^i \in U_v$  ( $U_v$  open in  $TM$ ) it is given by

$$\Omega_L = dq^1 \wedge \cdots \wedge dq^N \wedge dv^1 \wedge \cdots \wedge dv^N.$$

On the velocity phase-space manifold  $TM$  we can also define the *action*  $A : TM \rightarrow \mathbb{R}$  in local coordinates  $q^i$ ,  $v^i = \dot{q}^i \in U_v$  ( $U_v$  open in  $TM$ ) given by  $A = v^i L_{v^i}$ , so  $E = v^i L_{v^i} - L$ . The Lagrangian vector-field  $X_L$  on  $TM$  is determined by the condition  $i_{X_L} \omega_L = dE$ . Classically, it is given by the second-order Lagrange equations (compare with (3.4))

$$\frac{d}{dt} \frac{\partial L}{\partial v^i} = \frac{\partial L}{\partial q^i}. \quad (3.7)$$

For a Lagrangian vector-field  $X_L$  on  $M$ , there is a base integral curve  $\gamma_0(t) = (q^i(t), v^i(t))$  iff  $\gamma_0(t)$  is a geodesic. This is given by the contravariant velocity equation

$$\dot{q}^i = v^i, \quad \dot{v}^i + \Gamma_{jk}^i v^j v^k = 0. \quad (3.8)$$

Here  $\Gamma_{jk}^i$  denote the Christoffel symbols of the Levi-Civita affine connection  $\nabla$  in an open chart  $U$  on  $M$ , defined on the Riemannian metric  $g = \langle, \rangle$  by (see Appendix, as well as section 2.5.1 above)

$$\Gamma_{jk}^i = g^{il} \Gamma_{jkl}, \quad \Gamma_{ijk} = \frac{1}{2} (\partial_{x^i} g_{jk} + \partial_{x^j} g_{ki} + \partial_{x^k} g_{ij}). \quad (3.9)$$

The l.h.s  $\dot{v}^i = \dot{v}^i + \Gamma_{jk}^i v^j v^k$  in the second part of (3.8) represents the *Bianchi covariant derivative* of the velocity with respect to  $t$ . *Parallel transport* on  $M$  is defined by  $\dot{v}^i = 0$ . When this applies,  $X_L$  is called the *geodesic spray* and its flow the *geodesic flow*.

For the dynamics in the gravitational potential field  $V : M \rightarrow \mathbb{R}$ , the Lagrangian  $L : TM \rightarrow \mathbb{R}$  has an extended form

$$L(v, q) = \frac{1}{2} g_{ij} v^i v^j - V(q),$$

A Lagrangian vector-field  $X_L$  is still defined by the second-order Lagrangian equations (3.7, 3.8).

A general form of the forced, non-conservative Lagrange's equations is given as

$$\frac{d}{dt} \frac{\partial L}{\partial v^i} - \frac{\partial L}{\partial q^i} = F_i(t, q^i, v^i).$$

Here the  $F_i(t, q^i, v^i)$  represent any kind of *covariant forces*, including dissipative and elastic joint forces, as well as muscular-like actuator drives and neural-like control forces, as a function of time, coordinates and momenta. In covariant form we have

$$\dot{q}^i = v^i, \quad g_{ij} (\dot{v}^i + \Gamma_{jk}^i v^j v^k) = F_j(t, q^i, v^i).$$

### 3.1.2 Basics of Poincaré Dynamics

#### The Euler–Poincaré Equations

Let  $G$  be a Lie group and let  $L : TG \rightarrow \mathbb{R}$  be a *left-invariant Lagrangian*. Let  $l : \mathfrak{g} \rightarrow \mathbb{R}$  be its restriction to the identity. For a curve  $g(t) \in G$ , let  $\xi(t) = g(t)^{-1} \cdot \dot{g}(t)$ ; that is,  $\xi(t) = T_{g(t)}L_{g(t)^{-1}}\dot{g}(t)$ . Then the following are equivalent [MR99]:

1.  $g(t)$  satisfies the Euler–Lagrange equations for  $L$  on  $G$ ;
2. The variational principle holds,

$$\delta \int L(g(t), \dot{g}(t)) dt = 0$$

for variations with fixed endpoints;

3. The *Euler–Poincaré equations* hold:

$$\frac{d}{dt} \frac{\partial l}{\partial \xi} = \text{Ad}_\xi^* \frac{\delta l}{\delta \xi};$$

4. The variational principle holds on  $\mathfrak{g}$ ,

$$\delta \int l(\xi(t)) dt = 0,$$

using variations of the form  $\delta \xi = \dot{\eta} + [\xi, \eta]$ , where  $\eta$  vanishes at the endpoints.

#### The Lagrange–Poincaré Equations

Here we follow [MR99] and drop Euler–Lagrange equations and variational principles from a general velocity phase-space  $TM$  to the quotient  $TM/G$  by an action of a Lie group  $G$  on  $M$ . If  $L$  is a  $G$ -invariant Lagrangian on  $TM$ , it induces a reduced Lagrangian  $l$  on  $TM/G$ . We introduce a connection  $A$  on the principal bundle  $M \rightarrow S = M/G$ , assuming that this quotient is nonsingular. This connection allows one to split the variables into a horizontal and vertical part. Let internal variables  $x^\alpha$  be coordinates for shape-space  $S = M/G$ , let  $\eta^a$  be coordinates for the Lie algebra  $\mathfrak{g}$  relative to a chosen basis, let  $l$  be the Lagrangian regarded as a function of the variables  $x^\alpha, \dot{x}^\alpha, \eta^a$  and let  $C_{ab}^a$  be the structure constants of the Lie algebra  $\mathfrak{g}$  of  $G$ .

If one writes the Euler–Lagrange equations on  $TM$  in a local principal bundle trivialization, with coordinates  $x^\alpha$  on the base and  $\eta^a$  in the fibre, then one gets the following system of *Hamel equations*:

$$\frac{d}{dt} \frac{\partial l}{\partial \dot{x}^\alpha} = \frac{\partial l}{\partial x^\alpha}, \quad \text{and} \quad \frac{d}{dt} \frac{\partial l}{\partial \eta^b} = \frac{\partial l}{\partial \eta^a} C_{ab}^a \eta^a.$$

However, this representation of the equations does not make global intrinsic sense. The introduction of a connection overcomes this, and one can intrinsically and globally split the original variational principle relative to horizontal and vertical variations. One gets from one form to the other by means of the velocity shift given by replacing  $\eta^a$  by the vertical part relative to the *affine connection*

$$\xi^a = A_\alpha^a \dot{x}^\alpha + \eta^a.$$

Here  $A_\alpha^a$  are the local coordinates of the connection  $A$ . This change of coordinates is motivated from the mechanical point of view, since the variables  $\xi^a$  have the interpretation of the locked angular velocity. The resulting *Lagrange-Poincaré equations* have the following form:

$$\begin{aligned} \frac{d}{dt} \frac{\partial l}{\partial \dot{x}^\alpha} - \frac{\partial l}{\partial x^\alpha} &= \frac{\partial l}{\partial \xi^a} \left( B_{\alpha\beta}^a \dot{x}^\beta + B_{\alpha d}^a \xi^d \right), \\ \frac{d}{dt} \frac{\partial l}{\partial \xi^b} &= \frac{\partial l}{\partial \xi^a} \left( B_{b\alpha}^a \dot{x}^\alpha + C_{db}^a \xi^d \right). \end{aligned}$$

In these equations,  $B_{\alpha\beta}^a$  are the coordinates of the curvature  $B$  of  $A$ ,

$$B_{d\alpha}^a = C_{db}^a A_\alpha^b, \quad \text{and} \quad B_{b\alpha}^a = -B_{\alpha b}^a.$$

The variables  $\xi^a$  may be regarded as the rigid part of the variables on the original configuration space, while  $x^\alpha$  are the internal variables.

### 3.2 Hamiltonian Formalism in Human-Like Biomechanics

In this section we present classical Hamiltonian formalism, as is used in contemporary biomechanics. Let  $(M, \omega)$  be a *symplectic manifold* and  $H \in C^k(M, \mathbb{R})$  a smooth real valued function on  $M$ . The vector-field  $X_H$  determined by the condition

$$i_{X_H} \omega + dH = 0,$$

is called *Hamiltonian vector-field* with *Hamiltonian energy function*  $H$ . A triple  $(M, \omega, H)$  is called a *Hamiltonian mechanical system* [MR99, Put93].

Nondegeneracy of  $\omega$  guarantees that  $X_H$  exists, but only in the finite-dimensional case.

Let  $\{q^1, \dots, q^n, p_1, \dots, p_n\}$  be *canonical coordinates* on  $M$ , i.e.,  $\omega = dp_i \wedge dq^i$ . Then in these coordinates

$$X_H = \left( \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q^i} - \frac{\partial H}{\partial q^i} \frac{\partial}{\partial p_i} \right).$$

As a consequence,  $((q^i(t)), (p_i(t)))$  is an integral curve of  $X_H$  (for  $i = 1, \dots, n$ ) iff *Hamilton's equations* hold,

$$\dot{q}^i = \partial_{p_i} H, \quad \dot{p}_i = -\partial_{q^i} H. \quad (3.10)$$

Let  $(M, \omega, H)$  be a Hamiltonian mechanical system and let  $\gamma(t)$  be an integral curve of  $X_H$ . Then  $H(\gamma(t))$  is constant in  $t$ . Moreover, if  $\phi_t$  is the flow of  $X_H$ , then  $H \circ \phi_t = H$  for each  $t$ .

Let  $(M, \omega, H)$  be a Hamiltonian mechanical system and  $\phi_t$  be the flow of  $X_H$ . Then, by the Liouville theorem, for each  $t$ ,  $\phi_t^* \omega = \omega$ , ( $\frac{d}{dt} \phi_t^* \omega = 0$ , so  $\phi_t^* \omega$  is constant in  $t$ ), that is,  $\phi_t$  is symplectic, and it preserves the volume  $\Omega_\omega$ .

A convenient criterion for symplectomorphisms is that they preserve the form of Hamilton's equations. More precisely, let  $(M, \omega)$  be a symplectic manifold and  $f : M \rightarrow M$  a diffeomorphism. Then  $f$  is symplectic iff for all  $H \in C^k(M, \mathbb{R})$  we have  $f^*(X_H) = X_{H \circ f}$ .

A vector-field  $X \in \mathcal{X}(M)$  on a symplectic manifold  $(M, \omega)$  is called locally Hamiltonian iff  $\mathcal{L}_X \omega = 0$ , where  $L$  denotes the *Lie derivative*. From the equality  $L_{[X, Y]} \omega = \mathcal{L}_X L_Y \omega - L_Y \mathcal{L}_X \omega$ , it follows that the locally Hamiltonian vector-fields on  $M$  form a Lie subalgebra of  $\mathcal{X}(M)$ .

Let  $(M, \omega)$  be a symplectic manifold and  $f, g \in C^k(M, \mathbb{R})$ . The *Poisson bracket* of  $f$  and  $g$  is the function

$$\{f, g\}_\omega = -\omega(X_f, X_g) = -\mathcal{L}_{X_f} g = \mathcal{L}_{X_g} f.$$

Also, for  $f_0 \in C^k(M, \mathbb{R})$ , the map  $g \mapsto \{f_0, g\}_\omega$  is a derivation. The connection between the Lie bracket and the Poisson bracket is

$$[X_f, X_g] = -X_{\{f, g\}_\omega} \iff d\omega = 0.$$

The real vector space  $C^k(M, \mathbb{R})$  together with the Poisson bracket on it forms an infinite-dimensional Lie algebra called the *algebra of classical observables*.

In canonical coordinates  $\{q^1, \dots, q^n, p_1, \dots, p_n\}$  on  $(M, \omega)$  the Poisson bracket of two functions  $f, g \in C^k(M, \mathbb{R})$  is given by

$$\{f, g\}_\omega = \frac{\partial f}{\partial q^i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q^i}.$$

From this definition follows:

$$\{q^i, q^j\}_\omega = 0, \quad \{p_i, p_j\}_\omega = 0, \quad \{q^i, p_j\}_\omega = \delta_j^i.$$

Let  $(M, \omega)$  be a symplectic manifold and  $f : M \rightarrow M$  a diffeomorphism. Then  $f$  is symplectic iff it preserves the Poisson bracket.

Let  $(M, \omega, H)$  be a Hamiltonian mechanical system and  $\phi_t$  the flow of  $X_H$ . Then for each function  $f \in C^k(M, \mathbb{R})$  we have the equations of motion in the Poisson bracket notation:

$$\frac{d}{dt} (f \circ \phi_t) = \{f \circ \phi_t, H\}_\omega = \{f, H\}_\omega \circ \phi_t.$$

Also,  $f$  is called a *constant of motion*, or a *first integral*, if it satisfies the following condition

$$\{f, H\}_\omega = 0.$$

If  $f$  and  $g$  are constants of motion then their Poisson bracket is also a constant of motion.

A Hamiltonian mechanical system  $(M, \omega, H)$  is said to be integrable if there exists  $n = \frac{1}{2} \dim(M)$  linearly-independent functions  $K_1 = H, K_2, \dots, K_n$  such that for each  $i, j = 1, 2, \dots, n$ :

$$\{K_i, H\}_\omega = 0, \quad \{K_i, K_j\}_\omega = 0.$$

### 3.2.1 Nonlinear Dynamics in Hamiltonian Form

#### Real 1-DOF Hamiltonian Dynamics

The basic structural unit of the biomechanics is a *uniaxial rotational joint*, geometrically representing a *constrained  $SO(2)$  group of plane rotations*. In other words, this is a one-DOF dynamical system, represented in a differential formulation as a *vector-field*, or in an integral form as a *phase-flow*, on a 2D phase-space manifold  $M$ , *cylinder  $\mathbb{R} \times S^1$* , being itself a *cotangent bundle  $T^*M$*  of the joint  *$SO(2)$ -configuration manifold, circle  $S^1$* .

A vector-field  $X(t)$  on the momentum phase-space manifold  $M$  can be given by a system of *canonical equations of motion*

$$\dot{q} = f(q, p, t, \mu), \quad \dot{p} = g(q, p, t, \mu), \quad (3.11)$$

where  $t$  is time,  $\mu$  is a parameter,  $q \in S^1, p \in \mathbb{R} \times S^1$  are *coordinates and momenta*, respectively, while  $f$  and  $g$  are smooth functions on the phase-space  $\mathbb{R} \times S^1$ .

If time  $t$  does not explicitly appear in the functions  $f$  and  $g$ , the vector-field  $X$  is called *autonomous*. In this case equation (3.11) simplifies as

$$\dot{q} = f(q, p, \mu), \quad \dot{p} = g(q, p, \mu). \quad (3.12)$$

By a *solution curve* of the vector-field  $X$  we mean a map  $x = (q, p)$ , from some interval  $I \subset \mathbb{R}$  into the phase-space manifold  $M$ , such that  $t \mapsto x(t)$ . The map  $x(t) = (q(t), p(t))$  geometrically represents a curve in  $M$ , and equations (3.11) or (3.12) give the tangent vector at each point of the curve.

To specify an *initial condition* on the vector-field  $X$ , by

$$x(t, t_0, x_0) = (q(t, t_0, q_0), p(t, t_0, p_0)),$$

geometrically means to distinguish a solution curve by a particular point  $x(t_0) = x_0$  in the phase-space manifold  $M$ . Similarly, it may be useful to explicitly display the parametric dependence of solution curves, as

$x(t, t_0, x_0, \mu) = (q(t, t_0, q_0, \mu_q), p(t, t_0, p_0, \mu_p))$ , where  $\mu_q, \mu_p$  denote  $q$ -dependent and  $p$ -dependent parameters, respectively.

The solution curve  $x(t, t_0, x_0)$  of the vector-field  $X$ , may be also referred as the *phase trajectory* through the point  $x_0$  at  $t = t_0$ . Its graph over  $t$  is referred to as an *integral curve*; more precisely, *graph*  
 $x(t, t_0, x_0) \equiv \{(x, t) \in M \times \mathbb{R} : x = x(t, t_0, x_0), t \in I \subset \mathbb{R}\}$ .

Let  $x_0 = (q_0, p_0)$  be a point on  $M$ . By the *orbit through*  $x_0$ , denoted  $O(x_0)$ , we mean the set of points in  $M$  that lie on a trajectory passing through  $x_0$ ; more precisely, for  $x_0 \in U$ ,  $U$  open in  $M$ , the orbit through  $x_0$  is given by  $O(x_0) = \{x \in \mathbb{R} \times S^1 : x = x(t, t_0, x_0), t \in I \subset \mathbb{R}\}$ .

Consider a general autonomous vector-field  $X$  on the phase-space manifold  $M$ , given by equation  $\dot{x} = f(x)$ ,  $x = (q, p) \in M$ . An *equilibrium solution*, *singularity*, or *fixed point* of  $X$  is a point  $\bar{x} \in M$  such that  $f(\bar{x}) = 0$ , i.e., a solution which does not change in time.

Any solution  $\bar{x}(t)$  of an autonomous vector-field  $X$  on  $M$  is *stable* if solutions starting ‘close’ to  $\bar{x}(t)$  at a given time remain close to  $\bar{x}(t)$  for all later times. It is *asymptotically stable* if nearby solutions actually converge to  $\bar{x}(t)$  as  $t \rightarrow \infty$ . In order to determine the stability of  $\bar{x}(t)$  we must understand the nature of solutions near  $\bar{x}(t)$ , which is done by *linearization* of the vector-field  $X$ . The solution of the linearized vector-field  $Y$  is asymptotically stable if all eigenvalues have negative real parts. In that case the fixed point  $x = \bar{x}$  of associated nonlinear vector-field  $X$  is also asymptotically stable. A fixed point  $\bar{x}$  is called *hyperbolic point* if none of the eigenvalues of  $Y$  have zero real part; in that case the orbit structure near  $\bar{x}$  is essentially the same for  $X$  and  $Y$ .

In the case of autonomous vector-fields on  $M$  we have also an important property of *Hamiltonian flow*. If  $x(t) = (q(t), p(t))$  is a solution of  $\dot{x} = f(x)$ ,  $x \in M$ , then so is  $x(t + \tau)$  for any  $\tau \in \mathbb{R}$ . Also, for any  $x_0 \in M$  there exists only one solution of an autonomous vector-field passing through this point. The autonomous vector-field

$$\dot{x} = f(x)$$

has the following properties (compare with the section (2.3.1) above):

1.  $x(t, x_0)$  is  $C^k$ ;
2.  $x(0, x_0) = x_0$ ; and
3.  $x(t + s, x_0) = x(t, x(s, x_0))$ .

These properties show that the solutions of an autonomous vector-field form a *one-parameter family of diffeomorphisms* of the phase-space manifold  $M$ . This is referred to as a *phase-flow* and denoted by  $\phi_t(x)$  or  $\phi(t, x)$ .

Consider a flow  $\phi(t, x)$  generated by vector-field  $\dot{x} = f(x)$ . A point  $x_0 = (q_0, p_0)$  on  $M$  is called an  $\omega$ -*limit point* of  $x = (q, p) \in M$ , denoted  $\omega(x)$ , if there exists a sequence  $\{t_i\}$ ,  $t_i \mapsto \infty$ , such that  $\phi(t_i, x) \mapsto x_0$ . Similarly,  $\alpha$ -*limit points* are defined by taking a sequence  $\{t_i\}$ ,  $t_i \mapsto -\infty$ . The set of all  $\omega$ -limit points of a flow is called the  $\omega$ -*limit set*. The  $\alpha$ -limit set is similarly defined.

A point  $x_0 = (q_0, p_0)$  on  $M$  is called *nonwandering* if for any open neighborhood  $U \subset M$  of  $x_0$ , there exists some  $t \neq 0$  such that  $\phi(t, U) \cap U \neq \emptyset$ . The set of all nonwandering points of a flow is called the *nonwandering set* of that particular map or flow.

A closed invariant subset  $A \subset M$  is called an *attracting set* if there is some open neighborhood  $U \subset M$  of  $A$  such that  $\phi(t, x) \in U$  and  $\phi(t, x) \mapsto \infty$  for any  $x \in U$  and  $t \geq 0$ . The *domain* or *basin of attraction* of  $A$  is given by  $\cup_{t \leq 0} \phi(t, U)$ . In practice, a way of locating attracting sets is to first find a *trapping region*, i.e., a closed, connected subset  $V \subset M$  such that for any  $t \geq 0$   $\phi(t, V) \subset V$ . Then  $\cap_{t \geq 0} \phi(t, V) = A$  is an *attracting set*.

As a first example of one-DOF dynamical systems, let us consider a vector-field  $x = (q, p) \in \mathbb{R} \times \mathbb{R}$  of a simple harmonic oscillator, given by equations

$$\dot{q} = p, \quad \dot{p} = -q. \quad (3.13)$$

Here, the *solution* passing through the point  $(q, p) = (1, 0)$  at  $t = 0$  is given by  $(q(t), p(t)) = (\cos t, -\sin t)$ ; the *integral curve* passing through  $(q, p) = (1, 0)$  at  $t = 0$  is given by  $\{(q, p, t) \in \mathbb{R} \times \mathbb{R} \times \mathbb{R} : (q(t), p(t)) = (\cos t, -\sin t)\}$ , for all  $t \in \mathbb{R}$ ; the *orbit* passing through  $(q, p) = (1, 0)$  is given by the circle  $q^2 + p^2 = 1$ .

A one-DOF dynamical system is called *Hamiltonian system* if there exists a *first integral* or a function of the dependent variables  $(q, p)$  whose level curves give the orbits of the vector-field  $X = X_H$ , i.e., a total-energy *Hamiltonian function*  $H = H(q, p) : U \rightarrow \mathbb{R}$ , ( $U$  open set on the phase-space manifold  $M$ ), such that the vector-field  $X_H$  is given by *Hamilton's canonical equations* (3.10). In (3.10), the first,  $\dot{q}$ -equation, is called the *velocity equation* and serves as a definition of the *momentum*, while the second,  $\dot{p}$ -equation is called the *force equation*, and represents the *Newtonian second law of motion*.

The simple harmonic oscillator (3.13) is a Hamiltonian system with a Hamiltonian function  $H = \frac{p^2}{2} + \frac{q^2}{2}$ . It has a *fixed point* – *center* (having purely imaginary eigenvalues) at  $(q, p) = (0, 0)$  and is surrounded by a one-parameter family of periodic orbits given by the Hamiltonian  $H$ .

A nice example of one-DOF dynamical system with a Hamiltonian structure is a *damped Duffing oscillator* (see, e.g., [Wig90]). This is a *plane* Hamiltonian vector-field  $x = (q, p) \in \mathbb{R}^2$ , given by Hamilton's equations

$$\dot{q} = p \equiv f(q, p), \quad \dot{p} = q - q^3 - \delta p \equiv g(q, p, \delta), \quad \delta \geq 0. \quad (3.14)$$

For the special parameter value  $\delta = 0$ , we have an *undamped* Duffing oscillator with a *first integral* represented by Hamiltonian function  $H = \frac{p^2}{2} - \frac{q^2}{2} + \frac{q^4}{4}$ , where  $\frac{p^2}{2}$  corresponds to the *kinetic energy* (with a mass scaled to unity), and  $-\frac{q^2}{2} + \frac{q^4}{4} \equiv V(x)$  corresponds to the *potential energy* of the oscillator.

In general, if the first integral, i.e., a Hamiltonian function  $H$ , is defined by  $H = \frac{p^2}{2} + V(x)$ , then the momentum is given by  $p = \pm\sqrt{2}\sqrt{H - V(x)}$ . All one-DOF Hamiltonian systems are *integrable* and all the solutions lie on *level*

curves of the Hamiltonian function, which are topologically equivalent with the circle  $S^1$ . This is actually a general characteristic of all  $n$ -DOF integrable Hamiltonian systems: their bounded motions lie on  $n$ D *invariant tori*  $T^n = S^1 \times \cdots \times S^1$ , or *homoclinic orbits*. The homoclinic orbit is sometimes called a *separatrix* because it is the boundary between two distinctly different types of motion.

For example, in case of a damped Duffing oscillator (3.14) with  $\delta \neq 0$ , we have

$$\partial_q f + \partial_p g = -\delta,$$

and according to the *Bendixon's criterion* for  $\delta > 0$  it has no closed orbits.

The vector-field  $X$  given by equations (3.14) has three fixed points given by  $(q, p) = (0, 0), (\pm 1, 0)$ . The *eigenvalues*  $\lambda_{1,2}$  of the associated linearized vector-field are given by  $\lambda_{1,2} = -\delta/2 \pm \frac{1}{2}\sqrt{\delta^2 + 4}$ , for the fixed point  $(0, 0)$ , and by  $\lambda_{1,2} = -\delta/2 \pm \frac{1}{2}\sqrt{\delta^2 - 8}$ , for the fixed point  $(\pm 1, 0)$ . Hence, for  $\delta > 0$ ,  $(0, 0)$  is *unstable* and  $(\pm 1, 0)$  are *asymptotically stable*; for  $\delta = 0$ ,  $(\pm 1, 0)$  are *stable in the linear approximation* (see, e.g., [Wig90]).

Another example of one-DOF Hamiltonian systems, representing the actual basis of the human  $SO(2)$ -joint dynamics, is a *simple pendulum* (again, all physical constants are scaled to unity), given by Hamiltonian function  $H = \frac{p^2}{2} - \cos q$ . This is the first integral of the *cylindrical* Hamiltonian vector-field  $(q, p) \in S^1 \times \mathbb{R}$ , defined by canonical equations

$$\dot{q} = p, \quad \dot{p} = -\sin q.$$

This vector-field has fixed points at  $(0, 0)$ , which is a center (i.e., the eigenvalues are purely imaginary), and at  $(\pm\pi, 0)$ , which are saddles, but since the phase-space manifold is the cylinder, these are really the same point.

The basis of human arm and leg dynamics represents the *coupling* of two uniaxial,  $SO(2)$ -joints. The study of two DOF Hamiltonian dynamics we shall start with the most simple case of two linearly coupled linear undamped oscillators with parameters scaled to unity. Under general conditions we can perform a change of variables to canonical coordinates (the ‘normal modes’)  $(q^i, p_i)$ ,  $i = 1, 2$ , so that the vector-field  $X_H$  is given by

$$\dot{q}^1 = p_1, \quad \dot{q}^2 = p_2, \quad \dot{p}_1 = -\omega_1^2 q^1, \quad \dot{p}_2 = -\omega_2^2 q^2.$$

This system is integrable, since we have two independent functions of  $(q^i, p_i)$ , i.e., Hamiltonians

$$H_1 = \frac{p_1^2}{2} + \frac{\omega_1^2 (q^1)^2}{2}, \quad H_2 = \frac{p_2^2}{2} + \frac{\omega_2^2 (q^2)^2}{2}.$$

The level curves of these functions are compact sets (topological circles); therefore, the orbits in the 4D phase-space  $\mathbb{R}^4$  actually lie on the two-torus  $T^2$ . By making the appropriate change of variables, it can be shown (see, e.g.,

[Wig90]) that the whole dynamics of the two linearly coupled linear undamped oscillators is actually contained in the equations

$$\dot{\theta}_1 = \omega_1, \quad \dot{\theta}_2 = \omega_2, \quad (\theta_1, \theta_2) \in S^1 \times S^1 \equiv T^2. \quad (3.15)$$

The flow on the two-torus  $T^2$ , generated by (3.15), is simple to compute and is given by

$$\theta_1(t) = \omega_1 t + \theta_{10}, \quad \theta_2(t) = \omega_2 t + \theta_{20}, \quad (\text{mod } 2\pi),$$

and  $\theta_1$  and  $\theta_2$  are called the longitude and latitude. However, orbits under this flow will depend on how  $\omega_1$  and  $\omega_2$  are related. If  $\omega_1$  and  $\omega_2$  are *commensurate* (i.e., the equation  $m\omega_1 + n\omega_2 = 0$ ,  $(n, m) \in Z$  has solutions), then every phase curve of (3.15) is closed. However, if  $\omega_1$  and  $\omega_2$  are *incommensurate* (i.e., upper equation has no solutions), then every phase curve of (3.15) is everywhere dense on  $T^2$ .

Somewhat deeper understanding of Hamiltonian dynamics is related to the method of *action-angle variables*. The easiest way to introduce this idea is to consider again a simple harmonic oscillator (3.13). If we transform equations (3.13) into polar coordinates using  $q = r \sin \theta$ ,  $p = r \cos \theta$ , then the equations of the vector-field become  $\dot{r} = 0$ ,  $\dot{\theta} = 1$ , having the obvious solution  $r = \text{const}$ ,  $\theta = t + \theta_0$ . For this example polar coordinates work nicely because the system (3.13) is linear and, therefore, all of the periodic orbits have the same period.

For the general, nonlinear one-DOF Hamiltonian system (3.10) we will seek a coordinate transformation that has the same effect. Namely, we will seek a coordinate transformation  $(q, p) \mapsto (\theta(q, p), I(q, p))$  with inverse transformation  $(\theta, I) \mapsto (q(I, \theta), p(I, \theta))$  such that the vector-field (3.10) in the action-angle  $(\theta, I)$  coordinates satisfies the following conditions: (i)  $\dot{I} = 0$ ; (ii)  $\theta$  changes linearly in time on the closed orbits with  $\dot{\theta} = \Omega(I)$ . We might even think of  $I$  and  $\theta$  heuristically as 'nonlinear polar coordinates'. In such a coordinate system Hamiltonian function takes the form  $H = H(I)$ , and also,  $\Omega(I) = \partial_I H$ , i.e., specifying  $I$  specifies a periodic orbit.

The action variable  $I(q, p)$  geometrically represents an area enclosed by any closed curve, which is constant in time. It is defined as an integral  $I = \frac{1}{2\pi} \int_H p dq$ , where  $H$  denotes the periodic orbit defined by  $H(q, p) = H = \text{const}$ . If the period of each periodic orbit defined by  $H(q, p) = H = \text{const}$  is denoted by  $T(H)$ , the angle variable  $\theta(q, p)$  is defined by

$$\theta(q, p) = \frac{2\pi}{T(H)} t(q, p),$$

where  $t = t(q, p)$  represents the time taken for the solution starting from  $(q_0, p_0)$  to reach  $(q, p)$ .

For the system with Hamiltonian  $H = \frac{p^2}{2} + V(x)$  and momentum  $p = \pm \sqrt{2\sqrt{H - V(x)}}$  the action is given by  $I = \frac{\sqrt{2}}{\pi} \int_{q_{min}}^{q_{max}} \sqrt{H - V(q)} dq$ , and the angle is given by  $\theta(q, p) = \frac{2\pi}{T(H)} \int_{q_{min}}^{q_{max}} \frac{dq}{\sqrt{2}\sqrt{H - V(q)}}$ .

Closely related to the action-angle variables is the *perturbation theory* (see [Nay73]). To explain the main idea of this theory, let us consider an  $\epsilon$ -*perturbed* vector-field periodic in  $t$  which can be in component form given as (with  $(q, p) \in \mathbb{R}^2$ )

$$\dot{q} = f_1(q, p) + \epsilon g_1(q, p, t, \epsilon), \quad \dot{p} = f_2(q, p) + \epsilon g_2(q, p, t, \epsilon). \quad (3.16)$$

Setting  $\epsilon = 0$  we get the *unperturbed* Hamiltonian system with a smooth scalar-valued function  $H(q, p)$  for which holds

$$f_1(q, p) = \frac{\partial H(q, p)}{\partial p}, \quad f_2(q, p) = -\frac{\partial H(q, p)}{\partial q},$$

so, the perturbed system (3.16) obtains the symmetric canonical form

$$\dot{q} = \frac{\partial H(q, p)}{\partial p} + \epsilon g_1(q, p, t, \epsilon), \quad \dot{p} = -\frac{\partial H(q, p)}{\partial q} + \epsilon g_2(q, p, t, \epsilon).$$

The perturbation  $(g_1, g_2)$  need not be Hamiltonian, although in the case where perturbation is Hamiltonian versus the case where it is not, the dynamics are very different.

Now, if we transform the coordinates of the perturbed vector-field using the action-angle transformation for the unperturbed Hamiltonian vector-field, we get

$$\begin{aligned} \dot{I} &= \epsilon \left( \frac{\partial I}{\partial q} g_1 + \frac{\partial I}{\partial p} g_2 \right) \equiv \epsilon F(I, \theta, t, \epsilon), \\ \dot{\theta} &= \Omega(I) + \epsilon \left( \frac{\partial \theta}{\partial q} g_1 + \frac{\partial \theta}{\partial p} g_2 \right) \equiv \Omega(I) + \epsilon G(I, \theta, t, \epsilon), \end{aligned} \quad (3.17)$$

where

$$\begin{aligned} F(I, \theta, t, \epsilon) &= \frac{\partial I}{\partial q}(q(I, \theta), p(I, \theta)) g_1((q(I, \theta), p(I, \theta)), t, \epsilon) \\ &\quad + \frac{\partial I}{\partial p}(q(I, \theta), p(I, \theta)) g_2((q(I, \theta), p(I, \theta)), t, \epsilon), \\ G(I, \theta, t, \epsilon) &= \frac{\partial \theta}{\partial q}(q(I, \theta), p(I, \theta)) g_1((q(I, \theta), p(I, \theta)), t, \epsilon) \\ &\quad + \frac{\partial \theta}{\partial p}(q(I, \theta), p(I, \theta)) g_2((q(I, \theta), p(I, \theta)), t, \epsilon). \end{aligned}$$

Here,  $F$  and  $G$  are  $2\pi$  periodic in  $\theta$  and  $T = 2\pi/\omega$  periodic in  $t$ .

Finally, we shall explain in brief the most important idea in the dynamical systems theory, the idea of *Poincaré maps*. The idea of reducing the study of continuous time systems (flows) to the study of an *associated discrete time*

*system (map)* is due to Poincaré who first utilized it in the end of the last century in his studies of the three body problem in celestial mechanics. Nowadays virtually any discrete time system that is associated with an ordinary differential equation is referred to as a Poincaré map [Wig90]. This technique offers several advantages in the study of dynamical systems, including dimensional reduction, global dynamics and conceptual clarity. However, construction of a Poincaré map requires some knowledge of the phase-space of a dynamical system. One of the techniques which can be used for construction of Poincaré maps is the perturbation method.

To construct the Poincaré map for the system (3.17), we have to rewrite it as an autonomous system

$$\dot{I} = \epsilon F(I, \theta, \phi, \epsilon), \quad \dot{\theta} = \Omega(I) + \epsilon G(I, \theta, \phi, \epsilon), \quad \dot{\phi} = \omega, \quad (3.18)$$

(where  $(I, \theta, \phi) \in \mathbb{R}^+ \times S^1 \times S^1$ ). We construct a global *cross-section*  $\Sigma$  to this vector-field defined as  $\Sigma^{\phi_0} = \{(I, \theta, \phi) | \phi = \phi_0\}$ . If we denote the  $(I, \theta)$  components of solutions of (3.18) by  $(I_\epsilon(t), \theta_\epsilon(t))$  and the  $(I, \theta)$  components of solutions of (3.18) for  $\epsilon = 0$  by  $(I_0, \Omega(I_0)t + \theta_0)$ , then the perturbed Poincaré map is given by

$$P_\epsilon : \Sigma^{\phi_0} \rightarrow \Sigma^{\phi_0}, \quad (I_\epsilon(0), \theta_\epsilon(0)) \mapsto (I_\epsilon(T), \theta_\epsilon(T)),$$

and the  $m$ th *iterate* of the Poincaré map is given by

$$P_\epsilon^m : \Sigma^{\phi_0} \rightarrow \Sigma^{\phi_0}, \quad (I_\epsilon(0), \theta_\epsilon(0)) \mapsto (I_\epsilon(mT), \theta_\epsilon(mT)).$$

Now we can approximate the solutions to the perturbed problem as linear, constant-coefficient approximation

$$I_\epsilon(t) = I_0 + \epsilon I_1(t) + O(\epsilon^2), \quad \theta_\epsilon(t) = \theta_0 + \Omega(I_0)t + \epsilon \theta_1(t) + O(\epsilon^2),$$

where we have chosen  $I_\epsilon(0) = I_0$ ,  $\theta_\epsilon(0) = \theta_0$ .

As a last example of one-DOF Hamiltonian dynamics we shall analyze a *damped, forced Duffing oscillator*, given by canonical equations [Wig90]

$$\dot{q} = p, \quad \dot{p} = q - q^3 - \delta p + \gamma \cos \omega t, \quad \delta, \gamma, \omega \geq 0, \quad (q, p) \in \mathbb{R}^2. \quad (3.19)$$

where  $\delta, \gamma$ , and  $\omega$  are real parameters physically meaning *dissipation*, *amplitude of forcing* and *frequency*, respectively.

The *perturbed* system (3.19) is given by

$$\dot{q} = p, \quad \dot{p} = q - q^3 + \epsilon(\gamma \cos \omega t - \delta p), \quad (3.20)$$

where  $\epsilon$ -perturbation is assumed small. Then the *unperturbed* system is given by

$$\dot{q} = p, \quad \dot{p} = q - q^3,$$

and is conservative with Hamiltonian function

$$H(q, p) = \frac{p^2}{2} - \frac{q^2}{2} + \frac{q^4}{4}. \quad (3.21)$$

In the unperturbed phase-space all orbits are given by the level sets of the Hamiltonian (3.21). There are three equilibrium points at the following coordinates:  $(q, p) = (\pm 1, 0)$  – centers, and  $(q, p) = (0, 0)$  – saddle. The saddle point is connected to itself by two homoclinic orbits given by

$$q_+^0(t) = (\sqrt{2}(\cosh t)^{-1}, -\sqrt{2}(\cosh t)^{-1} \tanh t), \quad q_-^0(t) = -q_+^0(t).$$

There are two families of *periodic orbits*  $q_{\pm}^k(t)$ , where  $k$  represents the *elliptic modulus* related to the Hamiltonian by  $H(q_{\pm}^k(t)) \equiv H(k) = \frac{k^2-1}{(2-k^2)^2}$ , inside the corresponding homoclinic orbits  $q_{\pm}^0(t)$ , with the period  $T(k) = 2K(k)\sqrt{2-k^2}$  ( $K(k)$  is the complete elliptic integral of the first kind).

Also, there exists a family of *periodic orbits* outside the homoclinic orbits with the period  $T(k) = 4K(k)\sqrt{k^2-1}$ .

The perturbed system (3.20) can be rewritten as a third-order autonomous system

$$\dot{q} = p, \quad \dot{p} = q - q^3 + \epsilon(\gamma \cos \phi - \delta p), \quad \dot{\phi} = \omega,$$

where  $(q, p, \phi) \in \mathbb{R}^2 \times S^1$ ,  $S^1$  is the circle of length  $2\pi/\omega$  and  $\phi(t) = \omega t + \phi_0$ . We form the global cross-section to the flow

$$\Sigma^{\phi_0} = \{(q, p, \phi) | \phi = \phi_0 \in [0, 2\pi/\omega]\}$$

and the associated Poincaré map is given by

$$P : \Sigma^{\phi_0} \rightarrow \Sigma^{\phi_0}, \quad (q(0), p(0)) \mapsto (q(2\pi/\omega), p(2\pi/\omega)).$$

A detailed analysis of the perturbed Poincaré map for the damped, forced Duffing oscillator is related to the *Melnikov function* and can be found in [Wig90].

### Complex One-DOF Hamiltonian Dynamics

*Global complex analysis* represents another powerful tool for analyzing the uniaxial joint dynamics, which can be easily generalized to  $n$ -DOF human-like musculo-skeletal chains. Setting  $z = q + ip$ ,  $z \in \mathbb{C}$ ,  $i = \sqrt{-1}$ , Hamilton's equations  $\dot{q} = \partial H / \partial p$ ,  $\dot{p} = -\partial H / \partial q$  may be written in *complex notation* as [AM78, MR99, Wig90]

$$\dot{z} = -2i \frac{\partial H}{\partial \bar{z}}. \quad (3.22)$$

Let  $U$  be an open set in the *complex phase-space manifold*  $M_{\mathbb{C}}$  (i.e., manifold  $M$  modelled on  $\mathbb{C}$ ). A  $C^0$  function  $\gamma : [a, b] \rightarrow U \subset M_{\mathbb{C}}$ ,  $t \mapsto \gamma(t)$  represents a *solution curve*  $\gamma(t) = q(t) + ip(t)$  of a complex Hamiltonian

system (3.22). For instance, the curve  $\gamma(\theta) = \cos \theta + i \sin \theta$ ,  $0 \leq \theta \leq 2\pi$  is the unit circle.  $\gamma(t)$  is a *parameterized curve*. We call  $\gamma(a)$  the *beginning point*, and  $\gamma(b)$  the *end point* of the curve. By a *point on the curve* we mean a point  $w$  such that  $w = \gamma(t)$  for some  $t \in [a, b]$ .

The derivative  $\dot{\gamma}(t)$  is defined in the usual way, namely

$$\dot{\gamma}(t) = \dot{q}(t) + i\dot{p}(t),$$

so that the usual rules for the derivative of a sum, product, quotient, and chain rule are valid. The *speed* is defined as usual to be  $|\dot{\gamma}(t)|$ . Also, if  $f : U \rightarrow M_C$  represents a *holomorphic*, or *analytic* function, then the composite  $f \circ \gamma$  is differentiable (as a function of the real variable  $t$ ) and  $(f \circ \gamma)'(t) = f'(\gamma(t))\dot{\gamma}(t)$ .

A *path* represents a sequence of  $C^1$ -curves,

$$\gamma = \{\gamma_1, \gamma_2, \dots, \gamma_n\},$$

such that the end point of  $\gamma_j$ , ( $j = 1, \dots, n$ ) is equal to the beginning point of  $\gamma_{j+1}$ . If  $\gamma_j$  is defined on the interval  $[a_j, b_j]$ , this means that

$$\gamma_j(b_j) = \gamma_{j+1}(a_{j+1}).$$

We call  $\gamma_1(a_1)$  the *beginning point* of  $\gamma_j$ , and  $\gamma_n(b_n)$  the *end point* of  $\gamma_j$ . The path is said to *lie in an open set*  $U \subset M_C$  if each curve  $\gamma_j$  lies in  $U$ , i.e., for each  $t$ , the point  $\gamma_j(t)$  lies in  $U$ .

An open set  $U$  is *connected* if given two points  $\alpha$  and  $\beta$  in  $U$ , there exists a path  $\gamma = \gamma_1, \gamma_2, \dots, \gamma_n$  in  $U$  such that  $\alpha$  is the beginning point of  $\gamma_1$  and  $\beta$  is the end point of  $\gamma_n$ ; in other words, if there is a path  $\gamma$  in  $U$  which joins  $\alpha$  to  $\beta$ . If  $U$  is a connected open set and  $f$  a holomorphic function on  $U$  such that  $f' = 0$ , then  $f$  is a constant. If  $g$  is a function on  $U$  such that  $f' = g$ , then  $f$  is called a *primitive* of  $g$  on  $U$ . Primitives can be either find out by integration or written down directly.

Let  $f$  be a  $C^0$ -function on an open set  $U$ , and suppose that  $\gamma$  is a curve in  $U$ , meaning that all values  $\gamma(t)$  lie in  $U$  for  $a \leq t \leq b$ . The *integral of  $f$  along  $\gamma$*  is defined as

$$\int_{\gamma} f = \int_{\gamma} f(z) = \int_a^b f(\gamma(t)) \dot{\gamma}(t) dt.$$

For example, let  $f(z) = 1/z$ , and  $\gamma(\theta) = e^{i\theta}$ . Then  $\dot{\gamma}(\theta) = ie^{i\theta}$ . We want to find the value of the integral of  $f$  over the circle,  $\int_{\gamma} dz/z$ , so  $0 \leq \theta \leq 2\pi$ . By definition, this integral is equal to  $\int_0^{2\pi} ie^{i\theta}/e^{i\theta} d\theta = i \int_0^{2\pi} d\theta = 2\pi i$ .

The *length*  $L(\gamma)$  is defined to be the integral of the speed,  $L(\gamma) = \int_a^b |\dot{\gamma}(t)| dt$ .

If  $\gamma = \gamma_1, \gamma_2, \dots, \gamma_n$  is a path, then the integral of a  $C^0$ -function  $f$  on an open set  $U$  is defined as  $\int_{\gamma} f = \sum_{i=1}^n \int_{\gamma_i} f$ , i.e., the sum of the integrals of  $f$

over each curve  $\gamma_i$  ( $i = 1, \dots, n$ ) of the path  $\gamma$ . The *length of a path* is defined as  $L(\gamma) = \sum_{i=1}^n L(\gamma_i)$ .

Let  $f$  be continuous on an open set  $U \subset M_C$ , and suppose that  $f$  has a primitive  $g$ , that is,  $g$  is holomorphic and  $g' = f$ . Let  $\alpha, \beta$  be two points in  $U$ , and let  $\gamma$  be a path in  $U$  joining  $\alpha$  to  $\beta$ . Then  $\int_\gamma f = g(\beta) - g(\alpha)$ ; this integral is independent of the path and depends only on the beginning and end point of the path.

A *closed path* is a path whose beginning point is equal to its end point. If  $f$  is a  $C^0$ -function on an open set  $U \subset M_C$  admitting a holomorphic primitive  $g$ , and  $\gamma$  is any closed path in  $U$ , then  $\int_\gamma f = 0$ .

Let  $\gamma, \eta$  be two paths defined over the same interval  $[a, b]$  in an open set  $U \subset M_C$ . Recall (see Introduction) that  $\gamma$  is *homotopic* to  $\eta$  if there exists a  $C^0$ -function  $\psi : [a, b] \times [c, d] \rightarrow U$  defined on a rectangle  $[a, b] \times [c, d] \subset U$ , such that  $\psi(t, c) = \gamma(t)$  and  $\psi(t, d) = \eta(t)$  for all  $t \in [a, b]$ . For each number  $s \in [c, d]$  we may view the function  $\psi_s(t) = \psi(t, s)$  as a continuous curve defined on  $[a, b]$ , and we may view the family of continuous curves  $\psi_s$  as a *deformation* of the path  $\gamma$  to the path  $\eta$ . It is said that the homotopy  $\psi$  *leaves the end points fixed* if we have  $\psi(a, s) = \gamma(a)$  and  $\psi(b, s) = \gamma(b)$  for all values of  $s \in [c, d]$ . Similarly, when we speak of a homotopy of closed paths, we assume that each path  $\psi_s$  is a closed path.

Let  $\gamma, \eta$  be paths in an open set  $U \subset M_C$  having the same beginning and end points. Assume that they are homotopic in  $U$ . Let  $f$  be holomorphic on  $U$ . Then  $\int_\gamma f = \int_\eta f$ . The same holds for closed homotopic paths in  $U$ . In particular, if  $\gamma$  is homotopic to a point in  $U$ , then  $\int_\gamma f = 0$ . Also, it is said that an open set  $U \subset M_C$  is *simply connected* if it is connected and if every closed path in  $U$  is homotopic to a point.

In the previous example we found that

$$\frac{1}{2\pi i} \int_\gamma \frac{1}{z} dz = 1,$$

if  $\gamma$  is a circle around the origin, oriented counterclockwise. Now we define for any closed path  $\gamma$  its *winding number* with respect to a point  $\alpha$  to be

$$W(\gamma, \alpha) = \frac{1}{2\pi i} \int_\gamma \frac{1}{z - \alpha} dz,$$

provided the path does not pass through  $\alpha$ . If  $\gamma$  is a closed path, then  $W(\gamma, \alpha)$  is an integer.

A closed path  $\gamma \in U \subset M_C$  is *homologous to 0 in U* if

$$\int_\gamma \frac{1}{z - \alpha} dz = 0,$$

for every point  $\alpha$  not in  $U$ , or in other words,  $W(\gamma, \alpha) = 0$  for every such point.

Similarly, let  $\gamma, \eta$  be closed paths in an open set  $U \subset M_C$ . We say that they are *homologous in  $U$* , and write  $\gamma \sim \eta$ , if  $W(\gamma, \alpha) = W(\eta, \alpha)$  for every point  $\alpha$  in the complement of  $U$ . We say that  $\gamma$  is *homologous to 0 in  $U$* , and write  $\gamma \sim 0$ , if  $W(\gamma, \alpha) = 0$  for every point  $\alpha$  in the complement of  $U$ .

If  $\gamma$  and  $\eta$  are closed paths in  $U$  and are homotopic, then they are homologous. If  $\gamma$  and  $\eta$  are closed paths in  $U$  and are close together, then they are homologous.

Let  $\gamma_1, \dots, \gamma_n$  be curves in an open set  $U \subset M_C$ , and let  $m_1, \dots, m_n$  be integers. A formal sum  $\gamma = m_1\gamma_1 + \dots + m_n\gamma_n = \sum_{i=1}^n m_i\gamma_i$  is called a *chain in  $U$* . The chain is called *closed* if it is a finite sum of closed paths. If  $\gamma$  is the chain as above, then  $\int_\gamma f = \sum_i m_i \int_{\gamma_i} f$ . If  $\gamma$  and  $\eta$  are closed chains in  $U$ , then  $W(\gamma + \eta, \alpha) = W(\gamma, \alpha) + W(\eta, \alpha)$ . We say that  $\gamma$  and  $\eta$  are *homologous in  $U$* , and write  $\gamma \sim \eta$ , if  $W(\gamma, \alpha) = W(\eta, \alpha)$  for every point  $\alpha$  in the complement of  $U$ . We say that  $\gamma$  is *homologous to 0 in  $U$* , and write  $\gamma \sim 0$ , if  $W(\gamma, \alpha) = 0$  for every point  $\alpha$  in the complement of  $U$ .

*Cauchy's theorem* states that if  $\gamma$  is a closed chain in an open set  $U \subset M_C$ , and  $\gamma$  is homologous to 0 in  $U$ , then  $\int_\gamma f = 0$ . If  $\gamma$  and  $\eta$  are closed chains in  $U$ , and  $\gamma \sim \eta$  in  $U$ , then  $\int_\gamma f = \int_\eta f$ .

It follows from Cauchy's theorem that if  $\gamma$  and  $\eta$  are homologous, then  $\int_\gamma f = \int_\eta f$  for all holomorphic functions  $f$  on  $U$  [AM78, Wig90].

### Library of Basic Hamiltonian Systems

In this subsection, mainly following [Put93], we present some basic Hamiltonian systems used by human-like biomechanics.

#### 1D Harmonic Oscillator

In this case we have  $\{p, q\}$  as canonical coordinates on  $\mathbb{R}^2$

$$\begin{aligned} M &= T^*\mathbb{R} \simeq \mathbb{R}^2, & \omega &= dp \wedge dq, \\ H &= \frac{1}{2}(p^2 + y), & X_H &= p \frac{\partial}{\partial q} - q \frac{\partial}{\partial p}, \end{aligned}$$

and Hamilton's equations read

$$\dot{q} = p, \quad \dot{p} = -q.$$

For each  $f, g \in C^k(\mathbb{R}^2, \mathbb{R})$  the Poisson bracket is given by

$$\{f, g\}_\omega = \frac{\partial f}{\partial q} \frac{\partial g}{\partial p} - \frac{\partial f}{\partial p} \frac{\partial g}{\partial q}.$$

*Complex Plane*

Let  $T^*\mathbb{R} \simeq \mathbb{R}^2$  have the canonical symplectic structure  $\omega = dp \wedge dq$ . Writing  $z = q + ip$ , we have

$$\omega = \frac{1}{2i} dz \wedge d\bar{z}, \quad X_H = i \left( \frac{\partial H}{\partial z} \frac{\partial}{\partial z} - \frac{\partial H}{\partial \bar{z}} \frac{\partial}{\partial \bar{z}} \right),$$

$$\{f, g\}_\omega = \frac{i}{2} \left( \frac{\partial f}{\partial z} \frac{\partial g}{\partial \bar{z}} - \frac{\partial f}{\partial \bar{z}} \frac{\partial g}{\partial z} \right),$$

so, the Hamilton's equations,  $\dot{q} = \partial_p H$ ,  $\dot{p} = -\partial_q H$ , become

$$\dot{z} = -2i \frac{\partial H}{\partial \bar{z}}.$$

*2D Harmonic Oscillator*

In this case we have  $\{q^1, y, p_1, p_2\}$  as canonical coordinates on  $\mathbb{R}^4$

$$M = T^*\mathbb{R}^2 \simeq \mathbb{R}^4, \quad \omega = dp_1 \wedge dq^1 + dp_2 \wedge dq^2,$$

$$H = \frac{1}{2} [p_1^2 + p_2^2 + (q^1)^2 + (y)^2].$$

The functions  $f = p_i p_j + q^i q^j$  and  $g = p_i q^j + p_j q^i$ , (for  $i, j = 1, 2$ ), are constants of motion.

*nD Harmonic Oscillator*

In this case we have ( $i = 1, \dots, n$ )

$$M = T^*\mathbb{R}^n \simeq \mathbb{R}^{2n}, \quad \omega = dp_i \wedge dq^i,$$

$$H = \frac{1}{2} \sum_{i=1}^n [p_i^2 + (q^i)^2].$$

The system is integrable in an open set of  $T^*\mathbb{R}^n$  with:

$$K_1 = H, \quad K_2 = p_2^2 + (y)^2, \quad \dots, \quad K_n = p_n^2 + (q^n)^2.$$

*Toda Molecule*

Consider three mass-points on the line with coordinates  $q^i$ , ( $i = 1, 2, 3$ ), and satisfying the ODEs:

$$\ddot{q}^i = -\partial_{q^i} U, \quad \text{where} \quad U = e^{q^1 - q^2} + e^{q^2 - q^3} - e^{q^3 - q^1}.$$

This is a Hamiltonian system with  $\{q^i, p_i\}$  as canonical coordinates on  $\mathbb{R}^6$ ,

$$M = T^*\mathbb{R}^3 \simeq \mathbb{R}^6, \quad \omega = dp_i \wedge dq^i,$$

$$H = \frac{1}{2} (p_1^2 + p_2^2 + p_3^2) + U.$$

The Toda molecule (3.2.1) is an integrable Hamiltonian system in an open set of  $T^*\mathbb{R}^3$  with:

$$\begin{aligned} K_1 &= H, & K_2 &= p_1 + p_2 + p_3, \\ K_3 &= \frac{1}{9} (p_1 + p_2 + p_3) (p_2 + p_3 - 2p_1) (p_3 + p_1 - 2p_2) - (p_1 + p_2 - 2p_3) e^{q^1 - q^2} \\ &\quad - (p_2 + p_3 - 2p_1) e^{q^2 - q^3} - (p_3 + p_1 - 2p_2) e^{q^3 - q^1}. \end{aligned}$$

### 3-Point Vortex Problem

The motion of three-point vortices for an ideal incompressible fluid in the plane is given by the equations:

$$\begin{aligned} \dot{q}^j &= -\frac{1}{2\pi} \sum_{i \neq j} \Gamma_i (p_j - p_i) / r_{ij}^2, \\ \dot{p}_j &= \frac{1}{2\pi} \sum_{i \neq j} \Gamma_i (q^i - q^j) / r_{ij}^2, \\ r_{ij}^2 &= (q^i - q^j)^2 + (p_j - p_i)^2, \end{aligned}$$

where  $i, j = 1, 2, 3$ , and  $\Gamma_i$  are three nonzero constants. This mechanical system is Hamiltonian if we take:

$$\begin{aligned} M &= T^*\mathbb{R}^3 \simeq \mathbb{R}^6, & \omega &= dp_i \wedge dq^i, & (i = 1, \dots, 3), \\ H &= -\frac{1}{4\pi} \sum_{i,j=1}^3 \Gamma_i \Gamma_j \ln(r_{ij}). \end{aligned}$$

Moreover, it is integrable in an open set of  $T^*\mathbb{R}^3$  with:

$$\begin{aligned} K_1 &= H, & K_2 &= \sum_{i=1}^3 \Gamma_i \left[ (q^i)^2 + p_i^2 \right], \\ K_3 &= \left( \sum_{i=1}^3 \Gamma_i q^i \right)^2 + K_2^2. \end{aligned}$$

### The Newton's Second Law as a Hamiltonian System

In the case of conservative forces, Newton's law of motion can be written on  $\mathbb{R}^{3n}$  as

$$m_i \ddot{q}^i = -\partial_{q^i} U, \quad (i = 1, 2, \dots, 3n).$$

Its symplectic formulation reads:

$$\begin{aligned} M &= T^*\mathbb{R}^3 \simeq \mathbb{R}^6, & \omega &= dp_i \wedge dq^i, \\ H &= \sum_{i=1}^{3n} \frac{p_i^2}{2m_i} + U. \end{aligned}$$

The Hamiltonian vector-field  $X_H$  is

$$X_H = \left( \frac{p_i}{m_i} \partial_{q^i} - \partial_{q^i} U \partial_{p_i} \right),$$

giving the Hamilton's equations

$$\dot{q}^i = \frac{p_i}{m_i}, \quad \dot{p}_i = -\partial_{q^i} U.$$

### *Rigid Body*

The configuration space of the *rigid body* is  $SO(3)$ , the group of proper orthogonal transformations of  $\mathbb{R}^3$  to itself, while the corresponding phase-space is its cotangent bundle,  $T^*SO(3)$ . The motion of a rigid body is a *geodesic* with respect to a *left-invariant Riemannian metric* (the inertia tensor) on  $SO(3)$ . The *momentum map*  $J : P \rightarrow \mathbb{R}^3$  for the *left*  $SO(3)$ -action is *right* translation to the identity. We identify  $\mathfrak{so}(3)^*$  with  $\mathfrak{so}(3)$  via the *Killing form* and identify  $\mathbb{R}^3$  with  $\mathfrak{so}(3)$  via the map  $v \mapsto \hat{v}$ , where  $\hat{v}(w) = v \times w$  ( $\times$  being the standard cross product). Points in  $\mathfrak{so}(3)^*$  are regarded as the left reduction of  $T^*SO(3)$  by  $G = SO(3)$  and are the angular momenta as seen from a *body-fixed frame*.

### *A Segment of a Human-Like Body*

A *rigid body with a fixed point* is a basic model of a single segment of the human (or robot) body. This is a left-invariant Hamiltonian mechanical system on the phase-space  $T^*SO(3)$ . The differentiable structure on  $SO(3)$  is defined using the traditional Euler angles  $\{\varphi, \psi, \theta\}$ .

More precisely, a local chart is given by [Put93]

$$(\varphi, \psi, \theta) \in \mathbb{R}^3 \mapsto A \in SO(3), \quad 0 < \varphi, \psi < 2\pi; \quad 0 < \theta < \pi,$$

where

$$A = \begin{bmatrix} \cos \psi \cos \varphi - \cos \theta \sin \varphi \sin \psi & \cos \psi \cos \varphi + \cos \theta \cos \varphi \sin \psi & \sin \theta \sin \psi \\ -\sin \psi \cos \varphi - \cos \theta \sin \varphi \sin \psi & -\sin \psi \sin \varphi + \cos \theta \cos \varphi \cos \psi & \sin \theta \cos \psi \\ \sin \theta \sin \varphi & -\sin \theta \cos \varphi & \cos \theta \end{bmatrix}$$

The corresponding conjugate momenta are denoted by  $p_\varphi, p_\psi, p_\theta$ , so  $\{\varphi, \psi, \theta, p_\varphi, p_\psi, p_\theta\}$  is the phase-space  $T^*SO(3)$ . Thus, we have

$$M = T^*SO(3), \quad \omega = dp_\varphi \wedge d\varphi + dp_\psi \wedge d\psi + dp_\theta \wedge d\theta, \quad H = \frac{1}{2}K,$$

$$K = \frac{[(p_\varphi - p_\psi \cos \theta) \sin \psi + p_\theta \sin \theta \cos \psi]^2}{I_1 \sin^2 \theta} + \frac{[(p_\varphi - p_\psi \cos \theta) \cos \psi - p_\theta \sin \theta \sin \psi]^2}{I_2 \sin^2 \theta} + \frac{p_\psi^2}{I_3},$$

where  $I_1, I_2, I_3$  are the moments of inertia, diagonalizing the inertia tensor of the body.

The Hamilton's equations are

$$\begin{aligned}\dot{\varphi} &= \frac{\partial H}{\partial p_\varphi}, & \dot{\psi} &= \frac{\partial H}{\partial p_\psi}, & \dot{\theta} &= \frac{\partial H}{\partial p_\theta}, \\ \dot{p}_\varphi &= -\frac{\partial H}{\partial \varphi}, & \dot{p}_\psi &= -\frac{\partial H}{\partial \psi}, & \dot{p}_\theta &= -\frac{\partial H}{\partial \theta}.\end{aligned}$$

For each  $f, g \in C^k(T^*SO(3), \mathbb{R})$  the Poisson bracket is given by

$$\begin{aligned}\{f, g\}_\omega &= \frac{\partial f}{\partial \varphi} \frac{\partial g}{\partial p_\varphi} - \frac{\partial f}{\partial p_\varphi} \frac{\partial g}{\partial \varphi} + \frac{\partial f}{\partial \psi} \frac{\partial g}{\partial p_\psi} - \frac{\partial f}{\partial p_\psi} \frac{\partial g}{\partial \psi} \\ &+ \frac{\partial f}{\partial \theta} \frac{\partial g}{\partial p_\theta} - \frac{\partial f}{\partial p_\theta} \frac{\partial g}{\partial \theta}.\end{aligned}$$

*The Heavy Top – Continued*

Recall (see (6.24) above) that the heavy top is by definition a rigid body moving about a fixed point in a 3D space [Put93]. The rigidity of the top means that the distances between points of the body are fixed as the body moves. In this case we have

$$\begin{aligned}M &= T^*SO(3), \\ \omega &= dp_\varphi \wedge d\varphi + dp_\psi \wedge d\psi + dp_\theta \wedge d\theta, \\ H &= \frac{1}{2}K + mgl \cos \theta, \\ K &= \frac{[(p_\varphi - p_\psi \cos \theta) \sin \psi + p_\theta \sin \theta \cos \psi]^2}{I_1 \sin^2 \theta} \\ &+ \frac{[(p_\varphi - p_\psi \cos \theta) \cos \psi - p_\theta \sin \theta \sin \psi]^2}{I_2 \sin^2 \theta} + \frac{p_\psi^2}{I_3},\end{aligned}$$

where  $I_1, I_2, I_3$  are the moments of inertia,  $m$  is the total mass,  $g$  is the gravitational acceleration and  $l$  is the length of the vector determining the center of mass at  $t = 0$ .

The Hamilton's equations are

$$\begin{aligned}\dot{\varphi} &= \frac{\partial H}{\partial p_\varphi}, & \dot{\psi} &= \frac{\partial H}{\partial p_\psi}, & \dot{\theta} &= \frac{\partial H}{\partial p_\theta}, \\ \dot{p}_\varphi &= -\frac{\partial H}{\partial \varphi}, & \dot{p}_\psi &= -\frac{\partial H}{\partial \psi}, & \dot{p}_\theta &= -\frac{\partial H}{\partial \theta}.\end{aligned}$$

For each  $f, g \in C^k(T^*SO(3), \mathbb{R})$  the Poisson bracket is given by

$$\begin{aligned}\{f, g\}_\omega &= \frac{\partial f}{\partial \varphi} \frac{\partial g}{\partial p_\varphi} - \frac{\partial f}{\partial p_\varphi} \frac{\partial g}{\partial \varphi} + \frac{\partial f}{\partial \psi} \frac{\partial g}{\partial p_\psi} - \frac{\partial f}{\partial p_\psi} \frac{\partial g}{\partial \psi} \\ &+ \frac{\partial f}{\partial \theta} \frac{\partial g}{\partial p_\theta} - \frac{\partial f}{\partial p_\theta} \frac{\partial g}{\partial \theta}.\end{aligned}$$

The Hamiltonian  $H$  is invariant under rotations about the  $z$ -axis, i.e.,  $\varphi$  is a cyclic variable, so  $p_\varphi$  is a constant of motion. The momentum map for this  $S^1$ -action is  $J(\varphi, \psi, \theta, p_\varphi, p_\psi, p_\theta) = p_\varphi$ . The reduced phase-space  $J^{-1}(p_\varphi)/S^1$  can be identified with  $T^*S^2$  and it is parameterized by  $\{\psi, \theta, p_\psi, p_\theta\}$ . The equations of motion for  $\psi, \theta$  are just Hamilton's equations for  $H$  with  $p_\varphi$  held constant.

### Two Coupled Pendula

The configuration space of the system of two coupled pendula in the plane is  $T^2 = \{(\theta_1, \theta_2)\}$ , where the  $\theta$ s are the two pendulum angles, the phase-space is  $T^*T^2$  with its canonical symplectic structure and the Hamiltonian  $H$  is given by [Put93]

$$H = \frac{1}{2}(p_\varphi^2 + p_\psi^2) + V(\sqrt{2}\psi),$$

where

$$\varphi = \frac{\theta_1 + \theta_2}{\sqrt{2}}, \quad \psi = \frac{\theta_1 - \theta_2}{\sqrt{2}}.$$

The group  $S^1$  acts on  $T^2$  by

$$\theta \cdot (\theta_1 + \theta_2) = (\theta + \theta_1, \theta + \theta_2)$$

and hence the induced momentum map for the lifted action to  $T^*T^2$  is given by

$$J(\varphi, \psi, p_\varphi, p_\psi) = p_\varphi.$$

Therefore, the reduced phase-space  $J^{-1}(p_\varphi)/S^1$  is symplectically diffeomorphic to  $T^*S^1$  with its canonical symplectic structure  $\omega_\mu = dp_\psi \wedge d\psi$ . The reduced Hamiltonian  $H_\mu$  is

$$H_\mu = \frac{1}{2}p_\psi^2 + V(\sqrt{2}\psi),$$

and Hamilton's equations for  $H_\mu$  are

$$\dot{\psi} = p_\psi, \quad \dot{p}_\psi = -\sqrt{2}\dot{V}(\sqrt{2}\psi).$$

### The Plane 2-Body Problem

The plane two body problem can be formulated as the triple  $(M, \omega, H)$  where [Put93]

$$\begin{aligned} M &= T^*((0, \infty) \times S^1), & \omega &= dp_r \wedge dr + dp_\theta \wedge d\theta, \\ H &= (p_r^2 + p_\theta^2)/r^2 - 1/r. \end{aligned}$$

The Lie group  $G = SO(2) \simeq S^1$  acts on the configuration space  $M = (0, \infty) \times S^1$  by rotations, i.e., if  $R_\varphi \in SO(2)$  then

$$\phi : (R_\varphi, (r, \theta)) \mapsto (r, \theta + \varphi, p_r, p_\theta).$$

The corresponding momentum map is

$$J(r, \theta, p_r, p_\theta) = p_\theta.$$

*The 3-Body Problem*

There is a vast literature on the *restricted three-body problem* (see [MH92]). Among other things, there are investigations of the equilibriums points and their stability, investigations of the existence, stability and bifurcation of periodic orbits, and investigations of collisions and ejection orbits. The restricted problem is said to be a limit of the *full three-body problem* as one of the masses tends to zero, and so to each result for the restricted problem there should be a corresponding result for the full three-body problem.

The restricted three-body problem is a Hamiltonian system of differential equations which describes the motion of an infinitesimal particle (the *satellite*) moving under the gravitational influence of two particles of finite mass (the *primaries*) which are moving on a circular orbit of the Kepler problem [MS00].

Since the motion of the primaries is given, the restricted problem has two DOF for the planar problem and three DOF for the spatial problem. However, the full problem has six DOF in the planar case and nine DOF in the spatial case. Thus, at first the restricted problem seems too small to reflect the full complexity of the full problem; but when the symmetries of the full problem are taken into account the dimension gap narrows considerably.

The Hamiltonian of the full problem is invariant under Euclidean motions, i.e., translations and rotations, which begets the integrals of linear and angular momentum. Translations and rotations give rise to ignorable coordinates. Holding the integrals fixed and dropping the ignorable coordinates reduces the full problem from six to three DOF in the planar case and from nine to four DOF in the spatial case. Thus the full problem on the reduced space is only one DOF larger than the restricted problem in either the planar or the spatial case [MS00].

The full 3-body problem in 3D space has 9 DOF. By placing the center of mass at the origin and setting linear momentum equal to zero the problem reduces one with six DOF. This is easily done using Jacobi coordinates. The Hamiltonian of the full 3-body problem in rotating (about the  $z$ -axis) Jacobi coordinates  $(u_0, u_1, u_2, v_0, v_1, v_2)$  is

$$H = \frac{\|v_0\|^2}{2M_0} - u_0^T J v_0 + \frac{\|v_1\|^2}{2M_1} - u_1^T J v_1 - \frac{m_0 m_1}{\|u_1\|} \\ + \frac{\|v_2\|^2}{2M_2} - u_2^T J v_2 - \frac{m_1 m_2}{\|u_2 - \alpha_0 u_1\|} - \frac{m_2 m_0}{\|u_2 + \alpha_1 u_1\|}$$

where  $u_i, v_i \in \mathbb{R}^3$ ,

$$M_0 = m_0 + m_1 + m_2, \quad M_1 = m_0 m_1 / (m_0 + m_1), \\ M_2 = m_2 (m_0 + m_1) / (m_0 + m_1 + m_2), \\ \alpha_0 = m_0 / (m_0 + m_1), \quad \alpha_1 = m_1 / (m_0 + m_1),$$

and  $J = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ . In these coordinates  $u_0$  is the center of mass,  $v_0$  is total linear momentum, and total angular momentum is

$$A = u_0 \times v_0 + u_1 \times v_1 + u_2 \times v_2.$$

See [MH92] for further details.

### n-DOF Hamiltonian Dynamics

Classically,  $n$ -DOF Hamiltonian dynamics combines the ideas of differential equations and variational principles (see [AM78, Arn89, MR99, Wig90]). As Hamilton first realized, many of the systems of mechanics and optics can be put into the special form (compare (3.10))

$$\dot{q}^i = \frac{\partial H}{\partial p_i}(q^i, p_i, t), \quad \dot{p}_i = -\frac{\partial H}{\partial q^i}(q^i, p_i, t), \quad (i = 1, \dots, n),$$

or an associated variational form (summing upon the repeated index is used in the following text)

$$\delta \int (p_i dq^i - H) dt = 0.$$

Here the state of the system is given as a point  $(q^1, \dots, q^n, p_1, \dots, p_n)$  in *phase-space*, the  $q$ 's are the configuration coordinates, the  $p$ 's are the momenta,  $t$  is time, and  $H = H(q^i, p_i, t)$  is a total-energy function called Hamiltonian. The variables  $(q^i, p_i)$  are called *canonical* coordinates.

If  $H = H(q^i, p_i)$  does not depend explicitly on time, the system is said to be *autonomous*. In this case, it is easy to verify that  $H$  is conserved. The search for other conserved quantities led to a new notion of solving Hamiltonian systems. Instead of finding formulae for the coordinates as a function of time, one searches for constants of the motion (*integrals*). If one can find  $n$  integrals  $I_i(q^i, p_i)$  which are in *involution*:

$$[I_i, I_j] = \frac{\partial I_i}{\partial q^k} \frac{\partial I_j}{\partial p_k} - \frac{\partial I_i}{\partial p_k} \frac{\partial I_j}{\partial q^k} = 0, \quad (i \neq j),$$

(here the square brackets denote the Poisson bracket) and *independent* (the vectors  $\nabla I_i$  are independent 'almost everywhere'), then associated variables  $\phi_i$  can be derived which evolve linearly in time:  $\dot{\phi}^i = \frac{\partial H}{\partial I_i}(I_i)$ .

Such a system is *integrable* in the sense of Liouville [Arn89]. If the sets  $I = \text{const}$  are bounded, then they are  $n$ D *tori*  $T^n$  in phase-space. Choosing irreducible cycles,  $\gamma_i$ , on the tori, one can define a preferred set of integrals  $J_i = \int_{\gamma_i} p_i dq^i$ , called *action variables*, for which the corresponding  $\phi_i$  are *angle variables* mod 1 on  $T^n$ . The quantities  $\omega^i(J) = \frac{\partial H}{\partial J_i}(J_i)$  are called the *frequencies* on  $T^n$ .

Another feature of Hamiltonian systems noticed by Liouville is the preservation of phase-space volume  $\int (dq)^n (dp)^n$ . A more general result is that Poincaré's integral  $\int p_i dq^i$  is conserved around any loop following the flow [Arn89]. This is the property that really distinguishes Hamiltonian differential equations from general ones.

The major problem with the notion of integrability is that *most systems are not integrable*. This was first appreciated when Poincaré proved that the *circular restricted three-body problem has no integral analytic in the mass ratio*. The perturbation expansions which gave excellent predictions of motion of the planets do not converge. The basic reason is that among the invariant tori of integrable systems is a dense subset on which the frequencies  $\omega^i$  are *commensurate*, i.e.  $m_i \omega^i = 0$  for some non-zero integer vector  $m_i$ ; however, most systems have no commensurate tori, because they can be destroyed by arbitrarily small perturbation.

Poincaré went on to examine what really does happen. The key technique he used was geometric analysis: instead of manipulating formulae for canonical transformations as Jacobi and others did, he pictured the *orbits* in phase-space. An important step in this *qualitative theory* of differential equations was the idea of *surface of section*. If  $\Sigma$  is a *codimension-one* surface (i.e., of dimension one less than that of the phase-space) transverse to a *flow*, then the sequence  $\{x_j\}$  of successive intersections of an orbit with  $\Sigma$  provides a lot of information about that orbit. For example, if  $\{x_j\}$  is periodic then it corresponds to a periodic orbit. If  $\{x_j\}$  is confined to a subset of codimension  $m$  on  $\Sigma$  then so is the orbit of the flow, etc.. The flow induces a mapping of  $\Sigma$  to itself; the map takes a point in  $\Sigma$  to the point at which it first returns to  $\Sigma$  (assuming there is one). Since the surface of section has one dimension less than the phase-space it is easier to picture the dynamics of the return map than the flow. In fact, for Hamiltonian systems one can do even better; since  $H$  is conserved,  $\Sigma$  decomposes into a one-parameter family of codimension two surfaces parameterized by the value of the energy, a reduction of two dimensions.

This led Poincaré to the ideas of *stable* and *unstable manifolds* for *hyperbolic* periodic orbits, which are extensions of the stable and unstable *eigenspaces* for associated linear systems, and their intersections, known as *hetero- and homo-clinic points*, whose orbits converge to one periodic orbit in the past and to another (or the same) in the future. He showed that having intersected once, the invariant manifolds must intersect infinitely often. Moreover the existence of one heteroclinic orbit implies the existence of an infinity of others.

The distance between the stable and unstable manifolds can be quantified by Melnikov's integral. This leads to a technique for proving the non-existence of integrals for a slightly perturbed, integrable Hamiltonian.

For integrable systems, nearby orbits separate linearly in time; however, dynamical systems can have exponentially separating orbits. Let  $\delta x$  be a tangent vector at the phase-space point  $x$  and  $\delta x_t$  be the evolved vector following

the orbit of  $x$ . Then, recall from section 2.3 above, the average rate of exponentiality of  $\delta x_t$  is the *Lyapunov exponent*  $\lambda$ ,

$$\lambda(x, \delta x) = \lim_{t \rightarrow \infty} 1/t \ln |\delta x_t|.$$

If  $\lambda$  is nonzero, then the predictions one can make will be valid for a time only logarithmic in the precision. Therefore, although deterministic in principle, a system need not be predictable in practice.

A concrete example of the complexity of behavior of typical Hamiltonian systems is provided by the ‘horseshoe’, a type of invariant set found near homoclinic orbits. Its points can be labelled by doubly infinite sequences of 0’s and 1’s corresponding to which half of a horseshoe shaped set the orbit is in at successive times. For every sequence, no matter how complicated, there is an orbit which has that symbol sequence. This implies, e.g., that a simple pendulum in a sufficiently strongly modulated time–periodic gravitational field has an initial condition such that the pendulum will turn over once each period when there is 1 in the sequence and not if there is a 0 for any sequence of 0’s and 1’s.

### 3.2.2 Hamiltonian Geometry in Human–Like Biomechanics

We will develop our Hamiltonian geometry on the configuration biomechanics manifold  $M$  in three steps, as follows (compare with section (2.6) above):

**Step A** Find a symplectic *momentum phase–space*  $(P, \omega)$ .

Recall that a symplectic structure on a smooth manifold  $M$  is a nondegenerate closed 2–form  $\omega$  on  $M$ , i.e., for each  $x \in M$ ,  $\omega(x)$  is nondegenerate, and  $d\omega = 0$ .

Let  $T_x^*M$  be a cotangent space to  $M$  at  $m$ . The cotangent bundle  $T^*M$  represents a union  $\cup_{m \in M} T_x^*M$ , together with the standard topology on  $T^*M$  and a natural smooth manifold structure, the dimension of which is twice the dimension of  $M$ . A 1–form  $\theta$  on  $M$  represents a section  $\theta : M \rightarrow T^*M$  of the cotangent bundle  $T^*M$ .

$P = T^*M$  is our momentum phase–space. On  $P$  there is a nondegenerate symplectic 2–form  $\omega$  is defined in local joint coordinates  $q^i, p_i \in U$ ,  $U$  open in  $P$ , as  $\omega = dq^i \wedge dp_i$  (‘ $\wedge$ ’ denotes the wedge or exterior product). In that case the coordinates  $q^i, p_i \in U$  are called canonical. In a usual procedure the canonical 1–form  $\theta$  is first defined as  $\theta = p_i dq^i$ , and then the canonical 2–form  $\omega$  is defined as  $\omega = -d\theta$ .

A *symplectic phase–space manifold* is a pair  $(P, \omega)$ .

**Step B** Find a *Hamiltonian vector–field*  $X_H$  on  $(P, \omega)$ .

Let  $(P, \omega)$  be a symplectic manifold. A vector–field  $X : P \rightarrow TP$  is called *Hamiltonian* if there is a smooth function  $F : P \rightarrow \mathbb{R}$  such that  $i_X \omega = dF$  ( $i_X \omega$  denotes the *interior product* or *contraction* of the vector–field  $X$  and the 2–form  $\omega$ ).  $X$  is *locally Hamiltonian* if  $i_X \omega$  is closed.

Let the smooth real-valued *Hamiltonian function*  $H : P \rightarrow \mathbb{R}$ , representing the total biomechanical energy  $H(q, p) = T(p) + V(q)$  ( $T$  and  $V$  denote kinetic and potential energy of the system, respectively), be given in local canonical coordinates  $q^i, p_i \in U$ ,  $U$  open in  $P$ . The *Hamiltonian vector-field*  $X_H$ , condition by  $i_{X_H}\omega = dH$ , is actually defined via symplectic matrix  $J$ , in a local chart  $U$ , as

$$X_H = J\nabla H = (\partial_{p_i}H, -\partial_{q^i}H), \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix},$$

where  $I$  denotes the  $n \times n$  identity matrix and  $\nabla$  is the gradient operator.

**Step C** Find a *Hamiltonian phase-flow*  $\phi_t$  of  $X_H$ .

Let  $(P, \omega)$  be a symplectic phase-space manifold and  $X_H = J\nabla H$  a Hamiltonian vector-field corresponding to a smooth real-valued Hamiltonian function  $H : P \rightarrow \mathbb{R}$ , on it. If a unique one-parameter group of diffeomorphisms  $\phi_t : P \rightarrow P$  exists so that  $\frac{d}{dt}|_{t=0} \phi_t x = J\nabla H(x)$ , it is called the *Hamiltonian phase-flow*.

A smooth curve  $t \mapsto (q^i(t), p_i(t))$  on  $(P, \omega)$  represents an *integral curve* of the Hamiltonian vector-field  $X_H = J\nabla H$ , if in the local canonical coordinates  $q^i, p_i \in U$ ,  $U$  open in  $P$ , *Hamilton's canonical equations* (3.10) hold.

An integral curve is said to be *maximal* if it is not a restriction of an integral curve defined on a larger interval of  $\mathbb{R}$ . It follows from the standard theorem on the *existence* and *uniqueness* of the solution of a system of ODEs with smooth r.h.s., that if the manifold  $(P, \omega)$  is Hausdorff, then for any point  $x = (q^i, p_i) \in U$ ,  $U$  open in  $P$ , there exists a maximal integral curve of  $X_H = J\nabla H$ , passing for  $t = 0$ , through point  $x$ . In case  $X_H$  is complete, i.e.,  $X_H$  is  $C^p$  and  $(P, \omega)$  is compact, the maximal integral curve of  $X_H$  is the Hamiltonian phase-flow  $\phi_t : U \rightarrow U$ .

The phase-flow  $\phi_t$  is *symplectic* if  $\omega$  is constant along  $\phi_t$ , i.e.,  $\phi_t^*\omega = \omega$  ( $\phi_t^*\omega$  denotes the *pull-back* of  $\omega$  by  $\phi_t$ ),  
iff  $\mathcal{L}_{X_H}\omega = 0$

( $\mathcal{L}_{X_H}\omega$  denotes the *Lie derivative* of  $\omega$  upon  $X_H$ ).

Symplectic phase-flow  $\phi_t$  consists of canonical transformations on  $(P, \omega)$ , i.e., diffeomorphisms in canonical coordinates  $q^i, p_i \in U$ ,  $U$  open on all  $(P, \omega)$  which leave  $\omega$  invariant. In this case the *Liouville theorem* is valid:  $\phi_t$  *preserves* the *phase volume* on  $(P, \omega)$ . Also, the system's total energy  $H$  is conserved along  $\phi_t$ , i.e.,  $H \circ \phi_t = H$ .

Recall that the Riemannian metrics  $g = \langle, \rangle$  on the configuration manifold  $M$  is a positive-definite quadratic form  $g : TM \rightarrow \mathbb{R}$ , in local coordinates  $q^i \in U$ ,  $U$  open in  $M$ , given by (3.5–3.6) above. Given the metrics  $g_{ij}$ , the system's Hamiltonian function represents a momentum  $p$ -dependent quadratic form  $H : T^*M \rightarrow \mathbb{R}$  – the system's kinetic energy  $H(p) = T(p) = \frac{1}{2} \langle p, p \rangle$ , in local canonical coordinates  $q^i, p_i \in U_p$ ,  $U_p$  open in  $T^*M$ , given by

$$H(p) = \frac{1}{2} g^{ij}(q, m) p_i p_j, \quad (3.23)$$

where  $g^{ij}(q, m) = g_{ij}^{-1}(q, m)$  denotes the *inverse* (contravariant) material *metric tensor*

$$g^{ij}(q, m) = \sum_{\chi=1}^n m_{\chi} \delta_{rs} \frac{\partial q^i}{\partial x^r} \frac{\partial q^j}{\partial x^s}.$$

$T^*M$  is an *orientable* manifold, admitting the standard *volume form*

$$\Omega_{\omega_H} = \frac{(-1)^{\frac{N(N+1)}{2}}}{N!} \omega_H^N.$$

For Hamiltonian vector-field,  $X_H$  on  $M$ , there is a base integral curve  $\gamma_0(t) = (q^i(t), p_i(t))$  iff  $\gamma_0(t)$  is a *geodesic*, given by the one-form *force equation*

$$\dot{p}_i \equiv \dot{p}_i + \Gamma_{jk}^i g^{jl} g^{km} p_l p_m = 0, \quad \text{with} \quad \dot{q}^k = g^{ki} p_i, \quad (3.24)$$

where  $\Gamma_{jk}^i$  denote *Christoffel symbols* of an *affine Levi-Civita connection* on  $M$ , defined upon the *Riemannian metric*  $g = \langle, \rangle$  by (3.9).

The l.h.s  $\dot{p}_i$  of the covariant momentum equation (3.24) represents the *intrinsic* or *Bianchi covariant derivative* of the momentum with respect to time  $t$ . Basic relation  $\dot{p}_i = 0$  defines the *parallel transport* on  $T^N$ , the simplest form of human-motion dynamics. In that case Hamiltonian vector-field  $X_H$  is called the *geodesic spray* and its phase-flow is called the *geodesic flow*.

For Earthly dynamics in the gravitational *potential* field  $V : M \rightarrow \mathbb{R}$ , the Hamiltonian  $H : T^*M \rightarrow \mathbb{R}$  (3.23) extends into potential form

$$H(p, q) = \frac{1}{2} g^{ij} p_i p_j + V(q),$$

with Hamiltonian vector-field  $X_H = J\nabla H$  still defined by canonical equations (3.10).

A general form of a *driven*, non-conservative Hamilton's equations reads:

$$\dot{q}^i = \partial_{p_i} H, \quad \dot{p}_i = F_i - \partial_{q^i} H, \quad (3.25)$$

where  $F_i = F_i(t, q, p)$  represent any kind of joint-driving *covariant torques*, including active neuro-muscular-like controls, as functions of time, angles and momenta, as well as passive dissipative and elastic joint torques. In the covariant momentum formulation (3.24), the non-conservative Hamilton's equations (3.25) become

$$\dot{p}_i \equiv \dot{p}_i + \Gamma_{jk}^i g^{jl} g^{km} p_l p_m = F_i, \quad \text{with} \quad \dot{q}^k = g^{ki} p_i.$$

### 3.2.3 Hamilton-Poisson Geometry in Biomechanics

Now, instead of using symplectic structures arising in Hamiltonian biomechanics, we propose the more general *Poisson manifold*  $(\mathfrak{g}^*, \{F, G\})$ . Here  $\mathfrak{g}^*$  is a

chosen Lie algebra with a  $(\pm)$  *Lie-Poisson bracket*  $\{F, G\}_{\pm}(\mu)$  and carries an abstract *Poisson evolution equation*  $\dot{F} = \{F, H\}$ . This approach is well-defined in both the finite- and the infinite-dimensional case. It is equivalent to the strong symplectic approach when this exists and offers a viable formulation for Poisson manifolds which are not symplectic (for technical details, see see [Wei90, AMR88, MR99, Put93, IP01a]).

Let  $E_1$  and  $E_2$  be Banach spaces. A continuous bilinear functional  $\langle, \rangle: E_1 \times E_2 \rightarrow \mathbb{R}$  is nondegenerate if  $\langle x, y \rangle = 0$  implies  $x = 0$  and  $y = 0$  for all  $x \in E_1$  and  $y \in E_2$ . We say  $E_1$  and  $E_2$  are in *duality* if there is a nondegenerate bilinear functional  $\langle, \rangle: E_1 \times E_2 \rightarrow \mathbb{R}$ . This functional is also referred to as an  $L^2$ -pairing of  $E_1$  with  $E_2$ .

Recall that a *Lie algebra* consists of a vector space  $\mathfrak{g}$  (usually a Banach space) carrying a bilinear skew-symmetric operation  $[\cdot, \cdot]: \mathfrak{g} \times \mathfrak{g} \rightarrow \mathfrak{g}$ , called the *commutator* or Lie bracket. This represents a pairing  $[\xi, \eta] = \xi\eta - \eta\xi$  of elements  $\xi, \eta \in \mathfrak{g}$  and satisfies *Jacobi identity*

$$[[\xi, \eta], \mu] + [[\eta, \mu], \xi] + [[\mu, \xi], \eta] = 0.$$

Let  $\mathfrak{g}$  be a (finite- or infinite-dimensional) Lie algebra and  $\mathfrak{g}^*$  its dual Lie algebra, that is, the vector space  $L^2$  paired with  $\mathfrak{g}$  via the inner product  $\langle, \rangle: \mathfrak{g}^* \times \mathfrak{g} \rightarrow \mathbb{R}$ . If  $\mathfrak{g}$  is finite-dimensional, this pairing reduces to the usual action (interior product) of forms on vectors. The standard way of describing any finite-dimensional Lie algebra  $\mathfrak{g}$  is to provide its  $n^3$  *structural constants*  $\gamma_{ij}^k$ , defined by  $[\xi_i, \xi_j] = \gamma_{ij}^k \xi_k$ , in some basis  $\xi_i$ ,  $(i = 1, \dots, n)$

For any two smooth functions  $F: \mathfrak{g}^* \rightarrow \mathbb{R}$ , we define the *Fréchet derivative*  $D$  on the space  $L(\mathfrak{g}^*, \mathbb{R})$  of all linear diffeomorphisms from  $\mathfrak{g}^*$  to  $\mathbb{R}$  as a map  $DF: \mathfrak{g}^* \rightarrow L(\mathfrak{g}^*, \mathbb{R})$ ;  $\mu \mapsto DF(\mu)$ . Further, we define the *functional derivative*  $\delta F/\delta\mu \in \mathfrak{g}$  by

$$DF(\mu) \cdot \delta\mu = \langle \delta\mu, \frac{\delta F}{\delta\mu} \rangle$$

with arbitrary ‘variations’  $\delta\mu \in \mathfrak{g}^*$ .

For any two smooth functions  $F, G: \mathfrak{g}^* \rightarrow \mathbb{R}$ , we define the  $(\pm)$  *Lie-Poisson bracket* by

$$\{F, G\}_{\pm}(\mu) = \pm \langle \mu, \left[ \frac{\delta F}{\delta\mu}, \frac{\delta G}{\delta\mu} \right] \rangle. \quad (3.1)$$

Here  $\mu \in \mathfrak{g}^*$ ,  $[\xi, \mu]$  is the Lie bracket in  $\mathfrak{g}$  and  $\delta F/\delta\mu, \delta G/\delta\mu \in \mathfrak{g}$  are the functional derivatives of  $F$  and  $G$ .

The  $(\pm)$  Lie-Poisson bracket (3.1) is clearly a bilinear and skew-symmetric operation. It also satisfies the Jacobi identity

$$\{\{F, G\}, H\}_{\pm}(\mu) + \{\{G, H\}, F\}_{\pm}(\mu) + \{\{H, F\}, G\}_{\pm}(\mu) = 0$$

thus confirming that  $\mathfrak{g}^*$  is a Lie algebra, as well as Leibniz’ rule

$$\{FG, H\}_{\pm}(\mu) = F\{G, H\}_{\pm}(\mu) + G\{F, H\}_{\pm}(\mu). \quad (3.26)$$

If  $\mathbf{g}$  is a finite-dimensional phase-space manifold with structure constants  $\gamma_{ij}^k$ , the  $(\pm)$  Lie-Poisson bracket (3.26) becomes

$$\{F, G\}_{\pm}(\mu) = \pm \mu_k \gamma_{ij}^k \frac{\delta F}{\delta \mu_i} \frac{\delta G}{\delta \mu_j}. \quad (3.27)$$

The  $(\pm)$  Lie-Poisson bracket represents a Lie-algebra generalization of the classical finite-dimensional Poisson bracket  $[F, G] = \omega(X_f, X_g)$  on the symplectic phase-space manifold  $(P, \omega)$  for any two real-valued smooth functions  $F, G : P \rightarrow \mathbb{R}$ .

As in the classical case, any two smooth functions  $F, G : \mathbf{g}^* \rightarrow \mathbb{R}$  are *in involution* if  $\{F, G\}_{\pm}(\mu) = 0$ .

The Lie-Poisson theorem states that a Lie algebra  $\mathbf{g}^*$  with a  $\pm$  Lie-Poisson bracket  $\{F, G\}_{\pm}(\mu)$  represents a Poisson manifold  $(\mathbf{g}^*, \{F, G\}_{\pm}(\mu))$ .

Given a smooth Hamiltonian function  $H : \mathbf{g}^* \rightarrow \mathbb{R}$  on the Poisson manifold  $(\mathbf{g}^*, \{F, G\}_{\pm}(\mu))$ , the time evolution of any smooth function  $F : \mathbf{g}^* \rightarrow \mathbb{R}$  is given by the abstract *Poisson evolution equation*

$$\dot{F} = \{F, H\}. \quad (3.28)$$

### Hamilton-Poisson Biomechanical Systems

Let  $(P, \{\})$  be a Poisson manifold and  $H \in C^k(P, \mathbb{R})$  a smooth real valued function on  $P$ . The vector-field  $X_H$  defined by

$$X_H(F) = \{F, H\},$$

is the Hamiltonian vector-field with energy function  $H$ . The triple  $(P, \{\}, H)$  we call the *Hamilton-Poisson biomechanical system* (HPBS) [MR99, Put93, IP01a]. The map  $F \mapsto \{F, H\}$  is a derivation on the space  $C^k(P, \mathbb{R})$ , hence it defines a vector-field on  $P$ . The map  $F \in C^k(P, \mathbb{R}) \mapsto X_F \in \mathcal{X}(P)$  is a Lie algebra anti-homomorphism, i.e.,  $[X_F, X_g] = -X_{\{F, g\}}$ .

Let  $(P, \{\}, H)$  be a HPBS and  $\phi_t$  the flow of  $X_H$ . Then for all  $F \in C^k(P, \mathbb{R})$  we have the *conservation of energy*:

$$H \circ \phi_t = H,$$

and the *equations of motion in Poisson bracket form*,

$$\frac{d}{dt}(F \circ \phi_t) = \{F, H\} \circ \phi_t = \{F \circ \phi_t, H\},$$

that is, the above Poisson evolution equation (3.28) holds. Now, the function  $F$  is constant along the integral curves of the Hamiltonian vector-field  $X_H$  iff

$$\{F, H\} = 0.$$

$\phi_t$  preserves the Poisson structure.

Next we present two main examples of HPBS.

*'Ball-and-Socket' Joint Dynamics in Euler Vector Form*

The dynamics of human body-segments, classically modelled *via* Lagrangian formalism (see 3.1.1 as well as [Hat77b, Iva91]), may be also prescribed by Euler's equations of rigid body dynamics. The equations of motion for a free rigid body, described by an observer fixed on the moving body, are usually given by *Euler's vector equation*

$$\dot{p} = p \times w. \quad (3.29)$$

Here  $p, w \in \mathbb{R}^3$ ,  $p_i = I_i w_i$  and  $I_i$  ( $i = 1, 2, 3$ ) are the principal moments of inertia, the coordinate system in the segment is chosen so that the axes are principal axes,  $w$  is the angular velocity of the body and  $p$  is the corresponding angular momentum.

The kinetic energy of the segment is the Hamiltonian function  $H : \mathbb{R}^3 \rightarrow \mathbb{R}$  given by [IP01a]

$$H(p) = \frac{1}{2} p \cdot w$$

and is a conserved quantity for (3.29).

The vector space  $\mathbb{R}^3$  is a Lie algebra with respect to the bracket operation given by the usual cross product. The space  $\mathbb{R}^3$  is paired with itself *via* the usual dot product. So if  $F : \mathbb{R}^3 \rightarrow \mathbb{R}$ , then  $\delta F / \delta p = \nabla F(p)$  and the  $(-)$  Lie-Poisson bracket  $\{F, G\}_-(p)$  is given *via* (3.27) by the triple product

$$\{F, G\}_-(p) = -p \cdot (\nabla F(p) \times \nabla G(p)).$$

Euler's vector equation (3.29) represents a generalized Hamiltonian system in  $\mathbb{R}^3$  relative to the Hamiltonian function  $H(p)$  and the  $(-)$  Lie-Poisson bracket  $\{F, G\}_-(p)$ . Thus the Poisson manifold  $(\mathbb{R}^3, \{F, G\}_-(p))$  is defined and the abstract Poisson equation is equivalent to Euler's equation (3.29) for a body segment and associated joint.

*Solitary Model of Muscular Contraction*

The basis of the molecular model of muscular contraction (see Appendix) is oscillations of Amid I peptide groups with associated dipole electric momentum inside a spiral structure of myosin filament molecules (see [Dav81, Dav91]).

There is a simultaneous resonant interaction and strain interaction generating a collective interaction directed along the axis of the spiral. The resonance excitation jumping from one peptide group to another can be represented as an exciton, the local molecule strain caused by the static effect of excitation as a phonon and the resultant collective interaction as a *soliton*.

The simplest model of Davydov's solitary particle-waves is given by the *nonlinear Schrödinger equation* [IP01a]

$$i\partial_t \psi = -\partial_{x^2} \psi + 2\chi |\psi|^2 \psi, \quad (3.30)$$

for  $-\infty < x < +\infty$ . Here  $\psi(x, t)$  is a smooth complex-valued wave function with initial condition  $\psi(x, t)|_{t=0} = \psi(x)$  and  $\chi$  is a nonlinear parameter. In the linear limit ( $\chi = 0$ ) (3.30) becomes the ordinary Schrödinger equation for the wave function of the free 1D particle with mass  $m = 1/2$ .

We may define the infinite-dimensional phase-space manifold  $\mathcal{P} = \{(\psi, \bar{\psi}) \in S(\mathbb{R}, \mathbf{C})\}$ , where  $S(\mathbb{R}, \mathbf{C})$  is the Schwartz space of rapidly-decreasing complex-valued functions defined on  $\mathbb{R}$ . We define also the algebra  $\chi(\mathcal{P})$  of observables on  $\mathcal{P}$  consisting of real-analytic functional derivatives  $\delta F/\delta\psi, \delta F/\delta\bar{\psi} \in S(\mathbb{R}, \mathbf{C})$ .

The Hamiltonian function  $H : \mathcal{P} \rightarrow \mathbb{R}$  is given by

$$H(\psi) = \int_{-\infty}^{+\infty} \left( \left| \frac{\partial\psi}{\partial x} \right|^2 + \chi|\psi|^4 \right) dx$$

and is equal to the total energy of the soliton. It is a conserved quantity for (4.3) (see [Sei95]).

The Poisson bracket on  $\chi(\mathcal{P})$  represents a direct generalization of the classical finite-dimensional Poisson bracket

$$\{F, G\}_+(\psi) = i \int_{-\infty}^{+\infty} \left( \frac{\delta F}{\delta\psi} \frac{\delta G}{\delta\bar{\psi}} - \frac{\delta F}{\delta\bar{\psi}} \frac{\delta G}{\delta\psi} \right) dx. \tag{3.31}$$

It manifestly exhibits skew-symmetry and satisfies Jacobi identity. The functionals are given by  $\delta F/\delta\psi = -i\{F, \bar{\psi}\}$  and  $\delta F/\delta\bar{\psi} = i\{F, \psi\}$ . Therefore the algebra of observables  $\chi(\mathcal{P})$  represents the Lie algebra and the Poisson bracket is the (+) Lie-Poisson bracket  $\{F, G\}_+(\psi)$ .

The nonlinear Schrödinger equation (3.30) for the solitary particle-wave is a Hamiltonian system on the Lie algebra  $\chi(\mathcal{P})$  relative to the (+) Lie-Poisson bracket  $\{F, G\}_+(\psi)$  and Hamiltonian function  $H(\psi)$ . Therefore the Poisson manifold  $(\chi(\mathcal{P}), \{F, G\}_+(\psi))$  is defined and the abstract Poisson evolution equation (3.28), which holds for any smooth function  $F : \chi(\mathcal{P}) \rightarrow \mathbb{R}$ , is equivalent to equation (3.30).

A more subtle model of soliton dynamics is provided by the *Korteweg-De Vries equation* [IP01a]

$$f_t - 6ff_x + f_{xxx} = 0, \quad (f_x = \partial_x f), \tag{3.32}$$

where  $x \in \mathbb{R}$  and  $f$  is a real-valued smooth function defined on  $\mathbb{R}$  (compare with (2.46) above). This equation is related to the ordinary Schrödinger equation by the inverse scattering method [Sei95, IP01a].

We may define the infinite-dimensional phase-space manifold  $\mathcal{V} = \{f \in S(\mathbb{R})\}$ , where  $S(\mathbb{R})$  is the Schwartz space of rapidly-decreasing real-valued functions  $\mathbb{R}$ . We define further  $\chi(\mathcal{V})$  to be the algebra of observables consisting of functional derivatives  $\delta F/\delta f \in S(\mathbb{R})$ .

The Hamiltonian  $H : \mathcal{V} \rightarrow \mathbb{R}$  is given by

$$H(f) = \int_{-\infty}^{+\infty} (f^3 + \frac{1}{2}f_x^2) dx$$

and provides the total energy of the soliton. It is a conserved quantity for (3.32) (see [Sei95]).

As a real-valued analogue to (3.31), the (+) Lie-Poisson bracket on  $\chi(\mathcal{V})$  is given *via* (3.26) by

$$\{F, G\}_+(f) = \int_{-\infty}^{+\infty} \frac{\delta F}{\delta f} \frac{d}{dx} \frac{\delta G}{\delta f} dx.$$

Again it possesses skew-symmetry and satisfies Jacobi identity. The functionals are given by  $\delta F/\delta f = \{F, f\}$ .

The Korteweg-De Vries equation (KdV1), describing the behavior of the molecular solitary particle-wave, is a Hamiltonian system on the Lie algebra  $\chi(\mathcal{V})$  relative to the (+) Lie-Poisson bracket  $\{F, G\}_+(f)$  and the Hamiltonian function  $H(f)$ . Therefore, the Poisson manifold  $(\chi(\mathcal{V}), \{F, G\}_+(f))$  is defined and the abstract Poisson evolution equation (3.28), which holds for any smooth function  $F : \chi(\mathcal{V}) \rightarrow \mathbb{R}$ , is equivalent to (3.32).

### 3.2.4 Completely Integrable Hamiltonian Systems

In order to integrate a system of  $2n$  ODEs, we must know  $2n$  first integrals. It turns out that if we are given a canonical system of ODEs, it is often sufficient to know only  $n$  first integrals [Arn89].

#### Liouville Theorem on Completely Integrable Systems

Recall that a function  $F$  is a first integral of a system  $\mathcal{E}$  with Hamiltonian function  $H$  iff  $H$  and  $F$  are in involution on the system's phase-space  $P$  (which is the cotangent bundle of the system's configuration manifold  $T^*M$ ), i.e., iff the Poisson bracket of  $H$  and  $F$  is identically equal to zero on  $P$ ,  $\{H, F\} \equiv 0$ .

Liouville proved that if, in a system  $\mathcal{E}$  with  $n$  DOF (i.e., with a  $2n$ D phase-space  $P = T^*M$ ),  $n$  independent first integrals in involution are known, then the system is integrable by quadratures.

Here is the exact formulation of the *Liouville theorem* [Arn89]: Suppose that we are given  $n$  functions in involution on a symplectic  $2n$ D manifold:

$$F_1, \dots, F_n; \quad \{F_i, F_j\} \equiv 0, \quad (i, j = 1, \dots, n).$$

Consider a level set of the functions  $F_i$ :

$$M_f = \{x : F_i(x) = f_i\}, \quad (i = 1, \dots, n).$$

Assume that the  $n$  functions  $F_i$  are independent on  $M_f$  (i.e., the  $n$  1-forms  $dF_i$  are linearly independent at each point of  $M_f$ ). Then

1.  $M_f$  is a smooth manifold, invariant under the phase-flow with Hamiltonian function  $H = F_1$ .

2. If the manifold  $M_f$  is compact and connected, then it is diffeomorphic to the  $n$ -torus

$$T^n = \{(\varphi^1, \dots, \varphi^n) \bmod 2\pi\}.$$

3. The phase-flow with Hamiltonian function  $H$  determines a conditionally periodic motion on  $M_f$ , i.e., in angular coordinates  $\varphi^i = (\varphi^1, \dots, \varphi^n)$  we have

$$\dot{\varphi}^i = \omega^i, \quad \omega^i = \omega^i(f_i), \quad (i = 1, \dots, n).$$

4. The canonical equations with Hamiltonian function  $H$  can be integrated by quadratures.

For the proof of this theorem see [Arn89].

As an example with 3 DOF, we consider a heavy symmetrical Lagrange top fixed at a point on its axis. Three first integrals are immediately obvious:  $H$ ,  $M_z$  and  $M_3$ . It is easy to verify that the integrals  $M_z$  and  $M_3$  are in involution. Furthermore, the manifold  $H = h$  in the phase-space is compact. Therefore, we can say without any calculations that the motion of the top is conditionally periodic: the phase trajectories fill up the 3D torus  $T^3$ , given by:  $H = c_1$ ,  $M_z = c_2$ ,  $M_3 = c_3$ . The corresponding three frequencies are called frequencies of fundamental rotation, precession, and nutation.

Other examples arise from the following observation: *if a canonical system can be integrated by the method of Hamilton–Jacobi, then it has  $n$  first integrals in involution.* The method consists of a canonical transformation  $(p_i, q^i) \rightarrow (P_i, Q^i)$  such that the  $Q^i$  are first integrals, while the functions  $Q^i$  and  $Q^i$  are in involution.

The Liouville theorem, as formulated above, covers all the problems of dynamics which have been integrated to the present day [Arn89].

### Action–Angle Variables

Under the hypothesis of the Liouville theorem, we can find symplectic coordinates  $(I_i, \varphi^i)$  such that the first integrals  $F_i$  depend only on  $I_i$  and  $\varphi^i$  (for  $i = 1, \dots, n$ ) are angular coordinates on the  $n$ -torus  $T^n \simeq M_f = \{x : F_i(x) = f_i\}$ , which is invariant with respect to the phase-flow. We choose angular coordinates  $\varphi^i$  on  $M_f$  so that the phase-flow with Hamiltonian function  $H = F_1$  takes an especially simple form [Arn89]:

$$\dot{\varphi}^i = \omega^i(f_i), \quad \varphi^i(t) = \varphi^i(0) + \omega^i t.$$

Now we look at a neighborhood of the  $n$ -manifold  $M_f = T^n$  in the system's  $2n$ D phase-space  $P$ .

In the coordinates  $(F_i, \varphi^i)$  the phase-flow with Hamiltonian function  $H = F_1$  can be written in the form of the simple system of  $2n$  ODEs

$$\dot{F}_i = 0, \quad \dot{\varphi}^i = \omega^i(F_i), \quad (i = 1, \dots, n), \quad (3.33)$$

which is easily integrated:  $F_i(t) = F_i(0)$ ,  $\varphi^i(t) = \varphi^i(0) + \omega^i(F_i(0))t$ .

Thus, in order to integrate explicitly the original canonical system of ODEs, it is sufficient to find the variables  $\varphi^i$  in explicit form. It turns out that this can be done using only quadratures. A construction of the variables  $\varphi^i$  is given below [Arn89].

In general, the variables  $(F_i, \varphi^i)$  are not symplectic coordinates. However, there are functions of  $F_i$ , which we denote by  $I_i = I_i(F_i)$ ,  $(i = 1, \dots, n)$ , such that the variables  $(I_i, \varphi^i)$  are symplectic coordinates: the original symplectic structure  $dp_i \wedge dq^i$  is expressed in them as  $dI_i \wedge d\varphi^i$ . The variables  $I_i$  have physical dimensions of action and are called action variables; together with the angle variables  $\varphi^i$  they form the *action-angle system of canonical coordinates* in a neighborhood of  $M_f = T^n$ .

The quantities  $I_i$  are first integrals of the system with Hamiltonian function  $H = F_1$ , since they are functions of the first integrals  $F_i$ . In turn, the variables  $F_i$  can be expressed in terms of  $I_i$  and, in particular,  $H = F_1 = H(I_i)$ . In action-angle variables, the ODEs of our flow (3.33) have the form

$$\dot{I}_i = 0, \quad \dot{\varphi}^i = \omega^i(I_i), \quad (i = 1, \dots, n).$$

A system with one DOF in the phase plane  $(p, q)$  is given by the Hamiltonian function  $H(p, q)$ . In order to construct the action-angle variables, we look for a canonical transformation  $(p, q) \rightarrow (I, \varphi)$  satisfying the two conditions:

$$I = I(h), \quad \oint_{M_h} d\varphi = 2\pi. \quad (3.34)$$

The *action variable* in the system with one DOF given by the Hamiltonian function  $H(p, q)$  is the quantity

$$I(h) = \frac{1}{2\pi} \Pi(h) = \frac{1}{2\pi} \oint_{M_h} pdq,$$

which is the area bounded by the phase curve  $H = h$  [Arn89]. Arnold states the following theorem: Set  $S(I, q) = \int_{q_0}^q pdq|_{H=h(I)}$  is a *generating function*. Then a canonical transformation  $(p, q) \rightarrow (I, \varphi)$  satisfying conditions (3.34) is given by

$$p = \frac{\partial S(I, q)}{\partial q}, \quad \varphi = \frac{\partial S(I, q)}{\partial I}, \quad H\left(\frac{\partial S(I, q)}{\partial q}, q\right) = h(I).$$

We turn now to systems with  $n$  DOF given in  $\mathbb{R}^{2n} = \{(p_i, q^i), i = 1, \dots, n\}$  by a Hamiltonian function  $H(p_i, q^i)$  and having  $n$  first integrals in involution  $F_1 = H, F_2, \dots, F_n$ . Let  $\gamma_1, \dots, \gamma_n$  be a basis for the 1D cycles on the torus  $M_f = T^n$  (the increase of the coordinate  $\varphi^i$  on the cycle  $\gamma_j$  is equal to  $2\pi$  if  $i = j$  and 0 if  $i \neq j$ ). We set

$$I_i(f_i) = \frac{1}{2\pi} \oint_{M_h} p_i dq^i, \quad (i = 1, \dots, n). \quad (3.35)$$

The  $n$  quantities  $I_i(f_i)$  given by formula (3.35) are called the *action variables* [Arn89].

We assume now that, for the given values  $f_i$  of the  $n$  integrals  $F_i$ , the  $n$  quantities  $I_i$  are independent,  $\det(\partial I_i / \partial f_i)|_{f_i} \neq 0$ . Then in a neighborhood of the torus  $M_f = T^n$  we can take the variables  $I_i, \varphi^i$  as symplectic coordinates, i.e., the transformation  $(p_i, q^i) \rightarrow (I_i, \varphi^i)$  is canonical, or [Arn89]

$$dp_i \wedge dq^i = dI_i \wedge d\varphi^i, \quad (i = 1, \dots, n).$$

Now, let  $m$  be a point on  $M_f$ , in a neighborhood of which the  $n$  variables  $q^i$  are coordinates of  $M_f$ , such that the submanifold  $M_f \subset \mathbb{R}^{2n}$  is given by  $n$  equations of the form  $p_i = p_i(I_i, q^i)$ ,  $q^i(m) = q_0^i$ . In a simply connected neighborhood of the point  $q_0^i$  a single-valued function is defined,

$$S(I_i, q^i) = \int_{q_0}^q p_i(I_i, q^i) dq^i,$$

and we can use it as the generating function of a canonical transformation  $(p_i, q^i) \rightarrow (I_i, \varphi^i)$ :

$$p_i = \frac{\partial S}{\partial q^i}, \quad \varphi^i = \frac{\partial S}{\partial I_i}.$$

### A Universal Model for Completely Integrable Systems

A Hamiltonian system on a  $2n$ D symplectic manifold  $M$  is said to be *completely integrable* if it has  $n$  first integrals in involution, which are functionally independent on some open dense submanifold of  $M$ . This definition of a completely integrable system is usually found, with some minor variants, in any modern text on symplectic mechanics [Arn89, AM78, LM87, MS95, Thi79].

Starting with this definition, one uses the so-called *Liouville–Arnold theorem* to introduce action–angle variables and write the Hamiltonian system in the form

$$\dot{I}^k = 0, \quad \dot{\phi}_k = \frac{\partial H}{\partial I_k} = \nu_k(I),$$

where  $k \in \{1, \dots, n\}$ . The corresponding flow is given by

$$I^k(t) = I^k(0), \quad \phi_k(t) = \phi_k(0) + \nu_k t. \quad (3.36)$$

The main interest in completely integrable systems relies on the fact that they can be integrated by quadratures [Arn89].

It is clear, however, that even if  $\nu_k dI^k$  is not an exact (or even a closed) 1-form, as long as  $\dot{\nu}_k = 0$ , the system can always be integrated by quadratures.

If we consider the Abelian Lie group  $\mathbb{R}^n$ , we can construct a Hamiltonian action of  $\mathbb{R}^n$  on  $T^*\mathbb{R}^n$  induced by the group addition:

$$\mathbb{R}^n \times T^*\mathbb{R}^n \rightarrow T^*\mathbb{R}^n.$$

This can be generalized to the Hamiltonian action [AGM97]

$$\mathbb{R}^n \times T^*(\mathbb{R}^k \times T^{n-k}) \rightarrow T^*(\mathbb{R}^k \times T^{n-k}),$$

of  $\mathbb{R}^n$ , where  $T^m$  stands for the  $m$ D torus, and reduces to  $\mathbb{R}^n \times T^*T^n$  or  $T^n \times T^*T^n$ , when  $k = 0$ .

By using the standard symplectic structure on  $T^*\mathbb{R}^n$ , we find the momentum map  $\mu : T^*\mathbb{R}^n \rightarrow (\mathbb{R}^n)^s$ ,  $(q, p) \mapsto p$ , induced by the natural action of  $\mathbb{R}^n$  on itself via translations, which is a Poisson map if  $(\mathbb{R}^n)^s$  is endowed with the (trivial) natural Poisson structure of the dual of a Lie algebra. It is now clear that any function on  $(\mathbb{R}^n)^s$ , when pulled back to  $T^*\mathbb{R}^n$  or  $T^*T^n$ , gives rise to a Hamiltonian system which is completely integrable (in the Liouville sense). Because the level sets of this function carry on the action of  $\mathbb{R}^n$ , the completely integrable system gives rise to a 1D subgroup of the action of  $\mathbb{R}^n$  on the given level set. The specific subgroup will, however, depend on the particular level set, i.e., the ‘frequencies’ are first integrals. The property of being integrable by quadratures is captured by the fact that it is a subgroup of the  $\mathbb{R}^n$ -action on each level set.

It is now clear, how we can preserve this property, while giving up the requirement that our system is Hamiltonian. We can indeed consider any 1-form  $\eta$  on  $(\mathbb{R}^n)^s$  and pull it back to  $T^*\mathbb{R}^n$  or  $T^*T^n$ , then associated vector-field  $\Gamma_\eta = \Lambda_0(\mu^s(\eta))$ , where  $\Lambda_0$  is the canonical Poisson structure in the cotangent bundle, is no more Hamiltonian, but it is still integrable by quadratures. In action-angle variables, if  $\eta = \nu_k dI^k$  is the 1-form on  $(\mathbb{R}^n)^s$ , the associated equations of motion on  $T^*T^n$  will be [AGM97]

$$\dot{I}^k = 0, \quad \dot{\phi}_k = \nu_k,$$

with  $\dot{\nu}_k = 0$ , therefore the flow will be as in (3.36), even though  $\partial_{I^j}\nu_k \neq \partial_{I^k}\nu_j$ .

We can now generalize this construction to any Lie group  $G$ . We consider the Hamiltonian action

$$G \times T^*G \rightarrow T^*G,$$

of  $G$  on the cotangent bundle, induced by the right action of  $G$  on itself. The associated momentum map

$$\mu : T^*G \simeq \mathcal{G}^s \times G \rightarrow \mathcal{G}^s.$$

It is a Poisson map with respect to the natural Poisson structure on  $\mathcal{G}^s$  (see e.g., [AGM94, LM87]).

Now, we consider any differential 1-form  $\eta$  on  $\mathcal{G}^s$  which is annihilated by the natural Poisson structure  $\Lambda_{\mathcal{G}^s}$  on  $\mathcal{G}^s$  associated with the Lie bracket. Such form will be called a *Casimir form*. We define the vector-field  $\Gamma_\eta = \Lambda_0(\mu^s(\eta))$ . Then, the corresponding dynamical system can be written as [AGM97]

$$g^{-1}\dot{g} = \eta(g, p) = \eta(p), \quad \dot{p} = 0,$$

since  $\omega_0 = d(\langle p, g^{-1}dg \rangle)$  (see [AGM94]). Here we interpret the covector  $\eta(p)$  on  $\mathcal{G}^s$  as a vector of  $\mathcal{G}$ . Again, our system can be integrated by quadratures, because on each level set, obtained by fixing  $p$ 's in  $\mathcal{G}^s$ , our dynamical system coincides with a one-parameter group of the action of  $G$  on that particular level set.

We give a familiar example: the rigid rotator and its generalizations [AGM97]. In the case of  $G = \text{SO}(3)$  the (right) momentum map

$$\mu : T^*\text{SO}(3) \longrightarrow \mathfrak{so}(3)^*$$

is a Poisson map onto  $\mathfrak{so}(3)^*$  with the linear Poisson structure

$$\Lambda_{\mathfrak{so}(3)^*} = \varepsilon^{ijk} p_i \partial_{p_j} \otimes \partial_{p_k}.$$

Casimir 1-forms for  $\Lambda_{\mathfrak{so}(3)^*}$  read  $\eta = FdH_0$ , where  $H_0 = \sum p_i^2/2$  is the ‘free Hamiltonian’ and  $F = F(p)$  is an arbitrary function. Clearly,  $FdH_0$  is not a closed form in general, but  $(p_i)$  are first integrals for the dynamical system  $\Gamma_\eta = \Lambda_0(\mu^s(\eta))$ . It is easy to see that

$$\Gamma_\eta = F(p)\Gamma_0 = F(p)p_i \widehat{X}_i,$$

where  $\widehat{X}_i$  are left-invariant vector-fields on  $\text{SO}(3)$ , corresponding to the basis  $(X_i)$  of  $\mathfrak{so}(3)$  identified with  $(dp_i)$ . Here we used the identification  $T^*\text{SO}(3) \simeq \text{SO}(3) \times \mathfrak{so}(3)^*$  given by the momentum map  $\mu$ . In other words, the dynamics is given by

$$\dot{p}_i = 0, \quad g^{-1}\dot{g} = F(p)p_i X_i \in \mathfrak{so}(3),$$

and it is completely integrable, since it reduces to left-invariant dynamics on  $\text{SO}(3)$  for every value of  $p$ . We recognize the usual isotropic rigid rotator, when  $F(p) = 1$ .

We can generalize our construction once more, replacing the cotangent bundle  $T^*G$  by its deformation, namely a group double  $D(G, \Lambda_G)$  associated with a Lie-Poisson structure  $\Lambda_G$  on  $G$  (see e.g., [Lu90]). This double, denoted simply by  $D$ , carry on a natural *Poisson tensor-field*  $\Lambda_D^+$  which is non-degenerate on the open-dense subset  $D^+ = G \cdot G^s \cap G^s \cdot G$  of  $D$  (here  $G^s \subset D$  is the dual group of  $G$  with respect to  $\Lambda_G$ ). We refer to  $D$  as being *complete* if  $D^+ = D$ . Identifying  $D$  with  $G \times G^s$  if  $D$  is complete (or  $D^+$  with an open submanifold of  $G \times G^s$  in general case; we assume completeness for simplicity) via the group product, we can write  $\Lambda_D^+$  in ‘coordinates’  $(g, u) \in G \times G^s$  in the form [AGM97]

$$\Lambda_D^+(g, u) = \Lambda_G(g) + \Lambda_{G^s}(u) - X_i^l(g) \wedge Y_i^r(u), \tag{3.37}$$

where  $X_i^l$  and  $Y_i^r$  are, respectively, the left- and right-invariant vector-fields on  $G$  and  $G^s$  relative to dual bases  $X_i$  and  $Y_i$  in the Lie algebras  $\mathcal{G}$  and  $\mathcal{G}^s$ , and where  $\Lambda_G$  and  $\Lambda_{G^s}$  are the corresponding Lie-Poisson tensors on  $G$  and

$G^s$  (see [Lu90]). It is clear now that the projections  $\mu_{G^*}$  and  $\mu_G$  of  $(D, \Lambda_D^+)$  onto  $(G, \Lambda_G)$  and  $(G^s, \Lambda_{G^*})$ , respectively, are Poisson maps. Note that we get the cotangent bundle  $(D, \Lambda_D^+) = (T^*G, \Lambda_0)$  if we put  $\Lambda_G = 0$ .

The group  $G$  acts on  $(D, \Lambda_D^+)$  by left translations which, in general are not canonical transformations. This is, however, a Poisson action with respect to the inner Poisson structure  $\Lambda_G$  on  $G$ , which is sufficient to develop the momentum map reduction theory (see [Lu91]). For our purposes, let us take a Casimir 1-form  $\eta$  for  $\Lambda_{G^*}$ , i.e.,  $\Lambda_{G^*}(\eta) = 0$ . By means of the momentum map

$\mu_{G^*} : D \rightarrow G^s$ , we define the vector-field on  $D$  [AGM97]:

$$\Gamma_\eta = \Lambda_D^+(\mu_{G^*}^s(\eta)).$$

In ‘coordinates’  $(g, u)$ , due to the fact that  $\eta$  is a Casimir, we get

$$\Gamma_\eta(g, u) = \langle Y_i^r, \eta \rangle (u) X_i^l(g),$$

so that  $\Gamma_\eta$  is associated with the *Legendre map*

$$L_\eta : D \simeq G \times G^s \rightarrow TG \simeq G \times \mathcal{G}, \quad L_\eta(g, u) = \langle Y_i^r, \eta \rangle (u) X_i,$$

which can be viewed also as a map  $L_\eta : G^s \rightarrow \mathcal{G}$ . Thus we get the following theorem [AGM97]: The dynamics  $\Gamma_\eta$  on the group double  $D(G, \Lambda_G)$ , associated with a 1-form  $\eta$  which is a Casimir for the Lie-Poisson structure  $\Lambda_{G^*}$  on the dual group, is given by the system of equations

$$\dot{u} = 0, \quad g^{-1}\dot{g} = \langle Y_i^r, \eta \rangle (u) X_i \in \mathcal{G},$$

and is therefore completely integrable by quadratures.

We have seen that if we concentrate on the possibility of integrating our system by quadratures, then we can do without the requirement that the system is Hamiltonian.

By considering again the equations of motion in action-angle variables, we have, classically,

$$\dot{I}^k = 0, \quad \dot{\phi}_k = \nu^k(I).$$

Clearly, if we have

$$\dot{I}^k = F_k(I), \quad \dot{\phi}_k = A_k^j(I)\phi_j, \tag{3.38}$$

and we are able to integrate the first equation by quadratures, we again have the possibility to integrate by quadratures the system (3.38), if only the matrices  $(A_k^j(I(t)))$  commute [AGM97]:

$$\phi(t) = \exp\left(\int_0^t A(I(s))ds\right)\phi_0.$$

Of course, because  $\phi_k$  are discontinues functions on the torus, we have to be more careful here. We show, however, how this idea works for double groups.

In the case when the 1-form  $\eta$  on  $G^s$  is not a Casimir 1-form for the Lie-Poisson structure  $\Lambda_{G^*}$ , we get, in view of (3.37),

$$\Gamma_\eta(g, u) = \langle Y_i^r, \eta \rangle (u) X_i^l(g) + \Lambda_{G^*}(\eta)(u).$$

Now, the momenta evolve according to the dynamics  $\Lambda_{G^*}(\eta)$  on  $G^s$  (which can be interpreted, as we will see later, as being associated with an interaction of the system with an external field) and ‘control’ the evolution of the field of velocities on  $G$  (being left-invariant for a fixed time) by a ‘variation of constants’. Let us summarize our observations in the following theorem [AGM97]: The vector-field  $\Gamma_\eta$  on the double group  $D(G, \Lambda_G)$ , associated with a 1-form  $\eta$  on  $G^s$ , defines the following dynamics

$$\dot{u} = \Lambda_{G^*}(\eta)(u), \quad g^{-1}\dot{g} = \langle Y_i^r, \alpha \rangle (u) X_i \in \mathcal{G}, \quad (3.39)$$

and is therefore completely integrable, if only we are able to integrate the equation (3.39) and  $\langle Y_i^r, \eta \rangle (u(t)) X_i$  lie in a commutative subalgebra of  $\mathcal{G}$  for all  $t$ .

Finally, we can weaken the assumptions of the previous theorem. It is sufficient to assume [AGM97] that

$$g^{-1}\dot{g}(t) = \exp(tX)A(t)\exp(-tX),$$

for some  $A(t)$ ,  $X \in \mathcal{G}$ , such that  $X + A(t)$  lie in a commutative subalgebra of  $\mathcal{G}$  for all  $t$  (e.g.,  $A(t) = \text{const}$ ), to assure that (3.39) is integrable by quadratures. Indeed, in the new variable

$$g_1(t) = \exp(-tX)g(t)\exp(tX),$$

the equation (3.39) reads

$$\dot{g}_1(t) = g_1(t)(X + A(t)) - Xg_1(t),$$

and, since the right- and the left-multiplications commute, we easily find that [AGM97]

$$g(t) = g_0 \exp\left(tX + \int_0^t A(s)ds\right) \exp(-tX).$$

This procedure is similar to what is known as the Dirac interaction picture in the quantum evolution.

Finally, it should be noted that the Hamiltonian dynamics of time-dependent mechanics is in [MS98, GM97] described in a different way as a particular Hamiltonian dynamics on fibre bundles.

### 3.2.5 Killing Vector and Tensor Fields in Biomechanics

Recall from section 2.5 above, that on a Riemannian biomechanical manifold  $(M, g)$  with the system’s kinetic energy metric tensor  $g = (g_{ij})$ , for any pair

of vectors  $V$  and  $T$ , the following relation holds<sup>1</sup>

$$\partial_s \langle V, T \rangle = \langle \nabla_s V, T \rangle + \langle V, \nabla_s T \rangle, \quad (3.40)$$

where  $\langle V, T \rangle = g_{ij} V^i T^j$ . If the curve  $\gamma(s)$  is a geodesic, for a generic vector  $X$  we have

$$\partial_s \langle X, \dot{\gamma} \rangle = \langle \nabla_s X, \dot{\gamma} \rangle + \langle X, \nabla_s \dot{\gamma} \rangle = \langle \nabla_s X, \dot{\gamma} \rangle \equiv \langle \nabla_{\dot{\gamma}} X, \dot{\gamma} \rangle, \quad (3.41)$$

where

$$(\nabla_{\dot{\gamma}} X)^i = \partial_s x^l \partial_{x^l} X^i + \Gamma_{jk}^i \partial_s x^j X^k,$$

so that in components it reads

$$\partial_s (X_i \dot{x}^i) = \dot{x}^i \nabla_i (X_j \dot{x}^j).$$

Using the fact that  $X_j \dot{x}^i \nabla_i \dot{x}^j = X_j \nabla_{\dot{\gamma}} \dot{\gamma}^j = 0$ , as well as the auto-parallelism of the geodesics, this can be rewritten as

$$\partial_s (X_i \dot{x}^i) = \frac{1}{2} \dot{x}^j \dot{x}^i (\nabla_i X_j + \nabla_j X_i), \quad (i, j = 1, \dots, N).$$

This means that the conservation of  $X_i \dot{x}^i$  along a geodesic, i.e.,  $\partial_s (X_i \dot{x}^i) = 0$ , is guaranteed by (see [CP02])

$$\nabla_{(i} X_{j)} \equiv \nabla_i X_j + \nabla_j X_i = 0. \quad (3.42)$$

If such a field exists on a manifold, it is called a *Killing vector-field* (see subsection 2.5.4 above). Recall that (3.42) is equivalent to  $\mathcal{L}_X g = 0$ , where  $\mathcal{L}$  is the Lie derivative. On the biomechanical manifolds  $(M, g)$ , being the unit vector  $\dot{q}^i$  – tangent to a geodesic – proportional to the canonical momentum  $p_i = \frac{\partial L}{\partial \dot{q}^i} = \dot{q}^i$ , the existence of a Killing vector-field  $X$  implies that the corresponding *momentum map* (see subsection 2.6.3 above),

$$J(q, p) = X_k(q) \partial_s q^k = \frac{1}{\sqrt{2(E - V(q))}} X_k(q) \dot{q}^k = \frac{1}{\sqrt{2T(q)}} X_k(q) p_k, \quad (3.43)$$

is a constant of motion along the geodesic flow. Thus, for an  $N$ DOF Hamiltonian system, a physical conservation law, involving a conserved quantity linear in the canonical momenta, can always be related with a symmetry on the manifold  $(M, g)$  due to the action of a Killing vector-field on the manifold. These are conservation laws of Noetherian kind (see subsection 1.1.4 above). The equation (3.42) is equivalent to the vanishing of the Poisson brackets

$$\{H, J\} = \left( \frac{\partial H}{\partial q^i} \frac{\partial J}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial J}{\partial q^i} \right) = 0, \quad (3.44)$$

<sup>1</sup> In this subsection, the overdot denotes the derivative upon the arc-length parameter  $s$ , namely  $\dot{(\ )} \equiv \partial_s \equiv d/ds$ , while  $\nabla_s$  is the covariant derivative along a curve  $\gamma(s)$ .

which is the standard definition of a constant of motion  $J(q, p)$  (see, e.g., [AM78]).

However, if a one-to-one correspondence is to exist between conserved physical quantities along a Hamiltonian flow and suitable symmetries of the biomechanical manifolds  $(M, g)$ , then *integrability* will be equivalent to the existence of a number of symmetries at least equal to the number of DOF, which is equal to  $\dim(M)$ . If a Lie group  $G$  acts on the phase-space manifold through completely canonical transformations, and there exists an associated momentum map, then every Hamiltonian having  $G$  as a symmetry group, with respect to its action, admits the momentum map as the constant of motion. These symmetries are usually referred to as *hidden symmetries* because, even though their existence is ensured by integrability, they are not easily recognizable [CP02].

Let us now extend what has been presented so far about Killing vector-fields, trying to generalize the form of the conserved quantity along a geodesic flow from  $J = X_i \dot{x}^i$  to  $J = K_{j_1 j_2 \dots j_r} \dot{x}^{j_1} \dot{x}^{j_2} \dots \dot{x}^{j_r}$ , with  $K_{j_1 j_2 \dots j_r}$  a tensor of rank  $r$ . Thus, we look for the conditions that entail

$$\partial_s(K_{j_1 j_2 \dots j_r} \dot{x}^{j_1} \dot{x}^{j_2} \dots \dot{x}^{j_r}) = \dot{x}^j \nabla_j (K_{j_1 j_2 \dots j_r} \dot{x}^{j_1} \dot{x}^{j_2} \dots \dot{x}^{j_r}) = 0. \quad (3.45)$$

In order to work out from this equation a condition for the existence of a suitable tensor  $K_{j_1 j_2 \dots j_r}$ , which is called a *Killing tensor-field*, let us first consider the  $2r$  rank tensor  $K_{j_1 j_2 \dots j_r} \dot{x}^{i_1} \dot{x}^{i_2} \dots \dot{x}^{i_r}$  and its covariant derivative along a geodesic [CP02]

$$\dot{x}^j \nabla_j (K_{j_1 j_2 \dots j_r} \dot{x}^{i_1} \dot{x}^{i_2} \dots \dot{x}^{i_r}) = \dot{x}^{i_1} \dot{x}^{i_2} \dots \dot{x}^{i_r} \dot{x}^j \nabla_j K_{j_1 j_2 \dots j_r}, \quad (3.46)$$

where we have again used  $\dot{x}^j \nabla_j \dot{x}^{i_k} = 0$  along a geodesic, and a standard covariant differentiation formula (see Appendix, as well as section 2.5 above). Now, by contraction on the indices  $i_k$  and  $j_k$  the  $2r$ -rank tensor in (3.46) provides a new expression for (3.45), which reads

$$\partial_s(K_{j_1 j_2 \dots j_r} \dot{x}^{j_1} \dot{x}^{j_2} \dots \dot{x}^{j_r}) = \dot{x}^{j_1} \dot{x}^{j_2} \dots \dot{x}^{j_r} \dot{x}^j \nabla_{(j} K_{j_1 j_2 \dots j_r)}, \quad (3.47)$$

where  $\nabla_{(j} K_{j_1 j_2 \dots j_r)} = \nabla_j K_{j_1 j_2 \dots j_r} + \nabla_{j_1} K_{j j_2 \dots j_r} + \dots + \nabla_{j_r} K_{j_1 j_2 \dots j_{r-1} j}$ . The vanishing of (3.47), entailing the conservation of  $K_{j_1 j_2 \dots j_r} \dot{x}^{j_1} \dot{x}^{j_2} \dots \dot{x}^{j_r}$  along a geodesic flow, is therefore guaranteed by the existence of a tensor-field fulfilling the conditions [CP02]

$$\nabla_{(j} K_{j_1 j_2 \dots j_r)} = 0. \quad (3.48)$$

These equations generalize (3.42) and give the definition of a Killing tensor-field on a Riemannian biomechanical manifold  $(M, g)$ . These  $N^{r+1}$  equations in  $(N+r-1)!/r!(N-1)!$  unknown independent components of the Killing tensor constitute an *overdetermined* system of equations. Thus, *a priori*, we can expect that the existence of Killing tensor-fields has to be rather exceptional.

If a Killing tensor-field exists on a Riemannian manifold, then the scalar

$$K_{j_1 j_2 \dots j_r} \dot{q}^{j_1} \dot{q}^{j_2} \dots \dot{q}^{j_r}$$

is a constant of motion for the geodesic flow on the same manifold. With the only difference of a more tedious combinatorics, also in this case it turns out that the equations (3.48) are equivalent to the vanishing of the Poisson brackets of  $J(q, p)$ , that is

$$\{H, J\} = 0 \quad \text{is equivalent to} \quad \nabla_{(j} K_{j_1 j_2 \dots j_r)} = 0.$$

Thus, the existence of Killing tensor-fields, obeying (3.48), on a biomechanical manifold  $(M, g)$  provide the rephrasing of integrability of Newtonian equations of motion or, equivalently, of standard Hamiltonian systems, within the Riemannian geometric framework.

The first natural question to address concerns the existence of a Killing tensor-field, on any biomechanical manifold  $(M, g)$ , to be associated with total energy conservation. Such a Killing tensor-field actually exists and coincides with the metric tensor  $g$ , in fact it satisfies by definition (3.48).

One of the simplest case of integrable system is represented by a decoupled system described by a generic Hamiltonian

$$H = \sum_{i=1}^N \left[ \frac{p_i^2}{2} + V_i(q^i) \right] = \sum_{i=1}^N H_i(q^i, p_i)$$

for which all the energies  $E_i$  of the subsystems  $H_i$ ,  $i = 1, \dots, N$ , are conserved. On the associated biomechanical manifold,  $N$  second order Killing tensor-fields exist, they are given by

$$K_{jk}^{(i)} = \delta_{jk} \{V_i(q^i)[E - V(q^i)] + \delta_j^i [E - V(q^i)]^2\}.$$

In fact, these tensor-fields fulfil (3.48), which explicitly reads [CP02]

$$\begin{aligned} & \nabla_k K_{lm}^{(i)} + \nabla_l K_{mk}^{(i)} + \nabla_m K_{kl}^{(i)} \\ &= \partial_{q^k} K_{lm}^{(i)} + \partial_{q^l} K_{mk}^{(i)} + \partial_{q^m} K_{kl}^{(i)} - 2\Gamma_{kl}^j K_{jm}^{(i)} - 2\Gamma_{km}^j K_{jl}^{(i)} - 2\Gamma_{lm}^j K_{jk}^{(i)} = 0. \end{aligned}$$

The conserved quantities  $J^{(i)}(q, p)$  are then obtained by saturation of the tensors  $K^{(i)}$  with the velocities  $\dot{q}^i$ ,

$$J^{(i)}(q, p) = K_{jk}^{(i)} \dot{q}^j \dot{q}^k = E_i.$$

### 3.3 Variational Formalism in Human-Like Biomechanics

As a summary of the holonomic Lagrangian and Hamiltonian methods developed so far, in this section we present variational formalism, to be used in conservative biomechanics, following *Hilbert's 19th and 23rd problems*.

### 3.3.1 Biomechanical Action Functional

*Biomechanical action* operates on four different biomechanical levels of organization, with the following top-down structure:

1. Level of a whole musculo-skeletal system;
2. Level of a single muscle;
3. Level of a single muscle-fibre, as a structural muscle-unit;
4. Molecular muscular level of nano-biomechanics.

All the macroscopic levels (1–3) of biomechanical organization are governed by *classical biomechanical action*. The molecular level (4) is governed by *quantum biomechanical action*.

The integral form of the general biomechanical action is called *biomechanical action functional* (BAF, for short), with physical dimension of energy  $\times$  time. We have defined BAF as a *time integral over the Lagrangian energy function*  $L(x^i(t), \dot{x}^i(t); t)$  (see Introduction, subsection 1.1.3),

$$S\{[x^i(t)]; t_1, t_2\} = \int_{t_1}^{t_2} dt L(x^i(t), \dot{x}^i(t); t). \quad (3.49)$$

Here,  $x^i$ ,  $i = 1, 2, \dots, N$  are generalized coordinates, i.e., points in  $ND$  biomechanical configuration space. Thus the set of trajectories  $(x^i(t))$  describes the behavior of the biomechanical system, and  $\dot{x}^i(t) = dx^i/dt$  determines its velocity along the path in the biomechanical configuration space. The endpoints of the trajectory are given by  $x^i(t_1) = x_1^i$ , and  $x^i(t_2) = x_2^i$ .

The *principle of stationary action* says (see [AM78, Arn89, MR99]): in response to infinitesimal variation of the integration path, the BAF is *stationary*, i.e.,  $\delta S = 0$ , for variations about correct path, provided the initial and final configurations are held fixed. On the other hand, if we permit infinitesimal changes of the trajectories  $x^i(t)$  at the initial and final times, including alterations of those times, the only contribution to  $\delta S$  comes from the endpoint variations, or

$$\delta S = G(t_2) - G(t_1). \quad (3.50)$$

Equation (3.50) is the most general formulation of the biomechanical action principle. The fixed values  $G_1 = G(t_1)$  and  $G_2 = G(t_2)$  depend only on the endpoint path variables at the respective terminal times.

Given a muscle-system with the BAF, the actual time evolution in biomechanical configuration space follows that path about which general variations produce only endpoint contributions. The explicit form of  $G$  is dependent upon the special representation of the biomechanical action principle.

### 3.3.2 Lagrangian Action

Each biomechanical point particle with mass  $m$  moves in a biophysical potential  $V(x^i, t)$ . Its Lagrangian function is defined as

$$L(x^i, \dot{x}^i; t) = \frac{m}{2} \dot{x}^i - V(x^i, t). \quad (3.51)$$

The dynamical variable  $x^i = x^i(t)$  denotes the actual classical trajectory of the particle which is parameterized by  $t$  with  $t_1 \leq t \leq t_2$ .

We consider the response of the biomechanical action functional (3.49) with respect to changes in the coordinates and in the time,  $\delta x^i(t)$  and  $\delta t$ , respectively.

If the time is not varied, we write  $\delta_0$  instead of  $\delta$ . The variation of  $x^i(t)$  is then given by

$$\delta x^i(t) = \delta_0 x^i(t) + \delta t \frac{d}{dt}(x^i(t)).$$

Similarly

$$\delta \dot{x}^i(t) = \delta_0 \dot{x}^i(t) + \delta t \frac{d}{dt}(\dot{x}^i(t)) = \frac{d}{dt}(\delta x^i) - \dot{x}^i \frac{d}{dt} \delta t.$$

The difference between  $\delta$  and  $\delta_0$  acting on  $t$ ,  $x^i(t)$  and  $\dot{x}^i(t)$  is expressed by the identity

$$\delta = \delta_0 + \delta t \frac{d}{dt},$$

Also, according to (3.49) we have

$$\delta L = \delta_0 L + \delta t \frac{d}{dt} L,$$

and the total variation of biomechanical Lagrangian is given by

$$\delta L = \frac{\partial L}{\partial x^i} \delta x^i + \frac{\partial L}{\partial \dot{x}^i} \delta \dot{x}^i + \frac{\partial L}{\partial t} \delta t.$$

Now, from (3.51) we substitute

$$\frac{\partial L}{\partial x^i} = -\frac{\partial V(x^i, t)}{\partial x^i}, \quad \frac{\partial L}{\partial \dot{x}^i} = \delta_k^i m \ddot{x}^k, \quad \frac{\partial L}{\partial t} = -\frac{\partial V(x^i, t)}{\partial t},$$

(where  $\delta^{ik} = \delta_k^i = \delta_{ik}$  is the Kronecker's symbol) so that we get,

$$\delta L = -\frac{\partial V}{\partial t} \delta t - \frac{\partial V}{\partial x^i} \delta x^i + m \dot{x}^i \frac{d}{dt} \delta x^i - m (\dot{x}^i)^2 \frac{d}{dt} \delta t.$$

Expression for the change of  $S$ ,  $\delta S$ , then becomes

$$\delta S = \int_{t_1}^{t_2} dt \left[ m \dot{x}^i \frac{d}{dt} \delta x^i - \frac{\partial V}{\partial t} \delta t - \frac{\partial V}{\partial x^i} \delta x^i + (L - m (\dot{x}^i)^2 \frac{d}{dt}) \delta t \right].$$

Using the definition of biomechanical mechanical energy

$$E = \frac{\partial L}{\partial \dot{x}^i} \dot{x}^i - L = \frac{m}{2} \left( \frac{dx^i}{dt} \right)^2 + V(x^i, t),$$

and reorganizing terms, we get

$$\begin{aligned} \delta S &= \int_{t_1}^{t_2} dt \frac{d}{dt} [m\dot{x}^i \delta x^i - E\delta t] \\ &+ \int_{t_1}^{t_2} dt \left[ -\delta x^i \left( m\ddot{x}^i + \delta^{ik} \frac{\partial V}{\partial x^k} \right) + \delta t \left( \frac{dE}{dt} - \frac{\partial V}{\partial t} \right) \right]. \end{aligned}$$

Since  $\delta x^i$  and  $\delta t$  are independent variations, the biomechanical action principle  $\delta S = G_2 - G_1$  implies the following laws:

$$\begin{aligned} \delta x^i : \quad m\ddot{x}^i &= -\delta^{ik} \frac{\partial V(x^i, t)}{\partial x^k}, & (\text{Newton's law of motion}), \\ \delta t : \quad \frac{dE}{dt} &= \frac{\partial V(x^i, t)}{\partial t}, \end{aligned}$$

so that for a static potential,  $\partial V/\partial t = 0$ , the law of the conservation of biomechanical energy follows:  $dE/dt = 0$ . Here we have

$$\text{Surface term :} \quad G = m\dot{x}^i \delta x^i - E\delta t.$$

### 3.3.3 Hamiltonian Action

As a function of the *total biomechanical energy*, given by *Hamiltonian*

$$H(x^i, p_i; t) = \frac{p_i^2}{2m} + V(x^i, t), \quad (3.52)$$

the biomechanical Lagrangian (3.51) can also be written as ( $p_i = \partial L/\partial \dot{x}^i$ ):

$$L = p_i \dot{x}^i - H(x^i, p_i; t).$$

Here the independent dynamical variables are  $x^i$  and  $p_i$ ;  $t$  is the independent time-parameter variable. Hence the change of BAF is

$$\begin{aligned} \delta S &= \delta \int_{t_1}^{t_2} dt [p_i \dot{x}^i - H(x^i, p_i; t)] \\ &= \int_{t_1}^{t_2} dt \left[ p_i \frac{d}{dt} \delta x^i + \dot{x}^i \delta p_i - \delta H - H \frac{d}{dt} \delta t \right]. \end{aligned}$$

Upon using

$$\delta H = \left( \frac{\partial H}{\partial x^i} \delta x^i + \frac{\partial H}{\partial p_i} \delta p_i + \frac{\partial H}{\partial t} \delta t \right),$$

where, according to (3.52):  $\partial H/\partial x^i = \partial V/\partial x^i$  and  $\partial H/\partial p_i = p_i/m$ , we get

$$\begin{aligned} \delta S &= \delta \int_{t_1}^{t_2} dt [p_i \delta x^i - H\delta t] \\ &+ \int_{t_1}^{t_2} dt \left[ -\delta x^i \left( \dot{p}_i + \frac{\partial V}{\partial x^i} \right) + \delta p_i \left( \dot{x}^i - \delta_j^i \frac{p_j}{m} \right) + \delta t \left( \dot{H} - \frac{\partial H}{\partial t} \right) \right]. \end{aligned}$$

The biomechanical action principle  $\delta S = G_2 - G_1$  then tells us that

$$\begin{aligned}\delta p_i : \quad \dot{x}^k &= \frac{\partial H}{\partial p_k} = \delta^{ik} \frac{p_k}{m}, \\ \delta x^i : \quad \dot{p}_k &= -\frac{\partial H}{\partial x^k} = -\frac{\partial V}{\partial x^i}.\end{aligned}$$

In this way we have obtained the *two* first-order Hamiltonian ODEs of motion. Also,

$$\begin{aligned}\delta t : \quad \dot{H} &= \frac{\partial H}{\partial t}, \quad \text{and} \\ \text{Surface term :} \quad G &= p_i \delta x^i - H \delta t.\end{aligned}$$

### 3.3.4 Hamiltonian–Action Formulation of Biomechanics

Recall from Chapter 2 that *Riemannian metric*  $g = \langle, \rangle$  on the configuration manifold  $M$  is a positive-definite quadratic form  $g : M \rightarrow \mathbb{R}$ , induced by the system's kinetic energy (see [Arn89, IS01, Iva02, Iva05]). In local coordinates  $q^i \in U$ ,  $U$  open in  $M$ ,  $g$  is given as

$$g|_{q,m} \mapsto g_{ij}(q, m) dq^i dq^j, \quad (3.53)$$

where  $g_{ij}(q, m)$  is the *material covariant metric tensor* of the musculo-skeletal system, defining a relation between external and internal joint coordinates, and including  $n$  segmental masses  $m_\chi$  as

$$g_{ij}(q, m) = \sum_{\chi=1}^n m_\chi \delta_{rs} \frac{\partial x^r}{\partial q^i} \frac{\partial x^s}{\partial q^j}.$$

Here  $\delta_{rs}$  is the Kronecker-delta,  $x^r$  are external coordinates,  $r, s = 1, \dots, 6n$ ,  $i, j = 1, \dots, N \equiv 6n - h$  (where  $h$  denotes a number of holonomic constraints).

The *autonomous Hamiltonian function*  $H : T^*M \rightarrow \mathbb{R}$  of the musculo-skeletal biomechanics is, in local canonical coordinates  $q^i, p_i \in U_p$  on the momentum phase-space manifold, i.e., cotangent bundle  $T^*M$ , given by equation

$$H(q, p) = \frac{1}{2} g^{ij}(q, m) p_i p_j + V(q), \quad (3.54)$$

where  $g^{ij}(q, m)$  denotes the *material contravariant metric tensor*, relating internal and external coordinates, and including  $n$  segmental masses  $m_\chi$  as

$$g^{ij}(q, m) = \sum_{\chi=1}^n m_\chi \delta_{rs} \frac{\partial q^i}{\partial x^r} \frac{\partial q^j}{\partial x^s}.$$

Now, consider the *space  $\Omega$  of paths*  $\gamma = \gamma(t)$  in the momentum phase-space manifold  $T^*M$ , starting at the zero section  $o_M$

$$\Omega = \{\gamma : [0, 1] \rightarrow T^*M \mid \gamma(0) \in o_M\}$$

as a fibration  $\pi_\Omega : \Omega \rightarrow M$  over the configuration manifold  $M$ , given by

$$\pi_\Omega(\gamma) = \pi_{T^*M}(\gamma(1)).$$

For the Hamiltonian function (3.54), the classical *action functional*  $\mathcal{I}_H : \Omega \rightarrow \mathbb{R}$  is defined by

$$\mathcal{I}_H = \int_\gamma p_i dq^i - \int_0^1 H(\gamma) dt. \quad (3.55)$$

If  $\xi$  is a vector-field along  $\gamma \in \Omega$ , the first variation of  $\mathcal{I}_H$  in  $\xi$ -direction equals

$$d\mathcal{I}_H(\gamma)\xi = \int_0^1 [\omega(\dot{\gamma}, \xi) - dH(\gamma)\xi] dt + \theta(\xi(1)),$$

where  $\omega = -d(p_i dq^i)$  is the *canonical symplectic 2-form* on  $T^*M$ . The *fibre derivative* of  $\mathcal{I}_H$  vanishes on the set of Hamiltonian orbits in  $T^*M$  given by

$$\mathcal{H}_{orb} \equiv \{\gamma \in \Omega \mid \dot{\gamma} \lrcorner \omega = dH(\gamma)\}.$$

For Hamiltonian vector-field,  $X_H = \left(\frac{\partial H}{\partial p_i}, -\frac{\partial H}{\partial q^i}\right)$  on  $M$ , there exists a base integral curve  $\gamma_0(t) = (q^i(t), p_i(t))$  iff  $\gamma_0(t)$  is a *geodesic*, given by *covariant force equation* (see [DRh84, Iva02, IP01b, Iva05])

$$\dot{q}^k = g^{ki} p_i, \quad \dot{\tilde{p}}_i \equiv \dot{p}_i + \Gamma_{jk}^i g^{jl} g^{km} p_l p_m = 0, \quad (3.56)$$

where  $\Gamma_{jk}^i$  denote Christoffel symbols of the Levi-Civita connection  $\nabla$  in an open chart  $U$  on  $M$ , defined upon the Riemannian metric  $g = \langle, \rangle$  as

$$\Gamma_{jk}^i = g^{il} \Gamma_{jkl}, \quad \Gamma_{jkl} = \frac{1}{2} (\partial_{q^j} g_{kl} + \partial_{q^k} g_{jl} - \partial_{q^l} g_{jk}). \quad (3.57)$$

The l.h.s  $\dot{\tilde{p}}_i$  of the covariant momentum equation (3.56) represents the *intrinsic* or *Bianchi covariant derivative* of the momentum with respect to time  $t$ . Basic relation  $\dot{\tilde{p}}_i = 0$  defines the *parallel transport* on  $M$ , the simplest form of biomechanics. In that case Hamiltonian vector-field  $X_H$  is called the *geodesic spray* and its phase-flow is called the *geodesic flow* (for technical details see [Iva02, IS01, IP01b, Iva05]).

Now, the general deterministic model of human-like biomechanics is given by dissipative, driven Hamiltonian equations,

$$\dot{q}^i = \partial_{p_i} H + \partial_{p_i} R, \quad (3.58)$$

$$\dot{p}_i = F_i - \partial_{q^i} H + \partial_{q^i} R, \quad (3.59)$$

$$q^i(0) = q_0^i, \quad p_i(0) = p_i^0, \quad (3.60)$$

including *contravariant* equation (3.58) – the *velocity vector-field*, and *covariant* equation (3.59) – the *force 1-form*, together with initial joint angles and

momenta (3.60). Here  $(i = 1, \dots, N)$ , and  $R = R(q, p)$  denotes the Raileigh nonlinear (biquadratic) dissipation function, and  $F_i = F_i(t, q, p)$  are covariant driving torques of *equivalent muscular actuators*, resembling muscular excitation and contraction dynamics in rotational joint form (see subsection (3.4.4) below). For technical details see [Hat78, IS01, IP01a, Iva91].

The velocity vector-field (3.58) and the force 1-form field (3.59) together define the generalized Hamiltonian vector-field  $X_H$ , which geometrically represents the *section* of the momentum phase-space manifold  $T^*M$ , which is itself the cotangent bundle of the biomechanical configuration manifold  $M$ , (Fig. 1); the Hamiltonian (total energy) function  $H = H(q, p)$  is its generating function.

As the configuration manifold  $M$  is Hausdorff, for  $(q^i, p_i) \in U_p, U_q$  open in  $T^*M$ , there exists a unique one-parameter group of diffeomorphisms on  $T^*M$ , the *Hamiltonian phase-flow* [IP01b, Iva02, Iva05]

$$\begin{aligned} \phi_t : G_1 \times T^*M &\rightarrow T^*M : (p(0), q(0)) \mapsto (p(t), q(t)), \\ (\phi_t \circ \phi_s &= \phi_{t+s}, \quad \phi_0 = \text{identity}), \end{aligned}$$

given by (3.58–3.60) such that

$$\frac{d}{dt} \Big|_{t=0} \phi_t x = J \nabla H(x) = X_H, \quad \text{with} \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix},$$

where  $I$  denotes the  $n \times n$  identity matrix and  $\nabla$  is the gradient operator.

If  $\phi_t^H$  is a *Hamiltonian isotopy* generated by  $H$ , then we have the embedded *Lagrangian submanifold* (see [Mil99])

$$\phi_1^H(o_M) = \{d\mathcal{I}_H(\gamma) \mid \gamma \in \Sigma_{\mathcal{I}_H}\}.$$

For stochastic and fuzzy-set generalizations or the deterministic biomechanics defined above, see [IS01, Iva02].

### 3.3.5 Maupertuis Stationary Action in Biomechanics

In this subsection we consider dynamics of Newtonian biomechanical systems, depending on the Riemannian material metric tensor (i.e. inertia matrix)  $G_{ij}$ , including all the segment masses (see Introduction), and thus described in terms of either quadratic Hamiltonians,  $H(p, q) = \frac{1}{2}G^{ij}(q)p_i p_j + V(q)$ , or quadratic Lagrangians,  $L(q, \dot{q}) = \frac{1}{2}G_{ij}(q)\dot{q}^i \dot{q}^j - V(q)$ .

According to the *Maupertuis principle of stationary action*, among all the possible *iso-energetic paths*  $\gamma(t)$  with fixed end points, the paths that make vanish the first variation of the action functional

$$S[\gamma] = \int_{\gamma(t)} p_i dq^i = \int_{\gamma(t)} \frac{\partial L}{\partial \dot{q}^i} \dot{q}^i dt, \quad (i = 1, \dots, N)$$

– are natural motions (see [CCC97, CP02]).

As the kinetic energy  $T$  represents a homogeneous quadratic function in the system's velocities  $\dot{q}^i$ , i.e.,  $T = \frac{1}{2}\dot{q}^i \frac{\partial L}{\partial \dot{q}^i}$ , the Maupertuis principle reads

$$\delta S[\gamma] = \delta \int_{\gamma(t)} 2T dt = 0. \quad (3.61)$$

The configuration space  $M$  of a system with  $N$ DOF is an  $ND$  smooth manifold and the Lagrangian coordinates  $q^i$  ( $i = 1, \dots, N$ ) can be used as local coordinates on  $M$ . The manifold  $M$  can be naturally given a proper Riemannian structure. By introducing the tensor

$$g_{ij} = 2[E - V(q)] G_{ij}, \quad (3.62)$$

the Maupertuis principle (3.61) becomes

$$\delta \int_{\gamma(t)} 2T dt = \delta \int_{\gamma(t)} \sqrt{g_{ij} \dot{q}^i \dot{q}^j} dt = \delta \int_{\gamma(s)} ds = 0,$$

so that the Newtonian motions fulfil the geodesic condition on the manifold  $M$ , provided we define  $ds$  as its arc-length. The so-called Jacobi (or kinetic energy) metric tensor  $g$  on  $M$  is defined through its components by (3.62). Denoting by  $\nabla$  the canonical Levi-Civita connection on  $(M, g)$  (see section 2.5 above), the geodesic equation

$$\nabla_{\dot{\gamma}} \dot{\gamma} = 0$$

becomes, in the local coordinates  $q^i \in M$  (see Appendix)

$$\ddot{q}^i + \Gamma_{jk}^i \dot{q}^j \dot{q}^k = 0, \quad (3.63)$$

where the Christoffel symbols  $\Gamma_{jk}^i$  are the components of the connection  $\nabla$  defined by

$$\begin{aligned} \Gamma_{jk}^i &= \frac{1}{2} g^{im} (\partial_{q^j} g_{km} + \partial_{q^k} g_{mj} - \partial_{q^m} g_{jk}) \\ &= -\frac{1}{2T} [\delta_k^i \partial_{q^j} V + \delta_j^i \partial_{q^k} V - \partial_{q^i} V a^{li} G_{jk}] + \frac{1}{2} G^{il} [\partial_{q^l} G_{jk} + \partial_{q^k} G_{lj} - \partial_{q^l} G_{jk}]. \end{aligned}$$

Consider the slightly special case,  $g_{ij} = 2[E - V(q)] \delta_{ij}$ , so that

$$\Gamma_{jk}^i = -\frac{1}{2T} [\delta_{ik} \partial_{q^j} V + \delta_{ij} \partial_{q^k} V - \delta_{jk} \partial_{q^i} V]. \quad (3.64)$$

From the geodesic equation (3.63) we now get

$$\ddot{q}^i + \frac{1}{2(E - V)} [2\partial_{q^j} (E - V) \dot{q}^j \dot{q}^i - g^{ij} \partial_{q^j} (E - V) g_{km} \dot{q}^k \dot{q}^m] = 0,$$

and, using  $ds^2 = 2(E - V)^2 dt^2$ , these equations finally yield the expected Newtonian gradient form,

$$\ddot{q}^i = -\partial_{q^j} V.$$

### 3.3.6 Geometric Action

Recall that in the classical calculus of variations one studies functionals of the form

$$F_L(z) = \int_{\Omega} L(x, z, \nabla z) dx, \quad \Omega \subset \mathbb{R}^n, \quad (3.65)$$

where  $x = (x^1, \dots, x^n)$ ,  $dx = dx^1 \wedge \dots \wedge dx^n$ ,  $z = z(x) \in C^1(\bar{\Omega})$ , and the *Lagrangian*  $L = L(x, z, p)$  is a smooth function of  $x$ ,  $z$ , and  $p = (p_1, \dots, p_n)$ . The corresponding *Euler–Lagrange equation*, describing functions  $z(x)$  that are *stationary* for such a *functional*, is represented by the second-order PDE [BGG03]

$$\Delta z(x) = F'(z(x)).$$

For example, we may identify a function  $z(x)$  with its graph  $N \subset \mathbb{R}^{n+1}$ , and take the Lagrangian

$$L = \sqrt{1 + \|p\|^2},$$

whose associated functional  $F_L(z)$  equals the area of the graph, regarded as a hypersurface in Euclidean space. The Euler–Lagrange equation describing functions  $z(x)$  stationary for this functional is  $H = 0$ , where  $H$  is the mean curvature of the graph  $N$ .

To study these Lagrangians and Euler–Lagrange equations geometrically, we have to choose a class of admissible coordinate changes, and there are four natural candidates. In increasing order of generality, they are [BGG03]:

- Classical transformations, of the form  $x' = x'(x)$ ,  $z' = z'(z)$ ; in this situation, we think of  $(x, z, p)$  as coordinates on the space  $J^1(\mathbb{R}^n, \mathbb{R})$  of 1-jets of maps  $\mathbb{R}^n \rightarrow \mathbb{R}$  (see subsection (2.2.4) above).
- Gauge transformations, of the form  $x' = x'(x)$ ,  $z' = z'(x, z)$ ; here, we think of  $(x, z, p)$  as coordinates on the space of 1-jets of sections of a bundle  $\mathbb{R}^{n+1} \rightarrow \mathbb{R}^n$ , where  $x = (x^1, \dots, x^n)$  are coordinates on the base  $\mathbb{R}^n$  and  $z \in \mathbb{R}$  is a fibre coordinate.
- Point transformations, of the form  $x' = x'(x, z)$ ,  $z' = z'(x, z)$ ; here, we think of  $(x, z, p)$  as coordinates on the space of tangent hyperplanes

$$\{dz - p_i dx^i\}^\perp \subset T_{(x^i, z)}(\mathbb{R}^{n+1})$$

of the manifold  $\mathbb{R}^{n+1}$  with coordinates  $(x^1, \dots, x^n, z)$ .

- Contact transformations, of the form  $x' = x'(x, z, p)$ ,  $z' = z'(x, z, p)$ ,  $p' = p'(x, z, p)$ , satisfying the equation of differential 1-forms

$$dz' - p'_i dx^{i'} = f \cdot (dz - p_i dx^i)$$

for some function  $f(x, z, p) \neq 0$ .

Classical calculus of variations primarily concerns the following features of the functional  $F_L$  (3.65).

The first variation  $\delta F_L(z)$  is analogous to the derivative of a function, where  $z = z(x)$  is thought of as an independent variable in an infinite-dimensional space of functions. The analog of the condition that a point be critical is the condition that  $z(x)$  be stationary for all fixed-boundary variations. Formally, we write

$$\delta F_L(z) = 0,$$

which will give us a second-order scalar PDE for the unknown function  $z(x)$  of the form

$$\partial_z L - \partial_{x^i}(\partial_{p_i} L) = 0, \quad (3.66)$$

namely the *Euler-Lagrange equation* of the Lagrangian  $L(x, z, p)$ .

In this subsection we will study the PDE (3.66) in an invariant, geometric setting, following [BGG03]. As a motivation for this geometric approach, we note the fact that Lagrangian is invariant under the large class of *contact transformations*. Also, note that the Lagrangian  $L$  determines the functional  $F_L$ , but not vice versa. To see this, observe that if we add to  $L(x, z, p)$  a *divergence term* and consider

$$L'(x, z, p) = L(x, z, p) + \sum (\partial_{x^i} K^i(x, z) + \partial_z K^i(x, z) p^i)$$

for functions  $K^i(x, z)$ , then by the *Green's theorem*, the functionals  $F_L$  and  $F_{L'}$  differ by a constant depending only on values of  $z$  on  $\partial\Omega$ .  $L$  and  $L'$  have the same Euler-Lagrange equations.

Also, there is a relationship between symmetries of a Lagrangian  $L$  and conservation laws for the corresponding Euler-Lagrange equations, described by the *Noether theorem* (see subsection 1.1.4 above). A subtlety here is that the group of symmetries of an equivalence class of Lagrangians may be strictly larger than the group of symmetries of any particular representative. We will investigate how this discrepancy is reflected in the space of conservation laws, in a manner that involves global topological issues.

Finally, one considers the second variation  $\delta^2 F_L$ , analogous to the Hessian of a smooth function, usually with the goal of identifying local minima of the functional. There has been a great deal of analytic work done in this area for classical variational problems, reducing the problem of local minimization to understanding the behavior of certain Jacobi operators, but the geometric theory is not as well-developed as that of the first variation and the Euler-Lagrange equations.

Geometric BAF uses formalism of exterior differential systems introduced intuitively in (2.3.3) above, with *multi-index notation* [Gri83a, BGG03, BM82]. More precisely, an exterior differential system (EDS) is a pair  $(M, E)$  consisting of a smooth manifold  $M$  and a homogeneous, differentially closed ideal  $E \subseteq \Omega^*(M)$  in the algebra of smooth differential forms on  $M$ . Some of the EDSs that we study are differentially generated by the sections of a smooth subbundle  $I \subseteq T^*M$  of the cotangent bundle of  $M$ ; this subbundle, and sometimes its space of sections, is called a *Pfaffian system* on  $M$ . It will

be useful to use the notation  $\{\alpha, \beta, \dots\}$  for the (two-sided) *algebraic ideal* generated by forms  $\alpha, \beta, \dots$ , and to use the notation  $\{I\}$  for the algebraic ideal generated by the sections of a Pfaffian system  $I \subseteq T^*M$ . An *integral manifold* of an EDS  $(M, E)$  is a *submanifold immersion*  $\iota : N \hookrightarrow M$  for which  $\varphi_N \stackrel{\text{def}}{=} \iota^* \varphi = 0$  for all  $\varphi \in E$ . Integral manifolds of Pfaffian systems are defined similarly.

A differential form  $\varphi$  on the total space of a fibre bundle  $\pi : E \rightarrow B$  is said to be *semibasic* if its contraction with any vector-field tangent to the fibres of  $\pi$  vanishes, or equivalently, if its value at each point  $e \in E$  is the pull-back via  $\pi_e^*$  of some form at  $\pi(e) \in B$ . Some authors call such a form *horizontal*. A stronger condition is that  $\varphi$  be *basic*, meaning that it is locally (in open subsets of  $E$ ) the pull-back via  $\pi^*$  of a form on the base  $B$  [BGG03].

If  $(\omega^1, \dots, \omega^n)$  is an ordered basis for a vector space  $V$ , then corresponding to a *multi-index*  $I = (i_1, \dots, i_k)$  is the  $k$ -vector

$$\omega^I = \omega^{i_1} \wedge \dots \wedge \omega^{i_k} \in \bigwedge^k(V).$$

and for the complete multi-index we simply define [BGG03]

$$\omega = \omega^1 \wedge \dots \wedge \omega^n.$$

Letting  $(e_1, \dots, e_n)$  be a dual basis for  $V^*$ , we also define the  $(n - k)$ -vector

$$\omega_{(I)} = e_I \lrcorner \omega = e_{i_k} \lrcorner (e_{i_{k-1}} \lrcorner \dots (e_{i_1} \lrcorner \omega) \dots).$$

This  $\omega_{(I)}$  is, up to sign, just  $\omega^{I_c}$ , where  $I_c$  is a multi-index complementary to  $I$ .

Recall that a *contact manifold*  $(M, I)$  is a smooth manifold  $M$  of dimension  $2n + 1$ , with a distinguished line subbundle  $I \subset T^*M$  of the cotangent bundle which is non-degenerate in the sense that for any local 1-form  $\theta$  generating  $I$ ,

$$\theta \wedge (d\theta)^n \neq 0.$$

For example, A 1-jet is an equivalence class of functions having the same value and the same first derivatives at some designated point of the domain. On the space  $J^1(\mathbb{R}^n, \mathbb{R})$  of 1-jets of functions, we can take coordinates  $(x^i, z, p_i)$  corresponding to the jet at  $(x^i) \in \mathbb{R}^n$  of the linear function  $f(\bar{x}) = z + p_i(\bar{x}^i - x^i)$ . Then we define the *contact form*

$$\theta = dz - p_i dx^i,$$

for which

$$d\theta = -dp_i \wedge dx^i,$$

so the non-degeneracy condition  $\theta \wedge (d\theta)^n \neq 0$  is apparent. In fact, the *Pfaff theorem* [BGG03] implies that every contact manifold is locally isomorphic

to this example; that is, every contact manifold  $(M, I)$  has local coordinates  $(x^i, z, p_i)$  for which the form  $\theta = dz - p_i dx^i$  generates  $I$ .

Let  $(M, I)$  be a contact manifold of dimension  $2n + 1$ , and assume that  $I$  is generated by a global, non-vanishing section  $\theta \in \Gamma(I)$ ; this assumption only simplifies our notation, and would in any case hold on a double-cover of  $M$ . Sections of  $I$  generate the *contact differential ideal*

$$I = \{\theta, d\theta\} \subset \Omega^*(M)$$

in the exterior algebra of differential forms on  $M$ . A *Legendre submanifold* of  $M$  is an immersion  $\iota : N \hookrightarrow M$  of an  $n$ D submanifold  $N$  such that  $\iota^*\theta = 0$  for any contact form  $\theta \in \Gamma(I)$ ; in this case  $\iota^*d\theta = 0$  as well, so a Legendre submanifold is the same thing as an integral manifold of the differential ideal  $I$ . In Pfaff coordinates with  $\theta = dz - p_i dx^i$ , one such integral manifold is given by [BGG03]

$$N_0 = \{z = p_i = 0\}.$$

To see other Legendre submanifolds ‘near’ this one, note that any submanifold  $C^1$ -close to  $N_0$  satisfies the independence condition

$$dx^1 \wedge \cdots \wedge dx^n \neq 0,$$

and can therefore be described locally as a graph

$$N = \{(x^i, z(x), p_i(x))\}.$$

In this case, we have

$$\theta|_N = 0 \quad \text{iff} \quad p_i(x) = \partial_{x^i} z(x).$$

Therefore,  $N$  is determined by the function  $z(x)$ , and conversely, every function  $z(x)$  determines such an  $N$ ; we informally say that ‘the generic Legendre submanifold depends locally on one arbitrary function of  $n$  variables’. Legendre submanifolds of this form, with  $dx|_N \neq 0$ , will often be described as *transverse*.

Now, we are interested in functionals given by triples  $(M, I, \Lambda)$ , where  $(M, I)$  is a  $(2n + 1)$ D contact manifold, and  $\Lambda \in \Omega^n(M)$  is a differential form of degree  $n$  on  $M$ ; such a  $\Lambda$  will be referred to as a *Lagrangian* on  $(M, I)$  [BGG03]. We then define a functional on the set of smooth, compact Legendre submanifolds  $N \subset M$ , possibly with boundary  $\partial N$ , by

$$F_\Lambda(N) = \int_N \Lambda.$$

The classical variational problems described above may be recovered from this notion by taking  $M = J^1(\mathbb{R}^n, R) \cong R^{2n+1}$  with coordinates  $(x^i, z, p_i)$ ,  $I$  generated by  $\theta = dz - p_i dx^i$ , and  $\Lambda = L(x^i, z, p_i) dx$ . This formulation also admits certain functionals depending on second derivatives of  $z(x)$ , because

there may be  $dp_i$ -terms in  $\Lambda$ . Later, we will restrict attention to a class of functionals which, possibly after a contact transformation, can be expressed without second derivatives.

Suppose given a Lagrangian  $\Lambda \in \Omega^n(M)$  on a contact manifold  $(M, I)$ , and a fixed-boundary variation of Legendre submanifold  $F : N \times [0, 1] \rightarrow M$ ; we wish to compute  $\frac{d}{dt}(\int_{N_t} \Lambda)$ .

To do this, first recall the calculation of the *Poincaré–Cartan form* for the equivalence class  $[\Lambda] \in \bar{H}^n$ . Because  $I^{n+1} = \Omega^{n+1}(M)$ , we can write [BGG03]

$$d\Lambda = \theta \wedge \alpha + d\theta \wedge \beta = \theta \wedge (\alpha + d\beta) + d(\theta \wedge \beta),$$

and then

$$\Pi = \theta \wedge (\alpha + d\beta) = d(\Lambda - \theta \wedge \beta). \quad (3.67)$$

We are looking for conditions on a *Legendre submanifold*  $f : N \hookrightarrow M$  to be *stationary* for  $[\Lambda]$  under all fixed-boundary variations, in the sense that  $\frac{d}{dt}\big|_{t=0}(\int_{N_t} \Lambda) = 0$  whenever  $F|_{t=0} = f$ . We compute [BGG03]

$$\partial_t \int_{N_t} \Lambda = \partial_t \int_{N_t} (\Lambda - \theta \wedge \beta) = \int_{N_t} L_{\partial_t}(\Lambda - \theta \wedge \beta) = \int_{N_t} \partial_t \lrcorner \Pi.$$

One might express this result as

$$\delta(F_\Lambda)_N(v) = \int_N v \lrcorner f^* \Pi,$$

where the variational vector-field  $v$ , lying in the space  $\Gamma_0(f^*TM)$  of sections of  $f^*TM$  vanishing along  $\partial N$ , plays the role of  $\partial_t$ . The condition  $\Pi \equiv 0 \pmod{\{I\}}$  allows us to write  $\Pi = \theta \wedge \Psi$  for some  $n$ -form  $\Psi$ , not uniquely determined, and we have [BGG03]

$$\frac{d}{dt}\bigg|_{t=0} \int_{N_t} \Lambda = \int_N g f^* \Psi,$$

where  $g = (\partial_t \lrcorner F^* \theta)|_{t=0}$ . It was shown previously that this  $g$  could locally be chosen arbitrarily in the interior  $N^\circ$ , so the necessary and sufficient condition for a Legendre submanifold  $f : N \hookrightarrow M$  to be stationary for  $F_\Lambda$  is that  $f^* \Psi = 0$ .

In the particular classical situation where  $M = \{(x^i, z, p_i)\}$ ,  $\theta = dz - p_i dx^i$ , and  $\Lambda = L(x, z, p) dx$ , we have [BGG03]

$$d\Lambda = L_z \theta \wedge dx + L_{p_i} dp_i \wedge dx = \theta \wedge L_z dx - d\theta \wedge L_{p_i} dx_{(i)},$$

so referring to (3.67),

$$\Pi = \theta \wedge (L_z dx - d(L_{p_i} dx_{(i)})) = \theta \wedge \Psi.$$

Now, for a transverse Legendre submanifold  $N = \{(x^i, z(x), z_{x^i}(x))\}$ , we have  $\Psi|_N = 0$  iff (3.66) is valid along  $N$ .

### 3.3.7 Feynman Quantum-Mechanical Action

So far we have analyzed the macroscopic biodynamic dynamics. To make description of the biodynamic action complete, in this section we give a glimpse of a deeper, microscopic, quantum biodynamic action.

Molecular model of biodynamic action describes oscillations of Amid I peptide groups with associated dipole electric momentum inside a spiral structure of myosin filament molecules. There is a simultaneous resonant interaction and strain interaction generating a collective interaction directed along the axis of the spiral. The resonance excitation jumping from one peptide group to another can be represented as an exciton, the local molecule strain caused by the static effect of excitation as a phonon and the resultant collective interaction as a *solitary particle-wave object*.

To find appropriate BAF for this particle-wave object, we start from the Lagrangian version of biodynamic action principle. To quantize the theory, we begin with the important concept of the *probability*, or *transition*, *amplitude*. The motion of a biodynamic particle between two space-time points is described here in a quantum-mechanical formulation of R.P. Feynman [FH65], by a phase carrying *transition amplitude*.<sup>2</sup> Furthermore, all possible particle paths between these two points contribute to the transition amplitude.

At time  $t_1$ , we have a probability amplitude  $\psi(\mathbf{r}_1, t_1)$  of finding the biodynamic particle at the location given by the radius-vector  $\mathbf{r}_1$ . Similarly,  $\psi(\mathbf{r}_2, t_2)$  is the probability amplitude of finding the particle at the location  $\mathbf{r}_2$  at time  $t_2$ .

With  $K(\mathbf{r}_2, t_2 | \mathbf{r}_1, t_1)$  we want to denote the transition amplitude for a particle that is emitted at  $\mathbf{r}_1$  at time  $t_1$ , and is being detected at  $\mathbf{r}_2$  at time  $t_2$ .

If a particle is selected by a screen with openings  $\mathbf{r}_1$  to be at  $(\mathbf{r}_1, t_1)$  with the amplitude  $\psi(\mathbf{r}_1, t_1)$ , then propagates, [i.e., is emitted at  $(\mathbf{r}_1, t_1)$  and goes to  $(\mathbf{r}_2, t_2)$ , which is described by the quantum mechanical amplitude

<sup>2</sup> Feynman summarizes his approach to quantum mechanics in [Fey48]: “Non-relativistic quantum mechanics is formulated here in a different way. It is, however, mathematically equivalent to the familiar formulation. In quantum mechanics the probability of an event which can happen in several different ways is the absolute square of a sum of complex contributions, one from each alternative way. The probability that a particle will be found to have a path  $x(t)$  lying somewhere within a region of space time is the square of a sum of contributions, one from each path in the region. The contribution from a single path is postulated to be an exponential whose (imaginary) phase is the classical action (in units of  $\hbar$ ) for the path in question. The total contribution from all paths reaching  $x, t$  from the past is the wave function  $\psi(x, t)$ . This is shown to satisfy Schrödinger equation. The relation to matrix and operator algebra is discussed. Applications are indicated, in particular to eliminate the coordinates of the field oscillators from the equations of quantum electrodynamics.” (compare to section A.3.1 in the Appendix).

$K(\mathbf{r}_2, t_2 | \mathbf{r}_1, t_1)$ ], and then is detected at  $(\mathbf{r}_2, t_2)$  – amplitude  $\psi(\mathbf{r}_2, t_2)$  – then the total amplitude  $\psi(\mathbf{r}_2, t_2)$  reads:

$$\psi(\mathbf{r}_2, t_2) = \int d^3\mathbf{r}_1 K(\mathbf{r}_2, t_2 | \mathbf{r}_1, t_1) \psi(\mathbf{r}_1, t_1).$$

This is the fundamental dynamical equation of the microscopic biodynamic theory. Our main concern now is to find  $K$ , the kernel of the integral micro-biodynamic equation. So we have to study  $K(\mathbf{r}_2, t_2 | \mathbf{r}_1, t_1)$ , the so-called *Feynman propagator* more closely.

In order to get from  $A(\mathbf{r}_1, t_1)$  to  $B(\mathbf{r}_2, t_2)$ , the biodynamic particle must have taken some path  $\gamma$ . Let  $\phi_{BA}[\gamma]$  be the amplitude for the path of the particle going from  $A$  to  $B$  along  $\gamma$ . Then it holds that

$$K(B|A) = \int [d\gamma] \phi_{BA}[\gamma], \quad (3.68)$$

where the integral (or the sum) has to be taken over all paths from  $A$  to  $B$ . Obviously, the integral is very complicated, as infinitely many paths exist between  $A$  and  $B$ . The r.h.s of (3.68) is called the *Feynman path integral*.

For example, when we allow all possible paths in the  $(x, t)$ –plane between two points  $a$  and  $b$ , then the path integral is written as

$$K(b, a) = \int [dx(t)] \phi_{ba}[x(t)]$$

and the integral is taken over all possible paths from  $a$  to  $b$ .

We have until now reduced our problem to finding the amplitude  $\phi_{BA}[\gamma]$ . But one cannot determine this amplitude from a fundamental physical principle! We shall therefore postulate  $\phi_{BA}[\gamma]$  according to Dirac [Dir30]. Here we again come into contact with the Lagrangian version of the biodynamic action principle, where we assigned a classical  $S$ –BAF to each path:

$$S[\gamma] = \int_{t_1}^{t_2} dt L(\mathbf{r}, \dot{\mathbf{r}}; t).$$

Following an idea of Dirac, Feynman uses the following expression for  $\phi_{BA}[\gamma]$ :

$$\phi_{BA}[\gamma] = \exp\{(i/\hbar)S[\gamma]\}.$$

With this we get the following formula for the Feynman propagator:

$$K(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) = \int_{r(t_1)=r_1}^{r(t_2)=r_2} [d\mathbf{r}(t)] \exp \left[ \frac{i}{\hbar} \int_{t_1}^{t_2} dt L(\mathbf{r}(t), \dot{\mathbf{r}}(t); t) \right].$$

We can see from this form of  $K = \int [d\mathbf{r}(t)] \exp[iS[\mathbf{r}(t)]/\hbar]$  that the plane is constructed in such a way that in the classical limit,  $S \gg \hbar$ , exactly the actual classical particle path results, for the classical path is constructed in such a

manner that  $S$  does not change in first order in the vicinity of the classical trajectory; i.e., the phase  $S/\hbar$  stays constant in an infinitesimal neighborhood of the classical path  $\mathbf{r}_{cl}(t)$ . Outside of this vicinity of  $\mathbf{r}_{cl}(t)$ , the phase, in case  $S_{cl}/\hbar \gg 1$ , will change rapidly, so that the corresponding amplitudes will be washed out by destructive interference.

Since the main contribution to the propagator comes from the infinitesimal strip around the classical path, as first approximation it holds that in the classical limit  $\hbar \rightarrow 0$ :

$$K(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) \sim \exp \left[ \frac{i}{\hbar} \int_{t_1}^{t_2} dt L(\mathbf{r}_{cl}(t), \dot{\mathbf{r}}_{cl}(t); t) \right].$$

For a typical classical problem, the strip is very ‘narrow’, but for a typical quantum mechanical problem, the strip is very ‘wide’. Consequently, the classical path loses its meaning in a typical quantum mechanical solution.

As a first example, look at a free particle. For 1D case we have

$$K(x_2, t_2; x_1, t_1) = \int_{x(t_1)=x_1}^{x(t_2)=x_2} [dx(t)] e^{\frac{i}{\hbar} S}$$

with

$$S = \int_{t_1}^{t_2} dt L(x, \dot{x}; t).$$

For the deviation  $y = y(t)$  from the classical path (with fixed ends), the action is given as

$$S = S_{cl} + \frac{m}{2} \int_{t_1}^{t_2} dt \dot{y}^2,$$

where the classical action is equal

$$S_{cl} = \frac{m}{2} \frac{(x_2 - x_1)^2}{t_2 - t_1}. \quad (3.69)$$

So for the kernel-propagator we get

$$K(x_2, t_2; x_1, t_1) = \exp \left[ \frac{i}{\hbar} \frac{m}{2} \frac{(x_2 - x_1)^2}{t_2 - t_1} \right] \times \int_{y(t_1)=0}^{y(t_2)=0} [dy(t)] \times \exp \left[ \frac{i}{\hbar} \int_{t_1}^{t_2} dt \frac{m}{2} \dot{y}^2(t) \right],$$

which explicitly gives

$$K(x_2, t_2; x_1, t_1) = \sqrt{\frac{m}{2\pi i \hbar (t_2 - t_1)}} \exp \left[ \frac{i}{\hbar} \frac{m}{2} \frac{(x_2 - x_1)^2}{t_2 - t_1} \right].$$

In three dimensions we get instead

$$K(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) = \sqrt{\left(\frac{m}{2\pi i \hbar (t_2 - t_1)}\right)^3} \exp\left[\frac{i}{\hbar} \frac{m}{2} \frac{(\mathbf{r}_2 - \mathbf{r}_1)^2}{t_2 - t_1}\right].$$

Now,  $K(x, t; 0, 0)$  represents the Schrödinger wave function for a free particle which was emitted at  $x_1 = 0$  at time  $t_1 = 0$  and at  $(x, t)$  is described by the probability amplitude  $\psi(x, t)$ :

$$\psi(x, t) = K(x, t; 0, 0) = \sqrt{\frac{m}{2\pi i \hbar t}} \exp\left[\frac{i}{\hbar} \frac{m}{2} \frac{x^2}{t}\right].$$

As a second example, we take the more general quadratic Lagrangian for a particle in a constant external field

$$L = a(t)x^2 + b(t)x\dot{x} + c(t)\dot{x}^2 + d(t)x + e(t)\dot{x} + f(t).$$

For the deviation  $y = y(t)$  from the classical path (with fixed ends), the action is given as

$$S = S_{cl} + \int_{t_1}^{t_2} dt (a(t)y^2 + b(t)y\dot{y} + c(t)\dot{y}^2),$$

where the classical action is equal

$$S_{cl} = \frac{m}{2} \frac{(x_2 - x_1)^2}{t_2 - t_1} + \frac{F(t_2 - t_1)}{2} (x_1 + x_2) - \frac{F^2(t_2 - t_1)^3}{24m}.$$

So the propagator of a particle in a constant external field is

$$K(x_2, t_2; x_1, t_1) = \sqrt{\frac{m}{2\pi i \hbar (t_2 - t_1)}} \times \exp\left\{\frac{i}{\hbar} \left[\frac{m}{2} \frac{(x_2 - x_1)^2}{t_2 - t_1} + \frac{F}{2} (x_1 + x_2)(t_2 - t_1) - \frac{F^2(t_2 - t_1)^3}{24m}\right]\right\}.$$

Now, the simplest, linear model of the solitary particle-wave object, representing a single muscle-fibre, is *quantum harmonic oscillator* (see [9, 10]). Lagrangian of the oscillator is given by

$$L = \frac{m}{2} \dot{x}^2 - \frac{m}{2} \omega^2 x^2,$$

so for the propagator we have ( $T = t_2 - t_1$ ):

$$K(x_2, T; x_1, 0) = A(T) e^{\frac{i}{\hbar} S_{cl}}.$$

The classical BAF is equal

$$S_{cl} = \frac{m\omega}{2 \sin(\omega T)} [(x_1^2 + x_2^2) \cos(\omega T) - 2x_1 x_2], \quad \omega T \neq n\pi, \quad n \in \mathbb{Z},$$

so the propagator for the micro-biodynamic quantum harmonic oscillator is ( $T = t_2 - t_1$ ):

$$K(x_2, T; x_1, 0) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega T)}} \times \exp\left\{\frac{i m \omega}{\hbar 2 \sin(\omega T)} [(x_1^2 + x_2^2) \cos(\omega T) - 2x_1x_2]\right\}.$$

See Appendix for technical details on the Feynman path–integral formalism. Also, its geometric and fields extensions are used in Chapter 6 below.

### 3.4 Nonholonomic Problems in Human–Like Biomechanics

In this section we present nonholonomic problems in contemporary biomechanics. For these problems, an ordinary Hamilton principle is not valid.

#### 3.4.1 Lagrangian Approach

We start with a biomechanical configuration manifold  $M$  with local coordinates denoted  $q^i$ ,  $i = 1, \dots, n$  and a distribution  $\mathcal{D}$  on  $M$  that describes the kinematic nonholonomic constraints. The distribution is given by the specification of a linear subspace  $\mathcal{D}_q \subset T_qM$  of the tangent space to  $M$  at each point  $q \in M$ . In this section we consider only homogeneous velocity constraints.

The dynamics of a nonholonomically constrained biomechanical system is governed by the *Lagrange–d’Alembert principle*. The principle states that the equations of motion of a curve  $q(t)$  in configuration space are obtained by setting to zero the variations in the integral of the Lagrangian subject to variations lying in the constraint distribution and that the velocity of the curve  $q(t)$  itself satisfies the constraints; that is,  $\dot{q}(t) \in \mathcal{D}_{q(t)}$ . Standard arguments in the calculus of variations show that this *constrained variational principle* is equivalent to the equations (see [KM97])

$$-\delta L : \left( \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} - \frac{\partial L}{\partial q^i} \right) \delta q^i = 0, \quad (3.70)$$

for all variations  $\delta q$  such that  $\delta q \in \mathcal{D}_q$  at each point of the underlying curve  $q(t)$ . These equations are often equivalently written as

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} - \frac{\partial L}{\partial q^i} = \lambda_i, \quad (3.71)$$

where  $\lambda_i$  is a set of *Lagrange multipliers* ( $i = 1, \dots, n$ ), representing the force of constraint. Intrinsically, this multiplier  $\lambda$  is a section of the cotangent bundle over  $q(t)$  that annihilates the constraint distribution. The Lagrange multipliers are often determined by using the condition that  $\dot{q}(t)$  lies in the distribution.

To explore the structure of the Lagrange–d’Alembert equations (3.71) in more detail, let  $\{\omega^a\}$ ,  $a = 1, \dots, k$  be a set of  $k$  independent one forms whose

vanishing describes the constraints; i.e., the distribution  $\mathcal{D}$ . One can introduce local coordinates  $q^i = (r^\alpha, s^a)$  where  $\alpha = 1, \dots, n-k$ , in which  $\omega^a$  has the form

$$\omega^a(q) = ds^a + A_\alpha^a(r, s) dr^\alpha.$$

In other words, we are locally writing the distribution as

$$\mathcal{D} = \{(r; s, \dot{r}; \dot{s}) \in TM : \dot{s} + A_\alpha^a \dot{r}^\alpha = 0\}. \quad (3.72)$$

The equations of motion (3.70) may be rewritten by noting that the allowed variations  $\delta q^i = (\delta r^\alpha; \delta s^a)$  satisfy  $\delta s^a + A_\alpha^a \delta r^\alpha = 0$ . Substitution into (3.70) gives

$$\left( \frac{d}{dt} \frac{\partial L}{\partial \dot{r}^\alpha} - \frac{\partial L}{\partial r^\alpha} \right) = A_\alpha^a \left( \frac{d}{dt} \frac{\partial L}{\partial \dot{s}^a} - \frac{\partial L}{\partial s^a} \right).$$

Equation (3.72) combined with the constraint equations

$$\dot{s}^a = -A_\alpha^a \dot{r}^\alpha,$$

gives a complete description of the equations of motion of the system; this procedure may be viewed as one way of eliminating the Lagrange multipliers. Using this notation, one finds that  $\lambda = \lambda_a \omega^a$ , where  $\lambda_a = \frac{d}{dt} \frac{\partial L}{\partial \dot{s}^a} - \frac{\partial L}{\partial s^a}$ .

Now, we construct the geometric structures on the tangent bundle  $TM$  corresponding to those on the Hamiltonian side from the preceding subsection and formulate a similar procedure for obtaining the equations of motion.

First of all, we can define the energy function  $E$  simply as  $E = H \circ \mathbb{F}L$  (where  $\mathbb{F}L$  is the *fiber derivative*, or *Legendre transformation* defined above) and pull back to  $TM$  the canonical 2-form on  $T^*M$  and denote it by  $\Omega_L$ .

We define the distribution  $\mathcal{C} = (T\tau_M)^{-1}(\mathcal{D}) \subset TTM$ , where  $\tau_M : TM \rightarrow M$ . In coordinates, the distribution  $\mathcal{C}$  consists of vectors annihilated by the form  $\tau_M^* \omega^a$ :

$$\mathcal{C} = \{u \in TTM \mid \langle \tau_M^* \omega^a, u \rangle = 0\}.$$

When  $\mathcal{C}$  is restricted to the constraint submanifold  $\mathcal{D} \subset TM$ , we get the constraint distribution  $\mathcal{K}$ :

$$\mathcal{K} = \mathcal{C} \cap T\mathcal{D}.$$

Clearly  $\mathcal{M} = \mathbb{F}L(\mathcal{D})$  and  $\mathcal{H} = T\mathbb{F}L(\mathcal{K})$ .

The dynamics is given by a vector-field  $X_{\mathcal{K}}$  on the manifold  $\mathcal{D}$  which takes values in  $\mathcal{K}$  and satisfies the equation

$$X_{\mathcal{K}} \lrcorner \Omega_{\mathcal{K}} = dE_{\mathcal{K}},$$

where  $dE_{\mathcal{K}}$  and  $\Omega_{\mathcal{K}}$  are the restrictions of  $dE_{\mathcal{D}}$  and  $\Omega_{\mathcal{D}}$  respectively to the distribution  $\mathcal{K}$  and where  $E_{\mathcal{D}}$  and  $\Omega_{\mathcal{D}}$  are the restrictions of  $E$  and  $\Omega_L$  to  $\mathcal{D}$ .

Consider a configuration space  $M$ , a hyperregular Lagrangian  $L$  and a distribution  $\mathcal{D}$  that describes the kinematic nonholonomic constraints. The  $\mathcal{K}$ -valued vector-field  $X_{\mathcal{K}}$  on  $\mathcal{D}$  given by the equation

$$X_{\mathcal{K}} \lrcorner \Omega_{\mathcal{K}} = dE_{\mathcal{K}}$$

defines dynamics that are equivalent to the Lagrange–d’Alembert equations together with the constraints.

### 3.4.2 Hamiltonian Approach

The approach starts on the Lagrangian side with a configuration space  $M$  and a Lagrangian  $L$  of the form kinetic energy minus potential energy, i.e.,

$$L(q, \dot{q}) = \frac{1}{2} \langle \dot{q}, \dot{q} \rangle - V(q),$$

where  $\langle, \rangle$  is a metric on  $M$  defining the kinetic energy and  $V$  is a potential energy function. We do not restrict ourselves to Lagrangians of this form.

As above, our nonholonomic constraints are given by a distribution  $\mathcal{D} \subset TM$ . We also let  $\mathcal{D}^\circ \subset T^*M$  denote the annihilator of this distribution. As above, the basic equations are given by the Lagrange–d’Alembert principle.

The *Legendre transformation*  $\mathbb{F}L : TM \rightarrow T^*M$ , assuming that it is a diffeomorphism, is used to define the Hamiltonian  $H : T^*M \rightarrow \mathbb{R}$  in the standard fashion (ignoring the constraints for the moment):

$$H = \langle p, \dot{q} \rangle - L = p_i \dot{q}^i - L.$$

Here, the momentum is  $p = \mathbb{F}L(v_q) = \partial L / \partial \dot{q}$ . Under this change of variables, the equations of motion are written in the Hamiltonian form as (see [KM97])

$$\dot{q}^i = \partial_{p_i} H, \quad \dot{p}_i = -\partial_{q^i} H + \lambda_a \omega_i^a, \quad (3.73)$$

where  $i = 1, \dots, n$ , together with the constraint equations.

The *constrained Hamilton–d’Alembert equations* (3.73) can be rewritten as

$$X \lrcorner \Omega = dH + \lambda_a \pi_M^* \omega^a,$$

where  $X$  is the vector–field on  $T^*M$  governing the dynamics,  $\Omega$  is the canonical symplectic form on  $T^*M$ , and  $\pi_M : T^*M \rightarrow M$  is the cotangent bundle projection. We may write  $X$  in coordinates as  $X = \dot{q}^i \partial_{q^i} + \dot{p}_i \partial_{p_i}$ .

It is desirable to model the Hamiltonian equations without the Lagrange multipliers by a vector–field on a submanifold of  $T^*M$ . First, we define the set  $M = \mathbb{F}L(D) \subset T^*M$ ; so that the constraints on the Hamiltonian side are given by  $p \in M$ . Besides  $M$ , another basic object we deal with is defined as

$$\mathcal{F} = (T \pi_M)^{-1}(D) \subset TT^*M.$$

Using a basis  $\omega^a$  of the annihilator  $\mathcal{D}^\circ$ , we can write these spaces as

$$\mathcal{M} = \{p \in T^*M \mid \omega^a((\mathbb{F}L)^{-1}(p)) = 0\},$$

and

$$\mathcal{F} = \{u \in TT^*M \mid \langle \pi_M^* \omega^a, u \rangle = 0\}.$$

Finally, we define

$$\mathcal{H} = \mathcal{F} \cap T\mathcal{M}.$$

Using natural coordinates  $(q^i, p_i, \dot{q}^i, \dot{p}_i)$  on  $TT^*M$ , we see that the distribution  $\mathcal{F}$  naturally lifts the constraint on  $\dot{q}$  from  $TM$  to  $TT^*M$ . On the other hand, the space  $\mathcal{M}$  puts the associated constraints on the variable  $p$  and therefore the intersection  $\mathcal{H}$  puts the constraints on both variables.

To eliminate the Lagrange multipliers, we regard the Hamiltonian equations as a vector-field on the constraint submanifold  $\mathcal{M} \subset T^*M$  which takes values in the constraint distribution  $\mathcal{H}$ .

A result is that  $\Omega_{\mathcal{H}}$ , the restriction of the canonical 2-form  $\Omega$  of  $T^*M$  fiberwise to the distribution  $\mathcal{H}$  of the constraint submanifold  $\mathcal{M}$ , is nondegenerate. Note that  $\Omega_{\mathcal{H}}$  is not a true 2-form on a manifold, so it does not make sense to speak about it being closed. We speak of it as a fibre-restricted two form to avoid any confusion. Of course it still makes sense to talk about it being nondegenerate; it just means nondegenerate as a bilinear form on each fibre of  $\mathcal{H}$ . The dynamics is then given by the vector-field  $X_{\mathcal{H}}$  on  $\mathcal{M}$  which takes values in the constraint distribution  $\mathcal{H}$  and is determined by the condition

$$X_{\mathcal{H}} \lrcorner \Omega_{\mathcal{H}} = dH_{\mathcal{H}},$$

where  $dH_{\mathcal{H}}$  is the restriction of  $dH_{\mathcal{M}}$  to  $\mathcal{H}$ .

### 3.4.3 Biomechanical Example: Bicycle Dynamics

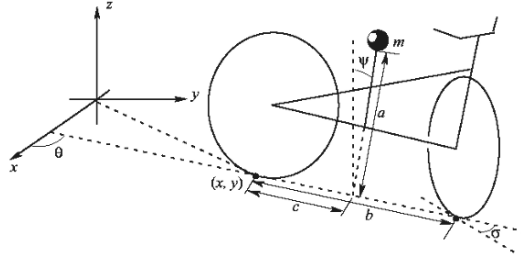
In engineering terminology bicycle represents an *underactuated balance mechanical system* with *nonholonomic rolling constraints* [KM97]. Such a system is beyond the reach of the Hamilton's action principle, and therefore cannot be described neither by Lagrangian, nor by Hamiltonian dynamics. It is governed by the Lagrange-d'Alembert principle.

The dynamics of an  $n$ -DOF nonholonomic mechanical system with  $k$  constraints, like a bicycle, are governed by the constrained Lagrange-d'Alembert equations (3.71), or Hamilton-d'Alembert equations (3.73). We will follow the later case here. The covariant term  $\lambda_a \omega_i^a$  in (3.73) denotes a set of Lagrange multipliers ( $i = 1, \dots, n$ ), representing the forces of constraint, where  $\{w_i^a\}$ ,  $a = 1, \dots, k$  is a set of  $k$  independent differential 1-forms whose vanishing describes the constraints, and coefficients  $\lambda_a$  are defined through coordinates of the constraints  $s^\alpha$  as

$$\lambda_a = \frac{d}{dt} \frac{\partial L}{\partial \dot{s}^\alpha} - \frac{\partial L}{\partial s^\alpha}.$$

For simplicity, a point mass bicycle is considered, with the wheels having negligible inertia moments, mass, and width, rolling without side or longitudinal slip, and having a fixed steering axis that is perpendicular to the

ground. Under such simplifications, the configuration manifold of the bicycle is  $M = SE(2) \times T^2$ , the direct product of the special 2D Euclidean group and the two-dimensional torus, parameterized by generalized coordinates  $q^i = \{x, y, \theta, \psi, \phi\}$  (see Figure 3.1).



**Fig. 3.1.** Simple model of a bicycle with coordinates used in the text.

Consider a ground fixed inertial reference frame with  $x$  and  $y$  axis in the ground plane and  $z$ -axis perpendicular to the ground plane in the direction opposite to gravity. The intersection of the vehicle's plane of symmetry with the ground plane forms a contact line. The contact line is rotated about the  $z$ -direction by a yaw angle  $\theta$ . The contact line is considered directed, with its positive direction from the rear to the front of the vehicle. The yaw angle  $\theta$  is zero when the contact line is in the  $x$ -direction. The angle that the bicycle's plane of symmetry makes with the vertical direction is the roll angle  $\psi \in (-\frac{\pi}{2}, \frac{\pi}{2})$ . Front and rear wheel contacts are constrained to have velocities parallel to the lines of intersection of their respective wheel planes and the ground plane, but free to turn about an axis through the wheel/ground contact and parallel to the  $z$ -axis. Let  $\sigma \in (-\frac{\pi}{2}, \frac{\pi}{2})$  be the steering angle between the front wheel plane/ground plane intersection and the contact line. With  $\sigma$  we associate a moment of inertia  $J$  which depends both on  $\psi$  and  $\sigma$ . We will parameterize the steering angle by  $\phi = \tan \sigma/b$ .

Kinetic energy  $KE : TM \rightarrow \mathbb{R}$  is given by

$$KE = \frac{1}{2}J(\psi, \phi)\dot{\phi}^2 + \frac{m}{2} \left( (\cos \theta \dot{x} + \sin \theta \dot{y} + a \sin \psi \dot{\theta})^2 + ((-\sin \theta \dot{x} + \cos \theta \dot{y} - a \cos \psi \dot{\psi} + c\dot{\theta})^2 + (-a \sin \psi \dot{\psi})^2 \right),$$

where  $m$  is the mass of the bicycle, considered for simplicity to be a point mass, and  $J(\psi, \phi)$  is the moment of inertia associated with the steering action. Potential energy  $PE : M \rightarrow \mathbb{R}$  is given by

$$PE = -mga \cos \psi.$$

The nonholonomic constraints associated with the front and rear wheels, assumed to roll without slipping, are expressed by

$$\dot{\theta} - \phi(\cos \theta \dot{x} + \sin \theta \dot{y}) = 0, \quad -\sin \theta \dot{x} + \cos \theta \dot{y} = 0,$$

which determine the *kinematic constraint distribution*

$$\mathcal{D}_q = \text{span}\{\partial_\psi, \partial_\phi, \cos \theta \partial_x + \sin \theta \partial_y + \phi \partial_\theta\}.$$

Using the nonholonomic momentum map on  $\mathcal{D}_q$ , the reduced Hamilton's equations of the bicycle motion are derived in the form (see [KM97])

$$\begin{aligned} \dot{\psi} &= \frac{1}{ma} \left( \frac{K}{F} \frac{p_\psi}{a} + \frac{c\phi \cos \psi}{F} p \right), & \dot{\phi} &= \frac{p_\phi}{J}, \\ \dot{p}_\psi &= mga \sin \psi + \frac{1}{2J^2} p_\phi^2 \frac{\partial J}{\partial \psi} + m(1 + a\phi \sin \psi) a\phi \cos \psi \xi^2 + mca\phi \sin \psi \xi \dot{\psi}, \\ \dot{p}_\phi &= \frac{1}{2J^2} \frac{\partial J}{\partial \phi} p_\phi^2, \\ \dot{p} &= -\frac{\gamma \cos \psi (1 + a\phi \sin \psi)}{F} \frac{p_\psi}{a} \dot{\phi} + \frac{a \sin \psi (1 + a\phi \sin \psi) + \gamma^2 \phi \sin^2 \psi}{F} p \dot{\phi}, \end{aligned}$$

where

$$\begin{aligned} \xi &= \frac{c\phi \cos \psi}{K} \dot{\psi} + \frac{1}{mK} p = \frac{c\phi \cos \psi}{mF} \frac{p_\psi}{a} + \frac{1}{mF} p, \\ K &= (1 + a\phi \sin \psi)^2 + \gamma^2 \phi^2, \\ F &= (1 + a\phi \sin \psi)^2 + \gamma^2 \phi^2 \sin^2 \psi. \end{aligned}$$

### 3.4.4 Constraint Dirac-Hamiltonian Dynamics

#### Dirac's Form of Classical Mechanics

Let  $q^i$  be coordinates in an  $ND$  configuration space  $Q$ . We restrict our presentation to autonomous systems, as explicit time dependencies can always be treated by considering the time as additional coordinate in an extended configuration space [Sei99]. The dynamics of a mechanical system described by a Lagrangian  $L(q, \dot{q})$  are given by the Euler-Lagrange's equations [Gol80]

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} = 0, \quad (i = 1, \dots, N). \quad (3.74)$$

If the Hessian  $\partial^2 L / \partial \dot{q}^i \partial \dot{q}^j$  is singular, some equations in (3.74) are not of second order and the system is *constrained*.

Recall that introduction of the canonically conjugate momenta

$$p_i = \frac{\partial L}{\partial \dot{q}^i}(q, \dot{q}) \quad (3.75)$$

leads to the Hamiltonian formalism. For a constrained system (3.75) cannot be solved for all velocities  $\dot{q}^i$ . Instead one obtains by elimination some *primary constraints*

$$\phi_\alpha(q, p) = 0, \quad \alpha = 1, \dots, A \leq N.$$

The *canonical Hamiltonian* of the system is given by

$$H_c(q, p) = p_i \dot{q}^i - L(q, \dot{q}). \quad (3.76)$$

For an unconstrained system it is obvious that  $H_c$  can be considered as a function of  $(q, p)$  only, since  $\dot{q}^i$  can be eliminated using (3.75). Due to the special form of the r.h.s of (3.76), this is also possible in a constrained system, but the resulting  $H_c$  is uniquely defined only *on* the constraint manifold. Thus the formalism remains unchanged, if we add an arbitrary linear combination of the constraint functions  $\phi$  [Sei99]. This leads to the *total Hamiltonian*

$$H_t(q, p) = H_c + u^\alpha \phi_\alpha, \quad (3.77)$$

where the multipliers  $u$  are *a priori* arbitrary functions of  $(q, p)$ .

Recall from subsection 3.2.3 above, that the standard Hamiltonian formalism is based on the canonical *Poisson bracket* of two phase-space functions  $F(q, p), G(q, p)$ :

$$\{F, G\} = \frac{\partial F}{\partial q} \frac{\partial G}{\partial p} - \frac{\partial G}{\partial q} \frac{\partial F}{\partial p}, \quad (3.78)$$

which is linear in its arguments, skew-symmetric ( $\{F, G\} = -\{G, F\}$ ), and satisfies the Jacobi identity  $\{F, \{G, H\}\} + \{G, \{H, F\}\} + \{H, \{F, G\}\} = 0$ . (3.78) gives the structure of a symplectic manifold to any biomechanical phase space. Coordinate transformations  $(q, p) \mapsto (Q, P)$  that preserve this structure are called *canonical*.

Using *constrained variational calculus* (see [Sei99]), one can show that the Euler-Lagrange equations (3.74) are equivalent to the following first order system [Dir50, Dir58]:

$$\dot{q} = \frac{\partial H_c}{\partial p} + u^\alpha \frac{\partial \phi_\alpha}{\partial p}, \quad \dot{p} = -\frac{\partial H_c}{\partial q} - u^\alpha \frac{\partial \phi_\alpha}{\partial q}, \quad \phi_\alpha = 0. \quad (3.79)$$

The differential part of (3.79) is not Hamiltonian. However, we can use the Hamiltonian system

$$\dot{q} = \{q, H_t\}, \quad \dot{p} = \{p, H_t\}, \quad \phi_\alpha = 0, \quad (3.80)$$

as the r.h.s of the ODEs in (3.79) and (3.80) differ only by linear combinations of the constraint functions. More generally, the time evolution of any phase-space function  $F(q, p)$  can be written as

$$\dot{F} = \{F, H_t\}. \quad (3.81)$$

In a consistent theory the constraints  $\phi_\alpha = 0$  must be preserved by the evolution of the system. This leads to the conditions

$$\dot{\phi}_\alpha = \{\phi_\alpha, H_t\} \approx 0. \quad (3.82)$$

The  $\approx$  signals a *weak equality*; it may hold only after taking the constraints into account. By a standard argument in differential geometry [Sei99] this implies that the Poisson bracket in (3.82) must be a linear combination of the constraint functions. There are three possibilities:

1. It yields modulo the constraints an equation of the form  $1 = 0$ ;
2. It becomes  $0 = 0$ ; and
3. We obtain a new equation  $\psi(q, p) = 0$ .

The first possibility (1) implies inconsistent equations of motion; they do not possess any solution. The second possibility (2) is the desired outcome. The third possibility (3) splits into two subcases. If  $\psi$  depends on some of the multipliers  $u$ , we consider it as an equation determining one of them. Otherwise we have a *secondary constraint*. We must then check whether all secondary constraints are preserved by repeating the procedure until either we encounter case (1) or all constraints lead to case (2). This is the *Dirac algorithm* [Dir50, Dir58].

The Dirac algorithm is sometimes surprisingly subtle [Sei99]. We consider here only a trivial example with the Lagrangian  $L = \frac{1}{2}(\dot{q}^1)^2 - V(q^1, q^2)$ . The momenta are  $p_1 = \dot{q}^1$  and  $p_2 = 0$ . Thus there is one primary constraint function  $\phi_1 = p_2$ . The total Hamiltonian is  $H_t = \frac{1}{2}p_1^2 + V(q^1, q^2) + up_2$  with a multiplier  $u$ . (3.82) leads to the secondary constraint function  $\phi_2 = \{\phi_1, H_t\} = -V_{q^2}$ . Applying (3.82) again yields  $\{\phi_2, H_t\} = -V_{q^1q^2}p_1 - V_{q^2q^2}u = 0$ . If we assume that  $V_{q^2q^2}$  does not vanish, the Dirac algorithm stops here, as this condition determines the multiplier  $u$ .

From the point of view of ODEs, the Dirac theory is a special case of the general problem of *completing* a system of ODEs [ST95]. This problem is also closely related to the concept of an *index* of a differential algebraic equation. Essentially, the (differential) index corresponds to the number of iterations needed in the Dirac algorithm [Sei99].

### Hamilton–Dirac Equations

Let  $\chi_\alpha$  ( $\alpha = 1, \dots, K$ ) denote all constraint functions, primary ones and those obtained with the Dirac algorithm. They can be divided into two classes by studying the  $K \times K$  matrix of their Poisson brackets

$$C_{\alpha\beta} = \{\chi_\alpha, \chi_\beta\}. \quad (3.83)$$

As  $C$  is skew-symmetric, its rank  $M$  is even. Let us assume for simplicity that after a simple relabelling of the  $\chi_\alpha$  the top left  $M \times M$  submatrix of  $C$  is regular (in general we must redefine the constraint functions by taking linear combinations to achieve this). Then we call the constraint functions  $\chi_1, \dots, \chi_M$  *second class*.

The Poisson bracket of a *first class* constraint function  $\psi$  with any other constraint function  $\chi$  (primary or higher) vanishes weakly,

for all  $\chi : \{\psi, \chi\} \approx 0$ .

In our case the constraint functions  $\chi_{M+1}, \dots, \chi_K$  are first class (again we may have to redefine them by taking linear combinations). Obviously this classification can be performed only after all constraints have been found.

First class constraints generate *gauge symmetries* [Sei99]. One example is the following system, which came up in a study of *Chern–Simons quantum mechanics*:

$$L = \frac{1}{2} (\dot{q}^1 - q^3 q^2)^2 + \frac{1}{2} (\dot{q}^2 + q^3 q^1)^2. \quad (3.84)$$

It describes a charged particle moving in a plane under the influence of a perpendicular constant magnetic field. There is one primary constraint function  $\phi_1 = p_3$  generating one secondary constraint function  $\phi_2 = q^2 p_1 - q^1 p_2$ . Both are first class and essentially generate the rotational symmetry of the system.

First class constraints lead to arbitrary functions in the general solution of the equations of motion; these are under-determined [ST95]. In the example described by the Lagrangian (3.84),  $q^3$  remains arbitrary. In the sequel we will always assume that no first class constraints are present. This is no real restriction, as they appear very rarely in finite-dimensional systems. Furthermore they can always be transformed into second class constraints by a gauge fixing, i.e., by adding further constraints removing the under-determinacy.

Second class constraints signal the presence of unphysical or redundant DOF; as mentioned above, their number  $M$  is always even. A trivial example is  $q^1 = p_1 = 0$ . If there are no first class constraints, the matrix  $C$  defined by (3.83) is regular (otherwise we take the submatrix of  $C$  corresponding to the second class constraint functions) and we can introduce the *Dirac bracket* [Dir50] of two phase-space functions  $F, G$ , by

$$\{F, G\}^* = \{F, G\} - \{F, \chi_\alpha\} (C^{-1})^{\alpha\beta} \{\chi_\beta, G\}. \quad (3.85)$$

In the case of our trivial example this means that in (3.78) we simply omit the differentiations with respect to  $q^1, p_1$ .

The Dirac bracket possesses exactly the same algebraic properties as the canonical Poisson bracket (3.78): it is linear, skew-symmetric and satisfies the Jacobi identity. Hence it can be used instead of (3.78) to define a symplectic structure on the phase-space. We will show now that, restricted to the constraint manifold, both brackets generate the same dynamics.

Consider for any function  $F(q, p)$  the dynamics defined by

$$\dot{F} = \{F, H_c\}^*. \quad (3.86)$$

We prove in two steps that for initial data on the constraint manifold these dynamics are equivalent to the original ones defined by (3.81). It suffices to show that the r.h.s of the respective equations of motion (3.81) and (3.86) are weakly equal, as for such initial data the trajectories never leave the constraint manifold.

As our first step we show that the evolution (3.86) is weakly equal to the one generated by the total Hamiltonian  $H_t$  using Dirac brackets:

$$\begin{aligned}\{F, H_t\}^* &= \{F, H_t\} - \{F, \chi_\alpha\}(C^{-1})^{\alpha\beta}\{\chi_\beta, H_t\} \\ &\approx \{F, H_c\} - \{F, \chi_\alpha\}(C^{-1})^{\alpha\beta}\{\chi_\beta, H_c\} \\ &\quad + u^\gamma (\{F, \chi_\gamma\} - \{F, \chi_\alpha\}(C^{-1})^{\alpha\beta}\{\chi_\beta, \chi_\gamma\}) \\ &= \{F, H_c\}^*.\end{aligned}$$

Here in the second line we used the fact that all Poisson brackets involving the multipliers  $u$  are multiplied by constraint functions, and in the last line the definition (3.83) of  $C$ .

As second step we note that on the constraint manifold the Dirac and Poisson brackets generate the same dynamics with  $H_t$ :

$$\{F, H_t\}^* = \{F, H_t\} - \{F, \chi_\alpha\}(C^{-1})^{\alpha\beta}\{\chi_\beta, H_t\} \approx \{F, H_t\},$$

as after completion of the Dirac algorithm  $\{\chi_\beta, H_t\}$  is for all  $\beta$  a linear combination of constraint functions. We are thus lead to the *Hamilton-Dirac equations*

$$\begin{aligned}\dot{q} = \{q, H_c\}^* &= \frac{\partial H_c}{\partial p} - \frac{\partial \chi_\alpha}{\partial p}(C^{-1})^{\alpha\beta}\{\chi_\beta, H_c\}, \\ \dot{p} = \{p, H_c\}^* &= -\frac{\partial H_c}{\partial q} + \frac{\partial \chi_\alpha}{\partial q}(C^{-1})^{\alpha\beta}\{\chi_\beta, H_c\}.\end{aligned}\tag{3.87}$$

For historical correctness one should remark that Dirac did not consider (3.87). He used the total Hamiltonian  $H_t$  instead of the canonical  $H_c$ . But we proved above that the corresponding equations of motion are weakly equal. Computationally the use of  $H_c$  is more efficient, as it leads to simpler equations.

The Dirac bracket effectively eliminates the second class constraints, as they become *distinguished* or *Casimir functions*: the Dirac bracket of any phase-space function  $F$  with a second class constraint function vanishes strongly, i. e. everywhere in phase-space, as again by the definition (3.83) of  $C$

$$\{F, \chi_\gamma\}^* = \{F, \chi_\gamma\} - \{F, \chi_\alpha\}(C^{-1})^{\alpha\beta}\{\chi_\beta, \chi_\gamma\} = 0.\tag{3.88}$$

### The Extended Hamiltonian

The distinction into first and second class constraints is an intrinsic one, i. e. it has a geometric meaning. In contrast, the distinction into primary and secondary (or higher) constraints is to some extent artificial and depends on the precise form of the Lagrangian  $L$ . There might exist an equivalent Lagrangian, i. e. one describing the same system, yielding different primary constraints.

Furthermore, if one looks at the argument for introducing the total Hamiltonian, one sees that one could also apply it to secondary constraints. These

considerations lead to the *extended Hamiltonian*  $H_e$ , which is the canonical Hamiltonian  $H_c$  plus a linear combination of all constraint functions and not just the primary ones.

Assuming that all constraint functions  $\chi$  are second class, we make the ansatz (see [Sei99])

$$H_e = H_c + v^\alpha \chi_\alpha. \quad (3.89)$$

Recall that the  $v$  should not be considered as new variables but as so far unknown functions of  $(q, p)$ . Demanding  $\{\chi_\alpha, H_e\} \approx 0$  yields the condition

$$\{\chi_\alpha, H_e\} = \{\chi_\alpha, H_c\} + \{\chi_\alpha, v^\beta\} \chi_\beta + \{\chi_\alpha, \chi_\beta\} v^\beta \approx 0. \quad (3.90)$$

If we discard the Poisson brackets with  $v$ , since they are multiplied by constraint functions, (3.90) becomes a system of linear equations with the particular solution

$$v^\alpha = -(C^{-1})^{\alpha\beta} \{\chi_\beta, H_c\}, \quad (3.91)$$

with  $C$  given by (3.83). Further solutions of the weak equation (3.90) are obtained by adding an arbitrary linear combination of constraint functions to each of the  $v^\alpha$ .

This suggests the following equations of motion:

$$\dot{q} = \{q, H_e\}, \quad \dot{p} = \{p, H_e\}. \quad (3.92)$$

We will see below that they yield the correct dynamics, as (3.92) is weakly equal to the Hamilton–Dirac equations (3.87).

The extended Hamiltonian leads to considerably more involved equations of motion than the Hamilton–Dirac approach. The multipliers and thus  $H_e$  depend on the matrix  $C^{-1}$  also appearing in the Dirac bracket (3.85). In the equations of motion (3.92) there arise terms from the Poisson brackets of the dynamical variables with the entries of  $C^{-1}$ , and these terms are typically rather complicated.

Leimkuhler and Reich [LR94] considered a simplification which they called the ‘weakly Hamiltonian Dirac formulation’. It arises by discarding the terms containing the Poisson brackets with the multipliers. This is allowed, since they vanish weakly. Using the solution (3.91) for the multipliers, we get as equations of motion

$$\begin{aligned} \dot{q} &= \{q, H_e\} \approx \{q, H_c\} - \{q, \chi_\alpha\} (C^{-1})^{\alpha\beta} \{\chi_\beta, H_c\}, \\ \dot{p} &= \{p, H_e\} \approx \{p, H_c\} - \{p, \chi_\alpha\} (C^{-1})^{\alpha\beta} \{\chi_\beta, H_c\}. \end{aligned}$$

Thus we recover the Hamilton–Dirac equations (3.87). Leimkuhler and Reich claimed that they were not Hamiltonian. We can now correct this statement. Although (3.87) is not Hamiltonian with respect to the canonical Poisson bracket, it is with respect to the Dirac bracket.

The above derivation of the extended Hamiltonian  $H_e$  is a special case of a more general construction [Sun82]. With any phase-space function  $A$  we

can associate a function  $A^* \approx A$  such that  $\{A^*, \chi\} \approx 0$  for all constraint functions  $\chi$ :

$$A^* = A - \chi_\alpha (C^{-1})^{\alpha\beta} \{\chi_\beta, A\}. \quad (3.93)$$

Using (3.91) for the multipliers, we find that  $H_e = H_c^*$ . The Dirac bracket of two functions  $A, B$  is weakly equal to the Poisson bracket of their associated quantities:

$$\{A, B\}^* \approx \{A^*, B^*\}.$$

### Constraint Stability

We discuss the stability of the constraint manifold for three formulations of the equations of motion:

1. The classical one (3.80) based on the total Hamiltonian  $H_t$ ;
2. The Hamilton–Dirac equations (3.87); and
3. The equations of motion (3.92) for the extended Hamiltonian  $H_e$ .

We assume that we are given the canonical Hamiltonian  $H_c$  on a  $2ND$  phase-space and that after completion of the Dirac algorithm there are  $K = 2k$  second class constraints  $\chi_\alpha(q, p) = 0$ .

Let  $T : (q, p) \mapsto (Q, P)$  be a canonical transformation such that in the new coordinates the constraints are given by  $Q^a = P_a = 0$  for  $a = 1, \dots, k$ .<sup>3</sup> At least locally, such a transformation always exists [Sei99]. Independent of which formulation is used, the transformed equations of motion can be split into two subsystems:

$$\begin{pmatrix} \dot{Q}^a \\ \dot{P}_b \end{pmatrix} = \begin{pmatrix} U_c^a(Q^i, P_i) Q^c + V^{ac}(Q^i, P_i) P_c \\ W_{bc}(Q^i, P_i) Q^c + Z_b^c(Q^i, P_i) P_c \end{pmatrix}, \quad \begin{pmatrix} \dot{Q}^r \\ \dot{P}_s \end{pmatrix} = \begin{pmatrix} F^r(Q^i, P_i) \\ G_s(Q^i, P_i) \end{pmatrix}. \quad (3.94)$$

The first part of (3.94) reflects that for all consistent formulations of the equations of motion the time derivative of any constraint function must vanish weakly and can thus be written as a linear combination of the constraint functions

$$\dot{\chi}_\alpha = M_\alpha^\beta(q^i, p_i) \chi_\beta. \quad (3.95)$$

Considering the variables  $(Q^r, P_r)$  as parameters, the origin is a fixed point of the first subsystem of (3.94) and its stability properties can be used as a measure for the stability of the constraint manifold.

Entering the constraints  $Q^a = P_a = 0$  into the second part of (3.94) yields a *Hamiltonian state-space form*. If we do not use the constraints, we get a perturbed state-space form, allowing for a perturbation theoretic analysis of the stability of the constraint manifold. However, we will not pursue this approach here, but concentrate on the stability of the origin in the first subsystem of (3.94).

<sup>3</sup> For the remainder of this section we adopt the following convention: indices  $a, b, c$  always run from 1 to  $k$ , indices  $r, s$  from  $k+1$  to  $N$ , and indices  $i, j$  from 1 to  $N$ .

The stability analysis of a Hamiltonian system differs in several aspects from that of a general dynamical system. Its linearization yields a Hamiltonian matrix. If  $\lambda$  is an eigenvalue of such a matrix,  $\bar{\lambda}$ ,  $-\lambda$  and  $-\bar{\lambda}$  are also eigenvalues [Arn89]. Hence a fixed point can be linearly stable iff all eigenvalues are zero or purely imaginary and their algebraic and geometric multiplicities are equal [MacK86].

Furthermore, no asymptotically stable fixed points exist. A stable fixed point is never hyperbolic, and the *Hartman–Grobman theorem* cannot be applied. Actually, linear stability is neither sufficient nor necessary for nonlinear stability. The only simple criterion for nonlinear stability is the theorem of Dirichlet [SM71]: if the eigenvalues are as above and the Hessian of the Hamiltonian with respect to all canonical variables is definite at the fixed point, then it is nonlinearly stable. Otherwise the stability can be only established with a normal form computation [Arn89, SM71].

For the Hamilton–Dirac equations (3.87) the stability analysis is easy. According to (3.88) the constraint functions  $\chi_\alpha$  are distinguished functions

$$\dot{\chi}_\alpha = \{\chi_\alpha, H_c\}^* = 0. \quad (3.96)$$

Hence the constraint functions are first integrals of the flow generated by (3.87), and in (3.94) the matrices  $U$ ,  $V$ ,  $W$  and  $Z$  vanish. This implies that the origin is stable. Obviously, there is no need to distinguish between linear and nonlinear stability.

This result has the following geometric meaning. The constraint functions  $\chi$  foliate the phase-space into disjoint submanifolds  $\mathcal{M}_\epsilon$  defined by  $\chi_\alpha(q, p) = \epsilon_\alpha$  with constants  $\epsilon$ . Exact solutions of the Hamilton–Dirac equations (3.87) lie completely on the submanifold  $\mathcal{M}_\epsilon$  determined by the initial data. The equations do not ‘see’ the values  $\epsilon$ ; especially  $\epsilon = 0$  is not distinguished.<sup>4</sup> Numerical errors are neither damped nor amplified by the dynamics. They lead to different values  $\bar{\epsilon}$ , and without further errors the trajectory would stay on the submanifold  $\mathcal{M}_{\bar{\epsilon}}$ .

For many constraint functions this result implies that the constraint manifold  $\mathcal{M}_0$  is *orbitally stable*<sup>5</sup> though not attractive. For example, if the submanifolds  $\mathcal{M}_\epsilon$  are compact, there obviously exists a constant upper bound (depending only on  $\epsilon$ ) for  $\text{dist}(X, \mathcal{M}_0)$  with  $X \in \mathcal{M}_\epsilon$ . The same holds for the important (for applications) case where the constraint functions  $\chi$  are quadratic.

In order to study the equations of motion derived with the total and extended Hamiltonian, respectively, we denote by  $\tilde{H}_c$ ,  $\tilde{H}_t$  and  $\tilde{H}_e$  the Hamiltonians transformed by  $\Gamma$ , by  $A_c$ ,  $A_t$  and  $A_e$  their Hessians with respect to

<sup>4</sup> This is also evident from the fact that the Dirac bracket depends only on the derivatives of the constraint functions and not on the functions themselves.

<sup>5</sup> A manifold  $\mathcal{M}$  is called orbitally stable for a dynamical system  $\dot{z} = f(z)$ , if for every  $\epsilon > 0$  there exists a  $\delta > 0$  such that for any solution  $z(t)$  satisfying  $\text{dist}(z(0), \mathcal{M}) < \delta$  the inequality  $\text{dist}(z(t), \mathcal{M}) < \epsilon$  holds [Sei99].

the variables  $(Q^a, P_a)$  evaluated at the origin, and by  $J = \begin{pmatrix} 0 & I_k \\ -I_k & 0 \end{pmatrix}$  the  $K \times K$  symplectic matrix. For the classical equations of motion (3.80) it is not possible to make any general statements. Linear stability is decided by the eigenvalues of  $B_t = JA_t$ . However, (numerical) experience shows that usually the origin is unstable. Otherwise the drift off the constraint manifold would not be a serious problem.

In the approach based on the extended Hamiltonian the precise form of the relevant matrices depends crucially on the chosen solution of the linear system (3.90) for the multipliers  $v$ . Leimkuhler and Reich [LR94] showed for the special case of the pendulum that the origin is a center if the  $v$  are determined using (3.91), whereas for another choice of  $v$  it becomes a saddle point. In principle, one could use the stability analysis as a guideline for choosing the precise form of the multipliers. But this seems hardly feasible in practice.

Using (3.91) for the multipliers, we find that

$$M_\alpha^\beta = -\{\chi_\alpha, (C^{-1})^{\beta\gamma}\{\chi_\gamma, H_c\}\} \quad (3.97)$$

(as above,  $C_{\alpha\beta} = \{\chi_\alpha, \chi_\beta\}$ ) and in the transformed coordinates  $(Q, P)$

$$U_b^a = -\frac{\partial^2 \tilde{H}_c}{\partial Q^a \partial P_b}, \quad V^{ab} = -\frac{\partial^2 \tilde{H}_c}{\partial Q^a \partial Q^b}, \quad W_{ab} = \frac{\partial^2 \tilde{H}_c}{\partial P_a \partial P_b}, \quad Z = -U^t. \quad (3.98)$$

Evaluated at the origin, the block matrix  $\begin{pmatrix} U & V \\ W & Z \end{pmatrix}$  becomes  $B_c = JA_c$ .

Thus the stability depends not only on the choice of the multipliers  $v$  but also on the precise form of the canonical Hamiltonian  $H_c$ . Recall from section 3.4.4 that  $H_c$  is uniquely defined only on the constraint manifold. We can add arbitrary linear combinations of the primary constraint functions to it, and such modifications change the matrix  $B_c$ . The Hamilton–Dirac equations are less sensitive to such changes; they affect only the second and not the first subsystem of (3.94), and thus only the perturbed state–space form but not the stability of the constraint manifold.

### Regular Systems with Imposed Constraints

For applications the most important case of a constrained system is described by a regular Lagrangian  $L_0$  and subject to  $k$  externally imposed holonomic constraints  $\phi_\alpha(q) = 0$ . In principle, this situation *cannot* be treated within the Dirac formalism, as it covers only singular Lagrangians. Therefore one introduces Lagrange multipliers  $\lambda^\alpha$  and considers the Lagrangian  $L = L_0 + \lambda^\alpha \phi_\alpha$ . In contrast to the multipliers  $u$  in the Dirac theory, the  $\lambda$  must be considered as additional dynamical variables and not as undetermined functions. Now  $L$  is obviously singular, as it does not depend on the ‘velocities’  $\dot{\lambda}$ .

For the Hamiltonian formalism we must introduce canonically conjugate momenta  $\pi_\alpha$  for the  $\lambda^\alpha$ . The primary constraints are simply given by  $\pi = 0$ .

If we denote by  $H_0$  the Hamiltonian for the regular system, the canonical Hamiltonian of the constrained system is  $H_c = H_0 - \lambda^\alpha \phi_\alpha$ ; the total one is  $H_t = H_c + u^\alpha \pi_\alpha$ . The Dirac algorithm yields the secondary constraints  $\phi_\alpha = 0$  and the tertiary constraints  $\psi_\alpha = \{\phi_\alpha, H_0\} = 0$ . The next step determines  $\lambda$ :

$$\{\psi_\alpha, H_0\} - \lambda^\beta \{\psi_\alpha, \phi_\beta\} = 0. \quad (3.99)$$

The fifth and last step yields  $u = 0$ .

This rather long derivation can be shortened by *not* introducing the total Hamiltonian  $H_t$  and the momenta  $\pi$ . Starting with  $H_c$  and imposing  $\phi = 0$  as primary constraints leads to equivalent results, as in the end  $\pi = u = 0$ . The standard approach is to take the Hamiltonian equations of motion for  $H_c$  and augment them by the constraints to get the following *differential algebraic equation* (see (3.79)):

$$\dot{q} = \frac{\partial H_0}{\partial p}, \quad \dot{p} = -\frac{\partial H_0}{\partial q} + \lambda^\alpha \frac{\partial \phi_\alpha}{\partial q}, \quad \phi_\alpha = 0. \quad (3.100)$$

By differentiating the last equation in (3.100) twice, one can derive exactly the same equation (3.99) for  $\lambda$  as in the Dirac theory. With  $Q_{\alpha\beta} = \{\phi_\alpha, \psi_\beta\}$  it has the solution

$$\lambda^\alpha \approx (Q^{-1})^{\alpha\beta} \{\psi_\beta, H_0\}. \quad (3.101)$$

The main problem in using Dirac brackets is the inversion of the matrix  $C$  of the Poisson brackets of the constraint functions. For a larger number  $K$  of constraints one can no longer do this symbolically. Thus one must numerically invert a  $K \times K$  matrix at each evaluation of the equations of motion. In our special case we have  $K = 2k$ , and  $C$  can be partitioned into four  $k \times k$  submatrices:

$$C = \begin{pmatrix} 0 & Q \\ -Q^t & S \end{pmatrix}, \quad (3.102)$$

where  $Q$  is as above and  $S_{\alpha\beta} = \{\psi_\alpha, \psi_\beta\}$ . The inversion of such a matrix can be reduced to the inversion of one  $k \times k$  matrix plus two matrix multiplications, as

$$C^{-1} = \begin{pmatrix} Q^{-t} S Q^{-1} & -Q^{-t} \\ Q^{-1} & 0 \end{pmatrix}. \quad (3.103)$$

The Hamilton-Dirac equations now take the following form:

$$\begin{aligned} \dot{q} &= \frac{\partial H_0}{\partial p} - (Q^{-1})^{\alpha\beta} \frac{\partial \psi_\alpha}{\partial p} \psi_\beta, \\ \dot{p} &= -\frac{\partial H_0}{\partial q} - (Q^{-1})^{\alpha\beta} \frac{\partial \phi_\alpha}{\partial q} \{\psi_\beta, H_0\} \\ &\quad + \left[ (Q^{-t} S Q^{-1})^{\alpha\beta} \frac{\partial \phi_\alpha}{\partial q} + (Q^{-1})^{\alpha\beta} \frac{\partial \psi_\alpha}{\partial q} \right] \psi_\beta. \end{aligned} \quad (3.104)$$

Taking (3.101) into account, we see that they differ from (3.100) only by some terms multiplied by  $\psi$ . Thus both formulations are weakly equal.

For the extended Hamiltonian we make the following ansatz:

$$H_e = H_0 - \lambda^\alpha \phi_\alpha + \mu^\alpha \psi_\alpha.$$

For  $\lambda$  we recover the result (3.101); for  $\mu$  we get

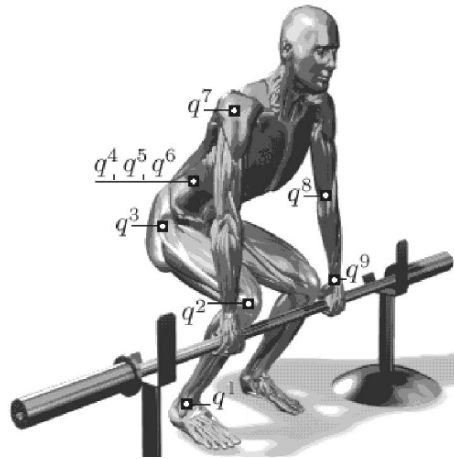
$$\mu^\alpha = (Q^{-1})^{\alpha\beta} \psi_\beta. \quad (3.105)$$

Thus  $\mu$  vanishes weakly and could be taken as zero. But then  $H_e = H_t$ , and we get as equations of motion the classical ones (3.100) plus terms  $(\partial\lambda^\alpha/\partial q)\phi_\alpha$  and  $(\partial\lambda^\alpha/\partial p)\phi_\alpha$ , respectively (compare (3.79) and (3.80)).

The multipliers  $\lambda$  depend on derivatives of the momentum constraint functions  $\psi$ . Since they occur in the extended Hamiltonian  $H_e$ , we need three differentiations of the original constraint functions  $\phi$  to set up the equations of motion, as opposed to the Hamilton–Dirac equations where two differentiations suffice.

### Biomechanics of Load–Lifting

As a simple practical example of the basic biomechanics equations in Hamiltonian form, we give here a 9 DOF, muscle-driven, lumped–spinal biomechanical model for 3D *symmetrical load–lifting* (see Figure 3.2; for biomechanical details, see [IS01]).



**Fig. 3.2.** A 9–DOF, muscle–driven, lumped–spinal biomechanical model for 3D symmetrical load–lifting.

The model is formulated under the following assumptions.

- Mechanical assumptions:

1. 3D load-lifting with symmetrical-hands is considered;
  2. All described joint motions, except L5/S1 swivel-joint, are reduced to uniaxial,  $SO(2)$  rotational groups;
  3. Distributed-parameter spine dynamics (according to the ergonomics literature) is represented by the lumped L5/S1 swivel-joint dynamics, and further decomposed into 3 uniaxial rotations: flexion-extension in the sagittal plane, lateral bending in the frontal plane and twisting in the horizontal plane; and
  4. In each  $SO(2)$ -joint an *equivalent muscle torque* is generated by an antagonistic muscle-pair of flexor-extensor type. Input variables are equivalent muscle torques and output variables are time evolutions of joint angles and associated angular momenta.
- Anatomical assumptions:  
Humanoid's joint-angles (see Figure 3.2) are defined as:  $q^1$  – ankle (flexion-extension),  $q^2$  – knee (flexion-extension),  $q^3$  – hip (flexion-extension),  $q^4$  – L5/S1-sagittal plane (flexion-extension),  $q^5$  – L5/S1-horizontal plane (twisting),  $q^6$  – L5/S1-frontal plane (lateral flexion),  $q^7$  – shoulder (flexion-extension),  $q^8$  – elbow (flexion-extension), and  $q^9$  – wrist (flexion-extension).
  - Biomechanical assumptions:  
The global load lifting-dynamical system can be separated into 3 parts:
    1. Pure mechanical, rigid skeleton dynamics, defining conservative motion of body segments influenced by inertial, gravitational and Coriolis forces;
    2. Active muscular (force-velocity-time) biomechanics, defining the excitation/contraction synergy of representative (i.e., equivalent) skeletal muscles;
    3. Passive nonlinear joint damping, representing anatomical-synovial dissipation.

Under above assumptions, the basic biomechanics equations in vector form read

$$\dot{\mathbf{q}} = \partial H / \partial \mathbf{p} + \partial R / \partial \mathbf{p}, \quad (3.106)$$

$$\dot{\mathbf{p}} = \mathbf{F} - \partial H / \partial \mathbf{q} + \partial R / \partial \mathbf{q}. \quad (3.107)$$

Without active muscular drives (i.e., for  $\mathbf{F} = 0$ ), the system (3.106–3.107) reduces:

1. with  $R = 0$ , to the conservative Hamiltonian system;
2. with  $H = 0$ , to the pure gradient system;

#### *Momentum Phase-Space*

The joint-angles  $q^i$  (Figure 3.2) now all represent the plane-rotational Lie-groups  $SO(2)^i$  ( $i = 1, \dots, 9$ ), and their 9-times tensor product gives a 9D torus  $T^9$ , which is an Abelian Lie group of all nondegenerate diagonal  $9 \times 9$ -matrices.

Consequently, the load lifting momentum phase-space is defined as an 18D cotangent bundle  $T^*T^9$ , including both the joint angles  $\mathbf{q} = q^i$  and the corresponding angular momenta  $\mathbf{p} = p_i$ , the canonically conjugate variables which are infinitesimal generators of joint rotations and consequently belong to the cotangent Lie-algebras  $so(2)_i^*$ ; otherwise they represent the impulses of the total joint-torques:

$$\mathbf{p} = \int_{t_0}^{t_1} \left( \mathbf{F}(\tau, \mathbf{q}, \mathbf{p}) - \frac{\partial H}{\partial \mathbf{q}} + \frac{\partial R}{\partial \mathbf{q}} \right) d\tau.$$

Thus, the biomechanical configuration manifold  $M$  is now reduced to the 9D torus  $T^9$  (with the active joint angles depicted on Figure 3.2) and the biomechanical momentum phase-space manifold  $T^*M$  is now reduced to the 18D cotangent bundle  $T^*T^9$ .

#### *Conservative Skeleton Dynamics*

On the load-lifting momentum phase-space manifold  $M = T^*T^9$  we have the natural action of the autonomous Hamiltonian (kinetic energy  $T$  plus potential energy  $V$ ) generating function  $H : M \rightarrow \mathbb{R}$ . The biomechanics Hamiltonian vector-field  $X_H$  on  $M$ , representing the conservative dynamical system of load-lifting, is now defined as  $X_H = (\partial H / \partial \mathbf{p}, -\partial H / \partial \mathbf{q})$ , representing the infinitesimal generator of the action  $\phi_t$  of the one-parameter group  $G_1$  of canonical diffeomorphisms on  $M$ , i.e., *autonomous conservative (symplectic) phase-flow*

$$\begin{aligned} \phi_t : G_1 \times M &\rightarrow M : (p(0), q(0)) \rightarrow (p(t), q(t)), \\ (\phi_t \circ \phi_s &= \phi_{t+s}, \quad \phi_0 = \text{identity}), \end{aligned} \quad (3.108)$$

determined by autonomous, conservative Hamilton's equations (in vector notation)

$$\dot{\mathbf{q}} = \partial H / \partial \mathbf{p}, \quad \dot{\mathbf{p}} = -\partial H / \partial \mathbf{q}.$$

To determine potential and kinetic energies, we define the two corresponding position vectors  $r_j^V$  and  $r_j^T$ , respectively

$$r_j^V = \sum_{i=1}^9 \sum_{i=1}^j \sigma_i L_i (1 - \cos q^i), \quad r_j^T = \sum_{i=1}^9 \sum_{i=1}^j L_i \cos q^i,$$

where  $\sigma = [-1, -1, -1, -1, 0, -1, 1, 1, 1]$  and  $L_i$  denote human segmental lengths. Using  $r_j^V$  and  $r_j^T$ , we get for the potential energy

$$V(q) = g m_j r_j^V,$$

(where  $g$  denotes gravitational acceleration, and  $m_i$  are segmental masses) and for the kinetic energy

$$T(q, p) = \frac{1}{2} g^{ij}(q) p_i p_j = \frac{1}{2} \left\{ [m_i(r_j^T)^2]^{-1} + [J_i]^{-1} \right\} p_i p_j,$$

where  $g^{ij} = g^{ij}(q, m)$ , corresponding to the term in the curly braces, is the contravariant metric tensor (i.e., inverse inertia matrix).

The autonomous conservative Hamilton's equations are derived in the following expanded form

$$\dot{q}^i = p_i \left\{ [J_i]^{-1} + \left[ m_i \left( \sum_{k=1}^i L_k \cos q^k \right)^2 \right]^{-1} \right\}, \tag{3.109}$$

$$\begin{aligned} \dot{p}_i = & -g \sum_{k=i}^{10-i} L_k m_k \sin q^k \tag{3.110} \\ & - \sum_{k=i}^{10-i} L_k \sin q^k p_i p_k \left[ m_i \left( \sum_{k=1}^i L_k \cos q^k \right)^3 \right]^{-1}. \end{aligned}$$

The basic characteristic of the conservative Hamiltonian system (3.109–3.110) is that its symplectic phase-flow  $\phi_t$  (3.108) consists of canonical transformations *preserving the phase-space volume*, i.e., *Liouville measure* vol, defined as

$$\text{vol} = dq^1 \wedge \dots \wedge dq^9 \wedge dp_1 \wedge \dots \wedge dp_9,$$

as proposed by the Liouville theorem (see [Arn89]).

However, the preservation of volume *causes structural instability* of the conservative Hamiltonian system (3.109–3.110), i.e., the *phase-space spreading effect* by which small phase regions  $R_t(\in M)$  will tend to get distorted from the initial one  $R_o(\in M)$  (during the conservative Hamiltonian system evolution). The problem is much more serious in higher dimensions than in lower dimensions, since there are so many ‘directions’ in which the region can locally spread (see [Pen89]). So, regardless of stability and accuracy of the supposed numerical integrator, the solutions of the conservative ODEs (3.109–3.110) necessarily diverges for any initial angles and momenta, and the flow  $\phi_t$  (3.108) could not be obtained.

*Dynamics of Joints and Muscles*

**Joint dynamics**, is described here by  $(q, p)$ -quadratic form of the *Rayleigh – Van der Pol's dissipation function* (see [IS01])

$$R = \frac{1}{2} \sum_{i=1}^9 p_i^2 [a_i + b_i(q^i)^2], \tag{3.111}$$

where  $a_i$  and  $b_i$  denote dissipation parameters. Its partial derivatives  $\partial R / \partial p$  give rise to viscous forces in the joints which are linear in  $p_i$  and quadratic in  $q^i$ . It is based on the unforced Van der Pol's oscillator

$$\ddot{x} - (a + b x^2) \dot{x} + x = 0,$$

where the damping force  $F^{dmp}(\dot{x}) = -\partial R/\partial \dot{x}$  is given by the Rayleigh's dissipation function  $R = \frac{1}{2} (a + b x^2) \dot{x}^2$  – with the velocity term  $\dot{x}$  replaced by our momentum term  $p^2$ .

Thus, by including the biquadratic dissipation (3.111) into the symplectic phase-flow  $\phi_t$  (3.108), we try somehow to bound its naturally-unbounded diverging phase-trajectories, and hence to stabilize it in some kind of a *relaxation oscillatory regime*, which is quite natural for both biological and biomechanical systems (see [IS01]).

**Muscular dynamics**, giving the driving torques  $F_i = F_i(t, q, p)$  for the biomechanics in general, as well as for our load-lifting task in particular, should describe the internal *excitation* and *contraction* dynamics [IS01] of *equivalent muscular actuators*, anatomically represented by resulting action of *antagonistic muscle-pairs* for each uniaxial (i.e.,  $SO(2)$ ) human joint. We attempt herein to describe the equivalent muscular dynamics in the simplest possible way (e.g., Hatze used 51 nonlinear first-order ODEs to derive his arguably most elaborate, myocybernetic model [Hat78]), and yet to include the main excitation and contraction relations.

- *Excitation dynamics* can be described by *impulse torque-time relation*

$$\begin{aligned} F_i^{imp} &= F_i^0 (1 - e^{-t/\tau_i}) && \text{if stimulation} > 0 \\ F_i^{imp} &= F_i^0 e^{-t/\tau_i} && \text{if stimulation} = 0, \end{aligned}$$

where  $F_i^0$  denote the maximal isometric muscular torques applied at  $i$ -th joint ( $i = 1, \dots, 9$ ), while  $\tau_i$  denote the time characteristics of particular muscular actuators. This is a rotational-joint form of the solution of the Wilkie's *muscular active-state element equation* [Wil56]

$$\dot{x} + \beta x = \beta S A, \quad x(0) = 0, \quad 0 < S < 1,$$

where  $x = x(t)$  represents the active state of the muscle,  $\beta$  denotes the element gain,  $A$  corresponds to the maximum tension the element can develop, and  $S = S(r)$  is the 'desired' active state as a function of motor unit stimulus rate  $r$ .

- *Contraction dynamics* has classically been described by the Hill's *hyperbolic force-velocity relation* [Hil38], which we propose here in the rotational  $(q, p)$ -form

$$F_i^{Hill} = \frac{(F_i^0 b_i - a_i p_i)}{(p_i - b_i)}, \quad (i = 1, \dots, 9),$$

where  $a_i$  (having dimension of torque) and  $b_i$  (having dimension of momentum) denote the *rotational Hill's parameters* (see [IS01]), corresponding to the energy dissipated during the contraction and the phosphagenic energy conversion rate, respectively.

Therefore, we can describe the excitation/contraction dynamics for the  $i$ -th equivalent muscle-joint actuator, i.e., antagonistic muscle pair (e.g., flexion/extension in the  $i$ -th joint) by the simple impulse-hyperbolic product-relation

$$F_i(t, q, p) = F_i^{imp} \times F_i^{Hill}, \quad (i = 1, \dots, 9).$$

*Total Load-Lifting Dynamics*

In this way, the total load lifting dynamics on  $M = T^*T^9$  is represented by the *dissipative, muscle-driven Hamiltonian phase-flow*

$$\begin{aligned} \phi_{md_t} : G_1 \times M &\rightarrow M : (p(0), q(0)) \rightarrow (p(t), q(t)), & (3.112) \\ (\phi_{md_t} \circ \phi_{md_s} &= \phi_{md_{t+s}}, \quad \phi_{md_0} = \text{identity}), \end{aligned}$$

generated by the Hamiltonian vector-field  $X_H$  on  $M$  given by *dissipative, driven Hamilton's equations* (3.106–3.107).

Here  $G_1$  is the one-parameter Lie group of muscle-driven and dissipative transformations of the momentum phase-space manifold  $M = T^*T^9$ . Therefore, the autonomous Hamiltonian function  $H(q, p) = T(q, p) + V(q)$  is conserved during the load lifting, but the flow  $\phi_{md_t}$  (3.112) is not conserved. This is a biomechanical ‘escape’ from the Liouville theorem. The dynamical equations (3.106–3.107) can be expanded as

$$\dot{q}^i = p_i \left\{ [J_i]^{-1} + \left[ m_i \left( \sum_{k=1}^i L_k \cos q^k \right)^2 \right]^{-1} + b_i q^i p_i \right\}, \quad (3.113)$$

$$\begin{aligned} \dot{p}_i &= F_i + p_i \left( a_i + b_i q^{i(2)} \right) - g \sum_{k=i}^{10-i} L_k m_k \sin q^k & (3.114) \\ &- \sum_{k=i}^{10-i} L_k \sin q^k p_i p_k \left[ m_i \left( \sum_{k=1}^i L_k \cos q^k \right)^3 \right]^{-1}. \end{aligned}$$

In the velocity-equation (3.113), the terms denote rotational velocities, translational velocities and velocity dampings for the  $i$ th joint ( $i = 1, \dots, 9$ ), respectively. The force-equation (3.114) contains terms of inertial torques (as differences between active-internal muscular torques and passive-external gravitational, Coriolis and centrifugal torques), plus passive-internal joint-damping torques. In the velocity-equation, the last segment-length  $L_i$  should, in every iteration, be replaced by the segmental centre-mass proximal distance  $a_i$ . Also, the  $L_i$ -terms with indices 4, 5, 6 are mutually exclusive; e.g., when vertical lifting is simulated, both  $L_5$  and  $L_6$  are zero. In the force-equation, the gravitational term is zero for the 5th (horizontal twisting) joint.

The system (3.113–3.114) is geometrically analogous to the *redundant manipulator* (a load-body with 6 external DOF, representing the *special Euclidean group of motions* is being lifted using 9 internal DOF – joint angles

representing  $SO(2)$  rotational groups). Consequently, to each position of the load-body corresponds an infinite number of angle trajectories. So, the dissipative, driven phase-flow (3.112) has an infinite number of possible trajectories starting within the ‘small’ region of initial conditions (joint angles and momenta); for this reason, it is extremely sensitive to changes of anthropomorphic parameters and initial conditions. However, this is the *general characteristics* of the biomechanics [IS01, Iva91]: *many DOF and highly nonlinear synergy even for very simple tasks*. Consequently, the utilization of energy is also mechanically inefficient. However, from the point of view of information and control, it is highly efficient.

### 3.5 Lie Functors in Human-Like Biomechanics

In this section we present several Lie functors, as they are used in modern biomechanical research, all being different formulations of the *covariant force law*,  $F_i = mg_{ij}a^j$ , and giving different Lie representations of the fundamental *covariant force functor*  $\mathcal{F}_* : TT^*M \rightarrow TTM$  (see section 2.7 above).

#### 3.5.1 Lie-Lagrangian Biomechanical Functor

Now we develop the *Lie-Lagrangian biomechanics functor* using a modern, nonlinear formulation of the classical robotics structure:

$$\begin{array}{ccccc} \textit{Kinematics} & \rightarrow & \textit{Dynamics} & \rightarrow & \textit{Control} \\ \textit{Lie groups} & \rightarrow & \textit{Exterior Lagrangian} & \rightarrow & \textit{Lie derivative} \end{array}$$

The conservative part of generalized Lagrangian formalism, as used in biomechanics, is derived from Lagrangian conservative energy function. It describes the motion of the conservative skeleton, which is free of control and dissipation. According to the Liouville theorem, this conservative dynamics is structurally unstable due to the phase-space spreading effect, caused by the growth of entropy (see [Iva91, IS01]). The dissipative part is derived from nonlinear dissipative function, and describes quadratic joint dampings, which prevent entropy growth. Its driving part represents equivalent muscular torques  $F_i$  acting in all DOF (or just in active joints, as used in the affine input control), in the form of force-time and force-velocity signals.

#### Joint Kinematics

Recall from Chapter 2 that human joints represented by internal coordinates  $x^i$  ( $i = 1, \dots, n$ ), constitute an  $n$ D smooth biomechanical configuration manifold  $M$  (see Figure 2.1). Now we are going to perform some categorical transformations on the biomechanical configuration manifold  $M$ . If we apply the *functor Lie* to the *category*  $\bullet[SO(k)^i]$  of rotational Lie groups  $SO(k)^i$  and

their homomorphisms we get the category  $\bullet[so(k)_i]$  of corresponding *tangent* Lie algebras  $so(k)_i$  and their homomorphisms. If we further apply the *isomorphic* functor **Dual** to the category  $\bullet[so(k)_i]$  we get the dual category  $\ast[so(k)_i^\ast]$  of *cotangent*, or, *canonical* Lie algebras  $so(k)_i^\ast$  and their homomorphisms. To go directly from  $\bullet[SO(k)^i]$  to  $\ast[so(k)_i^\ast]$  we use the canonical functor **Can** [IS01, Iva02, IB05, Iva05]. Therefore we have a commutative triangle

$$\begin{array}{ccc}
 & \bullet[SO(k)^i] & \\
 \text{Lie} \swarrow & & \searrow \text{Can} \\
 \bullet[so(k)_i] & \xrightarrow[\cong]{\text{Dual}} & \ast[so(k)_i^\ast]
 \end{array}$$

$\mathcal{LGA}$

Both the tangent algebras  $so(k)_i$  and the cotangent algebras  $so(k)_i^\ast$  contain infinitesimal group generators, angular velocities  $\dot{x}^i = \dot{x}^{\phi_i}$  in the first case and canonical angular momenta  $p_i = p_{\phi_i}$  in the second. As Lie group generators, angular velocities and angular momenta satisfy the respective commutation relations  $[\dot{x}^{\phi_i}, \dot{x}^{\psi_i}] = \epsilon_{\theta}^{\phi\psi} \dot{x}^{\theta_i}$  and  $[p_{\phi_i}, p_{\psi_i}] = \epsilon_{\phi\psi}^{\theta} p_{\theta_i}$ , where the structure constants  $\epsilon_{\theta}^{\phi\psi}$  and  $\epsilon_{\phi\psi}^{\theta}$  constitute totally antisymmetric third–order tensors.

In this way, the functor  $\text{Dual}_G : \text{Lie} \cong \text{Can}$  establishes a geometric duality between kinematics of angular velocities  $\dot{x}^i$  (involved in Lagrangian formalism on the tangent bundle of  $M$ ) and that of angular momenta  $p_i$  (involved in Hamiltonian formalism on the cotangent bundle of  $M$ ). This is analyzed below. In other words, we have two functors **Lie** and **Can** from a category of Lie groups (of which  $\bullet[SO(k)^i]$  is a subcategory) into a category of their Lie algebras (of which  $\bullet[so(k)_i]$  and  $\ast[so(k)_i^\ast]$  are subcategories), and a natural equivalence (functor isomorphism) between them defined by the functor  $\text{Dual}_G$ . (As angular momenta  $p_i$  are in a bijective correspondence with angular velocities  $\dot{x}^i$ , every component of the functor  $\text{Dual}_G$  is invertible.)

Applying the functor **Lie** to the biomechanical configuration manifold  $M$  (Fig. 1), we get the product–tree of the same anthropomorphic structure, but having tangent Lie algebras  $so(k)_i$  as vertices, instead of the groups  $SO(k)^i$ . Again, applying the functor **Can** to  $M$ , we get the product–tree of the same anthropomorphic structure, but this time having cotangent Lie algebras  $so(k)_i^\ast$  as vertices.

The functor **Lie** defines the *second–order Lagrangian formalism on the tangent bundle  $TM$*  (i.e., the *velocity phase–space manifold*) while the functor **Can** defines the *first order canonical Hamiltonian formalism on the cotangent bundle  $T^*M$*  (i.e., the *momentum phase–space manifold*). As these two formalisms are related by the isomorphic functor **Dual**, they are equivalent. In this section we shall follow the Lagrangian functor **Lie**, using the powerful formalism of exterior differential systems and integral variational principles [Gri83a, BM82].

For the parallel, Hamiltonian treatment along the functor **Can**, more suitable for chaos theory and stochastic generalizations, see [IS01, Iva02].

**Exterior Lagrangian Dynamics**

Let  $\Omega^p(M) = \sum \omega_I dx^I$  denote the space of differential  $p$ -forms on  $M$ . That is, if multi-index  $I \subset \{1, \dots, n\}$  is a subset of  $p$  elements then we have a  $p$ -form  $dx^I = dx_1^i \wedge dx_2^i \wedge \dots \wedge dx_p^i$  on  $M$ . We define the exterior derivative on  $M$  as  $d\omega = \sum \frac{\partial \omega^I}{\partial x_p} dx_p \wedge dx^I$  (compare with (3.3.6) above).

Now, from exterior differential systems point of view (see subsection 2.3.3 above as well as [Gri83a]), human-like motion represents an  $n$  DOF neuro-musculo-skeletal system  $\Xi$ , evolving in time on its  $n$ D configuration manifold  $M$ , (with local coordinates  $x^i, i = 1, \dots, n$ ) as well as on its tangent bundle  $TM$  (with local coordinates  $(x^i; \dot{x}^i)$ ).

For the system  $\Xi$  we will consider a *well-posed variational problem*  $(I, \omega; \varphi)$ , on an associated  $(2n + 1)$ -D jet manifold  $X = J^1(\mathbb{R}, M) \cong \mathbb{R} \times TM$ , with local canonical variables  $(t; x^i; \dot{x}^i)$  (compare with section 3.3 above).

Here,  $(I, \omega)$  is called a *Pfaffian exterior differential system* on  $X$  (see [Gri83a]), given locally as

$$\begin{cases} \theta^i = dx^i - \dot{x}^i \omega = 0 \\ \omega \equiv dt \neq 0 \end{cases}, \tag{3.115}$$

with the structure equations

$$d\theta^i = -d\dot{x}^i \wedge \omega.$$

Integral manifolds  $N \in J^1(\mathbb{R}, M)$  of the Pfaffian system  $(I, \omega)$  are locally one-jets  $t \rightarrow (t, x(t), \dot{x}(t))$  of curves  $x = x(t) : \mathbb{R} \rightarrow M$ .

$\varphi$  is a 1-form

$$\varphi = L\omega, \tag{3.116}$$

where  $L = L(t, x, \dot{x})$  is the system's *Lagrangian* function defined on  $X$ , having both coordinate and velocity partial derivatives, respectively denoted by  $L_{x^i} \equiv \partial_{x^i} L$ , and  $L_{\dot{x}^i} \equiv \partial_{\dot{x}^i} L$ .

A variational problem  $(I, \omega; \varphi)$  is said to be *strongly non-degenerate*, or *well-posed* [Gri83a], if the determinant of the matrix of mixed velocity partials of the Lagrangian is positive definite, i.e.,

$$\det \|L_{\dot{x}^i \dot{x}^j}\| > 0.$$

The *extended Pfaffian system*

$$\begin{cases} \theta^i = 0 \\ dL_{\dot{x}^i} - L_{x^i} \omega = 0 \\ \omega \neq 0 \end{cases}.$$

generates classical *Euler-Lagrange equations*

$$\frac{d}{dt}L_{\dot{x}^i} = L_{x^i}, \tag{3.117}$$

describing the *control-free and dissipation-free, conservative skeleton dynamics*.

If an *integral manifold*  $N$  satisfies the Euler-Lagrange equations (3.117) of a well-posed variational problem on  $X$  then

$$\frac{d}{dt} \left( \int_{N_t} \varphi \right)_{t=0} = 0$$

for any *admissible variation*  $N_t \in N$  that satisfies the *endpoint conditions*  $\omega = \theta^i = 0$ .

**Theorem:** *Under the above conditions, both the Lagrangian dynamics with initial conditions*

$$\begin{cases} \frac{d}{dt}L_{\dot{x}^i} = L_{x^i} \\ x(t_0) = x_0, \quad \dot{x}(t_0) = \dot{x}_0 \end{cases}$$

*and the Lagrangian dynamics with endpoint conditions*

$$\begin{cases} \frac{d}{dt}L_{\dot{x}^i} = L_{x^i} \\ x(t_0) = x_0, \quad x(t_1) = x_1 \end{cases}$$

*have unique solutions.* For the proof, see [Gri83a].

Now, if  $M$  is a smooth Riemannian manifold, its metric  $g = \langle . \rangle$  is locally given by a positive definite quadratic form (see Appendix as well as Chapter 2)

$$ds^2 = g_{ij}(x) dx^i dx^j, \tag{3.118}$$

where the metric tensor is a  $C^k$  symmetric matrix  $g(x) = \|g_{ij}(x)\|$ .

*Kinetic energy* of the system  $\Xi$  is a function  $T = T(x, \dot{x})$  on the tangent bundle  $TM$ , which induces a positive definite quadratic form in each fibre  $T_x M \subset TM$ . In local coordinates, it is related to the Riemannian metric (3.118) by

$$T \omega^2 = \frac{1}{2} ds^2.$$

If potential energy of the system  $\Xi$  is a function  $U = U(x)$  on  $M$ , then the autonomous Lagrangian is defined as  $L(x, \dot{x}) = T(x, \dot{x}) - U(x)$ , i.e., kinetic minus potential energy.

The condition of well-posedness is satisfied, as

$$\det \|L_{\dot{x}^i \dot{x}^j}\| = \det \|g_{ij}(x)\| > 0.$$

Now, the *covariant Euler-Lagrange equations* (3.117) expand as

$$\frac{d}{dt} (g_{ij}(x(t)) \dot{x}^j(t)) = \frac{1}{2} \left( \frac{\partial g_{jk}(x(t))}{\partial x^i} \dot{x}^j(t) \dot{x}^k(t) \right) - F_i(x(t)), \tag{3.119}$$

where  $F_i(x(t)) = \frac{\partial U(x(t))}{\partial \dot{x}^i}$  denote the *gradient force 1-forms*.

Letting  $\|g^{ij}(x)\|$  be the inverse matrix to  $\|g_{ij}(x)\|$  and introducing the *Christoffel symbols*

$$\Gamma_{jk}^i = g^{il}\Gamma_{jkl}, \quad \Gamma_{jkl} = \frac{1}{2} \left( \frac{\partial g_{kl}}{\partial x^j} + \frac{\partial g_{jl}}{\partial x^k} - \frac{\partial g_{jk}}{\partial x^l} \right)$$

the equations (3.119) lead to the classical *contravariant form* (see [Iva91, IP01b])

$$\ddot{x}^i(t) + \Gamma_{jk}^i(x(t)) \dot{x}^j(t) \dot{x}^k(t) = -F^i(x(t)), \quad (3.120)$$

where  $F^i(x(t)) = g^{ij}(x) \frac{\partial U(x(t))}{\partial \dot{x}^j}$  denote the *gradient force vector-fields*.

The above theorem implies that both the Lagrangian dynamics with initial conditions

$$\begin{cases} \ddot{x}^i(t) + \Gamma_{jk}^i(x(t)) \dot{x}^j(t) \dot{x}^k(t) = -F^i(x(t)) \\ x(t_0) = x_0, \quad \dot{x}(t_0) = \dot{x}_0 \end{cases} \quad (3.121)$$

and the Lagrangian dynamics with endpoint conditions

$$\begin{cases} \ddot{x}^i(t) + \Gamma_{jk}^i(x(t)) \dot{x}^j(t) \dot{x}^k(t) = -F^i(x(t)) \\ x(t_0) = x_0, \quad x(t_1) = x_1 \end{cases} \quad (3.122)$$

have unique solutions. We consider the system (3.121) to be the valid basis of human-like dynamics, and the system (3.122) to be the valid basis of the finite biomechanics control.

Now, recall from Chapter 3, that any smooth  $n$ -manifold  $M$  gives rise to an  $n$ -category  $\Pi_n(M)$ , its fundamental  $n$ -groupoid. In  $\Pi_n(M)$ , 0-cells are *points* in  $M$ ; 1-cells are *paths* in  $M$  (i.e., parameterized smooth maps  $f : [0, 1] \rightarrow M$ ); 2-cells are *smooth homotopies* (denoted by  $\simeq$ ) of *paths* relative to endpoints (i.e., parameterized smooth maps  $h : [0, 1] \times [0, 1] \rightarrow M$ ); 3-cells are *smooth homotopies of homotopies* of paths in  $M$  (i.e., parameterized smooth maps  $j : [0, 1] \times [0, 1] \times [0, 1] \rightarrow M$ ). Categorical *composition* is defined by *pastings* paths and homotopies. In this way, the *recursive homotopy dynamics* emerges (see next page).

On the other hand, to describe the biomechanically realistic biodynamics, we have to generalize (3.120), so to include any other type of *external* contravariant forces (including excitation and contraction dynamics of muscular-like actuators, as well as nonlinear dissipative joint forces) to the r.h.s of (3.120); in this way we get the *general form of contravariant Lagrangian dynamics*

$$\ddot{x}^i(t) + \Gamma_{jk}^i(x(t)) \dot{x}^j(t) \dot{x}^k(t) = \mathcal{F}^i(t, x(t), \dot{x}(t)), \quad (3.123)$$

or, in exterior, *covariant form*

$$\frac{d}{dt} L_{\dot{x}^i} - L_{x^i} = \mathcal{F}_i(t, x(t), \dot{x}(t)). \quad (3.124)$$

**Recursive homotopy dynamics:**

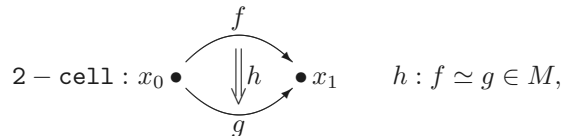
0 – cell :  $x_0 \bullet \quad x_0 \in M$ ;    in the higher cells below:  $t, s \in [0, 1]$ ;

1 – cell :  $x_0 \bullet \xrightarrow{f} \bullet x_1 \quad f : x_0 \simeq x_1 \in M$ ,  
 $f : [0, 1] \rightarrow M, f : x_0 \mapsto x_1, x_1 = f(x_0), f(0) = x_0, f(1) = x_1$ ;

e.g., linear path:  $f(t) = (1 - t)x_0 + tx_1$ ;    or

e.g., Euler-Lagrangian  $f$  – dynamics with endpoint conditions  $(x_0, x_1)$  :

$$\frac{d}{dt}f_{x^i} = f_{x^i}, \quad \text{with } x(0) = x_0, \quad x(1) = x_1, \quad (i = 1, \dots, n);$$



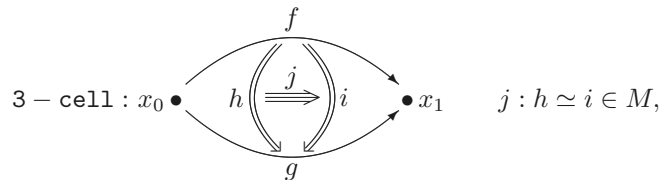
$h : [0, 1] \times [0, 1] \rightarrow M, h : f \mapsto g, g = h(f(x_0))$ ,

$h(x_0, 0) = f(x_0), h(x_0, 1) = g(x_0), h(0, t) = x_0, h(1, t) = x_1$

e.g., linear homotopy:  $h(x_0, t) = (1 - t)f(x_0) + tg(x_0)$ ;    or

e.g., homotopy between two Euler-Lagrangian  $(f, g)$  – dynamics with the same endpoint conditions  $(x_0, x_1)$  :

$$\frac{d}{dt}f_{x^i} = f_{x^i}, \quad \text{and} \quad \frac{d}{dt}g_{x^i} = g_{x^i} \quad \text{with } x(0) = x_0, \quad x(1) = x_1;$$



$j : [0, 1] \times [0, 1] \times [0, 1] \rightarrow M, j : h \mapsto i, i = j(h(f(x_0)))$

$j(x_0, t, 0) = h(f(x_0)), j(x_0, t, 1) = i(f(x_0))$ ,

$j(x_0, 0, s) = f(x_0), j(x_0, 1, s) = g(x_0)$ ,

$j(0, t, s) = x_0, j(1, t, s) = x_1$

e.g., linear composite homotopy:  $j(x_0, t, s) = (1 - t)h(f(x_0)) + ti(f(x_0))$ ;

or, homotopy between two homotopies between above two Euler-

Lagrangian  $(f, g)$  – dynamics with the same endpoint conditions  $(x_0, x_1)$ .

### 3.5.2 Lie–Hamiltonian Biomechanical Functor

The three fundamental and interrelated obstacles facing any researcher in the field of human-like musculo-skeletal dynamics, could be identified as [IS01]:

1. *Deterministic chaos*,
2. *Stochastic forces*, and
3. *Imprecision of measurement* of the system numbers (SN): inputs, parameters and initial conditions.

Recall that the deterministic chaos is manifested as an irregular and unpredictable time evolution of purely deterministic nonlinear systems. If a nonlinear system is started twice, from slightly different initial conditions, its time evolution differs exponentially, while in case of a linear system, the difference in time evolution is linear.

Again, recall that the stochastic dynamics is based on the concept of *Markov process*<sup>6</sup>, which represents the probabilistic analogue to the deterministic dynamics. The property of a *Markov chain* of prime importance for human-motion dynamics is the existence of an *invariant distribution of states*: we start with an initial state  $x_0$  whose absolute probability is 1. Ultimately the states should be distributed according to a specified distribution.

Recall that *Brownian dynamics* represents the phase-space trajectories of a collection of particles that individually obey *Langevin rate equations* (see [Gar85]) in the field of force (i.e., the particles interact with each other via some deterministic force). For one free particle the Langevin equation of motion is given by

$$m\dot{v} = R(t) - \beta v,$$

where  $m$  denotes the mass of the particle and  $v$  its velocity. The r.h.s represents the coupling to a *heat bath*; the effect of the random force  $R(t)$  is to heat the particle. To balance overheating (on the average), the particle is subjected to *friction*  $\beta$ .

Noe, between pure deterministic (in which all DOF of the system in consideration are explicitly taken into account, leading to classical dynamical equations like Hamilton's) and pure stochastic dynamics (Markov process), there is so-called *hybrid dynamics*, particularly the Brownian dynamics, in which some of DOF are represented only through their *stochastic influence* on others.

System theory and artificial intelligence have long investigated the topic of *uncertainty* in measurement, modelling and simulation. Research in artificial intelligence has enriched the spectrum of available techniques to deal with uncertainty by proposing a theory of possibility, based on the theory of fuzzy sets (see [Yag87, DP80, Cox92, Cox94]). The field of qualitative reasoning and

<sup>6</sup> Recall that the Markov process is characterized by a *lack of memory*, i.e., the statistical properties of the immediate future are uniquely determined by the present, regardless of the past (see [Gar85]).

simulation [BK92] is also interested in modelling incompletely known systems where qualitative values are expressed by intervals. Qualitative simulation techniques, however, reveal a low predictive power in presence of complex models. In this section we have combined qualitative and quantitative methods, in spirit of [Bon95, IS01].

In this section we will deal with the general biomechanics from the point of view that mathematically and logically approaches a *general theory of systems*, i.e., that *makes the unique framework* for both linear and nonlinear, discrete and continuous, deterministic and stochastic, crisp and fuzzy, SISO and MIMO-systems, and *generalizes the robot dynamics* elaborated in the literature (see [VJ69, VJF70, VFJ70, VS72, VS73, IN92, Hur93, SGL93, SK93, Lie94, CHP96, SBM96, Has98, SRB99, PP98, Yos84, Ser89]), including all necessary DOF to match the physiologically realistic human-like motion. Yet, we wish *to avoid* all the mentioned fundamental system *obstacles*. To achieve this goal we have formulated the general *biomechanics functor machine*, covering a union of the three intersected frameworks:

1. Muscle-driven, dissipative, Hamiltonian (nonlinear, both discrete and continuous) MIMO-system;
2. Stochastic forces (including dissipative fluctuations and ‘Master’ jumps); and
3. Fuzzy system numbers.

### The Abstract Functor Machine

In this section we define the *abstract functor machine* [IS01] (formalism used is modified from [AAM76]) by a two-step generalization of the Kalman’s modular theory of linear MIMO-systems (compare with Chapter 5). The first generalization puts the Kalman’s theory into the category **Vect** of vector spaces and linear operators (see [MacL71] for technical details about categorical language), thus formulating the unique, categorical formalism valid both for the discrete- and continual MIMO-systems.

We start with the unique, *continual-sequential state equation*

$$\dot{x}(t+1) = Ax(t) + Bu(t), \quad y(t) = Cx(t), \quad (3.125)$$

where the finite-dimensional vector spaces of *state*  $X \ni x$ , *input*  $U \ni u$ , and *output*  $Y \ni y$  have the corresponding linear operators, respectively  $A : X \rightarrow X$ ,  $B : U \rightarrow X$ , and  $C : X \rightarrow Y$ . The modular system theory comprises the *system dynamics*, given by a pair  $(X, A)$ , together with a *reachability map*  $e : U \rightarrow X$  of the pair  $(B, A)$ , and an *observability map*  $m : X \rightarrow Y$  of the pair  $(A, C)$ . If the reachability map  $e$  is surjection the system dynamics  $(X, A)$  is called *reachable*; if the observability map  $m$  is injection the system dynamics  $(X, A)$  is called *observable*. If the system dynamics  $(X, A)$  is both reachable and observable, a *composition*  $r = m \circ e : U \rightarrow Y$  defines the *total system’s response*, which is given by solution of equation (3.125). If the unique

solution to the continual-sequential state equation exists, it gives the answer to the (minimal) *realization problem*: find the system  $S$  that realizes the given response  $r = m \circ e : U \rightarrow Y$  (in the smallest number of discrete states and in the shortest time).

In categorical language, the system dynamics in the category  $\mathbf{Vect}$  is a pair  $(X, A)$ , where  $X \in \mathbf{Ob}(\mathbf{Vect})$  is an object in  $\mathbf{Vect}$  and  $A : X \rightarrow X \in \mathbf{Mor}(\mathbf{Vect})$  is a  $\mathbf{Vect}$ -morphism. A *decomposable system* in  $\mathbf{Vect}$  is such a sextuple  $S \equiv (X, A, U, B, Y, C)$  that  $(X, A)$  is the system dynamics in  $\mathbf{Vect}$ , a  $\mathbf{Vect}$ -morphism  $B : U \rightarrow X$  is an *input map*, and a  $\mathbf{Vect}$ -morphism  $C : X \rightarrow Y$  is an *output map*. Any object in  $\mathbf{Vect}$  is characterized by mutually *dual*<sup>7</sup> notions of its *degree* (a number of its input morphisms) and its *codegree* (a number of its output morphisms). Similarly, any decomposable system  $S$  in  $\mathbf{Vect}$  has a *reachability map* given by an epimorphism  $e = A \circ B : U \rightarrow X$  and its dual *observability map* given by a monomorphism  $m = C \circ A : X \rightarrow Y$ ; their composition  $r = m \circ e : U \rightarrow Y$  in  $\mathbf{Mor}(\mathbf{Vect})$  defines the total system's response in  $\mathbf{Vect}$  given by the unique solution of the continual-sequential state equation (3.125).

The second generalization gives an extension of the continual-sequential MIMO-system theory: from the linear category  $\mathbf{Vect}$  – to an arbitrary nonlinear category  $\mathcal{K}$ . We do this extension (see [IS01]) by formally applying the *action* of the *nonlinear process-functor*  $\mathcal{F} : \mathcal{K} \Rightarrow \mathcal{K}$  on the decomposable system  $S \equiv (X, A, U, B, Y, C)$  in  $\mathbf{Vect}$ . Under the action of the process functor  $\mathcal{F}$  the linear system dynamics  $(X, A)$  in  $\mathbf{Vect}$  transforms into a nonlinear  $\mathcal{F}$ -dynamics  $(\mathcal{F}[X], \mathcal{F}[A])$  in  $\mathcal{K}$ , creating the *functor machine* in  $\mathcal{K}$  represented by a *nonlinear decomposable system*

$\mathcal{F}[S] \equiv (\mathcal{F}[X], \mathcal{F}[A], \mathcal{F}[U], \mathcal{F}[B], \mathcal{F}[Y], \mathcal{F}[C])$ . The reachability map transforms into the *input process*  $\mathcal{F}[e] = \mathcal{F}[A] \circ \mathcal{F}[B] : \mathcal{F}[U] \rightarrow \mathcal{F}[X]$ , while its dual, observability map transforms into the *output process*  $\mathcal{F}[m] = \mathcal{F}[C] \circ \mathcal{F}[A] : \mathcal{F}[X] \rightarrow \mathcal{F}[Y]$ . In this way the total response of the linear system  $r = m \circ e : U \rightarrow Y$  in  $\mathbf{Mor}(\mathbf{Vect})$  transforms into the *nonlinear system behavior*  $\mathcal{F}[r] = \mathcal{F}[m] \circ \mathcal{F}[e] : \mathcal{F}[U] \rightarrow \mathcal{F}[Y]$  in  $\mathbf{Mor}(\mathcal{K})$ . Obviously,  $\mathcal{F}[r]$ , if exists, is given by a nonlinear  $\mathcal{F}$ -transform of the linear state equation (3.125).

The purpose of this section is to formulate a nonlinear  $\mathcal{F}$ -transform for the linear state equation (3.125) for biomechanics, i.e., the biomechanics functor machine. In subsequent sections we give a three-step development of a fuzzy-stochastic-Hamiltonian formulation for the biomechanics functor machine  $\mathcal{F}[S]$ , with a corresponding nonlinear system behavior  $\mathcal{F}[r]$ .

<sup>7</sup> Recall that in categorical language *duality* means reversing the (arrows of) morphisms; the knowledge of one of the two mutually dual terms automatically implies the knowledge of the other.

### Muscle-Driven, Dissipative, Hamiltonian Biomechanics

In this section we choose the functor  $\mathbf{Can}$ , as the first order Hamiltonian formalism is more suitable for both stochastic and fuzzy generalizations to follow. Recall that the general deterministic Hamiltonian biomechanics, representing the canonical functor  $\mathbf{Can} : \mathcal{S}^\bullet[SO(n)^i] \Rightarrow \mathcal{S}^\bullet[so(n)_i^*]$ , is given by dissipative, driven  $\delta$ -Hamiltonian equations (3.58–3.59), i.e.,

$$\dot{q}^i = \frac{\partial H}{\partial p_i} + \frac{\partial R}{\partial p_i}, \quad (3.126)$$

$$\dot{p}_i = F_i - \frac{\partial H}{\partial q^i} + \frac{\partial R}{\partial q^i}, \quad (3.127)$$

$$q^i(0) = q_0^i, \quad p_i(0) = p_i^0, \quad (3.128)$$

including *contravariant* equation (3.126) – the *velocity vector-field*, and *covariant* equation (3.127) – the *force 1-form*, together with initial joint angles and momenta (3.128). Here ( $i = 1, \dots, N$ ), and  $R = R(q, p)$  denotes the Raileigh nonlinear (biquadratic) dissipation function, and  $F_i = F_i(t, q, p)$  are covariant driving torques of *equivalent muscular actuators*, resembling muscular excitation and contraction dynamics in rotational form.

The velocity vector-field (3.126) and the force 1-form (3.127) together define the generalized Hamiltonian vector-field  $X_H$ , which geometrically represents the *section* of the momentum phase-space manifold  $T^*M$ , which is itself the cotangent bundle of the biomechanical configuration manifold  $M$ ; the Hamiltonian (total energy) function  $H = H(q, p)$  is its generating function.

As a Lie group, the configuration manifold  $M$  is Hausdorff [AMR88, MR99, Pos86]. Therefore, for  $x = (q^i, p_i) \in U_p, U_q$  open in  $T^*M$ , there exists a unique one-parameter group of diffeomorphisms  $\phi_{\delta_t} : T^*M \rightarrow T^*M$ , the generalized deterministic  $\delta$ -Hamiltonian phase-flow

$$\begin{aligned} \phi_{\delta_t} : G_1 \times T^*M &\rightarrow T^*M : (p(0), q(0)) \mapsto (p(t), q(t)), \\ (\phi_{\delta_t} \circ \phi_{\delta_s} &= \phi_{\delta_{t+s}}, \quad \phi_{\delta_0} = \text{identity}), \end{aligned} \quad (3.129)$$

given by (3.126–3.128) such that

$$\left. \frac{d}{dt} \right|_{t=0} \phi_{\delta_t} x = J\nabla H(x).$$

The  $\delta$ -Hamiltonian system (3.126–3.128), with its  $\delta$ -Hamiltonian phase-flow  $\phi_{\delta_t}$  (3.129), i.e., the canonical functor  $\mathbf{Can}$ , represents our first, continual-deterministic model for the biomechanics functor machine  $\mathcal{F}[S]$  with the nonlinear system behavior  $\mathcal{F}[r]$ . In the two subsequent sections we generalize this model to include discrete stochastic forces and fuzzy SN.

**3.5.3 Stochastic-Lie-Hamiltonian Biomechanical Functor**

In terms of the Markov stochastic process, we can interpret the deterministic  $\delta$ -Hamiltonian biomechanical system (3.126–3.128) as deterministic drift corresponding to the *Liouville equation*. Thus, we can naturally (in the sense of Langevin) add the covariant vector  $\sigma_i(t)$  of stochastic forces (diffusion fluctuations and discontinuous-Master jumps)  $\sigma_i(t) = B_{ij}[q^i(t), t] dW^j(t)$  to the canonical force equation. In this way we get *stochastic  $\sigma$ -Hamiltonian biomechanical system*, a *stochastic transformation Stoch[Can]* of the canonical functor Can,

$$dq^i = \left( \frac{\partial H}{\partial p_i} + \frac{\partial R}{\partial p_i} \right) dt, \tag{3.130}$$

$$dp_i = \left( F_i - \frac{\partial H}{\partial q^i} + \frac{\partial R}{\partial q^i} \right) dt + \sigma_i(t), \tag{3.131}$$

$$\sigma_i(t) = B_{ij}[q^i(t), t] dW^j(t), \quad q^i(0) = q_0^i, \quad p_i(0) = p_i^0.$$

In our low-dimensional example-case of symmetrical 3D load-lifting (see (3.4.4)), the velocity and force  $\sigma$ -Hamiltonian biomechanics equations (3.130–3.131) become

$$dq^i = \left( p_i \left\{ [J_i]^{-1} + \left[ m_i \left( \sum_{j=1}^i L_j \cos q^j \right)^2 \right]^{-1} \right\} + \frac{\partial R}{\partial p_i} \right) dt,$$

$$dp_i = B_{ij}[q^i(t), t] dW^j(t) + \left( F_i - g \sum_{j=i}^{10-i} L_j m_j \sin q^j \right.$$

$$\left. - \sum_{j=i}^{10-i} L_j \sin q^j p_j p_j \left[ m_i \left( \sum_{k=1}^i L_k \cos q^k \right)^3 \right]^{-1} + \frac{\partial R}{\partial q^i} \right) dt.$$

Recall that Ito quadratic cotangent bundle  $I^*Q^N$  is defined as a Whitney sum

$$I^*Q^N = T^*Q^N \oplus SQ^N,$$

where  $SQ^N$  corresponds to *stochastic tensor bundle*, whose elements are 2nd-order tensor-fields composed of continual diffusion fluctuations and discontinuous jumps at every point of the manifold  $Q^N$ . On  $I^*Q^N$  is defined a non-degenerate, stochastic 2-form  $\alpha$  which is closed, i.e.,  $d\alpha = 0$ , and exact, i.e.,  $\alpha = d\beta$ , where 1-form  $\beta$  represents a section  $\beta : Q^N \rightarrow I^*Q^N$  of the Ito bundle  $I^*Q^N$ .

Now, the stochastic Hamiltonian vector-field  $\Xi_H$  represents a section  $\Xi_H : Q^N \rightarrow IQ^N$  of the *Ito quadratic tangent bundle*  $IQ^N$ , also defined as a Whitney sum

$$IQ^N = TM \oplus SQ^N.$$

The quadratic character of Ito stochastic fibre-bundles corresponds to the second term (trace of the 2nd-order tensor-field) of associate *stochastic Taylor expansion* (see [Elw82, May81]).

Through stochastic  $\sigma$ -Hamiltonian biomechanical system (3.130–3.131), the deterministic  $\delta$ -Hamiltonian phase-flow  $\phi_{\delta t}$  (3.129), extends into stochastic  $\sigma$ -Hamiltonian phase-flow  $\phi_{\sigma t}$

$$\begin{aligned} \phi_{\sigma t} : G_1 \times I^*M &\rightarrow I^*M : (p(0), q(0)) \mapsto (p(t), q(t)), \\ (\phi_{\sigma t} \circ \phi_{\sigma s} &= \phi_{\sigma(t+s)}, \quad \phi_{\sigma 0} = \text{identity}), \end{aligned} \quad (3.132)$$

where  $I^*M$  denotes *Ito quadratic cotangent bundle* (see [Elw82, May81]) of biomechanical configuration manifold  $M$ .

Besides the  $\sigma$ -Hamiltonian phase-flow  $\phi_{\sigma t}$  (3.132), including  $N$  individual random-phase trajectories, we can also define (see [Elw82]) an *average* or *mean*  $\langle \sigma \rangle$ -Hamiltonian flow  $\langle \phi \rangle_{\sigma t}$

$$\begin{aligned} \langle \phi \rangle_{\sigma t} : G_1 \times I^*M &\rightarrow I^*M : (\langle p(0) \rangle, \langle q(0) \rangle) \mapsto (\langle p(t) \rangle, \langle q(t) \rangle), \\ (\langle \phi \rangle_{\sigma t} \circ \langle \phi \rangle_{\sigma s} &= \langle \phi \rangle_{\sigma(t+s)}, \quad \langle \phi \rangle_{\sigma 0} = \text{identity}), \end{aligned}$$

which stochastically corresponds to the trajectory of the center of mass in the human-like dynamics, approximatively lumbo-sacral spinal  $SO(3)$ -joint.

The necessary conditions for existence of a unique *non-anticipating solution* of the  $\sigma$ -Hamiltonian biomechanical system in a fixed time interval are *Lipschitz condition* and *growth condition* (see [Elw82, May81]). For constructing an approximate solution a simple iterative Cauchy-Euler procedure could be used to calculate  $(q_{k+1}^i, p_i^{k+1})$  from the knowledge of  $(q_k^i, p_i^k)$  on the mesh of time points  $t^k$ ,  $k = 1, \dots, s$ , by adding discrete  $\delta$ -Hamiltonian drift-terms  $A^i(q_k^i)\Delta t^k$  and  $A_i(p_i^k)\Delta t^k$ , as well as a stochastic term  $B_{ij}(q_i^k, t^k)\Delta W_k^j$ .

$\sigma$ -Hamiltonian biomechanical system (3.130–3.131), with its  $\sigma$ -Hamiltonian phase-flow  $\phi_{\sigma t}$  (3.132), i.e., the functor **Stoch[Can]**, represents our second, continual-discrete stochastic model for the biomechanics functor machine  $\mathcal{F}[S]$  with the nonlinear system behavior  $\mathcal{F}[r]$ . In the next section we generalize this model once more to include fuzzy SN.

### 3.5.4 Fuzzy-Stochastic-Lie-Hamiltonian Functor

Generally, a *fuzzy differential equation* model (FDE-model, for short) is a symbolic description expressing a state of incomplete knowledge of the continuous world, and is thus an abstraction of an infinite set of ODEs models. Qualitative simulation (see [BK92]) predicts the set of possible behaviors consistent with a FDE model and an initial state. Specifically, as a FDE we consider an ordinary deterministic (i.e., *crisp*) differential equation (CDE) in which some of the parameters (i.e., coefficients) or initial conditions are *fuzzy numbers*, i.e. uncertain and represented in a *possibilistic* form. As a *solution*

of a FDE we consider a time evolution of a *fuzzy region of uncertainty* in the system's phase-space, which corresponds to its the *possibility distribution*.

Recall that a fuzzy number is formally defined as a convex, normalized *fuzzy set* [DP80, Cox92, Cox94]. The concept of fuzzy numbers is an extension of the notion of real numbers: it encodes approximate quantitative knowledge. It is not probabilistic, but rather a possibilistic distribution. The mathematics of fuzzy numbers is founded on the *extension principle*, introduced by Zadeh [Yag87]. This principle provides a general method for extending standard mathematical concepts in order to deal with fuzzy quantities [DP80].

Let  $\Phi : Y^1 \times Y^2 \times \dots \times Y^n \rightarrow Z$  be a deterministic map such that  $z = \Phi(y^1, y^2, \dots, y^n)$  for all  $z \in Z, y^i \in Y^i$ . The extension principle allows us to induce from  $n$  input fuzzy sets  $\bar{y}^i$  on  $Y^i$  an output fuzzy set  $\bar{z}$  on  $Z$  through  $\Phi$  given by

$$\mu_{\bar{z}}(t) = \sup_{t=\Phi(s^1, \dots, s^n)} \min(\mu_{\bar{y}^1}(s^1), \dots, \mu_{\bar{y}^n}(s^n)),$$

or  $\mu_{\bar{z}}(t) = 0$  if  $\Phi^{-1}(t) = \emptyset,$

where  $\Phi^{-1}(t)$  denotes the inverse image of  $t$  and  $\mu_{\bar{y}^i}$  is the membership function of  $\bar{y}^i, (i = 1, \dots, n)$ .

The extension principle provides a method to compute the fuzzy value of a fuzzy map but, in practice, its application is not feasible because of the infinite number of computations it would require. The simplest way of efficiently applying the extension principle is in the form of iterative repetition of several crisp Hamiltonian simulations (see [Bon95, IS01, PI04]), within the range of included fuzzy SN.

Fuzzification of the crisp deterministic  $\delta$ -Hamiltonian biomechanical system (3.126–3.128) gives the fuzzified  $\mu$ -Hamiltonian biomechanical system, namely  $\delta$ -Hamiltonian biomechanical system with fuzzy SN, i.e., the *fuzzy transformation Fuzzy[Can]* of the canonical functor **Can**

$$\dot{q}^i = \frac{\partial H(q, p, \sigma)}{\partial p_i} + \frac{\partial R}{\partial p_i}, \quad (3.133)$$

$$\dot{p}_i = \bar{F}_i(q, p, \sigma) - \frac{\partial H(q, p, \sigma)}{\partial q^i} + \frac{\partial R}{\partial q^i}, \quad (3.134)$$

$$q^i(0) = \bar{q}_0^i, \quad p_i(0) = \bar{p}_i^0, \quad (i = 1, \dots, N). \quad (3.135)$$

Here  $\sigma = \sigma_\mu$  (with  $\mu \geq 1$ ) denote fuzzy sets of conservative parameters (segment lengths, masses and moments of inertia), dissipative joint dampings and actuator parameters (amplitudes and frequencies), while the bar ( $\bar{\cdot}$ ) over a variable ( $\cdot$ ) denotes the corresponding fuzzified variable.

In our example-case of symmetrical 3D load-lifting, the fuzzified  $\mu$ -Hamiltonian biomechanical system (3.133–3.135) becomes

$$\begin{aligned} \dot{q}^i &= p_i \left\{ [\bar{J}_i]^{-1} + \left[ \bar{m}_i \left( \sum_{j=1}^i \bar{L}_j \cos q^j \right)^2 \right]^{-1} \right\} + \frac{\partial R}{\partial p_i}, \\ \dot{p}_i &= \bar{F}_i(t, q^i, p_i, \{\sigma\}_\mu) - g \sum_{j=i}^{10-i} \bar{L}_j \bar{m}_j \sin q^j \\ &\quad - \sum_{j=i}^{10-i} \bar{L}_j \sin q^j p_i p_j \left[ \bar{m}_i \left( \sum_{k=1}^i \bar{L}_k \cos q^k \right)^3 \right]^{-1} + \frac{\partial R}{\partial q^i} \\ q^i(0) &= \bar{q}_0^i, \quad p_i(0) = \bar{p}_i^0, \quad (i = 1, \dots, 9). \end{aligned}$$

In this way, the crisp  $\delta$ -Hamiltonian phase-flow  $\phi_{\delta_t}$  (3.129) extends into fuzzy-deterministic  $\mu$ -Hamiltonian phase-flow  $\phi_{\mu_t}$

$$\begin{aligned} \phi_{\mu_t} : G_1 \times T^*M &\rightarrow T^*M : (\bar{p}_i^0, \bar{q}_0^i) \mapsto (p(t), q(t)), \\ (\phi_{\mu_t} \circ \phi_{\mu_s} &= \phi_{\mu_{t+s}}, \quad \phi_{\mu_0} = \text{identity}). \end{aligned}$$

Similarly, fuzzification of crisp stochastic  $\sigma$ -Hamiltonian biomechanical system (3.130–3.131) gives fuzzy-stochastic  $[\mu\sigma]$ -Hamiltonian biomechanical system, namely stochastic  $\sigma$ -Hamiltonian biomechanical system with fuzzy SN, i.e., the *fuzzy-stochastic transformation* **Fuzzy[Stoch[Can]]** of the canonical functor **Can**

$$dq^i = \left( \frac{\partial H(q, p, \sigma)}{\partial p_i} + \frac{\partial R}{\partial p_i} \right) dt, \tag{3.136}$$

$$dp_i = B_{ij}[q^i(t), t] dW^j(t) + \left( \bar{F}_i(q, p, \sigma) - \frac{\partial H(q, p, \sigma)}{\partial q^i} + \frac{\partial R}{\partial q^i} \right) dt, \tag{3.137}$$

$$q^i(0) = \bar{q}_0^i, \quad p_i(0) = \bar{p}_i^0. \tag{3.138}$$

In our example-case of symmetrical 3D load-lifting, the velocity and force  $[\mu\sigma]$ -Hamiltonian biomechanics equations (3.136–3.137) become

$$\begin{aligned} dq^i &= \left( p_i \left\{ [\bar{J}_i]^{-1} + \left[ \bar{m}_i \left( \sum_{j=1}^i \bar{L}_j \cos q^j \right)^2 \right]^{-1} \right\} + \frac{\partial R}{\partial p_i} \right) dt, \\ dp_i &= B_{ij}[q^i(t), t] dW^j(t) + \left( \bar{F}_i(t, q^i, p_i, \{\sigma\}_\mu) - g \sum_{j=i}^{10-i} \bar{L}_j \bar{m}_j \sin q^j \right. \\ &\quad \left. - \sum_{j=i}^{10-i} \bar{L}_j \sin q^j p_i p_j \left[ \bar{m}_i \left( \sum_{k=1}^i \bar{L}_k \cos q^k \right)^3 \right]^{-1} + \frac{\partial R}{\partial q^i} \right) dt. \end{aligned}$$

In this way, the crisp stochastic  $\sigma$ -Hamiltonian phase-flow  $\phi_{\sigma_t}$  (3.132) extends into fuzzy-stochastic  $[\mu\sigma]$ -Hamiltonian phase-flow  $\phi_{[\mu\sigma]_t}$

$$\begin{aligned} \phi_{[\mu\sigma]_t} : G_1 \times I^*M &\rightarrow I^*M : (\bar{p}_i^0, \bar{q}_0^i) \mapsto (p(t), q(t)), \\ (\phi_{[\mu\sigma]_t} \circ \phi_{[\mu\sigma]_s} &= \phi_{[\mu\sigma]_{t+s}}, \quad \phi_{[\mu\sigma]_0} = \text{identity}). \end{aligned} \quad (3.139)$$

$[\mu\sigma]$ –Hamiltonian biomechanical system (3.136–3.138), with its phase–flow  $\phi_{[\mu\sigma]_t}$  (3.139), i.e., the functor **Fuzzy[Stoch[Can]]**, represents our final, continual–discrete and fuzzy–stochastic model for the biomechanics functor machine  $\mathcal{F}[S]$  with the nonlinear system behavior  $\mathcal{F}[r]$ .

### 3.6 Biomechanics of Spinal Injuries

According to the construction of the spinal manifold  $M$ , we have two general types of soft spinal injuries (excluding vertebral fractions), which agrees with the medical literature [WZ98]:

- The *intervertebral dislocations*, corresponding to translational movements in 25 gauge groups  $\mathbb{R}^3$ , and
- The *intervertebral disclinations*, corresponding to rotational movements in 25 gauge groups  $SO(3)$ .

Continuum mechanics of soft spinal defects comprises the following set of continuity equations [KE83]:

$$\begin{aligned} \dot{\alpha}^k &= -dJ^k - S^k, & \dot{Q}^k &= -dS^k, \\ d\alpha^k &= Q^k, & dQ^k &= 0, \end{aligned}$$

where  $k = 1, \dots, 25 \times 3$ ;  $\alpha^k, J^k, S^k$ , and  $Q^k$  denote respectively 2–form of dislocation density, 1–form of dislocation flux, 2–form of disclination flux, and 3–form of disclination density, all spanned along the 25 movable spinal joints.

Now, the above picture is common for *all* movable (in particular, synovial) human joints included in the full biomechanical manifold  $M$  (see Figure 2.2): at all joints soft injuries can be classified as dislocations and disclinations defined above.

Regarding the hard injuries, *bone fractures*, we can say that they are generally *caused by*  $SE(3)$ –jolts, applied externally on the human bones (in particular, vertebrae, see the following subsections).

#### Biomechanical Jerk Functions

The *covariant force law*,  $F_i = mg_{ij}a^j$ , together with its Hamiltonian formulation given in the previous section, has been applied for the prediction of spinal (and other neuro–musculo–skeletal) injuries. The *risk of spinal injuries* is measured using the *torque–jerk* quantity,  $\dot{T}_i = \dot{T}_i - \Gamma_{ik}^j T_j \dot{x}^k$ , measured in  $[Nm/s]$ , defined as the *absolute time derivative of the total torque*  $T_i = F_i(t, q^i, p_i)$  acting along the joint Euler angles, in each movable intervertebral joint. This

is the measure of the dynamism of the total torque: the sharper the shape of the torque, i.e., the more it approaches the shape of the Dirac's impulse  $\delta$ -function, both in time and along the spine, the higher is the risk of injury at that particular joint.

More precisely, by taking the absolute time derivative of the force equation (3.127),  $\dot{p}_i = T_i - \partial_{q^i} H + \partial_{q^i} R$ , we get the *deterministic biomechanical jerk function*,

$$\ddot{p}_i = \dot{T}_i - \overline{\partial_{q^i} H} + \overline{\partial_{q^i} R}, \quad (3.140)$$

while differentiation of the fuzzy-stochastic equation (3.137),  $dp_i = B_{ij}[q^i(t), t] dW^j(t) + (\bar{T}_i(q, p, \sigma) - \partial_{q^i} H(q, p, \sigma) + \partial_{q^i} R) dt$ , – gives the *fuzzy-stochastic biomechanical jerk function*,

$$\dot{dp}_i = B_{ij}[q^i(t), t] \overline{dW^j}(t) + (\dot{\bar{T}}_i(q, p, \sigma) - \overline{\partial_{q^i} H}(q, p, \sigma) + \overline{\partial_{q^i} R}) dt. \quad (3.141)$$

Biomechanical jerk functions (3.140–3.141) are the quantities that need to be controlled by the high-level, brain-like controller, both in humans and in humanoid robots.

In case of our spinal simulator, the torque-jerk functions (3.140–3.141) read

$$\ddot{p}_i = \dot{T}_i(t, \dot{q}^i, \dot{p}_i) - (\dot{p}_i p_j + \dot{p}_j p_i) \sum_{j=i}^{76-i} L_j \sin q^j \left[ m_i \left( \sum_{k=1}^i L_k \cos q^k \right)^3 \right]^{-1} \quad (3.142)$$

$$+ \overline{\partial_{q^i} R}, \quad \text{and}$$

$$\dot{dp}_i = B_{ij}[q^i(t), t] \overline{dW^j}(t) + \left( \dot{\bar{T}}_i(t, q^i, p_i, \{\sigma\}_\mu) \right. \quad (3.143)$$

$$\left. - (\dot{p}_i p_j + \dot{p}_j p_i) \sum_{j=i}^{76-i} \bar{L}_j \sin q^j \left[ \bar{m}_i \left( \sum_{k=1}^i \bar{L}_k \cos q^k \right)^3 \right]^{-1} + \overline{\partial_{q^i} R} \right) dt,$$

respectively.

Assuming well-behaved muscular actuators and weakly nonlinear (or even linear) joint dissipation functions, we see that both in the definition jerk functions (3.140–3.141) and in the expanded ones (3.142–3.143), the source of possible chaos can be the middle term with trigonometric couplings of joints, i.e.,

$$\overline{\partial_{q^i} H} = (\dot{p}_i p_j + \dot{p}_j p_i) \sum_{j=i}^{76-i} L_j \sin q^j \left[ m_i \left( \sum_{k=1}^i L_k \cos q^k \right)^3 \right]^{-1}. \quad (3.144)$$

This term needs sophisticated, brain-like chaos control.

Finally, for the purpose of biomedical engineering, when muscular actuators  $T_i^{MUS}$  are insufficient to perform adequately, they can be complemented by D.C. motor-drives, to form the so-called ‘hybrid joint actuators’  $T_i = T_i^{MUS} + T_k^{DC}$  (see, e.g., [VS82]). The D.C. motor-driven torques,  $T_k^{DC}$ , as implemented in standard hybrid joint actuators, are defined here in Hamiltonian form by

$$T_k^{DC} = i_k(t) - \dot{p}_k(t) - B_k p_k(t), \quad k = 1, \dots, N, \quad (3.145)$$

with

$$l_k i_k(t) + R_k i_k(t) + C_k p_k(t) = u_k(t),$$

where  $i_k(t)$  and  $u_k(t)$  denote currents and voltages in the rotors of the drives,  $R_k, l_k$  and  $C_k$  are resistances, inductances and capacitances in the rotors, respectively, while  $B_k$  correspond to the viscous dampings of the drives.

If we use a hybrid joint actuator  $T_i = T_i^{MUS} + T_k^{DC}$  – that resembles the brushless DC motor – then it can be chaotic itself [CD98].

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## Topology of Human–Like Biomechanics

In this Chapter we develop the basics of algebraic topology as is used in modern biomechanics. It includes both tangent (Lagrangian) and cotangent (Hamiltonian) topological variations on the central theme of our *covariant force law*,  $F_i = mg_{ij}a^j$ .

### 4.1 Category of (Co)Chain Complexes in Human–Like Biomechanics

In this section we present the category of (co)chain complexes, as used in modern biomechanics. The central concept in cohomology theory is the *category*  $\mathbf{S}^\bullet(\mathbb{C})$  of *generalized cochain complexes* in an Abelian category  $\mathbb{C}$  [Die88]. The *objects* of the category  $\mathbf{S}^\bullet(\mathbb{C})$  are infinite sequences

$$A^\bullet : \dots \longrightarrow A^{n-1} \xrightarrow{d^{n-1}} A^n \xrightarrow{d^n} A^{n+1} \longrightarrow \dots$$

where, for each  $n \in \mathbb{Z}$ ,  $A^n$  is an object of  $\mathbb{C}$  and  $d^n$  a morphism of  $\mathbb{C}$ , with the conditions

$$d^{n-1} \circ d^n = 0$$

for every  $n \in \mathbb{Z}$ . When  $A^n = 0$  for  $n < 0$ , one speaks of *cochain complexes*. The  $d^n$  are called *coboundary operators*.

The *morphisms* of the category  $\mathbf{S}^\bullet(\mathbb{C})$  are sequences  $f^\bullet = (f^n) : A^\bullet \rightarrow B^\bullet$  where, for each  $n \in \mathbb{Z}$ ,  $f^n : A^n \rightarrow B^n$  is a morphism of  $\mathbb{C}$ , and in the diagram

$$\begin{array}{ccccccc} \dots & \longrightarrow & A^{n-1} & \xrightarrow{d^{n-1}} & A^n & \xrightarrow{d^n} & A^{n+1} & \longrightarrow & \dots \\ & & & & f^{n-1} \downarrow & & f^n \downarrow & & f^{n+1} \downarrow \\ \dots & \longrightarrow & B^{n-1} & \xrightarrow{d^{n-1}} & B^n & \xrightarrow{d^n} & B^{n+1} & \longrightarrow & \dots \end{array} \quad (4.1)$$

all squares are commutative; one says the  $f^n$  commute with the coboundary operators. One has  $\text{Im } d^{n+1} \subset \text{Ker } d^n \subset A^n$  for every  $n \in \mathbb{Z}$ ; the quotient  $H^n(A^\bullet) = \text{Ker } d^n / \text{Im } d^{n+1}$  is called the  $n$ th cohomology object of  $A^\bullet$ . From (4.1) it follows that there is a morphism

$$H^n(f^\bullet) : H^n(A^\bullet) \rightarrow H^n(B^\bullet)$$

deduced canonically from  $f^\bullet$ , and

$$(A^\bullet, f^\bullet) \Rightarrow (H^n(A^\bullet), H^n(f^\bullet))$$

is a *covariant functor* from  $\mathbf{S}^\bullet(\mathbb{C})$  to  $\mathbb{C}$ .

The *cohomology exact sequence*: if three cochain complexes  $A^\bullet, B^\bullet, C^\bullet$  are elements of a short exact sequence of morphisms

$$0 \longrightarrow A^\bullet \longrightarrow B^\bullet \longrightarrow C^\bullet \longrightarrow 0$$

then there exists an infinite sequence of canonically defined morphisms  $d^n : H^n(C^\bullet) \rightarrow H^{n-1}(A^\bullet)$  such that the sequence

$$\dots \longrightarrow H^n(A^\bullet) \longrightarrow H^n(B^\bullet) \longrightarrow H^n(C^\bullet) \longrightarrow H^{n-1}(A^\bullet) \longrightarrow \dots$$

is *exact*, that is the *image* of each homomorphism in the sequence is exactly the *kernel* of the next one.

The *dual* to the category  $\mathbf{S}^\bullet(\mathbb{C})$  is the *category* of  $\mathbf{S}_\bullet(\mathbb{C})$  of *generalized chain complexes*. Its objects and morphisms are obtained by formal inversion of all arrows and lowering all indices.

#### 4.1.1 (Co)Homologies in Abelian Categories Related to $M$

Let  $\mathcal{M}^\bullet$  denote the Abelian category of cochains, (i.e.,  $p$ -forms) on the biomechanical configuration manifold  $M$  (see Figure 2.2). When  $\mathcal{C} = \mathcal{M}^\bullet$ , we have the category  $\mathcal{S}^\bullet(\mathcal{M}^\bullet)$  of generalized cochain complexes  $A^\bullet$  in  $\mathcal{M}^\bullet$ , and if  $A^n = 0$  for  $n < 0$  we have a subcategory  $\mathcal{S}_{DR}^\bullet(\mathcal{M}^\bullet)$  of the *De Rham differential complexes* in  $\mathcal{M}^\bullet$

$$A_{DR}^\bullet : 0 \rightarrow \Omega^0(M) \xrightarrow{d} \Omega^1(M) \xrightarrow{d} \Omega^2(M) \dots \xrightarrow{d} \Omega^n(M) \xrightarrow{d} \dots$$

Here  $A^n = \Omega^n(M)$  is the vector space over  $\mathbb{R}$  of all  $p$ -forms  $\omega$  on  $M$  (for  $p = 0$  the smooth functions on  $M$ ) and  $d_n = d : \Omega^{n-1}(M) \rightarrow \Omega^n(M)$  is the exterior differential. A form  $\omega \in \Omega^n(M)$  such that  $d\omega = 0$  is a closed form or  $n$ -cocycle. A form  $\omega \in \Omega^n(M)$  such that  $\omega = d\theta$ , where  $\theta \in \Omega^{n-1}(M)$ , is an exact form or  $n$ -coboundary. Let  $Z^n(M) = \text{Ker } d$  (resp.  $B^n(M) = \text{Im } d$ ) denote a real vector space of cocycles (resp. coboundaries) of degree  $n$ . Since  $d_{n+1} \circ d_n = d^2 = 0$ , we have  $B^n(M) \subset Z^n(M)$ . The quotient vector space

$$H_{DR}^n(M) = \text{Ker } d / \text{Im } d = Z^n(M) / B^n(M)$$

is the *De Rham cohomology group*. The elements of  $H_{DR}^n(M)$  represent equivalence sets of cocycles. Two cocycles  $\omega_1, \omega_2$  belong to the same equivalence set, or are cohomologous (written  $\omega_1 \sim \omega_2$ ) iff they differ by a coboundary  $\omega_1 - \omega_2 = d\theta$ . The de Rham's cohomology class of any form  $\omega \in \Omega^n(M)$  is  $[\omega] \in H_{DR}^n(M)$ . The De Rham differential complex (1) can be considered as a system of second-order DEs  $d^2\theta = 0, \theta \in \Omega^{n-1}(M)$  having a solution represented by  $Z^n(M) = \text{Ker } d$ .

Analogously let  $\mathcal{M}_\bullet$  denote the Abelian category of chains on the configuration manifold  $M$ . When  $\mathcal{C} = \mathcal{M}_\bullet$ , we have the category  $\mathcal{S}_\bullet(\mathcal{M}_\bullet)$  of generalized chain complexes  $A_\bullet$  in  $\mathcal{M}_\bullet$ , and if  $A_n = 0$  for  $n < 0$  we have a subcategory  $\mathcal{S}_\bullet^{\mathcal{C}}(\mathcal{M}_\bullet)$  of chain complexes in  $\mathcal{M}_\bullet$ .

$$A_\bullet : 0 \leftarrow C^0(M) \xleftarrow{\partial} C^1(M) \xleftarrow{\partial} C^2(M) \dots \xleftarrow{\partial} C^n(M) \xleftarrow{\partial} \dots$$

Here  $A_n = C^n(M)$  is the vector space over  $\mathbb{R}$  of all finite chains  $C$  on the manifold  $M$  and  $\partial_n = \partial : C^{n+1}(M) \rightarrow C^n(M)$ . A finite chain  $C$  such that  $\partial C = 0$  is an  $n$ -cycle. A finite chain  $C$  such that  $C = \partial B$  is an  $n$ -boundary. Let  $Z_n(M) = \text{Ker } \partial$  (resp.  $B_n(M) = \text{Im } \partial$ ) denote a real vector space of cycles (resp. boundaries) of degree  $n$ . Since  $\partial_{n+1} \circ \partial_n = \partial^2 = 0$ , we have  $B_n(M) \subset Z_n(M)$ . The quotient vector space

$$H_n^C(M) = \text{Ker } \partial / \text{Im } \partial = Z_n(M) / B_n(M)$$

is the  $n$ -homology group. The elements of  $H_n^C(M)$  are equivalence sets of cycles. Two cycles  $C_1, C_2$  belong to the same equivalence set, or are homologous (written  $C_1 \sim C_2$ ), iff they differ by a boundary  $C_1 - C_2 = \partial B$ . The homology class of a finite chain  $C \in C^n(M)$  is  $[C] \in H_n^C(M)$ .

The dimension of the  $n$ -cohomology (resp.  $n$ -homology) group equals the  $n$ th Betti number  $b^n$  (resp.  $b_n$ ) of the manifold  $M$ . *Poincaré lemma* says that on an open set  $U \in M$  diffeomorphic to  $\mathbb{R}^N$ , all closed forms (cycles) of degree  $p \geq 1$  are exact (boundaries). That is, the Betti numbers satisfy  $b^p = 0$  (resp.  $b = 0$ ), for  $p = 1, \dots, n$ .

The *De Rham theorem* states the following. The map  $\Phi: H_n \times H^n \rightarrow \mathbb{R}$  given by  $([C], [\omega]) \rightarrow \langle C, \omega \rangle$  for  $C \in Z_n, \omega \in Z^n$  is a bilinear nondegenerate map which establishes the duality of the groups (vector spaces)  $H_n$  and  $H^n$  and the equality  $b_n = b^n$ .

#### 4.1.2 $M$ -Reduction and its Euler Characteristic

Recall (see subsection (2.4.4) above), that for the purpose of high-level control, the rotational biomechanical configuration manifold  $M$  (Figure 2.1), could be first, reduced to an  $n$ -torus, and second, transformed into an  $n$ -cube 'hyper-joystick', using the following topological techniques (see [Iva02, IP01b, Iva05]).

Let  $S^1$  denote the constrained unit circle in the complex plane, which is an Abelian Lie group. Firstly, we propose two reduction homeomorphisms, using the noncommutative semidirect product ' $\triangleright$ ' of the constrained  $SO(2)$ -groups:

$$SO(3) \gtrsim SO(2) \triangleright SO(2) \triangleright SO(2), \quad \text{and} \quad SO(2) \approx S^1.$$

Next, let  $I^n$  be the unit cube  $[0, 1]^n$  in  $\mathbb{R}^n$  and ‘ $\sim$ ’ an equivalence relation on  $\mathbb{R}^n$  obtained by ‘gluing’ together the opposite sides of  $I^n$ , preserving their orientation. Therefore, the manifold  $M$  can be represented as the quotient space of  $\mathbb{R}^n$  by the space of the integral lattice points in  $\mathbb{R}^n$ , that is an oriented and constrained  $n$ D torus  $T^n$ :

$$\mathbb{R}^n/Z^n = I^n/\sim \approx \prod_{i=1}^n S_i^1 \equiv \{(q^i, i = 1, \dots, N) : \text{mod } 2\pi\} = T^n. \quad (4.2)$$

Now, using the *De Rham theorem* and the *homotopy axiom* for the De Rham cohomologies, we can calculate the *Euler–Poincaré characteristics* for  $T^n$  as well as for its two bundles,  $TT^n$  and  $T^*T^n$ , as (see [Iva02, Iva05])

$$\chi(T^n, TT^n) = \sum_{p=1}^n (-1)^p b_p, \quad \text{where } b_p \text{ are the Betti numbers defined as}$$

$$b^0 = 1, \quad b^1 = n, \dots, \quad b^p = \binom{n}{p}, \dots, \quad b^{n-1} = n, \quad b^n = 1, \quad (p = 0, \dots, n).$$

## 4.2 Morse Theory in Human-Like Biomechanics

In this section we continue development of Morse theory, from Chapter 2.

### 4.2.1 Morse Geometry of $M$

Recall that on any smooth manifold  $M$  there exist many Riemannian metrics  $g$  (see subsection (3.53) above). Each of these metrics is *locally defined* in a particular point  $q \in M$  as a symmetric  $(0, 2)$  tensor-field such that  $g|_q : T_q M \times T_q M \rightarrow \mathbb{R}$  is a positively defined inner product for each point  $q \in M$ . In an open local chart  $U \in M$  containing the point  $q$ , this metric is given as  $g|_q \mapsto g_{ij}(q) dq^i dq^j$ . With each metric  $g|_q$  there is associated a *local geodesic* on  $M$ .

Now, two main *global geodesics problems* on the biomechanical configuration manifold  $M$  with the Riemannian metrics (3.53), can be formulated as follows (compare with subsection 2.5.2 above; also, see [Mil63, Die88]):

1. *Is there a minimal geodesic  $\gamma_0(t)$  between two points  $A$  and  $B$  on  $M$ ? In other words, does an arc of geodesic  $\gamma_0(t)$  with extremities  $A, B$  actually have minimum length among all rectifiable curves  $\gamma(t) = (q^i(t), p_i(t))$  joining  $A$  and  $B$ ?*
2. *How many geodesic arcs are there joining two points  $A$  and  $B$  on  $M$ ?*

Locally these problems have a *complete answer*: each point of the biomechanics manifold  $M$  has an open neighborhood  $V$  such that for any two distinct points  $A, B$  of  $V$  there is exactly one arc of a geodesic contained in  $V$  and joining  $A$  and  $B$ , and it is the *unique minimal geodesic* between  $A$  and  $B$ .

Recall (see subsection (2.5.2) above), that seven decades ago, Morse considered the set  $\Omega = \Omega(M; A, B)$  of *piecewise smooth paths* on a Riemannian manifold  $M$  having fixed extremities  $A, B$ , defined as continuous maps  $\gamma : [0, 1] \rightarrow M$  such that  $\gamma(0) = A$ ,  $\gamma(1) = B$ , and there were a finite number of points

$$t_0 = 0 < t_1 < t_2 < \dots < t_{m-1} < t_m = 1, \tag{4.3}$$

such that in every *closed interval*  $[t_i, t_{i+1}]$ ,  $\gamma$  was a  $C^k$ -function. The parametrization was always chosen such that for  $t_j \leq t \leq t_{j+1}$ ,

$$t - t_j = \frac{t_{j+1} - t_j}{l_j} \int_{t_j}^t \left\| \frac{d\gamma}{du} \right\| du, \quad \text{with} \quad l_j = \int_{t_j}^{t_{j+1}} \left\| \frac{d\gamma}{du} \right\| du. \tag{4.4}$$

In other words,  $t - t_j$  was proportional to the length of the image of  $[t_j, t]$  by  $\gamma$ . Then

$$L(\gamma) = \sum_{j=0}^m l_j,$$

the length of  $\gamma$ , was a function of  $\gamma$  in  $\Omega$ . A minimal arc from  $A$  to  $B$  should be a path  $\gamma$  for which  $L(\gamma)$  is *minimum* in  $\Omega$ , and a geodesic arc from  $A$  to  $B$  should be a path that is a ‘critical point’ for the function  $L$ . This at first has no meaning, since  $\Omega$  is not a differential manifold; the whole of Morse’s theory consists in showing that it is possible to substitute for  $\Omega$  genuine differential manifolds to which his results on critical points can be applied ([Mor34]).

To study the geodesics joining two points  $A, B$  it is convenient, instead of working with the length  $L(\gamma)$ , to work with the *energy of a path*  $\gamma : [A, B] \rightarrow M$ , defined by ([Die88])

$$E_A^B(\gamma) = \int_A^B \left\| \frac{d\gamma}{du} \right\|^2 du. \tag{4.5}$$

With the chosen parametrization (4.4),  $E(\gamma) = (B - A)L(\gamma)^2$ , and the extremals of  $E$  are again the geodesics, but the computations are easier with  $E$ .

Morse theory can be divided into several steps (see [Mil63]).

*Step 1* is essentially a presentation of the classical Lagrange method that brings to light the analogy with the critical points of a  $C^k$ -function on  $M$ . No topology is put on  $\Omega$ ; a *variation* of a path  $\gamma \in \Omega$  is a continuous map  $\alpha$  into  $M$ , defined in a product  $]-\varepsilon, \varepsilon[ \times [0, 1]$  with the following properties:

1.  $\alpha(0, t) = \gamma(t)$ ;
2.  $\alpha(u, 0) = A$ ,  $\alpha(u, 1) = B$  for  $-\varepsilon < u < \varepsilon$ ; and

3. There is a decomposition (4.3) such that  $\alpha$  is  $C^k$  in each set

$$] - \varepsilon, \varepsilon[ \times [t_i, t_{i+1}].$$

A *variation vector-field*  $t \mapsto W(t)$  is associated to each variation  $\alpha$ , where  $W(t)$  is a tangent vector in the tangent space  $T_{\gamma(t)}M$  to  $M$ , defined by

$$W(t) = \partial_u \alpha(0, t). \tag{4.6}$$

It is a continuous map of  $[0, 1]$  into the tangent bundle  $TM$ , *smooth* in each interval  $[t_i, t_{i+1}]$ . These maps are the substitute for the *tangent vectors* at the *point*  $\gamma$ ; they form an infinite-dimensional vector space written  $T\Omega(\gamma)$ .

More generally the interval  $] - \varepsilon, \varepsilon[$  can be replaced in the definition of a variation by a neighborhood of 0 in some  $\mathbb{R}^n$ , defining an *n-parameter variation*.

A *critical path*  $\gamma_0 \in \Omega$  for a function  $F : \Omega \rightarrow \mathbb{R}$  is defined by the condition that for every variation  $\alpha$  of  $\gamma_0$  the function

$$u \mapsto F(\alpha(u, \cdot))$$

is derivable for  $u = 0$  and its derivative is 0.

*Step 2* is a modern presentation of the formulas of Riemannian geometry, giving the *first variation* and *second variation* of the energy (4.5) of a path  $\gamma_0 \in \Omega$ , which form the basis of Jacobi results.

First consider an arbitrary path  $\omega_0 \in \Omega$ , its *velocity*  $\dot{\omega}(t) = d\omega/dt$ , and its *acceleration* in the Riemannian sense

$$\bar{\omega}(t) = \nabla_t \dot{\omega}(t),$$

where  $\nabla_t$  denotes the Bianchi covariant derivative, as defined in (3.56). They belong to  $T_{\omega(t)}M$  for each  $t \in [0, 1]$ , are defined and continuous in each interval  $[t_i, t_{i+1}]$  in which  $\omega$  is smooth, and have limits at both extremities. Now let  $\alpha$  be a variation of  $\omega$  and  $t \mapsto W(t)$  be the corresponding variation vector-field (4.6). The *first variation formula* gives the first derivative

$$\frac{1}{2} \frac{d}{du} E(\alpha(u, \cdot))|_{u=0} = - \sum_i (W(t_i) | \dot{\omega}(t_{i+}) - \dot{\omega}(t_{i-})) - \int_0^1 (W(t) | \bar{\omega}(t)) dt,$$

where  $(x|y)$  denotes the scalar product of two vectors in a tangent space. It follows from this formula that  $\gamma_0 \in \Omega$  is a critical path for  $E$  iff  $\gamma$  is a *geodesic*.

Next, fix such a geodesic  $\gamma$  and consider a two-parameter variation:

$$\alpha : U \times [0, 1] \rightarrow M,$$

where  $U$  is a neighborhood of 0 in  $\mathbb{R}^2$ , so that

$$\alpha(0, 0, t) = \gamma(t), \quad \partial_{u_1} \alpha(0, 0, t) = W_1(t), \quad \partial_{u_2} \alpha(0, 0, t) = W_2(t),$$

in which  $W_1$  and  $W_2$  are in  $T\Omega(\gamma)$ . The *second variation formula* gives the mixed second derivative

$$\begin{aligned} \frac{1}{2} \frac{\partial^2}{\partial u_1 \partial u_2} E(\alpha(u_1, u_2, \cdot))|_{(0,0)} &= - \sum_i (W_2(t_i) | \nabla_t W_1(t_i+) - \nabla_t W_1(t_i-)) \\ &\quad - \int_0^1 (W_2(t) | \nabla_t^2 W_1(t) + R(V(t) \wedge W_1(t)) \cdot V(t)) dt, \end{aligned} \tag{4.7}$$

where  $Z \mapsto R(X \wedge Y) \cdot Z$  is the curvature of the Levi-Civita connection (3.57). The l.h.s of (4.7) is thus a *bilinear symmetric form*

$$(W_1, W_2) \mapsto E_{**}(W_1, W_2)$$

on the product  $T\Omega(\gamma) \times T\Omega(\gamma)$ . For a one-parameter variation  $\alpha$

$$E_{**}(W, W) = \frac{1}{2} \frac{d^2}{du^2} E(\alpha(u, \cdot))|_{u=0},$$

from which it follows that if  $\gamma$  is a *minimal* geodesic in  $\Omega$ ,  $E_{**}(W, W) \geq 0$  in  $T\Omega(\gamma)$ . As usual, we shall speak of  $E_{**}$  indifferently as a symmetric bilinear form or as a quadratic form  $W \mapsto E_{**}(W, W)$ .

Formula (4.7) naturally leads to the junction with Jacobi work (see [Die88]): consider the smooth vector-fields  $t \mapsto J(t)$  along  $\gamma \in M$ , satisfying the equation

$$\nabla_t^2 J(t) + R(V(t) \wedge J(t)) \cdot V(t) = 0 \quad \text{for } 0 \leq t \leq 1. \tag{4.8}$$

With respect to a frame along  $\gamma$  moving by parallel translation on  $M$  this relation is equivalent to a system of  $n$  linear homogeneous ODEs of order 2 with  $C^k$ -coefficients; the solutions  $J$  of (4.8) are called the *Jacobi fields* along  $\gamma$  and form a vector space of dimension  $2n$ . If for a value  $a \in ]0, 1[$  of the parameter  $t$  there exists a Jacobi field along  $\gamma$  that is not identically 0 but *vanishes for*  $t = 0$  and  $t = a$ , then the points  $A = \gamma(0)$  and  $r = \gamma(a)$  are conjugate along  $\gamma$  with a *multiplicity* equal to the dimension of the vector space of Jacobi fields vanishing for  $t = 0$  and  $t = a$ .

Jacobi fields on the biomechanical configuration manifold  $M$  may also be defined as variation vector-fields for *geodesic variations* of the path  $\gamma \in M$ : they are  $C^k$ -maps

$$\alpha : ]-\varepsilon, \varepsilon[ \times [0, 1] \rightarrow M,$$

such that for any  $u \in ]-\varepsilon, \varepsilon[$ ,  $t \mapsto \alpha(u, t)$  is a geodesic and  $\alpha(0, t) = \gamma(t)$ .

It can be proved that the Jacobi fields along  $\gamma \in M$  that vanish at  $A$  and  $B$  (hence belong to  $T\Omega(\gamma)$ ) are exactly the vector-fields  $J \in T\Omega(\gamma)$  such that

$$E_{**}(J, W) = 0$$

for every  $W \in T\Omega(\gamma)$ . Although  $T\Omega(\gamma)$  is infinite-dimensional, the form  $E_{**}$  is again called *degenerate* if the vector space of the Jacobi fields vanishing at

$A$  and  $B$  is note reduced to 0 and the dimension of that vector space is called the *nullity* of  $E_{**}$ . Therefore,  $E_{**}$  is thus degenerate iff  $A$  and  $B$  are conjugate along  $\gamma$  and the nullity of  $E_{**}$  is the multiplicity of  $B$ .

*Step 3* is the beginning of Morse’s contributions (see [Mil63]). He first considered a *fixed* geodesic  $\gamma : [0, 1] \rightarrow M$  with extremities  $A = \gamma(0)$ ,  $B = \gamma(1)$  and the bilinear symmetric form  $E_{**} : T\Omega(\gamma) \times T\Omega(\gamma) \rightarrow \mathbb{R}$ . By analogy with the finite–dimensional quadratic form, the *index* of  $E_{**}$  is defined as the maximum dimension of a vector subspace of  $T\Omega(\gamma)$  in which  $E_{**}$  is *strictly negative* (i.e., nondegenerate and taking values  $E_{**}(W, W) < 0$  except for  $W = 0$ ). Morse’s central result gives the value of the index of  $E_{**}$  and is known as the *index theorem*.

Suppose a subdivision (4.3) is chosen such that each arc  $\gamma([t_{i-1}, t_i])$  is contained in an open set  $U_i \subset M$  such that any two points of  $U_i$  are joined by a unique geodesic arc contained in  $U_i$  that is *minimal*;  $\gamma([t_{i-1}, t_i])$  is such an arc. In the infinite–dimensional vector space  $T\Omega(\gamma)$ , consider the two vector subspaces:

1.  $T\Omega(\gamma; t_0, t_1, \dots, t_m)$  consisting of all continuous vector–fields  $t \mapsto W(t)$  along  $\gamma$ , vanishing for  $t = 0$  and  $t = 1$ , such that each restriction  $W|_{[t_{i-1}, t_i]}$  is a *Jacobi field* (hence smooth) along  $\gamma([t_{i-1}, t_i])$ ; that subspace is finite–dimensional;
2.  $T'$  consisting of the vector–fields  $t \mapsto W(t)$  along  $\gamma$ , such that  $W(t_0) = 0$ ,  $W(t_1) = 0, \dots, W(t_m) = 0$ .

$T\Omega(\gamma)$  is then the *direct sum*  $T\Omega(\gamma; t_0, t_1, \dots, t_m) \oplus T'$ ; these two subspaces are orthogonal for the bilinear form  $E_{**}$ , and  $E_{**}$  is *strictly positive* in  $T'$ , so that the index of  $E_{**}$  is equal to the index of its restriction to the subspace  $T\Omega(\gamma; t_0, t_1, \dots, t_m)$ .

To compute the nullity and index of  $E_{**}$ , due to this decomposition, apply their definitions either to vector subspaces of  $T\Omega(\gamma)$  or to vector subspaces of  $T\Omega(\gamma; t_0, t_1, \dots, t_m)$ . The computation of the index of  $E_{**}$  is done by considering the geodesic arc  $\gamma_\tau : [0, \tau] \rightarrow M$ , the restriction of  $\gamma$  to  $[0, \tau]$ , and its energy

$$E(\gamma_\tau) = \tau \int_0^\tau \left\| \frac{d\gamma}{du} \right\|^2 du.$$

$E_{**}^\tau$  is the corresponding quadratic form on  $T\Omega(\gamma_\tau)$ , and  $\lambda(\tau)$  is its index; one studies the variation of  $\lambda(\tau)$  when  $\tau$  varies from 0 to 1, and  $\lambda(1)$  is the index of  $E_{**}$ .

The index theorem says: *the index of  $E_{**}$  is the sum of the multiplicities of the points conjugate to  $A$  along  $B$  and distinct from  $B$ .*

We have seen that the dimension of  $T\Omega(\gamma; t_0, t_1, \dots, t_m)$  is finite; it follows that the index of  $E_{**}$  is always *finite*, and therefore the number of points conjugate to  $A$  along  $\gamma$  is also *finite*.

*Step 4* of Morse theory introduces a *topology* on the set  $\Omega = \Omega(M; A, B)$ . On the biomechanical configuration manifold  $M$  the usual topology can be

defined by a *distance*  $\rho(A, B)$ , the g.l.b. of the lengths of all piecewise smooth paths joining  $A$  and  $B$ . For any pair of paths  $\omega_1, \omega_2$  in  $\Omega(M; A, B)$ , consider the function  $d(\omega_1, \omega_2) \in M$

$$d(\omega_1, \omega_2) = \sup_{0 \leq t \leq 1} \rho(\omega_1(t), \omega_2(t)) + \sqrt{\int_0^1 (\dot{s}_1 - \dot{s}_2)^2 dt},$$

where  $s_1(t)$  (resp.  $s_2(t)$ ) is the length of the path  $\tau \mapsto \omega_1(\tau)$  (resp.  $\tau \mapsto \omega_2(\tau)$ ) defined in  $[0, t]$ . This distance on  $\Omega$  such that the function  $\omega \mapsto E_A^B(\omega)$  is *continuous* for that distance.

### 4.2.2 Morse Topology of $M$

#### Morse Functions and Boundary Operators on $M$

Let  $f : M \rightarrow \mathbb{R}$  represents a  $C^k$ -function on the biomechanical configuration manifold  $M$ . Recall that  $z = (q, p) \in M$  is the *critical point* of  $f$  if  $df(z) \equiv df[(q, p)] = 0$ . In local coordinates  $(x^1, \dots, x^n) = (q^1, \dots, q^n, p_1, \dots, p_n)$  in a neighborhood of  $z$ , this means  $\frac{\partial f}{\partial x^i}(z) = 0$  for  $i = 1, \dots, n$ . The Hessian of  $f$  at a critical point  $z$  defines a symmetric bilinear form  $\nabla df(z) = d^2 f(z)$  on  $T_z M$ , in local coordinates  $(x^1, \dots, x^n)$  represented by the matrix  $\left(\frac{\partial^2 f}{\partial x^i \partial x^j}\right)$ . Index and nullity of this matrix are called index and nullity of the critical point  $z$  of  $f$ .

Now, we assume that all critical points  $z_1, \dots, z_n$  of  $f \in M$  are nondegenerate in the sense that the Hessians  $d^2 f(z_i)$ ,  $i = 1, \dots, m$ , have maximal rank. Let  $z$  be such a critical point of  $f$  of *Morse index*  $s$  (= number of negative eigenvalues of  $d^2 f(z_i)$ , counted with multiplicity). The eigenvectors corresponding to these negative eigenvalues then span a subspace  $V_z \subset T_z M$  of dimension  $s$ . We choose an orthonormal basis  $e_1, \dots, e_s$  of  $V_z$  w.r.t. the the Riemannian metric (3.53) on  $M$  (induced by the system's kinetic energy), with dual basis  $dx^1, \dots, dx^s$ . This basis then defines an orientation of  $V_z$  which we may also represent by the  $s$ -form  $dx^1 \wedge \dots \wedge dx^s$ . We now let  $z'$  be another critical point of  $f$ , of Morse index  $s - 1$ . We consider paths  $\gamma(t)$  of the steepest descent of  $f$  from  $z$  to  $z'$ , i.e., integral curves of the vector-field  $-\nabla f(\gamma)$ . Thus  $\gamma(t)$  defines the *gradient flow* of  $f$

$$\dot{\gamma}(t) = -\nabla f(\gamma(t)), \quad \text{with} \quad \begin{cases} \lim_{t \rightarrow -\infty} \gamma(t) = z, \\ \lim_{t \rightarrow \infty} \gamma(t) = z' \end{cases} . \quad (4.9)$$

A path  $\gamma(t)$  obviously depends on the Riemannian metric (3.53) on  $M$  as

$$\nabla f = g^{ij} \partial_{x^i} f \partial_{x^j} f.$$

From [Sma60, Sma67] it follows that for a generic metric  $g$ , the Hessian  $\nabla df(y)$  has only nondegenerate eigenvalues. Having a metric  $g$  induced by the system's

kinetic energy, we let  $\tilde{V}_y \subset T_y M$  be the space spanned by the eigenvectors corresponding to the  $s - 1$  lowest eigenvalues. Since  $z'$  has Morse index  $s - 1$ ,  $\nabla df(z') = d^2 f(z')$  has precisely  $s - 1$  negative eigenvalues. Therefore,  $\tilde{V}_{z'} \equiv \lim_{t \rightarrow \infty} \tilde{V}_{\gamma(t)} = V_{z'}$ , while the unit tangent vector of  $\gamma$  at  $z'$ , i.e.,  $\lim_{t \rightarrow \infty} \frac{\dot{\gamma}(t)}{\|\dot{\gamma}(t)\|}$ , lies in the space of directions corresponding to positive eigenvalues and is thus orthogonal to  $V_{z'}$ . Likewise, the unit tangent vector  $v_z$  of  $\gamma$  at  $z$ , while contained in  $V_z$ , is orthogonal to  $\tilde{V}_z$ , because it corresponds to the largest one among the  $s$  negative eigenvalues of  $d^2 f(z)$ . Taking the interior product  $i(v_z) dx^1 \wedge \dots \wedge dx^s$  defines an orientation of  $\tilde{V}_z$ . Since  $\tilde{V}_y$  depends smoothly on  $y$ , we may transport the orientation of  $\tilde{V}_z$  to  $\tilde{V}_{z'}$  along  $\gamma$ . We then define  $n_\gamma = +1$  or  $-1$ , depending on whether this orientation of  $\tilde{V}_{z'}$  coincides with the chosen orientation of  $V_{z'}$  or not, and further define  $n(z, z') = \sum_\gamma n_\gamma$ , where the sum is taken over all such paths  $\gamma$  of the steepest descent from  $p$  to  $p'$ .

Now, let  $M^s$  be the set of critical points of  $f$  of Morse index  $s$ , and let  $H_f^s$  be the vector space over  $\mathbb{R}$  spanned by the elements of  $M^s$ . We define a boundary operator

$$\delta : H_f^{s-1} \rightarrow H_f^s, \quad \text{by putting, for } z' \in M^{s-1},$$

$$\delta(z') = \sum_{n \in M^s} n(z', z) z, \quad \text{and extending } \delta \text{ by linearity.}$$

This operator satisfies  $\delta^2 = 0$  and therefore defines a cohomology theory. Using Conley's continuation principle, Floer [Flo88] showed that the resulting cohomology theories resulting from different choices of  $f$  are canonically isomorphic.

Fields Medalist Edward Witten [Wit82] also considered the operators:

$$d_t = e^{-tf} de^{tf}, \quad \text{their adjoints : } d_t^* = e^{tf} de^{-tf},$$

$$\text{as well as their Laplacian: } \Delta_t = d_t d_t^* + d_t^* d_t.$$

For  $t = 0$ ,  $\Delta_0$  is the standard Hodge-De Rham Laplacian, whereas for  $t \rightarrow \infty$ , one has the following expansion

$$\Delta_t = dd^* + d^*d + t^2 \|df\|^2 + t \sum_{k,j} \frac{\partial^2 h}{\partial x^k \partial x^j} [i \partial_{x^k}, dx^j],$$

where  $(\partial_{x^k})_{k=1, \dots, n}$  is an orthonormal frame at the point under consideration. This becomes very large for  $t \rightarrow \infty$ , except at the critical points of  $f$ , i.e., where  $df = 0$ . Therefore, the eigenvalues of  $\Delta_t$  will concentrate near the critical points of  $f$  for  $t \rightarrow \infty$ , and we get an interpolation between De Rham cohomology and Morse cohomology.

### Morse Homology on $M$

Now, following [Mil99, IP05b], for any Morse function  $f$  on the configuration manifold  $M$  we denote by  $\text{Crit}_p(f)$  the set of its critical points of index  $p$

and define  $C_p(f)$  as a free Abelian group generated by  $\text{Crit}_p(f)$ . Consider the gradient flow generated by (4.9). Denote by  $\mathcal{M}_{f,g}(M)$  the set of all  $\gamma : \mathbb{R} \rightarrow M$  satisfying (4.9) such that

$$\int_{-\infty}^{+\infty} \left| \frac{d\gamma}{dt} \right|^2 dt < \infty.$$

Now, the spaces

$$\mathcal{M}_{f,g}(x^-, x^+) = \{ \gamma \in \mathcal{M}_{f,g}(M) \mid \gamma(t) \rightarrow x^\pm \text{ as } t \rightarrow \pm\infty \}$$

are smooth manifolds of dimension  $m(x^+) - m(x^-)$ , where  $m(x)$  denotes the Morse index of a critical point  $x$ . Note that

$$\mathcal{M}_{f,g}(x, y) \cong W_g^u(x) \cap W_g^s(y),$$

where  $W_g^s(y)$  and  $W_g^u(x)$  are the stable and unstable manifolds of the gradient flow (4.9). For generic  $g$  the intersection above is transverse (Morse–Smale condition). The group  $\mathbb{R}$  acts on  $\mathcal{M}_{f,g}(x, y)$  by  $\gamma \mapsto \gamma(\cdot + t)$ . We denote

$$\widehat{\mathcal{M}}_{f,g}(x, y) = \mathcal{M}_{f,g}(x, y) / \mathbb{R}.$$

The manifolds  $\widehat{\mathcal{M}}_{f,g}(x, y)$  can be given a coherent orientation  $\sigma$  (see [Sch93]). Now, we can define the boundary operator, as

$$\partial : C_p(f) \rightarrow C_{p-1}(f), \quad \partial x = \sum_{y \in \text{Crit}_{p-1}(f)} n(x, y) y,$$

where  $n(x, y)$  is the number of points in 0D manifold  $\widehat{\mathcal{M}}_{f,g}(x, y)$  counted with the sign with respect to the orientation  $\sigma$ . The proof of  $\partial \circ \partial = 0$  is based on gluing and cobordism arguments [Sch93]. Now Morse homology groups are defined by

$$H_p^{\text{Morse}}(f) = \text{Ker}(\partial) / \text{Im}(\partial).$$

For generic choices of Morse functions  $f_1$  and  $f_2$  the groups  $H_p(f_1)$  and  $H_p(f_2)$  are isomorphic. Furthermore, they are isomorphic to the singular homology group of  $M$ , i.e.,

$$H_p^{\text{Morse}}(f) \cong H_p^{\text{sing}}(M),$$

for generic  $f$  [Mil65].

The construction of isomorphism is given (see [Mil99, IP05b]) as

$$h_{\alpha\beta} : H_p(f^\alpha) \rightarrow H_p(f^\beta), \tag{4.10}$$

for generic Morse functions  $f^\alpha, f^\beta$ . Consider the ‘connecting trajectories’, i.e., the solutions of non-autonomous equation

$$\dot{\gamma} = -\nabla f_t^{\alpha\beta}, \tag{4.11}$$

where  $f_t^{\alpha\beta}$  is a homotopy connecting  $f^\alpha$  and  $f^\beta$  such that for some  $R > 0$

$$f_t^{\alpha\beta} \equiv \begin{cases} f^\alpha & \text{for } t \leq -R \\ f^\beta & \text{for } t \geq R \end{cases}.$$

For  $x^\alpha \in \text{Crit}_p(f^\alpha)$  and  $x^\beta \in \text{Crit}_p(f^\beta)$  denote

$$\mathcal{M}_{f^{\alpha\beta},g}(x^\alpha, x^\beta) = \{\gamma : \gamma \text{ satisfies (4.11) and } \lim_{t \rightarrow -\infty} \gamma = x^\alpha, \lim_{t \rightarrow \infty} \gamma = x^\beta\}.$$

As before,  $\mathcal{M}_{f^{\alpha\beta},g}$  is a smooth finite-dimensional manifold. Now, define

$$\begin{aligned} (h_{\alpha\beta})_\# &: C_p(f^\alpha) \rightarrow C_p(f^\beta), \quad \text{by} \\ (h_{\alpha\beta})_\# x^\alpha &= \sum_{x^\beta \in \text{Crit}_p(f^\beta)} n(x^\alpha, x^\beta) x^\beta, \quad \text{for } x^\alpha \in \text{Crit}_p(f^\alpha), \end{aligned}$$

where  $n(x^\alpha, x^\beta)$  is the algebraic number of points in 0D manifold  $\mathcal{M}_{f^{\alpha\beta},g}(x^\alpha, x^\beta)$  counted with the signs defined by the orientation of  $\mathcal{M}_{f^{\alpha\beta},g}$ . Homomorphisms  $(h_{\alpha\beta})_\#$  commute with  $\partial$  and thus define the homomorphisms  $h_{\alpha\beta}$  in homology which, in addition, satisfy  $h_{\alpha\beta} \circ h_{\beta\gamma} = h_{\alpha\gamma}$ .

Now, if we fix a Morse function  $f : M \rightarrow \mathbb{R}$  instead of a metric  $g$ , we establish the isomorphism (see [Mil99, IP05b])

$$h_{\alpha\beta} : H_p(g^\alpha, f) \rightarrow H_p(g^\beta, f)$$

between the two Morse homology groups defined by means of two generic metrics  $g^\alpha$  and  $g^\beta$  in a similar way, by considering the ‘connecting trajectories’,

$$\dot{\gamma} = -\nabla^{g_t^{\alpha\beta}} f. \quad (4.12)$$

Here  $g_t^{\alpha\beta}$  is a homotopy connecting  $g^\alpha$  and  $g^\beta$  such that for some  $R > 0$

$$g_t^{\alpha\beta} \equiv \begin{cases} g^\alpha & \text{for } t \leq -R, \\ g^\beta & \text{for } t \geq R, \end{cases}$$

and  $\nabla^g$  is a gradient defined by metric  $g$ .

Note that  $f$  is decreasing along the trajectories solving autonomous gradient equation (4.9). Therefore, the boundary operator  $\partial$  preserves the downward filtration given by level sets of  $f$ . In other words, if we denote

$$\begin{aligned} \text{Crit}_p^\lambda(f) &= \text{Crit}_p(f) \cap f^{-1}((-\infty, \lambda]), \quad \text{and} \\ C_p^\lambda(f) &= \text{free Abelian group generated by } \text{Crit}_p^\lambda(f), \end{aligned}$$

then the boundary operator  $\partial$  restricts to  $\partial^\lambda : C_p^\lambda(f) \rightarrow C_{p-1}^\lambda(f)$ . Obviously,  $\partial^\lambda \circ \partial^\lambda = 0$ , thus we can define the relative Morse homology groups

$$H_p^\lambda(f) = \text{Ker}(\partial^\lambda) / \text{Im}(\partial^\lambda).$$

Following the standard algebraic construction, we define (relative) Morse cohomology. We set

$$C_\lambda^p(f) = \text{Hom}(C_p^\lambda(f), \mathbb{Z}), \quad \text{and}$$

$$\delta^\lambda : C_\lambda^p(f) \rightarrow C_\lambda^{p+1}(f), \quad \langle \delta^\lambda a, x \rangle = \langle a, \partial^\lambda x \rangle$$

and define

$$H_\lambda^p(f) = \text{Ker}(\delta^\lambda) / \text{Im}(\delta^\lambda).$$

Since  $\text{Crit}_p(f)$  is finite, we have  $H_p^\lambda(f) = H_p(f)$  and  $H_\lambda^p(f) = H^p(f)$ .

### 4.3 Hodge–De Rham Theory in Human–Like Biomechanics

#### 4.3.1 Hodge Laplacian on $M$

A single biomechanical configuration manifold  $M$  can be equipped with many different Riemannian metrics  $g$  in local coordinates (apart from the one generated by its kinetic energy)

$$g = g_{ij}(u^1, u^2, \dots, u^n) du^i du^j.$$

Beltrami had shown that it is always possible for such a metric to define an operator (depending on the metric) that generalizes the usual Laplacian on  $\mathbb{R}^n$  and therefore gives rise to the notion of harmonic functions on the Riemannian manifold [BM82].

Hodge theory was described by H. Weyl as ‘one of the landmarks in the history of mathematics in the 20th century’. Hodge showed that it was possible to define a notion of *harmonic exterior differential form*: the metric  $g$  on  $M$  canonically defines a metric on the tangent bundle  $TM$ , hence also, by standard multilinear algebra, a metric on any bundle of tensors on  $M$ . In particular, let  $(\alpha, \beta) \mapsto g_p(\alpha, \beta)$  be the positive nondegenerate symmetric bilinear form defined on the vector space of  $p$ –forms on  $M$ . As  $M$  is orientable, this defines a *duality* between  $p$ –forms and  $(n - p)$ –forms: to each  $p$ –form  $\alpha$  is associated a  $(n - p)$ –form  $*\alpha$ , defined by the linear Hodge star operator  $*$  (see subsection 2.3.3), characterized by the relations

$$\beta \wedge (*\alpha) = g_p(\alpha, \beta) v, \quad **\alpha = (-1)^{p(n-p)}\alpha,$$

for all  $p$ –forms  $\alpha, \beta$ , where  $v$  is the volume form on the Riemannian manifold  $M$ . If  $d$  is the exterior derivative, it has a *transposed* (adjoint) operator for that duality, the codifferential  $\delta$ , defined as

$$\delta = -(* \circ d \circ *),$$

which maps  $p$ –forms onto  $(p - 1)$ –forms, such that

$$\delta\alpha = (-1)^{np+n+1} * d * \alpha.$$

The *Hodge Laplacian*, defined as [Gri83b, Voi02]

$$\Delta = d \circ \delta + \delta \circ d,$$

transforms  $p$ -forms into  $p$ -forms and generalizes Beltrami's Laplacian (2.18), which is the special case for  $p = 0$  (up to a sign). This defines *harmonic* (real or complex valued)  $p$ -forms as those for which  $\Delta\alpha = 0$ , or equivalently,  $d\alpha = \delta\alpha = 0$ .

In other words, let  $dv$  be the volume element of the chosen metric  $g$ . Then for every  $p$ -form  $\alpha$  we can define a *norm functional*

$$\|\alpha\| = \int_X (\alpha, *\alpha)_g dv,$$

for which the *Euler-Lagrange equation* becomes  $\Delta\alpha = 0$ .

Now, the  $p$ th Betti number of  $M$  can be defined as

$$b_p = \dim \text{Ker } \Delta_p,$$

so that the Euler-Poincaré characteristics of  $M$  is given by

$$\chi(M) = \sum_{p=0}^n (-1)^p b_p = \sum_{p=0}^n (-1)^p \dim \text{Ker } \Delta_p. \quad (4.13)$$

Finally, for any  $(p-1)$ -form  $\alpha$ ,  $(p+1)$ -form  $\beta$ , and harmonic  $p$ -form  $\gamma$  ( $\Delta\gamma = 0$ ) on the biomechanical configuration manifold  $M$ , the celebrated *Hodge-De Rham decomposition* of a  $p$ -form  $\omega$  [Gri83b, Voi02] gives

$$\omega = d\alpha + \delta\beta + \gamma.$$

Now, recall from section 2.5.3 (Chapter 2), that a large class of symplectic manifolds is given by the *Kähler manifolds*. Let  $M$  be a smooth manifold and  $g$  a Riemannian metric on  $M$ . Let  $J$  be a complex structure on  $M$ , that is,  $J : TM \rightarrow TM$ ,  $J^2 = -\text{Id}$ , and  $J$  is  $g$ -orthogonal.  $M$  is called a *Kähler manifold* if  $\nabla j = 0$ , where  $\nabla$  is the Levi-Civita connection of  $g$  and  $J$  is regarded as a  $(1,1)$  tensor-field. Define a 2-form  $\omega$  on  $M$  by  $\omega(X, Y) = g(JX, Y)$ , for each vector-field  $X, Y$  on  $M$ . Then  $(M, \omega)$  is a symplectic manifold.

*Hodge theory* takes place on the cohomology of the compact orientable configuration manifold  $M$  and reflects the subtle interplay of the following basic additional linear structures one can impose on  $M$ :

- Symplectic structure  $\omega \in \Gamma_{C^k}(M, \Lambda^2 T_M^\vee)$ , where  $\omega$  is nondegenerate,  $d\omega = 0$ .
- Riemannian structure  $g \in \Gamma_{C^k}(M, S^2 T_M^\vee)$ , where  $g$  is positive definite.
- Complex structure  $J \in \Gamma_{C^k}(M, \text{End}(T_M))$ , where  $J^2 = -\text{id}$ , and  $J$  is integrable.

The data  $(M, \omega, g, J)$  satisfy the *Kähler condition* if  $\omega, g$  and  $J$  are *compatible* in the sense that

$$\omega(\bullet, J(\bullet)) = g(\bullet, \bullet),$$

where  $\bullet$  is the strong compatibility condition allowing the comparison of different cohomology theories.

De Rham cohomology of  $(M, J)$  is defined as

$$H_{DR}^k(M) = \frac{\text{Ker} \left( \Omega^k(M) \xrightarrow{d} \Omega^{k+1}(M) \right)}{\text{Im} \left( \Omega^{k-1}(M) \xrightarrow{d} \Omega^k(M) \right)}.$$

De Rham cohomology classes are represented by harmonic (natural) differential forms.

Let  $(M, g)$  be a compact oriented (real or complex) Riemannian manifold. Let  $dv$  be the volume element of  $g$ . Then for every  $k$ -form  $\alpha$  we can define

$$\|\alpha\| = \int_M (\alpha, \bar{\alpha})_g dv.$$

The *Euler–Lagrange equation* for the norm functional turns out to be  $d\alpha = \delta\alpha = 0$ . A  $k$ -form  $\alpha \in \Omega^k(M)$  is called *harmonic* if it satisfies one of the following equivalent conditions:

- $\alpha$  is *closed* and  $\|\alpha\| \leq \|\alpha + d\beta\|$  for all  $\beta \in \Omega^{k-1}(M)$ .
- $d\alpha = \delta\alpha = 0$ .
- $\Delta\alpha = 0$ , where  $\Delta = d\delta + \delta d$  is the *Hodge Laplacian*.

Hodge–Weyl theorem [Gri83b, Voi02] states that *every De Rham cohomology class has a unique harmonic representative*.

### 4.3.2 Heat Kernel and Thermodynamics on $M$

Besides pure mechanical consideration of biomechanical system, there is another biophysical point of view – thermodynamical, compatible with the human motion [Hil38]. Namely, the *heat equation* on the biomechanical configuration manifold  $M$ ,

$$\partial_t a(t) = \Delta a(t), \quad \text{with initial condition } a(0) = \alpha,$$

has a unique solution for every  $t \in [0, \infty)$  and every  $p$ -form  $\alpha$  on  $M$ . If we think of  $\alpha$  as an *initial temperature distribution* on  $M$  then as the configuration manifold cools down, according to the classical heat equation, the temperature should approach a *steady state* which should be *harmonic* [Dav89].

To prove this, we define a *stationary* and hence *harmonic* operator  $H(\alpha) = \lim_{t \rightarrow \infty} a(t)$ . Also, a map  $\alpha \rightarrow G(\alpha)$  with

$$G(\alpha) = \int_0^\infty a(t) dt$$

is orthogonal to the space of harmonic forms and satisfies

$$\Delta G(\alpha) = \int_0^\infty \Delta a(t) dt = - \int_0^\infty \partial_t a(t) dt = \alpha - H(\alpha).$$

Here, the map  $\alpha \rightarrow H(\alpha)$  is called *harmonic projection* and the map  $\alpha \rightarrow G(\alpha)$  is called *Green's operator*.

In particular, for each  $p$ -form  $\alpha$  we get a *unique decomposition*

$$\alpha = H(\alpha) + \Delta G(\alpha).$$

This proves the existence of a *harmonic representative* in every De Rham cohomology class, as follows.

Let  $\alpha \in \Omega^p(M)$  be a closed form. Then

$$\alpha = H(\alpha) + dd^*G(\alpha) + d^*dG(\alpha).$$

But the three terms in this sum are orthogonal and so

$$\|d^*dG(\alpha)\| = \langle d^*dG(\alpha), \alpha \rangle = \langle dG(\alpha), d\alpha \rangle = 0,$$

since  $\alpha$  is closed. Thus  $H(\alpha)$  is *cohomologous* to  $\alpha$ .

This thermal reflection on the biomechanics topology complies with the basic biophysics of human muscles (see [Hil38]).

#### 4.4 Topological Duality in Human-Like Biomechanics

The present section uncovers the underlying dual geometro-topological structure beneath the general biomechanics. It presents a parallel development of Hamiltonian and Lagrangian formulations of biomechanics (see [IS01, Iva02, IP01b, IP01b, Iva05]), proves both differential-geometric and algebraic-topological dualities between these two formulations, and finally establishes a *unique functorial relation* between biomechanics geometry and biomechanics topology.

Lagrangian formulation of biomechanics is performed on the *tangent bundle*  $TM$ , while Hamiltonian formulation is performed on the *cotangent bundle*  $T^*M$ . Both *Riemannian* and *symplectic* geometry are used. The geometric duality (see [KMS93, BM82]) of Lie groups and algebras between these two biomechanics formulations is proved as an existence of natural equivalence between Lie and canonical functors. The topological duality (see [DP97]) between these two biomechanics formulations is proved as an existence of natural equivalence between Lagrangian and Hamiltonian functors in both *homology* and *cohomology* categories. In the case of reduced configuration manifold, the Betti numbers and Euler-Poincaré characteristic are given.

### 4.4.1 Geometric Duality Theorem for $M$

**Theorem.** There is a geometric duality between rotational Lagrangian and Hamiltonian biomechanical formulations on  $M$  (as given by Figure 2.1). In categorical terms, there is a unique natural geometric equivalence

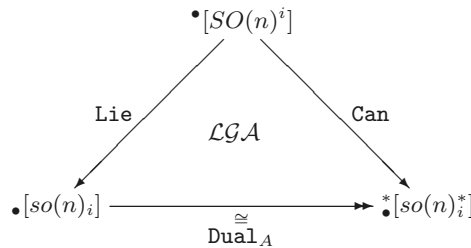
$$\text{Dual}_G : \text{Lie} \cong \text{Can}$$

in biomechanics (symbols are described in the next subsection).

**Proof.** The proof has two parts: Lie–functorial and geometric.

#### Lie–Functorial Proof

If we apply the functor **Lie** on the category  $\bullet[SO(n)^i]$  (for  $n = 2, 3$  and  $i = 1, \dots, N$ ) of rotational Lie groups  $SO(n)^i$  (and their homomorphisms) we get the category  $\bullet[so(n)_i]$  of corresponding *tangent* Lie algebras  $so(n)_i$  (and their homomorphisms). If we further apply the isomorphic functor **Dual** to the category  $\bullet[so(n)_i]$  we get the dual category  $\bullet^*[so(n)_i^*]$  of *cotangent*, or, *canonical* Lie algebras  $so(n)_i^*$  (and their homomorphisms). To go directly from  $\bullet[SO(n)^i]$  to  $\bullet^*[so(n)_i^*]$  we use the canonical functor **Can**. Therefore, we have a commutative triangle:



Applying the functor **Lie** on the biomechanical configuration manifold  $M$ , we get the product–tree of the same anthropomorphic structure, but having tangent Lie algebras  $so(n)_i$  as vertices, instead of the groups  $SO(n)^i$ . Again, applying the functor **Can** on  $M$ , we get the product–tree of the same anthropomorphic structure, but this time having cotangent Lie algebras  $so(n)_i^*$  as vertices. Both the tangent algebras  $so(n)_i$  and the cotangent algebras  $so(n)_i^*$  contain infinitesimal group generators: angular velocities  $\dot{q}^i = \dot{q}^{\phi_i}$  – in the first case, and canonical angular momenta  $p_i = p_{\phi_i}$  – in the second case [IS01]. As Lie group generators, both the angular velocities and the angular momenta satisfy the commutation relations:  $[\dot{q}^{\phi_i}, \dot{q}^{\psi_i}] = \epsilon_{\theta}^{\phi\psi} \dot{q}^{\theta_i}$  and  $[p_{\phi_i}, p_{\psi_i}] = \epsilon_{\phi\psi}^{\theta} p_{\theta_i}$ , respectively, where the structure constants  $\epsilon_{\theta}^{\phi\psi}$  and  $\epsilon_{\phi\psi}^{\theta}$  constitute the totally antisymmetric third–order tensors.

In this way, the functor  $\text{Dual}_G : \text{Lie} \cong \text{Can}$  establishes the unique geometric duality between kinematics of angular velocities  $\dot{q}^i$  (involved in *Lagrangian* formalism on the tangent bundle of  $M$ ) and kinematics of angular momenta  $p_i$

(involved in *Hamiltonian* formalism on the cotangent bundle of  $M$ ), which is analyzed below. In other words, we have two functors, **Lie** and **Can**, from the *category of Lie groups* (of which  $\bullet[SO(n)^i]$  is a subcategory) into the *category of (their) Lie algebras* (of which  $\bullet[so(n)_i]$  and  $\ast[so(n)_i^*]$  are subcategories), and a unique natural equivalence between them defined by the functor  $\text{Dual}_G$ . (As angular momenta  $p_i$  are in a bijective correspondence with angular velocities  $\dot{q}^i$ , every component of the functor  $\text{Dual}_G$  is invertible.) ■

### Geometric Proof

Geometric proof is given along the lines of Riemannian and symplectic geometry of mechanical systems, as follows (see 3.1 and 3.2.2 above, as well as [MR99, IS01, Iva02, IP01b, Iva05]). Recall that the Riemannian metric  $g = \langle, \rangle$  on the configuration manifold  $M$  is a positive-definite quadratic form  $g : TM \rightarrow \mathbb{R}$ , given in local coordinates  $q^i \in U$  ( $U$  open in  $M$ ) as

$$g_{ij} \mapsto g_{ij}(q, m) dq^i dq^j, \quad \text{where}$$

$$g_{ij}(q, m) = m_\mu \delta_{rs} \frac{\partial x^r}{\partial q^i} \frac{\partial x^s}{\partial q^j}$$

is the covariant material metric tensor  $g$ , defining a relation between internal and external coordinates and including  $n$  segmental masses  $m_\mu$ . The quantities  $x^r$  are external coordinates ( $r, s = 1, \dots, 6n$ ) and  $i, j = 1, \dots, N \equiv 6n - h$ , where  $h$  denotes the number of holonomic constraints.

The *Lagrangian* of the system is a quadratic form  $L : TM \rightarrow \mathbb{R}$  dependent on velocity  $v$  and such that  $L(v) = \frac{1}{2} \langle v, v \rangle$ . It is given by

$$L(v) = \frac{1}{2} g_{ij}(q, m) v^i v^j$$

in local coordinates  $q^i, v^i = \dot{q}^i \in U_v$  ( $U_v$  open in  $TM$ ). The *Hamiltonian* of the system is a quadratic form  $H : T^*M \rightarrow \mathbb{R}$  dependent on momentum  $p$  and such that  $H(p) = \frac{1}{2} \langle p, p \rangle$ . It is given by

$$H(p) = \frac{1}{2} g^{ij}(q, m) p_i p_j$$

in local canonical coordinates  $q^i, p_i \in U_p$  ( $U_p$  open in  $T^*M$ ). The inverse (contravariant) metric tensor  $g^{-1}$ , is defined as

$$g^{ij}(q, m) = m_\mu \delta_{rs} \frac{\partial q^i}{\partial x^r} \frac{\partial q^j}{\partial x^s}.$$

For any smooth function  $L$  on  $TM$ , the *fibre derivative*, or *Legendre transformation*, is a diffeomorphism  $\mathbb{F}L : TM \rightarrow T^*M$ ,  $\mathbb{F}L(w) \cdot v = \langle w, v \rangle$ , from the momentum phase-space manifold to the velocity phase-space manifold associated with the metric  $g = \langle, \rangle$ . In local coordinates  $q^i, v^i = \dot{q}^i \in U_v$  ( $U_v$  open in  $TM$ ),  $\mathbb{F}L$  is given by  $(q^i, v^i) \mapsto (q^i, p_i)$ .

Recall that on the momentum phase-space manifold  $T^*M$  exists:

- (i) A unique canonical 1-form  $\theta_H$  with the property that, for any 1-form  $\beta$  on the configuration manifold  $M$ , we have  $\beta^*\theta_H = \beta$ . In local canonical coordinates  $q^i, p_i \in U_p$  ( $U_p$  open in  $T^*M$ ) it is given by  $\theta_H = p_i dq^i$ .
- (ii) A unique nondegenerate Hamiltonian symplectic 2-form  $\omega_H$ , which is closed ( $d\omega_H = 0$ ) and exact ( $\omega_H = d\theta_H = dp_i \wedge dq^i$ ). Each body segment has, in the general  $SO(3)$  case, a sub-phase-space manifold  $T^*SO(3)$  with

$$\omega_H^{(sub)} = dp_\phi \wedge d\phi + dp_\psi \wedge d\psi + dp_\theta \wedge d\theta.$$

Analogously, on the velocity phase-space manifold  $TM$  exists:

- (i) A unique 1-form  $\theta_L$ , defined by the pull-back  $\theta_L = (\mathbb{F}L) * \theta_H$  of  $\theta_H$  by  $\mathbb{F}L$ . In local coordinates  $q^i, v^i = \dot{q}^i \in U_v$  ( $U_v$  open in  $TM$ ) it is given by  $\theta_L = L_{v^i} dq^i$ , where  $L_{v^i} \equiv \partial L / \partial v^i$ .
- (ii) A unique nondegenerate Lagrangian symplectic 2-form  $\omega_L$ , defined by the pull-back  $\omega_L = (\mathbb{F}L) * \omega_H$  of  $\omega_H$  by  $\mathbb{F}L$ , which is closed ( $d\omega_L = 0$ ) and exact ( $\omega_L = d\theta_L = dL_{v^i} \wedge dq^i$ ).

Both  $T^*M$  and  $TM$  are orientable manifolds, admitting the standard volumes given respectively by

$$\Omega_{\omega_H} = \frac{(-1)^{\frac{N(N+1)}{2}}}{N!} \omega_H^N, \quad \text{and} \quad \Omega_{\omega_L} = \frac{(-1)^{\frac{N(N+1)}{2}}}{N!} \omega_L^N,$$

in local coordinates  $q^i, p_i \in U_p$  ( $U_p$  open in  $T^*M$ ), resp.  $q^i, v^i = \dot{q}^i \in U_v$  ( $U_v$  open in  $TM$ ). They are given by

$$\begin{aligned} \Omega_H &= dq^1 \wedge \cdots \wedge dq^N \wedge dp_1 \wedge \cdots \wedge dp_N, \quad \text{and} \\ \Omega_L &= dq^1 \wedge \cdots \wedge dq^N \wedge dv^1 \wedge \cdots \wedge dv^N. \end{aligned}$$

On the velocity phase-space manifold  $TM$  we can also define the *action*  $A : TM \rightarrow \mathbb{R}$  by  $A(v) = \mathbb{F}L(v) \cdot v$  and the energy  $E = A - L$ . In local coordinates  $q^i, v^i = \dot{q}^i \in U_v$  ( $U_v$  open in  $TM$ ) we have  $A = v^i L_{v^i}$ , so  $E = v^i L_{v^i} - L$ . The Lagrangian vector-field  $X_L$  on  $TM$  is determined by the condition  $i_{X_L} \omega_L = dE$ . Classically, it is given by the second-order Lagrange equations

$$\frac{d}{dt} L_{v^i} = L_{q^i}. \quad (4.14)$$

The Hamiltonian vector-field  $X_H$  is defined on the momentum phase-space manifold  $T^*M$  by the condition  $i_{X_H} \omega = dH$ . The condition may be expressed equivalently as  $X_H = J \nabla H$ , where  $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$ .

In local canonical coordinates  $q^i, p_i \in U_p$  ( $U_p$  open in  $T^*M$ ) the vector-field  $X_H$  is classically given by the first-order Hamilton's canonical equations

$$\dot{q}^i = \partial_{p_i} H, \quad \dot{p}_i = -\partial_{q^i} H. \quad (4.15)$$

As a Lie group, the configuration manifold  $M$  is Hausdorff. Therefore for  $x = (q^i, p_i) \in U_p$  ( $U_p$  open in  $T^*M$ ) there exists a unique one-parameter group of diffeomorphisms  $\phi_t : T^*M \rightarrow T^*M$  such that  $\frac{d}{dt}|_{t=0} \phi_t x = J\nabla H(x)$ . This is termed *Hamiltonian phase-flow* and represents the maximal integral curve  $t \mapsto (q^i(t), p_i(t))$  of the Hamiltonian vector-field  $X_H$  passing through the point  $x$  for  $t = 0$ .

The flow  $\phi_t$  is *symplectic* if  $\omega_H$  is constant along it (that is,  $\phi_t^* \omega_H = \omega_H$ ) iff its Lie derivative vanishes (that is,  $\mathcal{L}_{X_H} \omega_H = 0$ ). A symplectic flow consists of canonical transformations on  $T^*M$ , that is, local diffeomorphisms that leave  $\omega_H$  invariant. By Liouville theorem, a symplectic flow  $\phi_t$  preserves the phase volume on  $T^*M$ . Also, the total energy  $H = E$  of the system is conserved along  $\phi_t$ , that is,  $H \circ \phi_t = H$ .

*Lagrangian flow* can be defined analogously (see [AM78, MR99]).

For a Lagrangian (resp. a Hamiltonian) vector-field  $X_L$  (resp.  $X_H$ ) on  $M$ , there is a base integral curve  $\gamma_0(t) = (q^i(t), v^i(t))$  (resp.  $\gamma_0(t) = (q^i(t), p_i(t))$ ) iff  $\gamma_0(t)$  is a geodesic. This is given by the contravariant velocity equation

$$\dot{q}^i = v^i, \quad \dot{v}^i + \Gamma_{jk}^i v^j v^k = 0, \quad (4.16)$$

in the former case, and by the covariant momentum equation

$$\dot{q}^k = g^{ki} p_i, \quad \dot{p}_i + \Gamma_{jk}^i g^{jl} g^{km} p_l p_m = 0, \quad (4.17)$$

in the latter. As before,  $\Gamma_{jk}^i$  denote the Christoffel symbols of an affine connection  $\nabla$  in an open chart  $U$  on  $M$ , defined by the Riemannian metric  $g = \langle, \rangle$  as:  $\Gamma_{jk}^i = g^{il} \Gamma_{jkl}$ ,  $\Gamma_{jkl} = \frac{1}{2} (\partial_{q^j} g_{kl} + \partial_{q^k} g_{jl} - \partial_{q^l} g_{jk})$ .

The l.h.s  $\dot{v}^i = \dot{v}^i + \Gamma_{jk}^i v^j v^k$  (resp.  $\dot{p}_i = \dot{p}_i + \Gamma_{jk}^i g^{jl} g^{km} p_l p_m$ ) in the second parts of (4.16) and (4.17) represent the *Bianchi covariant derivative* of the velocity (resp. momentum) with respect to  $t$ . Parallel transport on  $M$  is defined by  $\dot{v}^i = 0$ , (resp.  $\dot{p}_i = 0$ ). When this applies,  $X_L$  (resp.  $X_H$ ) is called the *geodesic spray* and its flow the *geodesic flow*.

For the dynamics in the gravitational potential field  $V : M \rightarrow \mathbb{R}$ , the Lagrangian  $L : TM \rightarrow \mathbb{R}$  (resp. the Hamiltonian  $H : T^*M \rightarrow \mathbb{R}$ ) has an extended form

$$L(v, q) = \frac{1}{2} g_{ij} v^i v^j - V(q),$$

$$\text{(resp. } H(p, q) = \frac{1}{2} g^{ij} p_i p_j + V(q)).$$

A Lagrangian vector-field  $X_L$  (resp. Hamiltonian vector-field  $X_H$ ) is still defined by the second-order Lagrangian equations (4.14, 4.16) (resp. first-order Hamiltonian equations (4.15, 4.17)).

The fibre derivative  $\mathbb{F}L : TM \rightarrow T^*M$  thus maps Lagrange's equations (4.14, 4.16) into Hamilton's equations (4.15, 4.17). Clearly there exists a diffeomorphism  $\mathbb{F}H : T^*M \rightarrow TM$ , such that  $\mathbb{F}L = (\mathbb{F}H)^{-1}$ . In local canonical coordinates  $q^i, p_i \in U_p$  ( $U_p$  open in  $T^*M$ ) this is given by  $(q^i, p_i) \mapsto (q^i, v^i)$

and thus maps Hamilton's equations (4.15, 4.17) into Lagrange's equations (4.14, 4.16).

A general form of the forced, non-conservative Hamilton's equations (resp. Lagrange's equations) is given as

$$\begin{aligned} \dot{q}^i &= \frac{\partial H}{\partial p_i}, & \dot{p}_i &= -\frac{\partial H}{\partial q^i} + F_i(t, q^i, p_i), \\ \text{(resp. } & \frac{d}{dt} \frac{\partial L}{\partial v^i} - \frac{\partial L}{\partial q^i} &= F_i(t, q^i, v^i)). \end{aligned}$$

Here the  $F_i(t, q^i, p_i)$  (resp.  $F_i(t, q^i, v^i)$ ) represent any kind of *covariant forces*, including dissipative and elastic joint forces, as well as actuator drives and control forces, as a function of time, coordinates and momenta. In covariant form we have

$$\begin{aligned} \dot{q}^k &= g^{ki} p_i, & \dot{p}_i &+ \Gamma_{jk}^i g^{jl} g^{km} p_l p_m = F_i(t, q^i, p_i), \\ \text{(resp. } & \dot{q}^i &= v^i, & \dot{v}^i + \Gamma_{jk}^i v^j v^k = g^{ij} F_j(t, q^i, v^i)). \quad \blacksquare \end{aligned}$$

This proves the existence of the unique natural geometric equivalence

$$\text{Dual}_G : \text{Lie} \cong \text{Can}$$

in the rotational biomechanics.

#### 4.4.2 Topological Duality Theorem for $M$

In this section we want to prove that the general biomechanics can be *equivalently* described in terms of two *topologically dual functors* **Lag** and **Ham**, from **Diff**, the *category of smooth manifolds* (and their smooth maps) of class  $C^p$ , into **Bund**, the *category of vector bundles* (and vector-bundle maps) of class  $C^{p-1}$ , with  $p \geq 1$ . **Lag** is physically represented by the second-order Lagrangian formalism on  $TM \in \text{Bund}$ , while **Ham** is physically represented by the first-order Hamiltonian formalism on  $T^*M \in \text{Bund}$ .

**Theorem.** There is a topological duality between Lagrangian and Hamiltonian formalisms on  $M$  (as given by Figure 2.1). In categorical terms, there is a unique natural topological equivalence

$$\text{Dual}_T : \text{Lag} \cong \text{Ham}$$

in the general biomechanics.

**Proof.** The proof has two parts: cohomological and homological.

#### Cohomological Proof

If  $\mathcal{C} = \mathcal{H}^\bullet \mathcal{M}$  (resp.  $\mathcal{C} = \mathcal{L}^\bullet \mathcal{M}$ ) represents the Abelian category of cochains on the momentum phase-space manifold  $T^*M$  (resp. the velocity phase-space

manifold  $TM$ ), we have the category  $\mathcal{S}^\bullet(\mathcal{H}^\bullet\mathcal{M})$  (resp.  $\mathcal{S}^\bullet(\mathcal{L}^\bullet\mathcal{M})$ ) of generalized cochain complexes  $A^\bullet$  in  $\mathcal{H}^\bullet\mathcal{M}$  (resp.  $\mathcal{L}^\bullet\mathcal{M}$ ) and if  $A^i = 0$  for  $i < 0$  we have a subcategory  $\mathcal{S}_{DR}^\bullet(\mathcal{H}^\bullet\mathcal{M})$  (resp.  $\mathcal{S}_{DR}^\bullet(\mathcal{L}^\bullet\mathcal{M})$ ) of De Rham differential complexes in  $\mathcal{S}^\bullet(\mathcal{H}^\bullet\mathcal{M})$  (resp.  $\mathcal{S}^\bullet(\mathcal{L}^\bullet\mathcal{M})$ )

$$\begin{aligned} A_{DR}^\bullet : 0 \rightarrow \Omega^0(T^*M) \xrightarrow{d} \Omega^1(T^*M) \xrightarrow{d} \\ \xrightarrow{d} \Omega^2(T^*M) \xrightarrow{d} \dots \xrightarrow{d} \Omega^N(T^*M) \xrightarrow{d} \dots \\ \text{(resp. } A_{DR}^\bullet : 0 \rightarrow \Omega^0(TM) \xrightarrow{d} \Omega^1(TM) \xrightarrow{d} \Omega^2(TM) \xrightarrow{d} \dots \\ \dots \xrightarrow{d} \Omega^N(TM) \xrightarrow{d} \dots), \end{aligned}$$

where  $A^N = \Omega^N(T^*M)$  (resp.  $A^N = \Omega^N(TM)$ ) is the vector space of all  $N$ -forms on  $T^*M$  (resp.  $TM$ ) over  $\mathbb{R}$ .

Let  $Z^N(T^*M) = \text{Ker}(d)$  (resp.  $Z^N(TM) = \text{Ker}(d)$ ) and  $B^N(T^*M) = \text{Im}(d)$  (resp.  $B^N(TM) = \text{Im}(d)$ ) denote respectively the real vector spaces of cocycles and coboundaries of degree  $N$ . Since  $d_{N+1}d_N = d^2 = 0$ , it follows that  $B^N(T^*M) \subset Z^N(T^*M)$  (resp.  $B^N(TM) \subset Z^N(TM)$ ). The quotient vector space

$$\begin{aligned} H_{DR}^N(T^*M) &= \text{Ker}(d)/\text{Im}(d) = Z^N(T^*M)/B^N(T^*M) \\ \text{(resp. } H_{DR}^N(TM) &= \text{Ker}(d)/\text{Im}(d) = Z^N(TM)/B^N(TM)), \end{aligned}$$

we refer to as the De Rham cohomology group (vector space) of  $T^*M$  (resp.  $TM$ ). The elements of  $H_{DR}^N(T^*M)$  (resp.  $H_{DR}^N(TM)$ ) are equivalence sets of cocycles. Two cocycles  $\omega_1$  and  $\omega_2$  are cohomologous, or belong to the same equivalence set (written  $\omega_1 \sim \omega_2$ ) iff they differ by a coboundary  $\omega_1 - \omega_2 = d\theta$ . Any form  $\omega_H \in \Omega^N(T^*M)$  (resp.  $\omega_L \in \Omega^N(TM)$ ) has a De Rham cohomology class  $[\omega_H] \in H_{DR}^N(T^*M)$  (resp.  $[\omega_L] \in H_{DR}^N(TM)$ ).

Hamiltonian symplectic form  $\omega_H = dp_i \wedge dq_i$  on  $T^*M$  (resp. Lagrangian symplectic form  $\omega_L = dL_{v^i} \wedge dq^i$  on  $TM$ ) is by definition both a closed 2-form or two-cocycle and an exact 2-form or two-coboundary. Therefore the 2D-De Rham cohomology group of human motion is defined as a quotient vector space

$$\begin{aligned} H_{DR}^2(T^*M) &= Z^2(T^*M)/B^2(T^*M) \\ \text{(resp. } H_{DR}^2(TM) &= Z^2(TM)/B^2(TM)). \end{aligned}$$

As  $T^*M$  (resp.  $TM$ ) is a compact Hamiltonian symplectic (resp. Lagrangian symplectic) manifold of dimension  $2N$ , it follows that  $\omega_H^N$  (resp.  $\omega_L^N$ ) is a volume element on  $T^*M$  (resp.  $TM$ ), and the  $2N$ D de Rham's cohomology class  $[\omega_H^N] \in H_{DR}^{2N}(T^*M)$  (resp.  $[\omega_L^N] \in H_{DR}^{2N}(TM)$ ) is nonzero. Since  $[\omega_H^N] = [\omega_H]^N$  (resp.  $[\omega_L^N] = [\omega_L]^N$ ), then  $[\omega_H] \in H_{DR}^2(T^*M)$  (resp.  $[\omega_L] \in H_{DR}^2(TM)$ ) and all of its powers up to the  $N$ -th must be zero as well. The existence of such an element is a necessary condition for  $T^*M$  (resp.  $TM$ ) to admit a Hamiltonian symplectic structure  $\omega_H$  (resp. Lagrangian symplectic structure  $\omega_L$ ).

The De Rham complex  $A_{DR}^\bullet$  on  $T^*M$  (resp.  $TM$ ) can be considered as a system of second-order ODEs  $d^2\theta_H = 0$ ,  $\theta_H \in \Omega^N(T^*M)$  (resp.  $d^2\theta_L = 0$ ,  $\theta_L \in \Omega^N(TM)$ ) having a solution represented by  $Z^N(T^*M)$  (resp.  $Z^N(TM)$ ). In local coordinates  $q^i$ ,  $p_i \in U_p$  ( $U_p$  open in  $T^*M$ ) (resp.  $q^i$ ,  $v^i \in U_v$  ( $U_v$  open in  $TM$ )) we have  $d^2\theta_H = d^2(p_i dq^i) = d(dp_i \wedge dq^i) = 0$ , (resp.  $d^2\theta_L = d^2(L_{v^i} dq^i) = d(dL_{v^i} \wedge dq^i) = 0$ ). ■

### Homological Proof

If  $\mathcal{C} = \mathcal{H}_\bullet\mathcal{M}$ , (resp.  $\mathcal{C} = \mathcal{L}_\bullet\mathcal{M}$ ) represents an Abelian category of chains on  $T^*M$  (resp.  $TM$ ), we have a category  $\mathcal{S}_\bullet(\mathcal{H}_\bullet\mathcal{M})$  (resp.  $\mathcal{S}_\bullet(\mathcal{L}_\bullet\mathcal{M})$ ) of generalized chain complexes  $\mathcal{A}_\bullet$  in  $\mathcal{H}_\bullet\mathcal{M}$  (resp.  $\mathcal{L}_\bullet\mathcal{M}$ ), and if  $A = 0$  for  $n < 0$  we have a subcategory  $\mathcal{S}_\bullet^C(\mathcal{H}_\bullet\mathcal{M})$  (resp.  $\mathcal{S}_\bullet^C(\mathcal{L}_\bullet\mathcal{M})$ ) of chain complexes in  $\mathcal{H}_\bullet\mathcal{M}$  (resp.  $\mathcal{L}_\bullet\mathcal{M}$ )

$$\begin{aligned} \mathcal{A}_\bullet : 0 \leftarrow C^0(T^*M) \xleftarrow{\partial} C^1(T^*M) \xleftarrow{\partial} C^2(T^*M) \xleftarrow{\partial} \dots \\ \dots \xleftarrow{\partial} C^m(T^*M) \xleftarrow{\partial} \dots \\ \text{(resp. } \mathcal{A}_\bullet : 0 \leftarrow C^0(TM) \xleftarrow{\partial} C^1(TM) \xleftarrow{\partial} C^2(TM) \xleftarrow{\partial} \dots \\ \dots \xleftarrow{\partial} C^m(TM) \xleftarrow{\partial} \dots). \end{aligned}$$

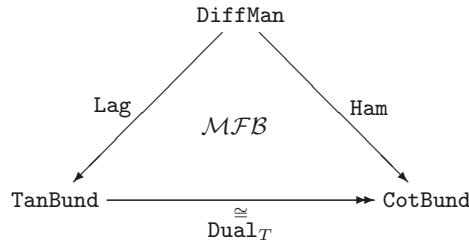
Here  $A_N = C^N(T^*M)$  (resp.  $A_N = C^N(TM)$ ) is the vector space of all finite chains  $C$  on  $T^*M$  (resp.  $TM$ ) over  $\mathbb{R}$ , and  $\partial_N = \partial : C^{N+1}(T^*M) \rightarrow C^N(T^*M)$  (resp.  $\partial_N = \partial : C^{N+1}(TM) \rightarrow C^N(TM)$ ). A finite chain  $C$  such that  $\partial C = 0$  is an  $N$ -cycle. A finite chain  $C$  such that  $C = \partial B$  is an  $N$ -boundary. Let  $Z_N(T^*M) = \text{Ker}(\partial)$  (resp.  $Z_N(TM) = \text{Ker}(\partial)$ ) and  $B_N(T^*M) = \text{Im}(\partial)$  (resp.  $B_N(TM) = \text{Im}(\partial)$ ) denote respectively real vector spaces of cycles and boundaries of degree  $N$ . Since  $\partial_{N-1}\partial_N = \partial^2 = 0$ , then  $B_N(T^*M) \subset Z_N(T^*M)$  (resp.  $B_N(TM) \subset Z_N(TM)$ ). The quotient vector space

$$\begin{aligned} H_N^C(T^*M) = Z_N(T^*M)/B_N(T^*M) \\ \text{(resp. } H_N^C(TM) = Z_N(TM)/B_N(TM)) \end{aligned}$$

represents an  $ND$  biomechanics homology group (vector space). The elements of  $H_N^C(T^*M)$  (resp.  $H_N^C(TM)$ ) are equivalence sets of cycles. Two cycles  $C_1$  and  $C_2$  are homologous, or belong to the same equivalence set (written  $C_1 \sim C_2$ ) iff they differ by a boundary  $C_1 - C_2 = \partial B$ . The homology class of a finite chain  $C \in C^N(T^*M)$  (resp.  $C \in C^N(TM)$ ) is  $[C] \in H_N^C(T^*M)$  (resp.  $[C] \in H_N^C(TM)$ ). ■

#### 4.4.3 Lagrangian Versus Hamiltonian Duality

In this way, we have proved a commutativity of a triangle:



which implies the existence of the unique natural topological equivalence

$$\text{Dual}_T : \text{Lag} \cong \text{Ham}$$

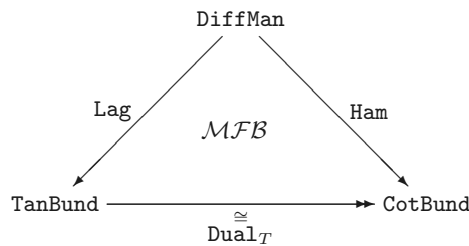
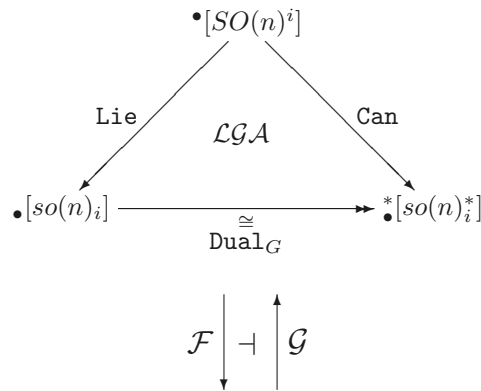
in the rotational biomechanics.

#### 4.4.4 Globally Dual Structure of Rotational Biomechanics

**Theorem.** Global dual structure of the rotational biomechanics is defined by the unique natural equivalence

$$\text{Dyn} : \text{Dual}_G \cong \text{Dual}_T.$$

**Proof.** This unique functorial relation, uncovering the natural equivalence between *geometric* and *topological* structures of biomechanics:



– has been established by parallel development of Lagrangian and Hamiltonian biomechanics formulations, i.e., functors  $\text{Lag}(\text{Lie})$  and  $\text{Ham}(\text{Can})$ .

## Nonlinear Control in Human–Like Biomechanics

In this Chapter we develop the basics of nonlinear control theory as is used in modern human–like biomechanics. It includes control variations on the central theme of our *covariant force law*,  $F_i = mg_{ij}a^j$ , and its associated *covariant force functor*  $\mathcal{F}_* : TT^*M \rightarrow TTM$  (see section 2.7 above).

### 5.1 The Basics of Classical Control and Stability

In this section we present the basics of classical control and stability theory, to be used in the subsequent sections.

#### 5.1.1 Brief Introduction into Feedback Control

The *basic formula of feedback control* reads

$$\textit{Sensing} + \textit{Computation} + \textit{Actuation} = \textit{Feedback Control} \quad (5.1)$$

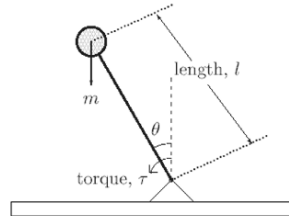
The formula (5.1) implies the *basic premise of control engineering*:

- Given a *system* to be controlled and the specifications of its *desired behavior*, construct a *feedback control law* to make the closed–loop system display its desired behavior.

The three basic goals of feedback control are (see [Mur97]):

1. *Stability*, which states that bounded inputs produce bounded outputs;
2. *Performance*, which defines how to achieve desired response; and
3. *Robustness*, which balances stability versus performance in the presence of unknown dynamics.

For example, consider the popular problem of stabilization of an *inverted pendulum* (see Figure 5.1), in which dynamics is governed by the Newtonian–like equation



**Fig. 5.1.** An inverted pendulum (see text for explanation).

$$J\ddot{\theta} - mgl \sin \theta = \tau,$$

and we want to start from a large angle, say  $\theta(0) = 60^\circ$  and move to the vertical upright position,  $\theta = 0$ .

One choice of a stabilizer is (see [Wil00])

$$\tau = -k_d\dot{\theta} - k_p\theta - mgl \sin \theta,$$

where  $\tau$  is the stabilizing torque, while  $k_d$  and  $k_p$  are positive constants. In this case closed loop dynamics is given by

$$J\ddot{\theta} + k_d\dot{\theta} + k_p\theta = 0,$$

which is globally stable and linear.

An alternative controller is given by

$$\tau = -k_d\dot{\theta} - 2mgl \sin \theta,$$

leading to the globally stable nonlinear closed-loop dynamics

$$J\ddot{\theta} + k_d\dot{\theta} + mgl \sin \theta = 0.$$

This example shows how the feedback and feedforward control amounts to modifying the dynamics of the plant into a desired form. It is further expanded as a difficult nonholonomic problem of a unicycle (5.2.2) below.

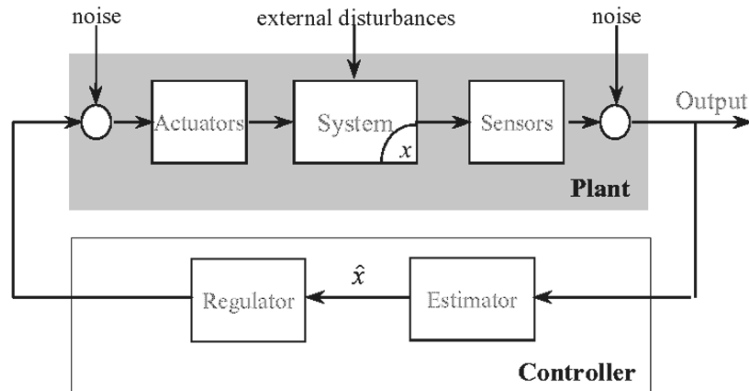
To summarize, the basic components of a feedback control system are (see Figure 5.2):

1. Plant, including (bio)physical system, actuation and sensing;
2. Controller, including state estimator and regulator; and
3. Feedback, including interconnection between plant output and controller input.

Control systems are usually represented using:

- Linear or nonlinear ODEs; and
- Block diagrams with transfer functions (Laplace transform based).

Historically, four periods can be distinguished in control theory (see [Mur97]):



**Fig. 5.2.** The basic components of a feedback control system (see text for explanation).

1. Classical control (1940–1960). This period is characterized by:
  - Frequency domain based tools; stability via gain and phase margins;
  - Mainly useful for single-input, single-output (SISO) systems;
  - Control is one of the main tools for the practicing engineer.
2. Modern control (1940–1960). In this period:
  - The so-called *state-space approach* was developed for linear control theory;
  - It works both for SISO and multi-input, multi-output (MIMO) systems;
  - Performance and robustness measures are often not made explicit.
3. Post-modern control (1940–1960). This period:
  - Generalizes ideas in classical control to MIMO context; and
  - Uses operator theory at its core, but can be easily interpreted in frequency domain.
4. Nonlinear control (1990–). This period is characterized by specialized techniques for control of nonlinear plants.

Now, as already stated, the *goal of a control system* is to enhance automation within a system while providing improved performance and robustness. For instance, we may develop a *cruise control system* for an automobile to release drivers from the tedious task of speed regulation while they are on long trips. In this case, the *output* of the *plant* is the sensed vehicle speed,  $y$ , and the *input* to the plant is the throttle angle,  $u$ . Typically, control systems are designed so that the *plant output follows some reference input* (the driver-specified speed in the case of our cruise control example) while achieving some level of *disturbance rejection*. For the cruise control problem, a disturbance would be a road grade variation or wind. Clearly we would want our

cruise controller to reduce the effects of such disturbances on the quality of the speed regulation that is achieved [SMO02].

In the area of *robust control* the focus is on the development of controllers that can maintain good performance even if we only have a poor model of the plant or if there are some plant parameter variations. In the area, of *adaptive control*, to reduce the effects of plant parameter variations, robustness is achieved by adjusting (i.e., adapting) the controller on-line. For instance, an adaptive controller for the cruise control problem would seek to achieve good speed tracking performance even if we do not have a good model of the vehicle and engine dynamics, or if the vehicle dynamics change over time (e.g., via a weight change that results from the addition of cargo, or due to engine degradation over time). At the same time it would try to achieve good disturbance rejection. Clearly, the performance of a good cruise controller should not degrade significantly as your automobile ages or if there are reasonable changes in the load the vehicle is carrying [SMO02].

We use *adaptive mechanisms* within the control laws when certain *parameters* within the plant dynamics are *unknown*. An adaptive controller is used to improve the closed-loop system robustness while meeting a set of performance objectives. If the plant uncertainty cannot be expressed in terms of unknown parameters, one may be able to reformulate the problem by expressing the uncertainty in terms of a *fuzzy system*, *neural network*, or some other *parameterized nonlinear system*, like an *adaptive Lie-derivative controller*. The uncertainty then becomes recast in terms of a new set of unknown parameters that may be adjusted using adaptive techniques.

When developing a *robust control design*, the focus is on *maintaining stability* even in the presence of *unmodelled plant dynamics* or *external disturbances*. The approach in robust control is to accept *a priori* that there will be model uncertainty, and try to cope with it.

The issue of robustness has been studied extensively in the control literature [SMO02]. When working with linear systems, one may define phase and gain margins which quantify the range of uncertainty a closed-loop system may withstand before becoming unstable. In the world of *nonlinear control design*, we often investigate the stability of a closed-loop system by studying the behavior of a *Lyapunov function candidate*. The Lyapunov function candidate is a mathematical function designed to provide a simplified measure of the control objectives allowing complex nonlinear systems to be analyzed using a scalar differential equation. When a controller is designed that drives the Lyapunov function to zero, the control objectives are met. If some system uncertainty tends to drive the Lyapunov candidate away from zero, we often simply add an additional stabilizing term to the control algorithm that dominates the effect of the uncertainty, thereby making the closed-loop system more robust.

Now, by adding a static term in the control law that simply dominates the plant uncertainty, it is often easy to simply stabilize an uncertain plant, however, driving the system error to zero may be difficult if not impossible.

Consider the case when the plant is defined by [SMO02]

$$\dot{x} = \theta x + u, \quad (5.2)$$

where  $x \in \mathbb{R}$  is the plant state that we wish to drive to the point  $x = 1$ ,  $u \in \mathbb{R}$  is the plant input, and  $\theta$  is an unknown constant. Since  $\theta$  is unknown, one may not define a static controller that causes  $x = 1$  to be a stable equilibrium point. In order for  $x = 1$  to be a stable equilibrium point, it is necessary that  $\dot{x} = 0$  when  $x = 1$ , so  $u(x) = -\theta$  when  $x = 1$ . Since  $\theta$  is unknown, however, we may not define such a controller. In this case, the best that a static nonlinear controller may do is to keep  $x$  bounded in some region around  $x = 1$ . If dynamics are included in the nonlinear controller, then it turns out that one may define a control system that does drive  $x \rightarrow 1$  even if  $\theta$  is unknown.

On the other hand, an adaptive controller can be designed so that it estimates some uncertainty within the system, then automatically designs a controller for the estimated plant uncertainty. In this way the control system uses information gathered on-line to reduce the model uncertainty, that is, to figure out exactly what the plant is at the current time so that good control can be achieved. Considering the system defined by (A.19), an adaptive controller may be defined so that an *estimate* of  $\theta$  is generated, which we denote by  $\hat{\theta}$ . If  $\theta$  were known, then including a term  $-\theta x$  in the control law would cancel the effects of the uncertainty. If  $\hat{\theta} \rightarrow \theta$  over time, then including the term  $-\hat{\theta}x$  in the control law would also cancel the effects of the uncertainty over time. This approach is referred to as *indirect adaptive control* [SMO02].

An indirect approach to adaptive control is made up of an *approximator* (often referred to as an *identifier* in the adaptive control literature) that is used to estimate unknown plant parameters and a certainty equivalence control scheme in which the plant controller is designed, assuming that the parameter estimates are their true values. Here the adjustable approximator is used to model some component of the system. Since the approximation is used in the control law, it is possible to determine if we have a good estimate of the plant dynamics. If the approximation is good (i.e., we know how the plant should behave), then it is easy to meet our control objectives. If, on the other hand, the plant output moves in the wrong direction, then we may assume that our estimate is incorrect and should be adjusted accordingly.

As an example of an indirect adaptive controller, consider the cruise control problem where we have an approximator that is used to estimate the vehicle mass and aerodynamic drag. Assume that the vehicle dynamics may be approximated by

$$m\dot{x} = -\rho x^2 + u,$$

where  $m$  is the vehicle mass,  $\rho$  is the coefficient of aerodynamic drag,  $x$  is the vehicle velocity, and  $u$  is the plant input. Assume that an approximator has been defined so that estimates of the mass and drag are found such that  $\hat{m} \rightarrow m$  and  $\hat{\rho} \rightarrow \rho$ . Then the control law

$$u = \hat{\rho}x^2 + \hat{m}v(t)$$

may be used so that  $\dot{x} = v(t)$  when  $\hat{m} = m$  and  $\hat{\rho} = \rho$ . Here  $v(t)$  may be considered a new control input that is defined to drive  $x$  to any desired value [SMO02].

### 5.1.2 Linear Stationary Systems and Operators

#### Basics of Kalman State-Space Theory

It is well-known that linear multiple input-multiple output (MIMO) control systems can always be put into Kalman canonical state-space form of order  $n$ , with  $m$  inputs and  $k$  outputs. In the case of *continual time systems* we have the state and output equations of the form<sup>1</sup>

$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{A}(t) \mathbf{x}(t) + \mathbf{B}(t) \mathbf{u}(t), \\ \mathbf{y}(t) &= \mathbf{C}(t) \mathbf{x}(t) + \mathbf{D}(t) \mathbf{u}(t),\end{aligned}\tag{5.3}$$

while in case of *discrete time systems* we have the state and output equations of the form

$$\begin{aligned}\mathbf{x}(n+1) &= \mathbf{A}(n) \mathbf{x}(n) + \mathbf{B}(n) \mathbf{u}(n), \\ \mathbf{y}(n) &= \mathbf{C}(n) \mathbf{x}(n) + \mathbf{D}(n) \mathbf{u}(n).\end{aligned}\tag{5.4}$$

Both in (5.3) and in (5.4) the variables have the following meaning:

$\mathbf{x}(t) \in \mathbb{X}$  is an  $n$ -vector of *state variables* belonging to the *state space*  $\mathbb{X} \subset \mathbb{R}^n$ ;

$\mathbf{u}(t) \in \mathbb{U}$  is an  $m$ -vector of *inputs* belonging to the *input space*  $\mathbb{U} \subset \mathbb{R}^m$ ;

$\mathbf{y}(t) \in \mathbb{Y}$  is a  $k$ -vector of *outputs* belonging to the *output space*  $\mathbb{Y} \subset \mathbb{R}^k$ ;

$\mathbf{A}(t) : \mathbb{X} \rightarrow \mathbb{X}$  is an  $n \times n$  matrix of *state dynamics*;

$\mathbf{B}(t) : \mathbb{U} \rightarrow \mathbb{X}$  is an  $n \times m$  matrix of *input map*;

$\mathbf{C}(t) : \mathbb{X} \rightarrow \mathbb{Y}$  is an  $k \times n$  matrix of *output map*;

$\mathbf{D}(t) : \mathbb{U} \rightarrow \mathbb{Y}$  is an  $k \times m$  matrix of *input-output transform*.

Input  $\mathbf{u}(t) \in \mathbb{U}$  can be empirically determined by trial and error; it is properly defined by optimization process called *Kalman regulator*, or more generally (in the presence of noise), by *Kalman filter* (even better, *extended Kalman filter* to deal with stochastic nonlinearities) [Kal60].

Now, the most common special case of the general Kalman model (5.3), with constant state, input and output matrices (and relaxed boldface vector-matrix notation), is the so-called *stationary linear model*. Such systems frequently serve as a baseline, against which other control systems are measured.

<sup>1</sup> In our covariant form, (5.4) reads

$$\dot{x}^i = a_j^i x^j + b_k^i u^k, \quad y^i = c_j^i x^j + d_k^i u^k, \quad (i, j = 1, \dots, n; k = 1, \dots, m).$$

We follow a common notational convention and let  $u$  denote the vector of *inputs*,  $y$  the vector of *outputs* and assume that they can be related through an intermediary *state* variable  $x$  according to the equations

$$\dot{x} = Ax + Bu, \quad y = Cx. \quad (5.5)$$

We refer to this as the deterministic *stationary linear model*. The stationary linear system (5.5) defines a variety of operators, in particular those related to: (i) regulators, (ii) end point controls, (iii) servomechanisms, and (iv) repetitive modes (see [Bro01]).

### Regulator Problem and the Steady State Operator

Consider a variable, or set of variables, associated with a dynamical system. They are to be maintained at some desired values in the face of changing circumstances. There exist a second set of parameters that can be adjusted so as to achieve the desired regulation. The effecting variables are usually called *inputs* and the affected variables called *outputs*. Specific examples include the regulation of the thrust of a jet engine by controlling the flow of fuel, as well as the regulation of the oxygen content of the blood using the respiratory rate.

Now, there is the steady state operator of particular relevance for the regulator problem. It is

$$y_\infty = -CA^{-1}Bu_\infty,$$

which describes the map from constant values of  $u$  to the equilibrium value of  $y$ . It is defined whenever  $A$  is invertible but the steady state value will only be achieved by a real system if, in addition, the eigenvalues of  $A$  have negative real parts. Only when the rank of  $CA^{-1}B$  equals the dimension of  $y$  can we steer  $y$  to an arbitrary steady state value and hold it there with a constant  $u$ . A nonlinear version of this problem plays a central role in robotics where it is called the *inverse kinematics problem* (see, e.g., [MLS94]).

### End Point Control Problem and the Adjustment Operator

Here we have inputs, outputs and trajectories. In this case the shape of the trajectory is not of great concern but rather it is the end point that is of primary importance. Standard examples include rendezvous problems such as one has in space exploration.

Now, the operator of relevance for the end point control problem, is the operator

$$x(T) = \int_0^T \exp[A(T - \sigma)] Bu(\sigma) d\sigma.$$

If we consider this to define a map from the  $m$ D  $L_2$  space  $L_2^m[0, T]$  (where  $u$  takes on its values) into  $\mathbb{R}^m$  then, if it is an onto map, it has a Moore–Penrose (least squares) inverse

$$u(\sigma) = B^T \exp[A^T(T - \sigma)] (W[0, T])^{-1} (x(T) - \exp(AT) x(0)),$$

with the symmetric positive definite matrix  $W$ , the *controllability Gramian*, being given by

$$W[0, T] = \int_0^T \exp[A(T - \sigma)] BB^T \exp[A^T(T - \sigma)] d\sigma.$$

### Servomechanism Problem and the Corresponding Operator

Here we have inputs, outputs and trajectories, as above, and an associated dynamical system. In this case, however, it is desired to cause the outputs to follow a trajectory specified by the input. For example, the control of an airplane so that it will travel along the flight path specified by the flight controller.

Now, because we have assumed that  $A$ ,  $B$  and  $C$  are constant

$$y(t) = C \exp(At) x(0) + \int_0^t C \exp[A(T - \tau)] Bu(\tau) d\tau,$$

and, as usual, the *Laplace transform*  $\mathcal{L}$ , defined as a pair of inverse maps  $\mathcal{L} = \{F, f\} : \mathbb{R} \rightleftharpoons \mathbb{C}$ ,

$$F(s) = \{\mathcal{L}f(t)\}(s) = \int_0^\infty e^{-st} f(t) dt, \quad (t \in \mathbb{R}, s \in \mathbb{C})$$

$$f(t) = \{\mathcal{L}^{-1}F(s)\}(t) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{st} F(s) ds,$$

– can be used to convert convolution to multiplication. This brings out the significance of the Laplace transform pair

$$C \exp(At) B \xleftrightarrow{\mathcal{L}} C(Is - A)^{-1} B \quad (5.6)$$

as a means of characterizing the input–output map of a linear model with constant coefficients.

### Repetitive Mode Problem and the Corresponding Operator

Here again one has some variable, or set of variables, associated with a dynamical system and some inputs which influence its evolution. The task has elements which are repetitive and are to be done efficiently. Examples from biology include the control of respiratory processes, control of the pumping action of the heart, control of successive trials in practicing an athletic event.

The relevant operator is similar to the servomechanism operator, however the constraint that  $u$  and  $x$  are periodic means that the relevant diagonalization is provided by Fourier series, rather than the Laplace transform. Thus, in the Fourier domain, we are interested in a set of complex matrices

$$G(iw_i) = C(iw_i - A)^{-1}B, \quad (w_i = 0, w_0, 2w_0, \dots)$$

More general, but still deterministic, models of the input–state–output relation are afforded by the *nonlinear affine control system* (see, e.g., [Isi89])

$$\dot{x}(t) = f(x(t)) + g(x(t))u(t), \quad y(t) = h(x(t));$$

and the still more general *fully nonlinear control system*

$$\dot{x}(t) = f(x(t), u(t)), \quad y(t) = h(x(t)).$$

### Feedback Changes the Operator

No idea is more central to automatic control than the idea of feedback. When an input is altered on the basis of the difference between the actual output of the system and the desired output, the system is said to involve *feedback*. Man made systems are often constructed by starting with a basic element such as a motor, a burner, a grinder, etc. and then adding sensors and the hardware necessary to use the measurement generated by the sensors to regulate the performance of the basic element. This is the *essence of feedback control*. Feedback is often contrasted with open loop systems in which the inputs to the basic element is determined without reference to any measurement of the trajectories. When the word feedback is used to describe naturally occurring systems, it is usually implicit that the behavior of the system can best be explained by pretending that it was designed as one sees man made systems being designed [Bro01].

In the context of linear systems, the effect of feedback is easily described. If we start with the stationary linear system (5.5) with  $u$  being the controls and  $y$  being the measured quantities, then the effect of feedback is to replace  $u$  by  $u - Ky$  with  $K$  being a matrix of feedback gains. The closed–loop equations are then

$$\dot{x} = (A - BKC)x + Bu, \quad y = Cx.$$

Expressed in terms of the Laplace transform pairs (5.6), feedback effects the transformation

$$(C \exp(At)B; C(Is - A)^{-1}B) \mapsto C \exp(A - BKC)^t B; C(Is - A + BKC)^{-1}B.$$

Using such a transformation, it is possible to alter the dynamics of a system in a significant way. The modifications one can effect by feedback include influencing the location of the eigenvalues and consequently the stability of the system. In fact, if  $K$  is  $m$  by  $p$  and if we wish to select a gain matrix  $K$  so that  $A - BKC$  has eigenvalues  $\lambda_1, \lambda_2, \dots, \lambda_n$ , it is necessary to insure that

$$\det \begin{pmatrix} C(I\lambda_i - A)^{-1}B & -I \\ I & K \end{pmatrix} = 0, \quad (i = 1, 2, \dots, n).$$

Now, if  $CB$  is invertible then we can use the relationship  $C\dot{x} = CAx + CBu$  together with  $y = Cx$  to write  $\dot{y} = CAx + CBu$ . This lets us solve for  $u$  and recast the system as

$$\begin{aligned}\dot{x} &= (A - B(CB)^{-1}CA)x + B(CB)^{-1}\dot{y}, \\ u &= (CB)^{-1}\dot{y} - (CB)^{-1}CAx.\end{aligned}$$

Here we have a set of equations in which the roles of  $u$  and  $y$  are reversed. They show how a choice of  $y$  determines  $x$  and how  $x$  determines  $u$  [Bro01].

### 5.1.3 Stability and Boundedness

Let a time-varying dynamical system may be expressed as

$$\dot{x}(t) = f(t, x(t)), \quad (5.7)$$

where  $x \in \mathbb{R}^n$  is an  $n$ D vector and  $f : \mathbb{R}^+ \times D \rightarrow \mathbb{R}^n$  with  $D = \mathbb{R}^n$  or  $D = B_h$  for some  $h > 0$ , where  $B_h = \{x \in \mathbb{R}^n : |x| < h\}$  is a ball centered at the origin with a radius of  $h$ . If  $D = \mathbb{R}^n$  then we say that the dynamics of the system are defined *globally*, whereas if  $D = B_h$  they are only defined *locally*. We do not consider systems whose dynamics are defined over disjoint subspaces of  $\mathbb{R}^n$ . It is assumed that  $f(t, x)$  is piecemeal continuous in  $t$  and Lipschitz in  $x$  for existence and uniqueness of state solutions. As an example, the linear system  $\dot{x}(t) = Ax(t)$  fits the form of (5.7) with  $D = \mathbb{R}^n$  [SMO02].

Assume that for every  $x_0$  the initial value problem

$$\dot{x}(t) = f(t, x(t)), \quad x(t_0) = x_0,$$

possesses a unique solution  $x(t, t_0, x_0)$ ; it is called a solution to (5.7) if  $x(t, t_0, x_0) = x_0$  and  $\frac{d}{dt}x(t, t_0, x_0) = f(t, x(t, t_0, x_0))$  [SMO02].

A point  $x_e \in \mathbb{R}^n$  is called an *equilibrium point* of (5.7) if  $f(t, x_e) = 0$  for all  $t \geq 0$ . An equilibrium point  $x_e$  is called an *isolated equilibrium point* if there exists an  $\rho > 0$  such that the ball around  $x_e$ ,  $B_\rho(x_e) = \{x \in \mathbb{R}^n : |x - x_e| < \rho\}$ , contains no other equilibrium points besides  $x_e$  [SMO02].

The equilibrium  $x_e = 0$  of (5.7) is said to be *stable in the sense of Lyapunov* if for every  $\epsilon > 0$  and any  $t_0 \geq 0$  there exists a  $\delta(\epsilon, t_0) > 0$  such that  $|x(t, t_0, x_0)| < \epsilon$  for all  $t \geq t_0$  whenever  $|x_0| < \delta(\epsilon, t_0)$  and  $x(t, t_0, x_0) \in B_h(x_e)$  for some  $h > 0$ . That is, the equilibrium is stable if when the system (5.7) starts close to  $x_e$ , then it will stay close to it. Note that stability is a property of an equilibrium, not a system. A system is stable if all its equilibrium points are stable. Stability in the sense of Lyapunov is a local property. Also, notice that the definition of stability is for a single equilibrium  $x_e \in \mathbb{R}^n$  but actually such an equilibrium is a trajectory of points that satisfy the differential equation in (5.7). That is, the equilibrium  $x_e$  is a solution to the differential equation (5.7),  $x(t, t_0, x_0) = x_e$  for  $t \geq 0$ . We call any set such that when the initial condition of (5.7) starts in the set and stays in the set for all  $t \geq 0$ ,

an *invariant set*. As an example, if  $x_e = 0$  is an equilibrium, then the set containing only the point  $x_e$  is an invariant set, for (5.7) [SMO02].

If  $\delta$  is independent of  $t_0$ , that is, if  $\delta = \delta(\epsilon)$ , then the equilibrium  $x_e$  is said to be *uniformly stable*. If in (5.7)  $f$  does not depend on time (i.e.,  $f(x)$ ), then  $x_e$  being stable is equivalent to it being uniformly stable. Uniform stability is also a local property.

The equilibrium  $x_e = 0$  of (5.7) is said to be *asymptotically stable* if it is stable and for every  $t_0 \geq 0$  there exists  $\eta(t_0) > 0$  such that  $\lim_{t \rightarrow \infty} |x(t, t_0, x_0)| = 0$  whenever  $|x_0| < \eta(t_0)$ . That is, it is asymptotically stable if when it starts close to the equilibrium it will converge to it. Asymptotic stability is also a local property. It is a stronger stability property since it requires that the solutions to the ordinary differential equation converge to zero in addition to what is required for stability in the sense of Lyapunov.

The equilibrium  $x_e = 0$  of (5.7) is said to be *uniformly asymptotically stable* if it is uniformly stable and for every  $\epsilon > 0$  and  $t_0 \geq 0$ , there exist a  $\delta_0 > 0$  independent of  $t_0$  and  $\epsilon$ , and a  $T(\epsilon) > 0$  independent of  $t_0$ , such that  $|x(t, t_0, x_0) - x_e| \leq \epsilon$  for all  $t \geq t_0 + T(\epsilon)$  whenever  $|x_0 - x_e| < \delta_0$ . Again, if in (5.7)  $f$  does not depend on time (i.e.,  $f(x)$ ), then  $x_e$  being asymptotically stable is equivalent to it being uniformly asymptotically stable. Uniform asymptotic stability is also a local property.

The set  $X_d \subset \mathbb{R}^n$  of all  $x_0 \in \mathbb{R}^n$  such that  $|x(t, t_0, x_0)| \rightarrow 0$  as  $t \rightarrow \infty$  is called the *domain of attraction* of the equilibrium  $x_e = 0$  of (5.7). The equilibrium  $x_e = 0$  is said to be *asymptotically stable in the large* if  $X_d \subset \mathbb{R}^n$ . That is, an equilibrium is asymptotically stable in the large if no matter where the system starts, its state converges to the equilibrium asymptotically. This is a global property as opposed to the earlier stability definitions that characterized local properties. This means that for asymptotic stability in the large, the local property of asymptotic stability holds for  $B_h(x_e)$  with  $h = \infty$  (i.e., on the whole state-space).

The equilibrium  $x_e = 0$  is said to be *exponentially stable* if there exists an  $\alpha > 0$  and for every  $\epsilon > 0$  there exists a  $\delta(\epsilon) > 0$  such that  $|x(t, t_0, x_0)| \leq \epsilon e^{-\alpha(t-t_0)}$ , whenever  $|x_0| < \delta(\epsilon)$  and  $t \geq t_0 \geq 0$ . The constant  $\alpha$  is sometimes called the *rate of convergence*. Exponential stability is sometimes said to be a ‘stronger’ form of stability since in its presence we know that system trajectories decrease exponentially to zero. It is a local property; here is its global version. The equilibrium point  $x_e = 0$  is *exponentially stable in the large* if there exists  $\alpha > 0$  and for any  $\beta > 0$  there exists  $\epsilon(\beta) > 0$  such that  $|x(t, t_0, x_0)| \leq \epsilon(\beta)e^{-\alpha(t-t_0)}$ , whenever  $|x_0| < \beta$  and  $t \geq t_0 \geq 0$ .

An equilibrium that is not stable is called *unstable*.

Closely related to stability is the concept of *boundedness*, which is, however, a global property of a system in the sense that it applies to trajectories (solutions) of the system that can be defined over all of the state-space [SMO02].

A solution  $x(t, t_0, x_0)$  of (5.7) is *bounded* if there exists a  $\beta > 0$ , that may depend on each solution, such that  $|x(t, t_0, x_0)| < \beta$  for all  $t \geq t_0 \geq 0$ . A

system is said to possess *Lagrange stability* if for each  $t_0 \geq 0$  and  $x_0 \in \mathbb{R}^n$ , the solution  $x(t, t_0, x_0)$  is bounded. If an equilibrium is asymptotically stable in the large or exponentially stable in the large then the system for which the equilibrium is defined is also Lagrange stable (but not necessarily vice versa). Also, if an equilibrium is stable, it does not imply that the system for which the equilibrium is defined is Lagrange stable since there may be a way to pick  $x_0$  such that it is near an unstable equilibrium and  $x(t, t_0, x_0) \rightarrow \infty$  as  $t \rightarrow \infty$ .

The solutions  $x(t, t_0, x_0)$  are *uniformly bounded* if for any  $\alpha > 0$  and  $t_0 \geq 0$ , there exists a  $\beta(\alpha) > 0$  (independent of  $t_0$ ) such that if  $|x_0| < \alpha$ , then  $|x(t, t_0, x_0)| < \beta(\alpha)$  for all  $t \geq t_0 \geq 0$ . If the solutions are uniformly bounded then they are bounded and the system is Lagrange stable.

The solutions  $x(t, t_0, x_0)$  are said to be *uniformly ultimately bounded* if there exists some  $B > 0$ , and if corresponding to any  $\alpha > 0$  and  $t_0 > 0$  there exists a  $T(\alpha) > 0$  (independent of  $t_0$ ) such that  $|x_0| < \alpha$  implies that  $|x(t, t_0, x_0)| < B$  for all  $t \geq t_0 + T(\alpha)$ . Hence, a system is said to be uniformly ultimately bounded if eventually all trajectories end up in a  $B$ -neighborhood of the origin.

#### 5.1.4 Lyapunov's Stability Method

A. M. Lyapunov invented two methods to analyze stability [SMO02]. In his *indirect method* he showed that if we linearize a system about an equilibrium point, certain conclusions about local stability properties can be made (e.g., if the eigenvalues of the linearized system are in the left half plane then the equilibrium is stable but if one is in the right half plane it is unstable).

In his *direct method* the stability results for an equilibrium  $x_e = 0$  of (5.7) depend on the existence of an appropriate *Lyapunov function*  $V : D \rightarrow \mathbb{R}$  where  $D = \mathbb{R}^n$  for global results (e.g., asymptotic stability in the large) and  $D = B_h$  for some  $h > 0$ , for local results (e.g., stability in the sense of Lyapunov or asymptotic stability). If  $V$  is continuously differentiable with respect to its arguments then the derivative of  $V$  with respect to  $t$  along the solutions of (5.7) is

$$\dot{V}(t, x) = \partial_t V + \partial_x V f(t, x).$$

As an example, suppose that (5.7) is autonomous, and let  $V(x)$  is a quadratic form  $V(x) = x^T P x$  where  $x \in \mathbb{R}^n$  and  $P = P^T$ . Then,  $\dot{V}(x) = \frac{\partial V}{\partial x} f(t, x) = \dot{x}^T P x + x^T P \dot{x} = 2x^T P \dot{x}$  [SMO02].

Lyapunov's direct method provides for the following ways to test for stability. The first two are strictly for local properties while the last two have local and global versions.

- *Stable*: If  $V(t, x)$  is continuously differentiable, positive definite, and  $\dot{V}(t, x) \leq 0$ , then  $x_e = 0$  is stable.

- *Uniformly stable*: If  $V(t, x)$  is continuously differentiable, positive definite, decrescent<sup>2</sup>, and  $V(t, x) \leq 0$ , then  $x_e = 0$  is uniformly stable.

<sup>2</sup> A  $C^0$ -function  $V(t, x) : \mathbb{R}^+ \times B_h \rightarrow \mathbb{R}$  ( $V(t, x) : \mathbb{R}^+ \times \mathbb{R}^n \rightarrow \mathbb{R}$ ) is said to be *decrescent* if there exists a strictly increasing function  $\gamma$  defined on  $[0, r)$  for some

- *Uniformly asymptotically stable*: If  $V(t, x)$  is continuously differentiable, positive definite, and decrescent, with negative definite  $\dot{V}(t, x)$ , then  $x_e = 0$  is uniformly asymptotically stable (uniformly asymptotically stable in the large if all these properties hold globally).

- *Exponentially stable*: If there exists a continuously differentiable  $V(t, x)$  and  $c, c_1, c_2, c_3 > 0$  such that

$$c_1 |x|^c \leq V(t, x) \leq c_2 |x|^c, \quad \dot{V}(t, x) \leq -c_3 |x|^c, \quad (5.8)$$

for all  $x \in B_h$  and  $t \geq 0$ , then  $x_e = 0$  is exponentially stable. If there exists a continuously differentiable function  $V(t, x)$  and equations (5.8) hold for some  $c, c_1, c_2, c_3 > 0$  for all  $x \in \mathbb{R}^n$  and  $t \geq 0$ , then  $x_e = 0$  is exponentially stable in the large [SMO02].

## 5.2 The Basis of Modern Geometric Control

In this section we present the basics of modern geometric control, as currently used in modern biomechanics.

### 5.2.1 Feedback Linearization

#### Exact Feedback Linearization

The idea of feedback linearization is to algebraically transform the nonlinear system dynamics into a fully or partly linear one so that the linear control techniques can be applied. Note that this is not the same as a conventional linearization using Jacobians. In this subsection we will present the modern, geometric, Lie-derivative based techniques for exact feedback linearization of nonlinear control systems.

#### *The Lie Derivative and Lie Bracket in Control Theory*

Recall (see (2.4.1) above) that given a scalar function  $h(x)$  and a vector-field  $f(x)$ , we define a new scalar function,  $\mathcal{L}_f h = \nabla h f$ , which is the Lie derivative of  $h$  w.r.t.  $f$ , i.e., the directional derivative of  $h$  along the direction of the vector  $f$ . Repeated Lie derivatives can be defined recursively:

$$\mathcal{L}_f^0 h = h, \quad \mathcal{L}_f^i h = \mathcal{L}_f \left( \mathcal{L}_f^{i-1} h \right) = \nabla \left( \mathcal{L}_f^{i-1} h \right) f, \quad (\text{for } i = 1, 2, \dots)$$

Or given another vector-field,  $g$ , then  $\mathcal{L}_g \mathcal{L}_f h(x)$  is defined as

$$\mathcal{L}_g \mathcal{L}_f h = \nabla (\mathcal{L}_f h) g.$$

---

$r > 0$  (defined on  $[0, \infty)$ ) such that  $V(t, x) \leq \gamma(|x|)$  for all  $t \geq 0$  and  $x \in B_h$  for some  $h > 0$ .

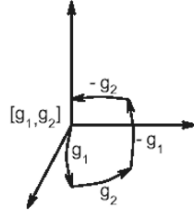
For example, if we have a control system

$$\dot{x} = f(x), \quad y = h(x),$$

with the state  $x = x(t)$  and the the output  $y$ , then the derivatives of the output are:

$$\dot{y} = \frac{\partial h}{\partial x} \dot{x} = \mathcal{L}_f h, \quad \text{and} \quad \ddot{y} = \frac{\partial \mathcal{L}_f h}{\partial x} \dot{x} = \mathcal{L}_f^2 h.$$

Also, recall that the curvature of two vector-fields,  $g_1, g_2$ , gives a non-zero Lie bracket (2.4.1),  $[g_1, g_2]$  (see Figure 5.3). Lie bracket motions can generate new directions in which the system can move.



**Fig. 5.3.** ‘Lie bracket motion’ is possible by appropriately modulating the control inputs (see text for explanation).

In general, the Lie bracket of two vector-fields,  $f(x)$  and  $g(x)$ , is defined by

$$[f, g] = Ad_f g = \nabla g f - \nabla f g = \frac{\partial g}{\partial x} f - \frac{\partial f}{\partial x} g,$$

where  $\nabla f = \partial f / \partial x$  is the Jacobian matrix. We can define Lie brackets recursively,

$$Ad_f^0 g = g, \quad Ad_f^i g = [f, Ad_f^{i-1} g], \quad (\text{for } i = 1, 2, \dots)$$

Lie brackets have the properties of bilinearity, skew-commutativity and Jacobi identity.

For example, if

$$f = \begin{pmatrix} \cos x_2 \\ x_1 \end{pmatrix}, \quad g = \begin{pmatrix} x_1 \\ 1 \end{pmatrix},$$

then we have

$$[f, g] = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \cos x_2 \\ x_1 \end{pmatrix} - \begin{pmatrix} 0 & -\sin x_2 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ 1 \end{pmatrix} = \begin{pmatrix} \cos x_2 + \sin x_2 \\ -x_1 \end{pmatrix}.$$

*Input/Output Linearization*

Given a single-input single-output (SISO) system

$$\dot{x} = f(x) + g(x)u, \quad y = h(x), \quad (5.9)$$

we want to formulate a linear-ODE relation between output  $y$  and a new input  $v$ . We will investigate (see [Isi89, SI89, Wil00]):

- How to generate a linear input/output relation.
- What are the internal dynamics and zero-dynamics associated with the input/output linearization?
- How to design stable controllers based on the I/O linearization.

This linearization method will be exact in a finite domain, rather than tangent as in the local linearization methods, which use Taylor series approximation. Nonlinear controller design using the technique is called exact feedback linearization.

*Algorithm for Exact Feedback Linearization*

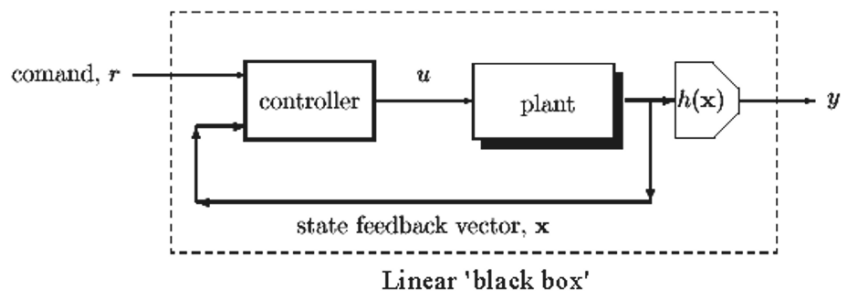
We want to find a nonlinear compensator such that the closed-loop system is linear (see Figure 5.4). We will consider only affine SISO systems of the type (5.9), i.e.  $\dot{x} = f(x) + g(x)u$ ,  $y = h(x)$ , and we will try to construct a *control law* of the form

$$u = p(x) + q(x)v, \quad (5.10)$$

where  $v$  is the setpoint, such that the *closed-loop nonlinear system*

$$\dot{x} = f(x) + g(x)p(x) + g(x)q(x)v, \quad y = h(x),$$

is linear from command  $v$  to  $y$ .



**Fig. 5.4.** Feedback linearization (see text for explanation).

The main idea behind the feedback linearization construction is to find a nonlinear change of coordinates which transforms the original system into

one which is linear and controllable, in particular, a chain of integrators. The difficulty is finding the output function  $h(x)$  which makes this construction possible.

We want to design an exact nonlinear feedback controller. Given the nonlinear affine system,  $\dot{x} = f(x) + g(x)u$ ,  $y = h(x)$ , we want to find the controller functions  $p(x)$  and  $q(x)$ . The unknown functions inside our controller (5.10) are given by:

$$\begin{aligned} p(x) &= \frac{-\left(\mathcal{L}_f^r h(x) + \beta_1 \mathcal{L}_f^{r-1} h(x) + \dots + \beta_{r-1} \mathcal{L}_f h(x) + \beta_r h(x)\right)}{\mathcal{L}_g \mathcal{L}_f^{r-1} h(x)}, \\ q(x) &= \frac{1}{\mathcal{L}_g \mathcal{L}_f^{r-1} h(x)}, \end{aligned} \quad (5.11)$$

which are comprised of Lie derivatives,  $\mathcal{L}_f h(x)$ . Here, the *relative order*,  $r$ , is the smallest integer  $r$  such that  $\mathcal{L}_g \mathcal{L}_f^{r-1} h(x) \neq 0$ . For linear systems  $r$  is the difference between the number of poles and zeros.

To obtain the *desired response*, we choose the  $r$  parameters in the  $\beta$  polynomial to describe how the output will respond to the setpoint,  $v$  (pole-placement).

$$\frac{d^r y}{dt^r} + \beta_1 \frac{d^{r-1} y}{dt^{r-1}} + \dots + \beta_{r-1} \frac{dy}{dt} + \beta_r y = v.$$

Here is the proposed algorithm [Isi89, SI89, Wil00]):

1. Given nonlinear SISO process,  $\dot{x} = f(x, u)$ , and output equation  $y = h(x)$ , then:
2. Calculate the relative order,  $r$ .
3. Choose an  $r$ th order desired linear response using pole-placement technique (i.e., select  $\beta$ ). For this could be used a simple  $r$ th order low-pass filter such as a Butterworth filter.
4. Construct the exact linearized nonlinear controller (5.11), using Lie derivatives and perhaps a symbolic manipulator (Mathematica or Maple).
5. Close the loop and obtain a linear input-output black-box (see Figure 5.4).
6. Verify that the result is actually linear by comparing with the desired response.

### Relative Degree

A nonlinear SISO system

$$\dot{x} = f(x) + g(x)u, \quad y = h(x),$$

is said to have *relative degree*  $r$  at a point  $x_o$  if (see [Isi89, NS90])

1.  $L_g L_f^k h(x) = 0$  for all  $x$  in a neighborhood of  $x_o$  and all  $k < r - 1$ ; and

2.  $L_g L_f^{r-1} h(x_o) \neq 0$ .

For example, *controlled Van der Pol oscillator* has the state space form

$$\dot{x} = f(x) + g(x)u = \begin{bmatrix} x_2 \\ 2\omega\zeta(1 - \mu x_1^2)x_2 - \omega^2 x_1 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} u.$$

Suppose the output function is chosen as  $y = h(x) = x_1$ . In this case we have

$$\begin{aligned} L_g h(x) &= \frac{\partial h}{\partial x} g(x) = [1 \ 0] \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 0, \quad \text{and} \\ L_f h(x) &= \frac{\partial h}{\partial x} f(x) = [1 \ 0] \begin{bmatrix} x_2 \\ 2\omega\zeta(1 - \mu x_1^2)x_2 - \omega^2 x_1 \end{bmatrix} = x_2. \end{aligned}$$

Moreover

$$L_g L_f h(x) = \frac{\partial(L_f h)}{\partial x} g(x) = [0 \ 1] \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 1,$$

and thus we see that the Vand der Pol oscillator system has relative degree 2 at any point  $x_o$ .

However, if the output function is, for instance  $y = h(x) = \sin x_2$ , then  $L_g h(x) = \cos x_2$ . The system has relative degree 1 at any point  $x_o$ , provided that  $(x_o)_2 \neq (2k+1)\pi/2$ . If the point  $x_o$  is such that this condition is violated, no relative degree can be defined.

As another example, consider a *linear system* in the state space form

$$\dot{x} = Ax + Bu, \quad y = Cx.$$

In this case, since  $f(x) = Ax$ ,  $g(x) = B$ ,  $h(x) = Cx$ , it is easily seen that

$$\begin{aligned} L_f^k h(x) &= C A^k x, \quad \text{and therefore,} \\ L_g L_f^k h(x) &= C A^k B. \end{aligned}$$

Thus, the integer  $r$  is characterized by the conditions

$$\begin{aligned} C A^k B &= 0, & \text{for all } k < r - 1 \\ C A^{r-1} B &\neq 0, & \text{otherwise.} \end{aligned}$$

It is well-known that the integer satisfying these conditions is exactly equal to the *difference* between the degree of the denominator polynomial and the degree of the numerator polynomial of the transfer function

$$H(s) = C(sI - A)^{-1}B$$

of the system.

### Approximative Feedback Linearization

Consider a SISO system

$$\dot{x} = f(x) + g(x)u, \quad (5.12)$$

where  $f$  and  $g$  are smooth vector-fields defined on a compact contractible region  $M$  of  $\mathbb{R}^n$  containing the origin. (Typically,  $M$  is a closed ball in  $\mathbb{R}^n$ .) We assume that  $f(0) = 0$ , i.e., that the origin is an equilibrium for  $\dot{x} = f(x)$ . The classical problem of feedback linearization can be stated as follows: find in a neighborhood of the origin a smooth change of coordinates  $z = \Phi(x)$  (a local diffeomorphism) and a smooth feedback law  $u = k(x) + l(x)u_{new}$  such that the closed-loop system in the new coordinates with new control is linear,

$$\dot{z} = Az + Bu_{new},$$

and controllable (see [BH96]). We usually require that  $\Phi(0) = 0$ . We assume that the system (5.12) has the *linear controllability* property

$$\dim(\text{span}\{g, Ad_f g, \dots, Ad_f^{n-1}g\}) = n, \quad \text{for all } x \in M \quad (5.13)$$

(where  $Ad_f^i$  are iterated Lie brackets of  $f$  and  $g$ ). We define the *characteristic distribution* for (5.12)

$$\mathcal{D} = \text{span}\{g, Ad_f g, \dots, Ad_f^{n-2}g\},$$

which is an  $(n-1)$ D smooth distribution by assumption of linear controllability (5.13). We call any nowhere vanishing 1-form  $\omega$  annihilating  $\mathcal{D}$  a characteristic 1-form for (5.12). All the characteristic 1-forms for (5.12) can be represented as multiples of some fixed characteristic 1-form  $\omega_0$  by a smooth nowhere vanishing function (zero-form)  $\beta$ . Suppose that there is a nonvanishing  $\beta$  so that  $\beta\omega_0$  is exact, i.e.,  $\beta\omega_0 = d\alpha$  for some smooth function  $\alpha$ , where  $d$  denotes the exterior derivative. Then  $\omega_0$  is called *integrable* and is called an integrating factor for  $\omega_0$ . The following result is standard in nonlinear control: Suppose that the system (5.12) has the linear controllability property (5.13) on  $M$ . Let  $\mathcal{D}$  be the characteristic distribution and  $\omega_0$  be a characteristic 1-form for (5.12). The following statements are equivalent:

1. Equation (5.12) is feedback linearizable in a neighborhood of the origin in  $M$ ;
2.  $\mathcal{D}$  is involutive in a neighborhood of the origin in  $M$ ; and
3.  $\omega_0$  is integrable in a neighborhood of the origin in  $M$ .

As is well known, a generic nonlinear system is not feedback linearizable for  $n > 2$ . However, in some cases, it may make sense to consider *approximate feedback linearization*.

Namely, if one can find a feedback linearizable system close to (5.12), there is hope that a control designed for the feedback linearizable system and applied to (5.12) will give satisfactory performance if the feedback linearizable

system is close enough to (5.12). The first attempt in this direction goes back to [Kre84], where it was proposed to apply to (5.12) a change of variables and feedback that yield a system of the form

$$\dot{z} = Az + B u_{new} + O(z, u_{new}),$$

where the term  $O(z, u_{new})$  contains higher-order terms. The aim was to make  $O(z, u_{new})$  of as high order as possible. Then we can say that the system (5.12) is approximately feedback linearized in a small neighborhood of the origin. Later [HT93] introduced a new algorithm to achieve the same goal with fewer steps.

Another idea has been investigated in [HSK92]. Roughly speaking, the idea was to neglect nonlinearities in (5.12) responsible for the failure of the involutivity condition in above theorem. This approach happened to be successful in the ball-and-beam system, when neglect of centrifugal force acting on ball yielded a feedback linearizable system. Application of a control scheme designed for the system with centrifugal force neglected to the original system gave much better results than applying a control scheme based on classical Jacobian linearization. This approach has been further investigated in [XH94, XH95] for the purpose of approximate feedback linearization about the manifold of constant operating points. However, a general approach to deciding which nonlinearities should be neglected to get the best approximation has not been set forth.

All of the above-mentioned work dealt with applying a change of coordinates and a preliminary feedback so that the resulting system looks like linearizable part plus nonlinear terms of highest possible order around an equilibrium point or an equilibrium manifold. However, in many applications one requires a large region of operation for the nonlinearizable system. In such a case, demanding the nonlinear terms to be neglected to be of highest possible order may, in fact, be quite undesirable. One might prefer that the nonlinear terms to be neglected be small in a uniform sense over the region of operation. In this section we propose an approach to approximate feedback linearization that uses a change of coordinates and a preliminary feedback to put a system (5.12) in a perturbed Brunovsky form,

$$\dot{z} = Az + B u_{new} + P(z) + Q(z) u_{new}, \quad (5.14)$$

where  $P(z)$  and  $Q(z)$  vanish at  $z = 0$  and are ‘small’ on  $M$ . We obtain upper bounds on uniform norms of  $P$  and  $Q$  (depending on some measures of noninvolutivity of  $\mathcal{D}$ ) on any compact, contractible  $M$ .

A different, indirect approach was presented in [BH96]. In this section, the authors present an approach for finding feedback linearizable systems that approximate a given SISO nonlinear system on a given compact region of the state-space. First, they it is shown that if the system is close to being involutive, then it is also close to being linearizable. Rather than working directly with the characteristic distribution of the system, the authors work with

characteristic 1-forms, i.e., with the 1-forms annihilating the characteristic distribution. It is shown that homotopy operators can be used to decompose a given characteristic 1-form into an exact and an antiexact part. The exact part is used to define a change of coordinates to a normal form that looks like a linearizable part plus nonlinear perturbation terms. The nonlinear terms in this normal form depend continuously on the antiexact part, and they vanish whenever the antiexact part does. Thus, the antiexact part of a given characteristic 1-form is a measure of nonlinearizability of the system. If the nonlinear terms are small, by neglecting them we get a linearizable system approximating the original system. One can design control for the original system by designing it for the approximating linearizable system and applying it to the original one. We apply this approach for design of locally stabilizing feedback laws for nonlinear systems that are close to being linearizable.

Let us start with approximating characteristic 1-forms by exact forms using *homotopy operators* (compare with (2.15) above). Namely, on any contractible region  $M$  one can define a linear operator  $H$  that satisfies

$$\omega = d(H\omega) + Hd\omega \quad (5.15)$$

for any form  $\omega$ . The homotopy identity (5.15) allows to decompose any given 1-form into the *exact part*  $d(H\omega)$  and an ‘error part’  $\epsilon = Hd\omega$ , which we call the *antiexact part of*  $\omega$ . For given  $\omega_0$  annihilating  $\mathcal{D}$  and a scaling factor  $\beta$  we define  $\alpha_\beta = H\beta\omega_0$  and  $\epsilon_\beta = Hd\beta\omega_0$ . The 1-form  $\epsilon_\beta$  measures how exact  $\omega_\beta = \beta\omega_0$  is. If it is zero, then  $\omega_\beta$  is exact and the system (5.12) is linearizable, and the zero-form  $\alpha_\beta$  and its first  $n - 1$  Lie derivatives along  $f$  are the new coordinates. In the case that  $\omega_0$  is not exactly integrable, i.e., when no exact integrating factor  $\beta$  exists, we choose  $\beta$  so that  $d\beta\omega_0$  is *smallest* in some sense (because this also makes  $\epsilon_\beta$  small). We call this  $\beta$  an *approximate integrating factor for*  $\omega_0$ . We use the zero-form  $\alpha_\beta$  and its first  $n - 1$  Lie derivatives along  $f$  as the new coordinates as in the linearizable case. In those new coordinates the system (5.12) is in the form

$$\dot{z} = Az + Bru + Bp + Eu,$$

where  $r$  and  $p$  are smooth functions,  $r \neq 0$  around the origin, and the term  $E$  (the obstruction to linearizability) depends linearly on  $\epsilon_\beta$  and some of its derivatives. We choose  $u = r^{-1}(u_{new} - p)$ , where  $u_{new}$  is a new control variable. After this change of coordinates and control variable the system is of the form (5.14) with  $Q = r^{-1}E$ ,  $P = -r^{-1}pE$ . We obtain estimates on the uniform norm of  $Q$  and  $P$  (via estimates on  $r$ ,  $p$ , and  $E$ ) in terms of the error 1-form  $\epsilon_\beta$ , for any fixed  $\beta$ , on any compact, contractible manifold  $M$ . Most important is that  $Q$  and  $P$  depend in a continuous way on  $\epsilon_\beta$  and some of its derivatives, and they vanish whenever  $\epsilon$  does (see [BH96]).

### 5.2.2 Controllability

#### Linear Controllability

A system is *controllable* if the set of all states it can reach from initial state  $x_0 = x(0)$  at the fixed time  $t = T$  contains a ball  $\mathcal{B}$  around  $x_0$ . Again, a system is *small time locally controllable* (STLC) iff the ball  $\mathcal{B}$  for  $t \leq T$  contains a neighborhood of  $x_0$ .<sup>3</sup>

In the case of a linear system in the standard state–space form (see subsection (3.5.2) above)

$$\dot{x} = Ax + Bu, \quad (5.16)$$

where  $A$  is the  $n \times n$  *state matrix* and  $B$  is the  $m \times n$  *input matrix*, all controllability definitions coincide, i.e.,

$$0 \rightarrow x(T), \quad x(0) \rightarrow 0, \quad x(0) \rightarrow x(T),$$

where  $T$  is either fixed or free.

*Rank condition* states: System (5.16) is controllable iff the matrix

$$W_n = (B \ AB \ \dots \ A^{n-1}B) \quad \text{has full rank.}$$

In the case of nonlinear systems the corresponding result is obtained using the formalism of Lie brackets, as Lie algebra is to nonlinear systems as matrix algebra is to linear systems.

#### Nonlinear Controllability

Nonlinear MIMO–systems are generally described by differential equations of the form (see [Isi89, NS90, Goo98]):

$$\dot{x} = f(x) + g_i(x) u^i, \quad (i = 1, \dots, n), \quad (5.17)$$

defined on a smooth  $n$ –manifold  $M$ , where  $x \in M$  represents the state of the control system,  $f(x)$  and  $g_i(x)$  are vector–fields on  $M$  and the  $u^i$  are control inputs, which belong to a set of *admissible controls*,  $u^i \in U$ . The system (5.17) is called *driftless*, or *kinematic*, or *control linear* if  $f(x)$  is identically zero; otherwise, it is called a *system with drift*, and the vector–field  $f(x)$  is called the *drift term*. The flow  $\phi_t^g(x_0)$  represents the solution of the differential equation  $\dot{x} = g(x)$  at time  $t$  starting from  $x_0$ . Geometric way to understand the *controllability* of the system (5.17) is to understand the geometry of the vector–fields  $f(x)$  and  $g_i(x)$ .

<sup>3</sup> The above definition of controllability tells us only whether or not something can reach an open neighborhood of its starting point, but does not tell us how to do it. That is the point of the *trajectory generation*.

*Example: Car-Parking Using Lie Brackets*

In this popular example, the driver has two different transformations at his disposal. He can turn the steering wheel, or he can drive the car forward or back. Here, we specify the state of a car by four coordinates: the  $(x, y)$  coordinates of the center of the rear axle, the direction  $\theta$  of the car, and the angle  $\phi$  between the front wheels and the direction of the car.  $L$  is the constant length of the car. Therefore, the configuration manifold of the car is 4D,  $M = (x, y, \theta, \phi)$ .

Using (5.17), the driftless car kinematics can be defined as:

$$\dot{x} = g_1(x) u_1 + g_2(x) u_2, \quad (5.18)$$

with two vector-fields  $g_1, g_2 \in \mathcal{X}^k(M)$ .

The infinitesimal transformations will be the vector-fields

$$g_1(x) \equiv \text{DRIVE} = \cos \theta \frac{\partial}{\partial x} + \sin \theta \frac{\partial}{\partial y} + \frac{\tan \phi}{L} \frac{\partial}{\partial \theta} \equiv \begin{pmatrix} \cos \theta \\ \sin \theta \\ \frac{1}{L} \tan \phi \\ 0 \end{pmatrix},$$

$$\text{and } g_2(x) \equiv \text{STEER} = \frac{\partial}{\partial \phi} \equiv \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

Now, STEER and DRIVE do not commute; otherwise we could do all your steering at home before driving of on a trip. Therefore, we have a Lie bracket

$$[g_2, g_1] \equiv [\text{STEER}, \text{DRIVE}] = \frac{1}{L \cos^2 \phi} \frac{\partial}{\partial \theta} \equiv \text{ROTATE}.$$

The operation  $[g_2, g_1] \equiv \text{ROTATE} \equiv [\text{STEER}, \text{DRIVE}]$  is the infinitesimal version of the sequence of transformations: steer, drive, steer back, and drive back, i.e.,

$$\{\text{STEER}, \text{DRIVE}, \text{STEER}^{-1}, \text{DRIVE}^{-1}\}.$$

Now, ROTATE can get us out of some parking spaces, but not tight ones: we may not have enough room to ROTATE out. The usual tight parking space restricts the DRIVE transformation, but not STEER. A truly tight parking space restricts STEER as well by putting your front wheels against the curb.

Fortunately, there is still another commutator available:

$$\begin{aligned} [g_1, [g_2, g_1]] &\equiv [\text{DRIVE}, [\text{STEER}, \text{DRIVE}]] = [[g_1, g_2], g_1] \equiv \\ [\text{DRIVE}, \text{ROTATE}] &= \frac{1}{L \cos^2 \phi} \left( \sin \theta \frac{\partial}{\partial x} - \cos \theta \frac{\partial}{\partial y} \right) \equiv \text{SLIDE}. \end{aligned}$$

The operation  $[[g_1, g_2], g_1] \equiv \text{SLIDE} \equiv [\text{DRIVE}, \text{ROTATE}]$  is a displacement at right angles to the car, and can get us out of any parking place. We just need

to remember to steer, drive, steer back, drive some more, steer, drive back, steer back, and drive back:

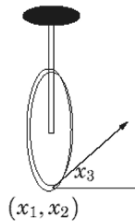
$$\{\text{STEER}, \text{DRIVE}, \text{STEER}^{-1}, \text{DRIVE}, \text{STEER}, \text{DRIVE}^{-1}, \text{STEER}^{-1}, \text{DRIVE}^{-1}\}.$$

We have to reverse steer in the middle of the parking place. This is not intuitive, and no doubt is part of the problem with parallel parking.

Thus from only two controls  $u_1$  and  $u_2$  we can form the vector-fields  $\text{DRIVE} \equiv g_1$ ,  $\text{STEER} \equiv g_2$ ,  $\text{ROTATE} \equiv [g_2, g_1]$ , and  $\text{SLIDE} \equiv [[g_1, g_2], g_1]$ , allowing us to move anywhere in the configuration manifold  $M$ . The car kinematics  $\dot{x} = g_1 u_1 + g_2 u_2$  is thus expanded as:

$$\begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{\theta} \\ \dot{\phi} \end{pmatrix} = \text{DRIVE} \cdot u_1 + \text{STEER} \cdot u_2 \equiv \begin{pmatrix} \cos \theta \\ \sin \theta \\ \frac{1}{L} \tan \phi \\ 0 \end{pmatrix} \cdot u_1 + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \cdot u_2.$$

The *parking theorem* says: One can get out of any parking lot that is larger than the car.



**Fig. 5.5.** The unicycle problem (see text for explanation).

*The Unicycle Example*

Now, consider the unicycle example (see Figure 5.5). Here we have

$$g_1 = \begin{pmatrix} \cos x_3 \\ \sin x_3 \\ 0 \end{pmatrix}, \quad g_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad [g_1, g_2] = \begin{pmatrix} \sin x_3 \\ -\cos x_3 \\ 0 \end{pmatrix}.$$

The unicycle system is full rank and therefore controllable.

**Controllability Condition**

Nonlinear controllability is an extension of linear controllability. The nonlinear MIMO system

$$\dot{x} = f(x) + g(x)u \quad \text{is controllable}$$

if the set of vector-fields  $\{g, [f, g], \dots, [f^{n-1}, g]\}$  is independent.

For example, for the kinematic car system of the form (5.18), the *nonlinear controllability criterion* reads: If the Lie bracket tree:

$$g_1, g_2, [g_1, g_2], [[g_1, g_2], g_1], [[g_1, g_2], g_2], [[[g_1, g_2], g_1], g_1], [[[g_1, g_2], g_1], g_2],$$

$$[[[g_1, g_2], g_2], g_1], [[[[g_1, g_2], g_2], g_2], \dots$$

– has *full rank* then the system is *controllable* [Isi89, NS90, Goo98]. In this case the combined input

$$(u_1, u_2) = \begin{cases} (1, 0), & t \in [0, \varepsilon] \\ (0, 1), & t \in [\varepsilon, 2\varepsilon] \\ (-1, 0), & t \in [2\varepsilon, 3\varepsilon] \\ (0, -1), & t \in [3\varepsilon, 4\varepsilon] \end{cases}$$

gives the motion  $x(4\varepsilon) = x(0) + \varepsilon^2 [g_1, g_2] + O(\varepsilon^3)$ , with the flow given by (see (2.20) below)

$$F_t^{[g_1, g_2]} = \lim_{n \rightarrow \infty} \left( F_{\sqrt{t/n}}^{-g_2} F_{\sqrt{t/n}}^{-g_1} F_{\sqrt{t/n}}^{g_2} F_{\sqrt{t/n}}^{g_1} \right)^n.$$

## Distributions

In control theory, the set of all possible directions in which the system can move, or the set of all points the system can reach, is of obvious fundamental importance. Geometrically, this is related to *distributions*.

A *distribution*  $\Delta \subset \mathcal{X}^k(M)$  on the manifold  $M$  is a subbundle of its tangent bundle  $TM$ , which assigns a subspace of the tangent space  $T_x M$  to each point  $x \in M$  in a smooth way. The dimension of  $\Delta(x)$  over  $\mathbb{R}$  at a point  $x \in M$  is called the rank of  $\Delta$  at  $x$ .

A distribution  $\Delta$  is involutive if, for any two vector-fields  $X, Y \in \Delta$ , their Lie bracket  $[X, Y] \in \Delta$ .

A function  $f \in C^k(M)$  is called an *integral* of  $\Delta$  if  $df(x) \in \Delta^0(x)$  for each  $x \in M$ . An *integral manifold* of  $\Delta$  is a submanifold  $N$  of  $M$  such that  $T_x N \subset \Delta(x)$  for each  $x \in N$ . A distribution  $\Delta$  is *integrable* if, for any  $x \in M$ , there is a submanifold  $N \subset M$ , whose dimension is the same as the rank of  $\Delta$  at  $x$ , containing  $x$  such that the tangent bundle,  $TN$ , is exactly  $\Delta$  restricted to  $N$ , i.e.,  $TN = \Delta|_N$ . Such a submanifold is called the *maximal integral manifold* through  $x$ .

It is natural to consider distributions generated by the vector-fields appearing in the sequence of flows (2.19). In this case, consider the distribution defined by

$$\Delta = \text{span}\{f; g_1 \dots g_m\},$$

where the span is taken over the set of smooth real-valued functions. Denote by  $\hat{\Delta}$  the *involutive closure* of the distribution  $\Delta$ , which is the closure of  $\Delta$

under bracketing. Then,  $\bar{\Delta}$  is the smallest subalgebra of  $\mathcal{X}^k(M)$  which contains  $\{f; g_1 \dots g_m\}$ . We will often need to ‘add’ distributions. Since distributions are, pointwise, vector spaces, define the sum of two distributions,

$$(\Delta_1 + \Delta_2)(x) = \Delta_1(x) + \Delta_2(x).$$

Similarly, define the intersection

$$(\Delta_1 \cap \Delta_2)(x) = \Delta_1(x) \cap \Delta_2(x).$$

More generally, we can arrive at a distribution via a *family of vector-fields*, which is simply a subset  $\mathcal{V} \subset \mathcal{X}^k(M)$ . Given a family of vector-fields  $\mathcal{V}$ , we may define a distribution on  $M$  by

$$\Delta_{\mathcal{V}}(x) = \langle X(x) | X \in \mathcal{V} \rangle_{\mathbb{R}}.$$

Since  $\mathcal{X}^k(M)$  is a Lie algebra, we may ask for the smallest Lie subalgebra of  $\mathcal{X}^k(M)$  which contains a family of vector-fields  $\mathcal{V}$ . It will be denoted as  $\overline{Lie}(\mathcal{V})$ , and will be represented by the set of vector-fields on  $M$  generated by repeated Lie brackets of elements in  $\mathcal{V}$ . Let  $\mathcal{V}^{(0)} = \mathcal{V}$  and then iteratively define a sequence of families of vector-fields by

$$\mathcal{V}^{(i+1)} = \mathcal{V}^{(i)} \cup \{[X, Y] | X \in \mathcal{V}^{(i)} = \mathcal{V} \text{ and } Y \in \mathcal{V}^{(i)}\}.$$

Now, every element of  $\overline{Lie}(\mathcal{V})$  is a linear combination of repeated Lie brackets of the form

$$[Z_k, [Z_{k-1}, [\dots, [Z_2, Z_1] \dots]]]$$

where  $Z_i \in \mathcal{V}$  for  $i = 1, \dots, k$ .

## Foliations

Related to integrable distributions are foliations.

Frobenius’ theorem asserts that integrability and involutivity are equivalent, at least locally. Thus, associated with an involutive distribution is a partition  $\Phi$  of  $M$  into disjoint connected immersed submanifolds called *leaves*. This partition  $\Phi$  is called a *foliation*. More precisely, a foliation  $\mathcal{F}$  of a smooth manifold  $M$  is a collection of disjoint immersed submanifolds of  $M$  whose disjoint union equals  $M$ . Each connected submanifold of  $\mathcal{F}$  is called a *leaf* of the foliation. Given an integrable distribution  $\Delta$ , the collection of maximal integral manifolds for  $\Delta$  defines a foliation on  $M$ , denoted by  $\mathcal{F}_D$ .

A foliation  $\mathcal{F}$  of  $M$  defines an equivalence relation on  $M$  whereby two points in  $M$  are equivalent if they lie in the same leaf of  $\mathcal{F}$ . The set of equivalence classes is denoted  $M/\mathcal{F}$  and is called the *leaf space* of  $\mathcal{F}$ . A foliation  $\mathcal{F}$  is said to be simple if  $M/\mathcal{F}$  inherits a manifold structure so that the projection from  $M$  to  $M/\mathcal{F}$  is a surjective submersion.

In control theory, foliation leaves are related to the set of points that a control system can reach starting from a given initial condition. A foliation  $\Phi$  of  $M$  defines an equivalence relation on  $M$  whereby two points in  $M$  are equivalent if they lie in the same leaf of  $\Phi$ . The set of equivalence classes is denoted  $M/\Phi$  and is called the *leaf space* of  $\Phi$ .

### Philip Hall Basis

Given a set of vector-fields  $\{g_1 \dots g_m\}$ , define the *length* of a *Lie product* as

$$l(g_i) = 1, \quad l([A, B]) = l(A) + l(B), \quad (\text{for } i = 1, \dots, m),$$

where  $A$  and  $B$  may be Lie products. A *Philip Hall basis* is an ordered set of Lie products  $H = \{B_i\}$  satisfying:

1.  $g_i \in H$ ,  $(i = 1, \dots, m)$ ;
2. If  $l(B_i) < l(B_j)$ , then  $B_i < B_j$ ; and
3.  $[B_i, B_j] \in H$  iff
  - (a)  $B_i, B_j \in H$  and  $B_i < B_j$ , and
  - (b) either  $B_j = g_k$  for some  $k$  or  $B_j = [B_l, B_r]$  with  $B_l, B_r \in H$  and  $B_l \leq B_i$ .

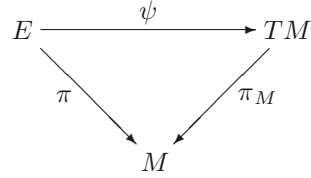
Essentially, the ordering aspect of the Philip Hall basis vectors accounts for skew symmetry and Jacobi identity to determine a basis.

## 5.3 Modern Control Techniques for Mechanical Systems

In this section we present modern control techniques for mechanical systems, as used in modern biomechanics research. Much of the existing work on control of mechanical systems has relied on the presence of specific structure. The most common examples of the types of structure assumed are symmetry (conservation laws) and constraints. While it may seem counter-intuitive that constraints may help in control theory, this is sometimes in fact the case. The reason is that the constraints provide extra forces (forces of constraint) which can be used to advantage. probably, the most interesting work is done from the Lagrangian (respectively Hamiltonian) perspective where we study systems whose Lagrangians are ‘kinetic energy minus potential energy’ (resp. ‘kinetic energy plus potential energy’). For these *simple mechanical control systems*, the controllability questions are different than those typically asked in nonlinear control theory. In particular, one is often more interested in what happens to configurations rather than states, which are configurations and velocities (resp. momenta) for these systems (see [Lew95, LM97]).

### 5.3.1 Abstract Control System

In general, a nonlinear control system  $\Sigma$  can be represented as a triple  $(\Sigma, M, f)$ , where  $M$  is the system’s *state-space* manifold with the tangent bundle  $TM$  and the general fibre bundle  $E$ , and  $f$  is a smooth map, such that the following bundle diagram commutes [Man98]



where  $\psi : (x, u) \mapsto (x, f(x, u))$ ,  $\pi_M$  is the natural projection of  $TM$  on  $M$ , the projection  $\pi : E \rightarrow M$  is a smooth fibre bundle, and the fibers of  $E$  represent the *input spaces*. If one chooses fibre-respecting coordinates  $(x, u)$  for  $E$ , then locally this definition reduces to  $\psi : (x, u) \mapsto (x, \psi(x, u))$ , i.e.,

$$\dot{x} = \psi(x, u).$$

The specific form of the map  $\psi$ , usually used in nonlinear control, is  $\psi : (x, u) \mapsto (x, f(x) + g(x, u))$ , with  $g(x, 0) = 0$ , producing standard nonlinear system equation

$$\dot{x} = f(x) + g(x, u).$$

### 5.3.2 Controllability of a Linear Control System

Consider a linear biomechanical control system:

$$\dot{x}(t) = Ax(t) + Bu(t), \quad (5.19)$$

where  $x \in \mathbb{R}^n$ ,  $u \in \mathbb{R}^m$ ,  $A \in L(\mathbb{R}^n, \mathbb{R}^n)$ , and  $B \in L(\mathbb{R}^m, \mathbb{R}^n)$ . One should think of  $t \mapsto u(t)$  as being a specified input signal, i.e., a function on the certain time interval,  $[0, T]$ . Now, control theory wants to design the signal to make the *state*  $t \mapsto x(t)$  do what we want. What this is may vary, depending on the situation at hand. For example, one may want to steer from an initial state  $x^i$  to a final state  $x_f$ , perhaps in an optimal way. Or, one may wish to design  $u : \mathbb{R}^n \rightarrow \mathbb{R}^m$  so that some state, perhaps  $x = 0$ , is stable for the dynamical system  $\dot{x}(t) = Ax + Bu(x)$ , which is called *state feedback* (often one asks that  $u$  be linear). One could also design  $u$  to be a function of both  $x$  and  $t$ , etc.

One of the basic control questions is *controllability*, which comes in many guises. Basically we are asking for ‘reachable’ points. In particular,

$$\mathcal{R}(0) = \text{span}_{\mathbb{R}}\{[B|AB|\dots|A^{n-1}B]\},$$

which is the smallest  $A$ -invariant subspace containing  $\text{Im}(B)$ , denotes the set of points reachable from  $0 \in \mathbb{R}^n$ . For the linear system (5.19), the basic controllability questions have definite answers. We want to do something similar for a class of simple mechanical systems [Lew95, LM97].

### 5.3.3 Affine Control System and Local Controllability

The nonlinear control system that we most often consider in human-like biomechanics has state-space  $M$ , a smooth  $n$ -manifold, and is *affine* in the controls. Thus it has the form (see [Lew95, LM97])

$$\dot{x} = f(x) + u^a g_a(x), \quad (x \in M), \quad (5.20)$$

where  $f, g_1, \dots, g_m$  are vector-fields on  $M$ . The *drift* vector-field  $f = f(x)$  describes how the system would evolve in the absence of any inputs. Each of the *control* vector-fields  $g_1, \dots, g_m$  specifies a direction in which one can supply actuation. To fully specify the control system properly, one should also specify the type of control action to be considered. Here we consider our controls to be taken from the set:  $U = \{u : \mathbb{R} \rightarrow \mathbb{R}^m \mid u \text{ is piecewise constant}\}$ . This class of controls is sufficient to deal with all analytic control systems. More generally, one may wish to consider measurable functions which take their values in a subset of  $\mathbb{R}^m$ .

Given an *affine control system* (5.20), it is possible to define a family of vector-fields on  $M$  by:  $V_\Sigma = \{f + u^a g_a \mid u \in \mathbb{R}^m\}$ .

A solution of the system (5.20) is a pair  $(\gamma, u)$ , where  $\gamma : [0, T] \rightarrow M$  is a piecewise smooth curve on  $M$  and  $u \in U$  such that

$$\dot{\gamma}(t) = f(\gamma(t)) + u^a(t) g_a(\gamma(t)), \quad \text{for each } t \in [0, T].$$

The *reachable set* from  $x_0$  in time  $T$  is

$$\begin{aligned} \mathcal{R}(x_0, T) &= \{x \mid \exists \gamma : [0, T] \rightarrow M \quad \text{and} \\ &\quad u : [0, T] \rightarrow \mathbb{R}^m \quad \text{satisfying (5.20)} \\ &\quad \text{with } \gamma(0) = x_0 \quad \text{and } \gamma(T) = x\}. \end{aligned}$$

Note that since the system has drift  $f$ , when we reach the point  $\gamma(T)$  we will not remain there if this is not an equilibrium point for  $f$ . Also, we have,  $\mathcal{R}(x_0, \leq T) = \cup_{0 < t \leq T} \mathcal{R}(x_0, T)$ .

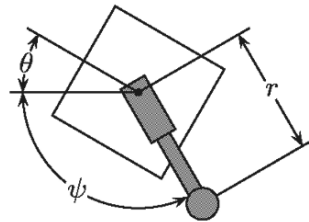
Let  $x_0 \in M$ , let  $V$  be a neighborhood of  $x_0$ , and let  $T > 0$ . We say that equation (5.20) represents a *locally accessible system* at  $x_0$  if  $\mathcal{R}(x_0, \leq T)$  contains an open subset of  $M$  for each  $V$  and for each  $T$  sufficiently small. Furthermore, we say that the system (5.20) is *small-time local controllability* (STLC, see [Sus83, Sus87]), if it is locally accessible and if  $x_0$  is in the interior of  $\mathcal{R}(x_0, \leq T)$  for each  $V$  and for each  $T$  sufficiently small.

### 5.3.4 Lagrangian Control Systems

#### Simple Mechanical Control Systems

As a motivation/prototype of a simple mechanical control system, consider a simple *robotic leg* (see Figure 5.6), in which inputs are: (1) an internal torque

$F^1$  moving the leg relative to the body and (2) a force  $F^2$  extending the leg. This system is ‘controllable’ in the sense that, starting from rest, one can reach any configuration from a given initial configuration. However, as a traditional control system, it is not controllable because of conservation of angular momentum. If one asks for the *states* (i.e., configurations and velocities) reachable from configurations with zero initial velocity, one finds that not all states are reachable. This is a consequence of the fact that angular momentum is conserved, even with inputs. Thus if one starts with zero momentum, the momentum will remain zero (this is what enables one to treat the system as *nonholonomic*). Nevertheless, all configurations are accessible. This suggests that the question of controllability is different depending on whether one is interested in configurations or states. We will be mainly interested in reachable configurations. Considering the system with just one of the two possible input forces is also interesting. In the case where we are just allowed to use  $F^2$ , the possible motions are quite simple; one can only move the ball on the leg back and forth. With just the force  $F^1$  available, things are a bit more complicated. But, for example, one can still say that no matter how you apply the force, the ball will never move ‘inwards’ [Lew95, LM97].



**Fig. 5.6.** A simple robotic leg (see text for explanation).

In general, simple mechanical control systems are characterized by:

- An  $n$ D configuration manifold  $M$ ;
- A Riemannian metric  $g$  on  $M$ ;
- A potential energy function  $V$  on  $M$ ; and
- $m$  linearly independent 1-forms,  $F^1, \dots, F^m$  on  $M$  (input forces; e.g., in the case of the simple robotic leg,  $F^1 = d\theta - d\psi$  and  $F^2 = dr$ ).

When we say these systems are not amenable to liberalization-based methods, we mean that their liberalizations at zero velocity are not controllable, and that they are not feedback linearizable. This makes simple mechanical control systems a non-trivial class of nonlinear control systems, especially from the point of view of control design.

As a basic example to start with, consider a *planar rigid body* (see Figure 5.7), with coordinates  $(x, y, \theta)$ . Inputs are (1) force pointing towards center of mass,  $F^1 = \cos \theta dx + \sin \theta dy$ , (2) force orthogonal to line to center of mass,

$F^2 = -\sin\theta dx + \cos\theta dy - h d\theta$ , and (3) torque at center of mass  $F^3 = d\theta$ . The planar rigid body, although seemingly quite simple, can be actually interesting. Clearly, if one uses all three inputs, the system is *fully actuated*, and so boring for investigating reachable configurations. But if one takes various combinations of one or two inputs, one gets a pretty nice sampling of what can happen for these systems. For example, all possible combinations of two inputs allow one to reach all configurations. Using  $F^1$  or  $F^3$  alone give simple, 1D reachable sets, similar to using  $F^2$  for the robotic leg (as we are always starting with zero initial velocity). However, if one is allowed to only use  $F^2$ , then it is not quite clear what to expect, at least just on the basis of intuition.

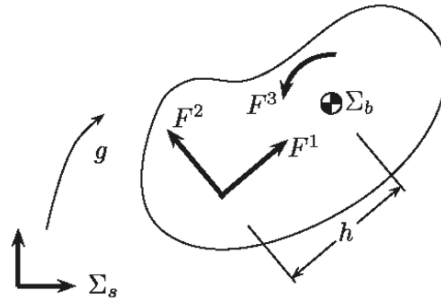


Fig. 5.7. Coordinate systems of a planar rigid body.

It turns out that our simplifying assumptions, i.e., zero initial velocity and restriction of our interest to configurations (i.e., as all problem data is on  $M$ , we expect answers to be describable using data on  $M$ ), makes our task much simpler. In fact, the computations without these assumptions have been attempted, but have yet to yield coherent answers.

Now, we are interested in how do the input 1-forms  $F^1, \dots, F^m$  interact with the unforced mechanics of the system as described by the kinetic energy Riemannian metric. That is, what is the analogue of linear system's ‘the smallest  $A$ -invariant subspace containing  $\text{Im}(B)$ ’ – for simple mechanical control systems?

### Motion and Controllability in Affine Connections

If we start with the local Riemannian metric form  $g \mapsto g_{ij}(q) dq^i dq^j$ , then we have a kinetic energy Lagrangian  $L(q, v) = g_{ij}(q) \dot{q}^i \dot{q}^j$ , and consequently the Euler-Lagrange equations (3.4) are given as [Lew98]

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} \equiv g_{ij} \ddot{q}^j + \left( \frac{\partial g_{ij}}{\partial q^k} - \frac{1}{2} \frac{\partial g_{jk}}{\partial q^i} \right) \dot{q}^j \dot{q}^k = u_a F_i^a, \quad (i = 1, \dots, n).$$

Now multiply this by  $g^{li}$  and take the symmetric part of the coefficient of  $\dot{q}^j \dot{q}^k$  to get  $\ddot{q}^l + \Gamma_{jk}^l \dot{q}^j \dot{q}^k = u^a Y_a^l$ ,  $l = 1, \dots, n$ , where  $\Gamma_{jk}^i$  are the Christoffel symbols

(3.9) for the Levi–Civita connection  $\nabla$  (see (2.5.1) above). So, the equations of motion are

$$\nabla_{\dot{\gamma}(t)} \dot{\gamma}(t) = u^a(t) Y_a(\gamma(t)),$$

where  $Y_a = (F^a)^\sharp$ ,  $a = 1, \dots, m$ . Here  $\sharp : T^*M \rightarrow TM$  is the ‘musical’ isomorphism associated with the Riemannian metric  $g$ .

Now, there is nothing to be gained by using a Levi–Civita connection, or by assuming that the vector–fields come from 1–forms. At this point, perhaps the generalization to an arbitrary affine connection seems like a senseless abstraction. However, as we shall see, this abstraction allows us to include another large class of mechanical control systems. So we will study the control system

$$\nabla_{\dot{\gamma}(t)} \dot{\gamma}(t) = u^a(t) Y_a(\gamma(t)) [+Y_0(\gamma(t))], \quad (5.21)$$

with  $\nabla$  a general affine connection on  $M$ , and  $Y_1, \dots, Y_m$  linearly independent vector–fields on  $M$ . The ‘optional’ term  $Y_0 = Y_0(\gamma(t))$  in (5.21) indicates how potential energy may be added. In this case  $Y_0 = -\text{grad} V$  (however, one loses nothing by considering a general vector–field instead of a gradient) [Lew98].

A *solution* to (5.21) is a pair  $(\gamma, u)$  satisfying (5.21) where  $\gamma : [0, T] \rightarrow M$  is a curve and  $u : [0; T] \rightarrow \mathbb{R}^m$  is bounded and measurable.

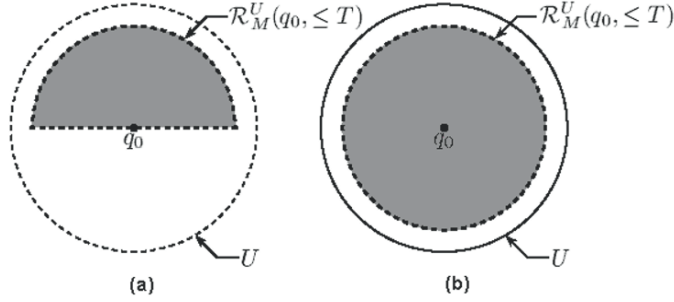
Let  $U$  be a neighborhood of  $q_0 \in M$  and denote by  $\mathcal{R}_M^U(q_0, T)$  those points in  $M$  for which there exists a solution  $(\gamma, u)$  with the following properties:

1.  $\gamma(t) \in U$  for  $t \in [0, T]$ ;
2.  $\dot{\gamma}(0) = 0_q$ ; and
3.  $\gamma(T) \in T_q M$ .

Also  $\mathcal{R}_M^U(q_0, \leq T) = \cup_{0 \leq t \leq T} \mathcal{R}_M^U(q_0, t)$ . Now, regarding the local controllability, we are only interested in points which can be reached without taking ‘large excursions’. Control problems which are local in this way have the advantage that they can be characterized by Lie brackets. So, we want to describe our *reachable set*  $\mathcal{R}_M^U(q, \leq T)$  for the simple mechanical control system (5.21). The system (5.21) is *locally configuration accessible* (LCA) at  $q$  if there exists  $T > 0$  so that  $\mathcal{R}_M^U(q, \leq t)$  contains a non–empty open subset of  $M$  for each neighborhood  $U$  of  $q$  and each  $t \in ]0, T]$ . Also, (5.21) is *locally configuration controllable* (LCC) at  $q$  if there exists  $T > 0$  so that  $\mathcal{R}_M^U(q, \leq t)$  contains a neighborhood of  $q$  for each neighborhood  $U$  of  $q$  and each  $t \in ]0, T]$ . Although sound very similar, the notions of local configuration accessibility and local configuration controllability are genuinely different (see Figure 5.8). Indeed, one need only look at the example of the robotic leg with the  $F^1$  input. In this example one may show that the system is LCA, but is not LCC [Lew98].

### Local Configuration Accessibility

The accessibility problem is solved by looking at Lie brackets. For this we need to recall the definition of the *vertical lift* [Lew98]:



**Fig. 5.8.** Difference between the notions of local configuration accessibility (a), and local configuration controllability (b).

$$\text{verlift}(Y(v_q)) = \left. \frac{d}{dt} \right|_{t=0} (v_q + tY(q)),$$

in local coordinates, if  $Y = Y^i \partial_{q^i}$ , then  $\text{verlift}(Y) = Y^i \partial_{v^i}$ . Now we can rewrite (5.21) in the first-order form:

$$\dot{v} = Z(v) + u^a \text{verlift}(Y_a(v)),$$

where  $Z$  is the geodesic spray for  $\nabla$ .

We evaluate all brackets at  $0_q$  (recall that  $T_{0_q}TM \simeq T_qM \oplus T_qM$ ). Here, the first component we think of as being the ‘horizontal’ bit which is tangent to the zero section in  $TM$ , and we think of the second component as being the ‘vertical’ bit which is the tangent space to the fibre of  $\tau_M : TM \rightarrow M$ .

To get an answer to the local configuration accessibility problem, we employ standard nonlinear control techniques involving Lie brackets. Doing so gives us our first look at the *symmetric product*,  $\langle X : Y \rangle = \nabla_X Y + \nabla_Y X$ . Our sample brackets suggest that perhaps the only things which appear in the bracket computations are symmetric products and Lie brackets of the input vector-fields  $Y_1, \dots, Y_m$ .

Here are some sample brackets:

- (i)  $[Z, \text{verlift}(Y_a)](0_q) = (-Y_a(q), 0)$ ;
- (ii)  $[\text{verlift}(Y_a), [Z, \text{verlift}(Y_b)]](0_q) = (0, \langle Y_a : Y_b \rangle(q))$ ;
- (iii)  $[[Z, \text{verlift}(Y_a)], [Z, \text{verlift}(Y_b)]](0_q) = (\langle Y_a, Y_b \rangle(q), 0)$ .

Now, let  $C_{ver}$  be the closure of  $\text{span}\{Y_1, \dots, Y_m\}$  under symmetric product. Also, let  $C_{hor}$  be the closure of  $C_{ver}$  under Lie bracket. So, we assume  $C_{ver}$  and  $C_{hor}$  to be distributions (i.e., of constant rank) on  $M$ . The closure of  $\text{span}\{Z, \text{verlift}(Y_1), \dots, \text{verlift}(Y_m)\}$  under Lie bracket, when evaluated at  $0_q$ , is then the distribution

$$q \mapsto C_{hor}(q) \oplus C_{ver}(q) \subset T_qM \oplus T_qM.$$

Proving that the involutive closure of  $\text{span}\{Z, \text{verlift}(Y_1), \dots, \text{verlift}(Y_m)\}$  is equal at  $0_q$  to  $C_{hor}(q) \oplus C_{ver}(q)$  is a matter of computing brackets, samples of which are given above, and seeing the patterns to suggest an inductive proof. The brackets for these systems are very structured. For example, the brackets of input vector-fields are identically zero. Many other brackets vanish identically, and many more vanish when evaluated at  $0_q$ .

$C_{hor}$  is integrable: let  $A_q$  be the maximal integral manifold through  $q \in M$ . Then,  $\mathcal{R}_M^U(q, \leq T)$  is contained in  $A_q$ , and  $\mathcal{R}_M^U(q, \leq T)$  contains a non-empty open subset of  $A_q$ . In particular, if  $\text{rank}(C_{hor}) = n$  then (5.21) is LCA [Lew95, LM97]. This theorem gives a ‘computable’ description of the reachable sets (in the sense that we can compute  $A_q$  by solving some over-determined nonlinear PDE’s). But it does not give the kind of insight that we had with the ‘smallest  $A$ -invariant subspace containing  $\text{Im}(B)$ ’.

Recall that a submanifold  $N$  of  $M$  is *totally geodesic* if every geodesic with initial velocity tangent to  $N$  remains on  $N$ . This can be weakened to distributions: a distribution  $D$  on  $M$  is *geodesically invariant* if for every geodesic  $\gamma : [0, T] \rightarrow M$ ,  $\dot{\gamma}(0) \in D_{\gamma(0)}$  implies  $\dot{\gamma}(t) \in D_{\gamma(t)}$  for  $t \in ]0, T]$ .

$D$  is geodesically invariant if it is closed under symmetric product [Lew98]. This theorem says that the symmetric product plays for geodesically invariant distributions the same role the Lie bracket plays for integrable distributions. This result was key in providing the geometric description of the reachable configurations.

An integrable distribution is *geodesically generated distribution* if it is the involutive closure of a geodesically invariant distribution. This basically means that one may reach all points on a leaf with geodesics lying in some subdistribution. The picture one should have in mind with the geometry of the reachable sets is a foliation of  $M$  by geodesically generated (immersed) submanifolds onto which the control system restricts if the initial velocity is zero. The idea is that when we start with zero velocity we remain on leaves of the foliation defined by  $C_{hor}$  [LM97]. Note that for cases when the affine connection possesses no geodesically invariant distributions, the system (5.21) is automatically LCA. This is true, for example, of  $S^2$  with the affine connection associated with its round metric.

Clearly  $C_{ver}$  is the smallest geodesically invariant distribution containing  $\text{span}\{Y_1, \dots, Y_m\}$ . Also,  $C_{hor}$  is geodesically generated by  $\text{span}\{Y_1, \dots, Y_m\}$ . Thus  $\mathcal{R}_M^U$  is contained in, and contains a non-empty open subset of, the distribution geodesically generated by  $\text{span}\{Y_1, \dots, Y_m\}$ . Note that the pretty decomposition we have for systems with no potential energy does not exist at this point for systems with potential energy.

### Local Configuration Controllability

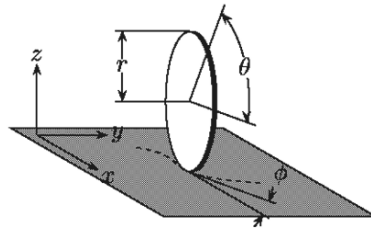
The problem of configuration controllability is harder than the one of configuration accessibility. Following [LM99], we will call a symmetric product in  $\{Y_1, \dots, Y_m\}$  *bad* if it contains an even number of each of the input vector-fields.

Otherwise we will call it *good*. The *degree* is the total number of vector-fields. For example,  $\langle\langle Y_a : Y_b \rangle\rangle : \langle Y_a : Y_b \rangle$  is bad and of degree 4, and  $\langle Y_a : \langle Y_b : Y_b \rangle \rangle$  is good and of degree 3. If each bad symmetric product at  $q$  is a linear combination of good symmetric products of lower degree, then (5.21) is LCC at  $q$ .

Now, the single-input case can be solved completely: The system (5.21) with  $m = 1$  is LCC iff  $\dim(M) = 1$  [LM99].

### Systems With Nonholonomic Constraints

Let us now add to the data a distribution  $D$  defining nonholonomic constraints. One of the interesting things about this affine connection approach is that we can easily integrate into our framework systems with nonholonomic constraints. As a simple example, consider a *rolling disk* (see Figure 5.9), with two inputs: (1) a ‘rolling’ torque,  $F^1 = d\theta$  and (2) a ‘spinning’ torque,  $F^2 = d\phi$ . It can be analyzed as a nonholonomic system (see [Lew99]).



**Fig. 5.9.** Rolling disk problem (see text for explanation).

The control equations for a simple mechanical control system with constraints are:

$$\nabla_{\dot{\gamma}(t)} \dot{\gamma}(t) = \lambda(t) + u^a(t) Y_a(\gamma(t)) [-\text{grad } V(\gamma(t))], \quad \dot{\gamma}(t) \in D_{\gamma(t)},$$

where  $\lambda(t) \in D_{\gamma(t)}^\perp$  are *Lagrange multipliers*.

### Examples

1. Recall that for the simple robotic leg (Figure 5.6) above,  $Y_1$  was internal torque and  $Y_2$  was extension force. Now, in the following three cases:

- (i) both inputs active – this system is LCA and LCC (satisfies sufficient condition);
- (ii)  $Y_1$  only, it is LCA but not LCC; and
- (iii)  $Y_2$  only, it is not LCA.

In these three cases,  $C_{hor}$  is generated by the following linearly independent vector-fields:

- (i) both inputs:  $\{Y_1, Y_2, [Y_1, Y_2]\}$ ;
- (ii)  $Y_1$  only:  $\{Y_1, \langle Y_1 : Y_1 \rangle, \langle Y_1 : \langle Y_1 : Y_1 \rangle \rangle\}$ ; and
- (iii)  $Y_2$  only:  $\langle Y_2 \rangle$ .

Recall that with both inputs the system was not accessible in  $TM$  as a consequence of conservation of angular momentum. With the input  $Y_2$  only, the control system behaves very simply when given zero initial velocity. The ball on the end of the leg just gets moved back and forth. This reflects the foliation of  $M$  by the maximal integral manifolds of  $C_{hor}$ , which are evidently 1D in this case. With the  $Y_1$  input, recall that the ball will always go ‘outwards’ no matter what one does with the input. Thus the system is not LCC. But apparently (since  $rank(C_{hor}) = \dim(M)$ ) one can reach a non-empty open subset of  $M$ . The behavior exhibited in this case is typical of what one can expect for single-input systems with no potential energy.

2. For the planar rigid body (Figure 5.7) above, we have the following five cases:

- (i)  $Y_1$  and  $Y_2$  active, this system is LCA and LCC (satisfies sufficient condition);
- (ii)  $Y_1$  and  $Y_3$ , it is LCA and LCC (satisfies sufficient condition);
- (iii)  $Y_1$  only or  $Y_3$  only, not LCA;
- (iv)  $Y_2$  only, LCA but not LCC; and
- (v)  $Y_2$  and  $Y_3$ : LCA and LCC (fails sufficient condition).

Now, with the inputs  $Y_1$  or  $Y_3$  alone, the motion of the system is simple. In the first case the body moves along the line connecting the point of application of the force and the center of mass, and in the other case the body simply rotates. The equations in  $(x, y, \theta)$  coordinates are

$$\ddot{x} = \frac{\cos \theta}{m} u^1 - \frac{\sin \theta}{m} u^2, \quad \ddot{y} = \frac{\sin \theta}{m} u^1 + \frac{\cos \theta}{m} u^2, \quad \ddot{\theta} = \frac{1}{J} (u^3 - hu^2),$$

which illustrates that the  $\theta$ -equation decouples when only  $Y_3$  is applied. We make a change of coordinates for the case where we have only  $Y_1$ :  $(\xi, \eta, \psi) = (x \cos \theta + y \sin \theta, -x \sin \theta + y \cos \theta, \theta)$ . In these coordinates we have

$$\ddot{\xi} - 2\dot{\eta}\dot{\psi} - \xi\dot{\psi}^2 = \frac{1}{m} u^1, \quad \ddot{\eta} + 2\dot{\xi}\dot{\psi} - \eta\dot{\psi}^2 = 0, \quad \dot{\psi} = 0,$$

which illustrates the decoupling of the  $\xi$ -equation in this case.

$C_{hor}$  has the following generators:

- (i)  $Y_1$  and  $Y_2$ :  $\{Y_1, Y_2, [Y_1, Y_2]\}$ ;
- (ii)  $Y_1$  and  $Y_3$ :  $\{Y_1, Y_3, [Y_1, Y_3]\}$ ;
- (iii)  $Y_1$  only or  $Y_3$  only:  $\{Y_1\}$  or  $\{Y_3\}$ ;
- (iv)  $Y_2$  only:  $\{Y_2, \langle Y_2 : Y_2 \rangle, \langle Y_2 : \langle Y_2 : Y_2 \rangle \rangle\}$ ;
- (v)  $Y_2$  and  $Y_3$ :  $\{Y_2, Y_3, [Y_2, Y_3]\}$ .

3. Recall that for the rolling disk (Figure 5.9) above,  $Y_1$  was ‘rolling’ input and  $Y_2$  was ‘spinning’ input. Now, in the following three cases:

- (i)  $Y_1$  and  $Y_2$  active, this system is LCA and LCC (satisfies sufficient condition);

- (ii)  $Y_1$  only: not LCA; and
- (iii)  $Y_2$  only: not LCA.

In these three cases,  $C_{hor}$  has generators:

- (i)  $Y_1$  and  $Y_2$ :  $\{Y_1, Y_2, [Y_1, Y_2], [Y_2, [Y_1, Y_2]]\}$ ;
- (ii)  $Y_1$  only:  $\{Y_1\}$ ; and
- (iii)  $Y_2$  only:  $\{Y_2\}$ .

The rolling disk passes the good/bad symmetric product test. Another way to show that it is LCC is to show that the inputs allow one to follow any curve which is admitted by the constraints. Local configuration controllability then follows as the constraint distribution for the rolling disk has an involutive closure of maximal rank [Lew99].

### Categorical Structure of Control Affine Systems

Control affine systems make a category  $\mathcal{CAS}$  (see [Elk99]). The category  $\mathcal{CAS}$  has the following data:

- An *object* in  $\mathcal{CAS}$  is a pair  $\Sigma = (M, \mathfrak{F} = \{f_0, f_1, \dots, f_m\})$  where  $\mathfrak{F}$  is a family of vector-fields

$$\dot{x}(t) = f_0(x(t)) + u^a(t)f_a(x(t))$$

on the manifold  $M$ .

- A *morphism* sending  $\Sigma = (M, \mathfrak{F} = \{f_0, f_1, \dots, f_m\})$  to  $\Sigma' = (M', \mathfrak{F}' = \{f'_0, f'_1, \dots, f'_{m'}\})$  is a triple  $(\psi, \lambda_0, \Lambda)$  where  $\psi: M \rightarrow M'$ ,  $\lambda_0: M \rightarrow \mathbb{R}^{m'}$ , and  $\Lambda: M \rightarrow L(\mathbb{R}^m, \mathbb{R}^{m'})$  are smooth maps satisfying:
  1.  $T_x\psi(f_a(x)) = \Lambda_a^\alpha(x)f'_\alpha(\psi(x))$ ,  $a \in \{1, \dots, m\}$ , and
  2.  $T_x\psi(f_0(x)) = f'_0(\psi(x)) + \lambda_0^\alpha f'_\alpha(\psi(x))$ .

This corresponds to a change of state-input by

$$(x, u) \mapsto (\psi(x), \lambda_0(x) + \Lambda(x)u).$$

Elkin [Elk99] discusses equivalence, inclusion, and factorization in the category  $\mathcal{CAS}$ . Using categorical language, he considers local equivalence for various classes of nonlinear control systems, including single-input systems, systems with involutive input distributions, and systems with three states and two inputs.

#### 5.3.5 Lie-Adaptive Control in Human-Like Biomechanics

In this subsection we develop the concept of *machine learning* in the framework of Lie derivative control formalism (see (5.2.1) above). Consider an  $n$ D, SISO system in the standard affine form (5.9), rewritten here for convenience:

$$\dot{x}(t) = f(x) + g(x)u(t), \quad y(t) = h(x), \quad (5.22)$$

As already stated, the feedback control law for the system (5.22) can be defined using Lie derivatives  $\mathcal{L}_f h$  and  $\mathcal{L}_g h$  of the system's output  $h$  along the vector-fields  $f$  and  $g$ .

If the SISO system (5.22) is a relatively simple (quasilinear) system with *relative degree*  $r = 1$  it can be rewritten in a quasilinear form

$$\dot{x}(t) = \gamma_i(t) f_i(x) + d_j(t) g_j(x) u(t), \quad (5.23)$$

where  $\gamma_i$  ( $i = 1, \dots, n$ ) and  $d_j$  ( $j = 1, \dots, m$ ) are system's parameters, while  $f_i$  and  $g_j$  are smooth vector-fields.

In this case the feedback control law for *tracking the reference signal*  $y_R = y_R(t)$  is defined as (see [Isi89, NS90])

$$u = \frac{-\mathcal{L}_f h + \dot{y}_R + \alpha(y_R - y)}{\mathcal{L}_g h}, \quad (5.24)$$

where  $\alpha$  denotes the feedback gain.

Obviously, the problem of reference signal tracking is relatively simple and straightforward if we know all the system's parameters  $\gamma_i(t)$  and  $d_j(t)$  of (5.23). The question is can we apply a similar control law if the system parameters are unknown?

Now we have much harder problem of *adaptive signal tracking*. However, it appears that the feedback control law can be actually cast in a similar form (see [SI89],[Gom94]):

$$\hat{u} = \frac{-\widehat{\mathcal{L}_f h} + \dot{y}_R + \alpha(y_R - y)}{\widehat{\mathcal{L}_g h}}, \quad (5.25)$$

where Lie derivatives  $\mathcal{L}_f h$  and  $\mathcal{L}_g h$  of (5.24) have been replaced by their estimates  $\widehat{\mathcal{L}_f h}$  and  $\widehat{\mathcal{L}_g h}$ , defined respectively as

$$\widehat{\mathcal{L}_f h} = \widehat{\gamma}_i(t) \mathcal{L}_{f_i} h, \quad \widehat{\mathcal{L}_g h} = \widehat{d}_j(t) \mathcal{L}_{g_j} h,$$

in which  $\widehat{\gamma}_i(t)$  and  $\widehat{d}_j(t)$  are the estimates for  $\gamma_i(t)$  and  $d_j(t)$ .

Therefore, we have the straightforward control law even in the uncertain case, provided that we are able to estimate the unknown system parameters. Probably the best known *parameter update law* is based on the so-called *Lyapunov criterion* (see [SI89]) and given by

$$\dot{\psi} = -\gamma \epsilon W, \quad (5.26)$$

where  $\psi = \{\gamma_i - \widehat{\gamma}_i, d_j - \widehat{d}_j\}$  is the parameter estimation error,  $\epsilon = y - y_R$  is the output error, and  $\gamma$  is a positive constant, while the matrix  $W$  is defined as:

$$W = [W_1^T W_2^T]^T, \quad \text{with}$$

$$W_1 = \begin{bmatrix} \mathcal{L}_{f_1} h \\ \vdots \\ \mathcal{L}_{f_n} h \end{bmatrix}, \quad W_2 = \begin{bmatrix} \mathcal{L}_{g_1} h \\ \vdots \\ \mathcal{L}_{g_m} h \end{bmatrix} \cdot \frac{-\widehat{\mathcal{L}_f h} + \dot{y}_R + \alpha(y_R - y)}{\widehat{\mathcal{L}_g h}}.$$

The proposed adaptive control formalism (5.25–5.26) can be efficiently applied wherever we have a problem of tracking a given signal with an output of a SISO-system (5.22–5.23) with unknown parameters.

### 5.3.6 Intelligent Robot Control: Interaction with Environment

Here we show a dynamic model of the robot interacting with the environment [KV98, KV03a, KV03b]. The robot dynamics is described by a vector differential equation

$$H(q)\ddot{q} + h(q, \dot{q}) + J^T(q)F = \tau,$$

where,  $q = q(t)$  is an  $n$ D vector of robot generalized coordinates;  $H(q)$  is an  $n \times n$  positive definite matrix of inertia moments of the manipulation mechanics;  $h(q, \dot{q})$  is an  $n$ D nonlinear function of centrifugal, Coriolis, and gravitational moments;  $\tau = \tau(t)$  is an  $n$ D vector of input control;  $J^T(q)$  is an  $n \times n$  Jacobian matrix connecting the velocities of robot end-effector and the velocities of robot generalized coordinates; and  $F = F(t)$  is an  $m$ D vector of generalized forces, or, of generalized forces and moments from the environment acting on the end-effector.

In the frame of robot joint coordinates, the model of environment dynamics can be presented in the form

$$M(q)\ddot{q} + L(q, \dot{q}) = S^T(q)F,$$

where  $M(q) \in \mathbb{R}^{n \times n}$  is a nonsingular matrix;  $L(q, \dot{q}) \in \mathbb{R}^n$  is a nonlinear vector function; and  $S^T(q) \in \mathbb{R}^{n \times n}$  is the matrix with  $\text{rank}(S) = n$ .

The end-effector of the manipulator is constrained on static geometric surfaces,  $\Phi(q) = 0$ , where  $\Phi(q) \in \mathbb{R}^m$  is the holonomic constraint function.

In practice, it is convenient to adopt a simplified model of the environment, taking into account the dominant effects, such as stiffness,  $F = K'(x - x_0)$ , or an environment damping during the tool motion,  $F = B'x$ , where  $K' \in \mathbb{R}^{n \times n}$ ,  $B' \in \mathbb{R}^{n \times n}$  are semidefinite matrices describing the environment stiffness and damping, respectively, and  $x_0 \in \mathbb{R}^n$  denotes the coordinate vector in Cartesian coordinates of the point of contact between the end-effector (tool) and a constraint surface. However, it is more appropriate to adopt the relationship defined by specification of the target impedance

$$F = M'\Delta\ddot{x} + B'\Delta\dot{x} + K'\Delta x, \quad \text{where} \quad \Delta x = x - x_0,$$

and  $M'$  is a positive definite inertia matrix. The matrices  $M'$ ,  $B'$ ,  $K'$  define the target impedance which can be selected to correspond to various objectives of the given manipulation task.

In the case of contact with the environment, the robot control task can be described as robot motion along a programmed trajectory  $q_p(t)$  representing a twice continuously differentiable function, when a desired force of interaction

$F_p(t)$  acts between the robot and the environment. Thus, the programmed motion  $q_p(t)$  and the desired interaction force  $F_p(t)$  must satisfy the following relation

$$F_p(t) \equiv f(q_p(t), \dot{q}_p(t), \ddot{q}_p(t)).$$

The control problem for robot interacting with dynamic environment is to define the control  $\tau(t)$  for  $t \geq t_0$ , that satisfies the target conditions

$$\lim_{t \rightarrow \infty} q(t) \rightarrow q_p(t), \quad \lim_{t \rightarrow \infty} F(t) \rightarrow F_p(t).$$

As a first example, the control algorithm based on stabilization of the robot motion with a preset quality of transient responses is considered, which has the form

$$\tau = H(q)[\ddot{q}_p - KP\eta - KD\dot{\eta}] + h(q, \dot{q}) + J^T(q)F.$$

The family of desired transient responses is specified by the vector differential equation

$$\ddot{\eta} = -KP\eta - KD\dot{\eta}, \quad \eta(t) = q(t) - q_p(t), \quad (5.27)$$

where  $KP \in \mathbb{R}^{n \times n}$  is the diagonal matrix of position feedback gains, and  $KD \in \mathbb{R}^{n \times n}$  is the diagonal matrix of velocity feedback gains. The right side of (5.27), i.e., PD-regulator is chosen such that the system defined by (5.27) is asymptotically stable in the whole. The values of matrices  $KP$  and  $KD$  can be chosen according to algebraic stability conditions.

The proposed control law represents a version of the well-known computed torque method including force term which uses dynamic robot model and the available on-line information from the position, velocity and force sensors. Here the model of robot environment does not have any influence on the performance of the control algorithm.

As the second example, control algorithm based on stabilization of the interaction force with a preset quality of transient responses is considered, which has the form

$$\begin{aligned} \tau = & H(q) M^{-1}(q) [-L(q, \dot{q}) + S^T(q) F] + h(q, \dot{q}) \\ & + J^T(q) \left\{ F_p - \int_{t_0}^t \left[ KFP \mu(\omega) + KFI \int_{t_0}^{\omega} \mu(\omega) dt \right] d\omega \right\}, \end{aligned}$$

where  $\mu(t) = F(t) - F_p(t)$ ;  $KFP \in \mathbb{R}^{n \times n}$  is the matrix of proportional force feedback gains; and  $KFI \in \mathbb{R}^{n \times n}$  is the matrix of integral force feedback gains. Here, it has been assumed that the interaction force in transient process should behave according to the following differential equation

$$\dot{\mu}(t) = Q(\mu), \quad Q(\mu) = -KFP \mu - KFI \int_{t_0}^t \mu dt. \quad (5.28)$$

PI force regulator (continuous vector function of  $Q$ ) is chosen such that the system defined by (5.28) is asymptotically stable in the whole. IN this case, environment dynamics model has explicit influence on the performance of contact control algorithm, also having influence on PI force local gains. It is clear that without knowing a sufficiently accurate environment model (parameters of matrices  $M(q), L(q, \dot{q}), S(q)$ ) it is not possible to determine the nominal contact force  $F_p(t)$ .

## 5.4 Neural Path Integral Motion Controller

Recall that human motion is naturally driven by synergistic action of more than 600 skeletal muscles. While the muscles generate driving torques in the moving joints, subcortical neural system performs both local and global (loco)motion control: first reflexly controlling contractions of individual muscles, and then orchestrating all the muscles into synergetic actions in order to produce efficient movements. While the local reflex control of individual muscles is performed on the *spinal control level*, the global integration of all the muscles into coordinated movements is performed within the *cerebellum*.

All hierarchical subcortical neuro-muscular physiology, from the bottom level of a single muscle fiber, to the top level of cerebellar muscular synergy, acts as a *temporal < out|in > reaction*, in such a way that the higher level acts as a command/control space for the lower level, itself representing an abstract image of the lower one:

1. At the *muscular level*, we have *excitation-contraction dynamics* [Hat78, Hat77b], in which *< out|in >* is given by the following sequence of nonlinear diffusion processes (see Appendix for details): *neural-action-potential*  $\rightsquigarrow$  *synaptic-potential*  $\rightsquigarrow$  *muscular-action-potential*  $\rightsquigarrow$  *excitation-contraction-coupling*  $\rightsquigarrow$  *muscle-tension-generating* [Iva91]. Its purpose is the generation of muscular forces, to be transferred into driving torques within the joint anatomical geometry.
2. At the *spinal level*, *< out|in >* is given by *autogenetic-reflex stimulus-response control* [Hou79]. Here we have a neural image of all individual muscles. The main purpose of the spinal control level is to provide both positive and negative feedbacks to stabilize generated muscular forces within the ‘homeostatic’ (or, more appropriately, ‘homeokinetic’) limits. The individual muscular actions are combined into flexor-extensor (or agonist-antagonist) pairs, mutually controlling each other. This is the mechanism of *reciprocal innervation of agonists and inhibition of antagonists*. It has a purely mechanical purpose to form the so-called *equivalent muscular actuators* (EMAs), which would generate driving torques  $T_i(t)$  for all movable joints.
3. At the *cerebellar level*, *< out|in >* is given by *sensory-motor integration* [HBB96]. Here we have an abstracted image of all autogenetic reflexes.

The main purpose of the cerebellar control level is integration and fine tuning of the action of all active EMAs into a synchronized movement, by *supervising* the individual autogenetic reflex circuits. At the same time, to be able to perform in new and unknown conditions, the cerebellum is continuously adapting its own neural circuitry by unsupervised (self-organizing) learning. Its action is subconscious and automatic, both in humans and in animals.

Naturally, we can ask the question: Can we assign a single  $\langle out|in \rangle$  measure to all these neuro-muscular stimulus-response reactions? We think that we can do it; so in this Letter, we propose the concept of *adaptive sensory-motor transition amplitude* as a unique measure for this temporal  $\langle out|in \rangle$  relation. Conceptually, this  $\langle out|in \rangle$  -*amplitude* can be formulated as the ‘*neural path integral*’ (see Appendix for details):

$$\langle out|in \rangle \equiv \langle motor|sensory \rangle_{amplitude} = \int \mathcal{D}[w, x] e^{iS[x]}. \quad (5.29)$$

Here, the integral is taken over all *activated* (or, ‘fired’) *neural pathways*  $x^i = x^i(t)$  of the cerebellum, connecting its input *sensory*-state with its output *motor*-state, symbolically described by *adaptive neural measure*  $\mathcal{D}[w, x]$ , defined by the weighted product (of discrete time steps)

$$\mathcal{D}[w, x] = \lim_{n \rightarrow \infty} \prod_{t=1}^n w^i(t) dx^i(t), \quad (5.30)$$

in which the *synaptic weights*  $w^i = w^i(t)$ , included in all active neural pathways  $x^i = x^i(t)$ , are updated by the unsupervised *Hebbian-like learning* rule [Heb49]:

$$w^i(t+1) = w^i(t) + \frac{\sigma}{\eta} (w_d^i(t) - w_a^i(t)), \quad (5.31)$$

where  $\sigma = \sigma(t)$ ,  $\eta = \eta(t)$  represent local neural *signal* and *noise* amplitudes, respectively, while superscripts *d* and *a* denote *desired* and *achieved* neural states, respectively. Theoretically, equations (5.29–6.7) define an  $\infty$ -*dimensional neural network*. Practically, in a computer simulation we can use  $10^7 \leq n \leq 10^8$ , roughly corresponding to the number of neurons in the cerebellum.

The exponent term  $S[x]$  in equation (5.29) represents the *autogenetic-reflex action*, describing reflexly-induced motion of all active EMAs, from their initial *stimulus*-state to their final *response*-state, along the family of extremal (i.e., Euler-Lagrangian) paths  $x_{\min}^i(t)$ . ( $S[x]$  is properly derived in (5.34–5.35) below.)

#### 5.4.1 Spinal Autogenetic Reflex Control

Recall (from Introduction) that at the spinal control level we have the autogenetic reflex *motor servo* [Hou79], providing the local, reflex feedback loops for

individual muscular contractions. A voluntary contraction force  $F$  of human skeletal muscle is reflexly excited (positive feedback  $+F^{-1}$ ) by the responses of its *spindle receptors* to stretch and is reflexly inhibited (negative feedback  $-F^{-1}$ ) by the responses of its *Golgi tendon organs* to contraction. Stretch and unloading reflexes are mediated by combined actions of several autogenetic neural pathways, forming the *motor servo*.

In other words, branches of the afferent fibers also synapse with with interneurons that inhibit motor neurons controlling the antagonistic muscles – *reciprocal inhibition*. Consequently, the stretch stimulus causes the antagonists to relax so that they cannot resist the shortening of the stretched muscle caused by the main reflex arc. Similarly, firing of the Golgi tendon receptors causes inhibition of the muscle contracting too strong and simultaneous *reciprocal activation* of its antagonist. Both mechanisms of reciprocal inhibition and activation performed by the autogenetic circuits  $+F^{-1}$  and  $-F^{-1}$ , serve to generate the well-tuned EMA-driving torques  $T_i$ .

Now, once we have properly defined the symplectic musculo-skeletal dynamics [Iva04] on the biomechanical (momentum) phase-space manifold  $T^*M^N$ , we can proceed in formalizing its hierarchical subcortical neural control. By introducing the *coupling Hamiltonians*  $H^m = H^m(q, p)$ , selectively corresponding *only* to the  $M \leq N$  *active joints*, we define the *affine Hamiltonian control function*  $H_{aff} : T^*M^N \rightarrow \mathbb{R}$ , in local canonical coordinates on  $T^*M^N$  given by (adapted from [NS90] for the biomechanical purpose)

$$H_{aff}(q, p) = H_0(q, p) - H^m(q, p) T_m, \quad (5.32)$$

$$(m = 1, \dots, M \leq N),$$

where  $T_m = T_m(t, q, p)$  are now *feedback torque one-forms* (different from the initial driving torques  $T_i$  acting in all the joints). Using the affine Hamiltonian function (5.32), we get the *affine Hamiltonian servo-system* [Iva04],

$$\begin{aligned} \dot{q}^i &= \frac{\partial H_0(q, p)}{\partial p_i} - \frac{\partial H^m(q, p)}{\partial p_i} T_m, \\ \dot{p}_i &= -\frac{\partial H_0(q, p)}{\partial q^i} + \frac{\partial H^m(q, p)}{\partial q^i} T_m, \\ q^i(0) &= q_0^i, \quad p_i(0) = p_i^0, \quad (i = 1, \dots, N; \quad m = 1, \dots, M \leq N). \end{aligned} \quad (5.33)$$

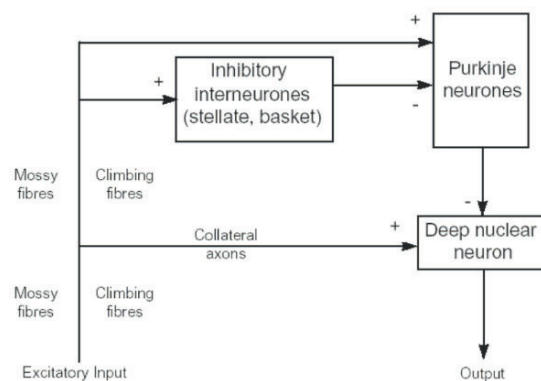
The affine Hamiltonian control system (5.33) gives our formal description for the autogenetic spinal motor-servo for all  $M \leq N$  activated (i.e., working) EMAs.

#### 5.4.2 Cerebellum – the Comparator

Having, thus, defined the spinal reflex control level, we proceed to model the top subcortical commander/controller, the *cerebellum*. It is a brain region anatomically located at the bottom rear of the head (the hindbrain), directly

above the brainstem, which is important for a number of subconscious and automatic motor functions, including motor learning. It processes information received from the motor cortex, as well as from proprioceptors and visual and equilibrium pathways, and provides ‘instructions’ to the motor cortex and other subcortical motor centers (like the basal nuclei), which result in proper balance and posture, as well as smooth, coordinated skeletal movements, like walking, running, jumping, driving, typing, playing the piano, etc. Patients with cerebellar dysfunction have problems with precise movements, such as walking and balance, and hand and arm movements. The cerebellum looks *similar in all animals*, from fish to mice to humans. This has been taken as evidence that it performs a common function, such as regulating motor learning and the timing of movements, in all animals. Studies of simple forms of motor learning in the vestibulo–ocular reflex and eye–blink conditioning are demonstrating that timing and amplitude of learned movements are encoded by the cerebellum.

The cerebellum is responsible for coordinating precisely timed  $\langle out|in \rangle$  activity by integrating motor output with ongoing sensory feedback (see Figure 5.10). It receives extensive projections from sensory–motor areas of the cortex and the periphery and directs it back to premotor and motor cortex [Ghe90]. This suggests a role in sensory–motor integration and the timing and execution of human movements. The cerebellum stores patterns of motor control for frequently performed movements, and therefore, its circuits are changed by experience and training. It was termed the *adjustable pattern generator* in the work of J. Houk and collaborators [HBB96]. Also, it has become the inspiring ‘brain–model’ in the recent robotic research [SA98, Sch98].



**Fig. 5.10.** Schematic  $\langle out|in \rangle$  organization of the primary cerebellar circuit. In essence, excitatory inputs, conveyed by collateral axons of Mossy and Climbing fibers activate directly neurones in the Deep cerebellar nuclei. The activity of these latter is also modulated by the inhibitory action of the cerebellar cortex, mediated by the Purkinje cells.

Comparing the number of its neurons ( $10^7 - 10^8$ ), to the size of conventional neural networks, suggests that artificial neural nets *cannot* satisfactorily model the function of this sophisticated ‘super-bio-computer’, as its dimensionality is virtually infinite. Despite a lot of research dedicated to its structure and function (see [HBB96] and references there cited), the real nature of the cerebellum still remains a ‘mystery’.

### 5.4.3 Hamiltonian Action and Neural Path Integral

Here, we propose a *quantum-like adaptive control* approach to modelling the ‘cerebellar mystery’. Corresponding to the affine Hamiltonian control function (5.32) we define the *affine Hamiltonian control action*,

$$S_{aff}[q, p] = \int_{t_{in}}^{t_{out}} d\tau [p_i \dot{q}^i - H_{aff}(q, p)]. \quad (5.34)$$

From the affine Hamiltonian action (5.34) we further derive the associated expression for the *neural phase-space path integral* (in normal units), representing the *cerebellar sensory-motor amplitude*  $\langle out|in \rangle$ ,

$$\begin{aligned} \langle q_{out}^i, p_i^{out} | q_{in}^i, p_i^{in} \rangle &= \int \mathcal{D}[w, q, p] e^{i S_{aff}[q, p]} \\ &= \int \mathcal{D}[w, q, p] \exp \left\{ i \int_{t_{in}}^{t_{out}} d\tau [p_i \dot{q}^i - H_{aff}(q, p)] \right\}, \\ \text{with} \quad \int \mathcal{D}[w, q, p] &= \int \prod_{\tau=1}^n \frac{w^i(\tau) dp_i(\tau) dq^i(\tau)}{2\pi}, \end{aligned} \quad (5.35)$$

where  $w_i = w_i(t)$  denote the cerebellar synaptic weights positioned along its neural pathways, being continuously updated using the Hebbian-like self-organizing learning rule (6.7). Given the transition amplitude  $\langle out|in \rangle$  (5.35), the *cerebellar sensory-motor transition probability* is defined as its absolute square,  $|\langle out|in \rangle|^2$ .

In (5.35),  $q_{in}^i = q_{in}^i(t)$ ,  $q_{out}^i = q_{out}^i(t)$ ;  $p_i^{in} = p_i^{in}(t)$ ,  $p_i^{out} = p_i^{out}(t)$ ;  $t_{in} \leq t \leq t_{out}$ , for all discrete time steps,  $t = 1, \dots, n \rightarrow \infty$ , and we are allowing for the affine Hamiltonian  $H_{aff}(q, p)$  to depend upon all the ( $M \leq N$ ) EMA-angles and angular momenta collectively. Here, we actually systematically took a discretized differential time limit of the form  $t_\sigma - t_{\sigma-1} \equiv d\tau$  (both  $\sigma$  and  $\tau$  denote discrete time steps) and wrote  $\frac{(q_\sigma^i - q_{\sigma-1}^i)}{(t_\sigma - t_{\sigma-1})} \equiv \dot{q}^i$ . For technical details regarding the path integral calculations on Riemannian and symplectic manifolds (including the standard regularization procedures), see [Kla97, Kla00].

Now, motor learning occurring in the cerebellum can be observed using functional MR imaging, showing changes in the cerebellar action potential, related to the motor tasks (see, e.g., [Mas02]). To account for these electrophysiological currents, we need to add the *source* term  $J_i(t)q^i(t)$  to the affine

Hamiltonian action (5.34), (the current  $J_i = J_i(t)$  acts as a source  $J_i A^i$  of the cerebellar electrical potential  $A^i = A^i(t)$ ),

$$S_{aff}[q, p, J] = \int_{t_{in}}^{t_{out}} d\tau [p_i \dot{q}^i - H_{aff}(q, p) + J_i q^i],$$

which, subsequently gives the cerebellar path integral with the action potential source, coming either from the motor cortex or from other subcortical areas.

Note that the standard *Wick rotation*:  $t \mapsto it$  (see [Kla97, Kla00]), makes all our path integrals real, i.e.,

$$\int \mathcal{D}[w, q, p] e^{i S_{aff}[q, p]} \quad \underline{Wick} \quad \int \mathcal{D}[w, q, p] e^{-S_{aff}[q, p]},$$

while their subsequent discretization gives the standard thermodynamic *partition functions*,

$$Z = \sum_j e^{-w_j E^j / T}, \quad (5.36)$$

where  $E^j$  is the energy eigenvalue corresponding to the affine Hamiltonian  $H_{aff}(q, p)$ ,  $T$  is the temperature–like environmental control parameter, and the sum runs over all energy eigenstates (labelled by the index  $j$ ). From (6.16), we can further calculate all statistical and thermodynamic system properties (see [Fey72]), as for example, *transition entropy*  $S = k_B \ln Z$ , etc.

## 5.5 Brain–Like Control Functor in Human–Like Biomechanics

In this final section we propose our most recent model [IB05] of the complete biomechanical *brain–like control functor*. This is a neuro–dynamical reflection on our *covariant force law*,  $F_i = m g_{ij} a^j$ , and its associated *covariant force functor*  $\mathcal{F}_* : TT^*M \rightarrow TTM$  (see section 2.7 above).

Traditional hierarchical robot control (see, e.g., [VS82]) consists of three levels: the *executive* control–level (at the bottom) performs tracking of nominal trajectories in internal–joint coordinates, the *strategic* control–level (at the top) performs ‘planning’ of trajectories of an end–effector in external–Cartesian coordinates, and the *tactical* control–level (in the middle) connects other two levels by means of inverse kinematics.

The modern version of the hierarchical robot control includes decision–making done by the neural (or, neuro–fuzzy) classifier to adapt the (manipulator) control to dynamically changing environment.

On the other hand, the so–called ‘intelligent’ approach to robot control typically represents a form of function approximation, which is itself based on some combination of neuro–fuzzy–genetic computations. Many special issues and workshops focusing on physiological models for robot control reflect the

increased attention for the development of *cerebellar models* [Sma99, SA98, Sch99, Sch98, Arb98] for learning robot control with functional decomposition, where the main result could be formulated as: *the cerebellum is more than just the function approximator*.

In this section we try to fit between these three approaches for humanoid control, emphasizing the role of muscle-like robot actuators. We propose a new, physiologically based, tensor-invariant, hierarchical force control (FC, for short) for the physiologically realistic biomechanics. We consider the muscular torque one-forms  $F_i$  as the most important component of human-like motion; therefore we propose the sophisticated hierarchical system for the subtle  $F_i$ -control: corresponding to the spinal, the cerebellar and cortical levels of human motor control.  $F_i$  are first set-up as testing input-signals to biomechanics, and then covariantly updated as feedback 1-forms  $u_i$  on each FC-level. On the spinal FC-level the nominal joint-trajectory tracking is proposed in the form of affine Hamiltonian control; here the driving torques are given corrections by spinal-reflex controls. On the cerebellar FC-level, the relation is established between canonical joint coordinates  $q^i$ ,  $p_i$  and gradient *neural-image coordinates*  $x^i$ ,  $y_i$ , representing bidirectional, self-organized, associative memory machine; here the driving torques are given the cerebellar corrections. On the cortical FC-level the topological ‘hyper-joystick’ is proposed as the central FC command-space, selector, with the fuzzy-logic feedback-control map defined on it, giving the cortical corrections to the driving torques.

The model of the spinal FC-level formulated here resembles *autogenetic motor servo*, acting on the spinal-reflex level of the human locomotor control. The model of the cerebellar FC-level formulated here mimics the self-organizing, associative function of the excitatory granule cells and the inhibitory Purkinje cells of the cerebellum [HBB96]. The model of the cortical FC-level presented in this section mimics the synergistic *regulation of locomotor conditioned reflexes* by the cerebellum [HBB96].

We believe that (already mentioned) extremely high order of the driving force redundancy in biomechanics justifies the formulation of the three-level force control system. Also, both brain-like control systems can be easily extended to provide  $SE(3)$ -based force control for moving inverse kinematics (IK) chains of legs and arms.

### Functor Control Machine

In this subsection we define the functor control-machine (compare with section (3.5) above), for the learning control with functional decomposition, by a two-step generalization of the Kalman’s theory of linear MIMO-feedback systems. The first generalization puts the Kalman’s theory into the pair of mutually dual linear categories  $\mathbf{Vect}$  and  $\mathbf{Vect}^*$  of vector spaces and linear operators, with a ‘loop-functor’ representing the closed-loop control, thus formulating the unique, categorical formalism valid both for the discrete and continual MIMO-systems.

We start with the unique, *feedforward continual-sequential state equation*

$$\dot{x}(t+1) = Ax(t) + Bu(t), \quad y(t) = Cx(t), \quad (5.37)$$

where the finite-dimensional vector spaces of *state*  $X \ni x$ , *input*  $U \ni u$ , and *output*  $Y \ni y$  have the corresponding linear operators, respectively  $A : X \rightarrow X$ ,  $B : U \rightarrow X$ , and  $C : X \rightarrow Y$ . The modular system theory comprises the *system dynamics*, given by a pair  $(X, A)$ , together with a *reachability map*  $e : U \rightarrow X$  of the pair  $(B, A)$ , and an *observability map*  $m : X \rightarrow Y$  of the pair  $(A, C)$ . If the reachability map  $e$  is surjection the system dynamics  $(X, A)$  is called *reachable*; if the observability map  $m$  is injection the system dynamics  $(X, A)$  is called *observable*. If the system dynamics  $(X, A)$  is both reachable and observable, a *composition*  $r = m \circ e : U \rightarrow Y$  defines the *total system's response*, which is given by solution of equation (5.37). If the unique solution to the continual-sequential state equation exists, it gives the answer to the (minimal) *realization problem*: find the system  $S$  that realizes the given response  $r = m \circ e : U \rightarrow Y$  (in the smallest number of discrete states and in the shortest time).

The inverse map  $r^{-1} = e^{-1} \circ m^{-1} : Y \rightarrow U$  of the total system's response  $r : U \rightarrow Y$  defines the linear *feedback operator*  $K : Y \rightarrow U$ , given by standard feedback equation

$$u(t) = Ky(t). \quad (5.38)$$

In categorical language, the feedforward system dynamics in the category  $\mathbf{Vect}$  is a pair  $(X, A)$ , where  $X \in \mathbf{Ob}(\mathbf{Vect})$  is an object in  $\mathbf{Vect}$  and  $A : X \rightarrow X \in \mathbf{Mor}(\mathbf{Vect})$  is a  $\mathbf{Vect}$ -morphism. A *feedforward decomposable system* in  $\mathbf{Vect}$  is such a sextuple  $S \equiv (X, A, U, B, Y, C)$  that  $(X, A)$  is the system dynamics in  $\mathbf{Vect}$ , a  $\mathbf{Vect}$ -morphism  $B : U \rightarrow X$  is an *input map*, and a  $\mathbf{Vect}$ -morphism  $C : X \rightarrow Y$  is an *output map*. Any object in  $\mathbf{Vect}$  is characterized by mutually dual notions of its *degree* (a number of its input morphisms) and its *codegree* (a number of its output morphisms). Similarly, any decomposable system  $S$  in  $\mathbf{Vect}$  has a *reachability map* given by an epimorphism  $e = A \circ B : U \rightarrow X$  and its dual *observability map* given by a monomorphism  $m = C \circ A : X \rightarrow Y$ ; their composition  $r = m \circ e : U \rightarrow Y$  in  $\mathbf{Mor}(\mathbf{Vect})$  defines the total system's response in  $\mathbf{Vect}$  given by the unique solution of the continual-sequential state equation (5.37) [IS01].

The dual of the total system's response, defined by the feedback equation (5.38), is the *feedback morphism*  $K = e^{-1} \circ m^{-1} : Y \rightarrow U$  belonging to the dual category  $\mathbf{Vect}^*$ .

In this way, the linear, closed-loop, continual-sequential MIMO-system (5.37–5.38) represents the *linear iterative loop functor*  $\mathcal{L} : \mathbf{Vect} \Rightarrow \mathbf{Vect}^*$ .

Our second generalization represents a *natural system process*  $\Xi[\mathcal{L}]$ , that transforms the linear loop functor  $\mathcal{L} : \mathbf{Vect} \Rightarrow \mathbf{Vect}^*$  – into the *nonlinear loop functor*  $\mathcal{NL} : \mathcal{CAT} \Rightarrow \mathcal{CAT}^*$  between two mutually dual nonlinear categories  $\mathcal{CAT}$  and  $\mathcal{CAT}^*$ . We apply the natural process  $\Xi$ , separately

1. To the feedforward decomposable system  
 $S \equiv (X, A, U, B, Y, C)$  in  $\mathbf{Vect}$ , and
2. To the feedback morphism  $K = e^{-1} \circ m^{-1} : Y \rightarrow U$  in  $\mathbf{Vect}^*$ .

Under the action of the natural process  $\Xi$ , the linear feedforward system dynamics  $(X, A)$  in  $\mathbf{Vect}$  transforms into a nonlinear feedforward  $\Xi$ -dynamics  $(\Xi[X], \Xi[A])$  in  $\mathcal{CAT}$ , represented by a *nonlinear feedforward decomposable system*,  $\Xi[S] \equiv (\Xi[X], \Xi[A], \Xi[U], \Xi[B], \Xi[Y], \Xi[C])$ .

The reachability map transforms into the *input process*  $\Xi[e] = \Xi[A] \circ \Xi[B] : \Xi[U] \rightarrow \Xi[X]$ , while its dual, observability map transforms into the *output process*  $\Xi[m] = \Xi[C] \circ \Xi[A] : \Xi[X] \rightarrow \Xi[Y]$ . In this way the total response of the linear system  $r = m \circ e : U \rightarrow Y$  in  $\mathbf{Mor}(\mathbf{Vect})$  transforms into the *nonlinear system behavior*,  $\Xi[r] = \Xi[m] \circ \Xi[e] : \Xi[U] \rightarrow \Xi[Y]$  in  $\mathbf{Mor}(\mathcal{CAT})$ . Obviously,  $\Xi[r]$ , if exists, is given by a nonlinear  $\Xi$ -transform of the linear state equations (5.37–5.38).

Analogously, the linear feedback morphism  $K = e^{-1} \circ m^{-1} : Y \rightarrow U$  in  $\mathbf{Mor}(\mathbf{Vect}^*)$  transforms into the nonlinear feedback morphism  $\Xi[K] = \Xi[e^{-1}] \circ \Xi[m^{-1}] : \Xi[Y] \rightarrow \Xi[U]$  in  $\mathbf{Mor}(\mathcal{CAT}^*)$ .

In this way, the natural system process  $\Xi : \mathcal{L} \Rightarrow \mathcal{NL}$  is established. That means that the nonlinear loop functor  $L = \Xi[\mathcal{L}] : \mathcal{CAT} \Rightarrow \mathcal{CAT}^*$  is defined out of the linear, closed-loop, continual-sequential MIMO-system (5.37).

In this section we formulate the nonlinear loop functor  $L = \Xi[\mathcal{L}] : \mathcal{CAT} \Rightarrow \mathcal{CAT}^*$  for various hierarchical levels of muscular-like FC.

### Spinal Control Level

Our first task is to establish the nonlinear loop functor  $L = \Xi[\mathcal{L}] : \mathcal{EX} \Rightarrow \mathcal{EX}^*$  on the category  $\mathcal{EX}$  of spinal FC-level.

Recall that our dissipative, driven  $\delta$ -Hamiltonian biomechanical system on the configuration manifold  $M$  is, in local canonical-symplectic coordinates  $q^i, p_i \in U_p$  on the momentum phase-space manifold  $T^*M$ , given by autonomous equations

$$\dot{q}^i = \frac{\partial H_0}{\partial p_i} + \frac{\partial R}{\partial p_i}, \quad (i = 1, \dots, N) \quad (5.39)$$

$$\dot{p}_i = F_i - \frac{\partial H_0}{\partial q^i} + \frac{\partial R}{\partial q^i}, \quad (5.40)$$

$$q^i(0) = q_0^i, \quad p_i(0) = p_i^0, \quad (5.41)$$

including contravariant equation (5.39) – the velocity vector-field, and covariant equation (5.40) – the force 1-form, together with initial joint angles  $q_0^i$  and momenta  $p_i^0$ . Here the physical Hamiltonian function  $H_0 : T^*M \rightarrow \mathbb{R}$  represents the total biomechanical energy function, in local canonical coordinates  $q^i, p_i \in U_p$  on  $T^*M$  given by

$$H_0(q, p) = \frac{1}{2} g^{ij} p_i p_j + V(q),$$

where  $g^{ij} = g^{ij}(q, m)$  denotes the contravariant material metric tensor.

Now, the *control Hamiltonian function*  $H_\gamma : T^*M \rightarrow \mathbb{R}$  of FC is in local canonical coordinates on  $T^*M$  defined by [NS90]

$$H_\gamma(q, p, u) = H_0(q, p) - q^i u_i, \quad (i = 1, \dots, N) \quad (5.42)$$

where  $u_i = u_i(t, q, p)$  are feedback-control 1-forms, representing the spinal FC-level  $u$ -corrections to the covariant torques  $F_i = F_i(t, q, p)$ .

Using  $\delta$ -Hamiltonian biomechanical system (5.39–5.41) and the control Hamiltonian function (5.42), control  $\gamma_\delta$ -Hamiltonian FC-system can be defined as

$$\begin{aligned} \dot{q}^i &= \frac{\partial H_\gamma(q, p, u)}{\partial p_i} + \frac{\partial R(q, p)}{\partial p_i}, \\ \dot{p}_i &= F_i - \frac{\partial H_\gamma(q, p, u)}{\partial q^i} + \frac{\partial R(q, p)}{\partial q^i}, \\ o^i &= -\frac{\partial H_\gamma(q, p, u)}{\partial u_i}, \quad (i = 1, \dots, N) \\ q^i(0) &= q_0^i, \quad p_i(0) = p_i^0, \end{aligned}$$

where  $o^i = o^i(t)$  represent FC natural outputs which can be different from commonly used joint angles.

If nominal reference outputs  $o_R^i = o_R^i(t)$  are known, the simple PD *stiffness-servo* [Whi87] could be formulated, via *error function*  $e(t) = o^j - o_R^j$ , in covariant form

$$u_i = K_o \delta_{ij} (o^j - o_R^j) + K_\delta \delta_{ij} (\dot{o}^j - \dot{o}_R^j), \quad (5.43)$$

where  $K$ s are the control-gains and  $\delta_{ij}$  is the Kronecker tensor.

If natural outputs  $o^i$  *actually are* the joint angles and nominal canonical trajectories ( $q_R^i = q_R^i(t)$ ,  $p_i^R = p_i^R(t)$ ) are known, then the stiffness-servo (5.43) could be formulated in canonical form as

$$u_i = K_q \delta_{ij} (q^i - q_R^i) + K_p (p_i - p_i^R).$$

Now, using the fuzzified  $\mu$ -Hamiltonian biomechanical system with fuzzy system numbers (i.e, imprecise segment lengths, masses and moments of inertia, joint dampings and muscular actuator parameters)

$$\dot{q}^i = \frac{\partial H_0(q, p, \sigma_\mu)}{\partial p_i} + \frac{\partial R}{\partial p_i}, \quad (5.44)$$

$$\dot{p}_i = \bar{F}_i - \frac{\partial H_0(q, p, \sigma_\mu)}{\partial q^i} + \frac{\partial R}{\partial q^i}, \quad (5.45)$$

$$q^i(0) = \bar{q}_0^i, \quad p_i(0) = \bar{p}_i^0, \quad (i = 1, \dots, N), \quad (5.46)$$

(see 3.5.4 above) and the control Hamiltonian function (5.42),  $\gamma_\mu$ -Hamiltonian FC-system can be defined as

$$\begin{aligned}\dot{q}^i &= \frac{\partial H_\gamma(q, p, u, \sigma_\mu)}{\partial p_i} + \frac{\partial R(q, p)}{\partial p_i}, \\ \dot{p}_i &= \bar{F}_i - \frac{\partial H_\gamma(q, p, u, \sigma_\mu)}{\partial q^i} + \frac{\partial R(q, p)}{\partial q^i}, \\ \dot{\sigma}^i &= -\frac{\partial H_\gamma(q, p, u, \sigma_\mu)}{\partial u_i}, \quad q^i(0) = \bar{q}_0^i, \quad p_i(0) = \bar{p}_i^0,\end{aligned}$$

where  $\bar{\sigma}^i = \bar{\sigma}^i(t)$  represent the fuzzified natural outputs.

Finally, applying stochastic forces (diffusion fluctuations  $B_{ij}[q^i(t), t]$  and discontinuous jumps in the form of ND Wiener process  $W^j(t)$ ), i.e., using the fuzzy-stochastic  $[\mu\sigma]$ -Hamiltonian biomechanical system

$$dq^i = \left( \frac{\partial H_0(q, p, \sigma_\mu)}{\partial p_i} + \frac{\partial R}{\partial p_i} \right) dt, \quad (5.47)$$

$$\begin{aligned}dp_i &= B_{ij}[q^i(t), t] dW^j(t) + \\ &\quad \left( \bar{F}_i - \frac{\partial H_0(q, p, \sigma_\mu)}{\partial q^i} + \frac{\partial R}{\partial q^i} \right) dt, \quad (5.48)\end{aligned}$$

$$q^i(0) = \bar{q}_0^i, \quad p_i(0) = \bar{p}_i^0. \quad (5.49)$$

(see 3.5.4 above), and the control Hamiltonian function (5.42),  $\gamma_{\mu\sigma}$ -Hamiltonian FC-system can be defined as

$$\begin{aligned}dq^i &= \left( \frac{\partial H_\gamma(q, p, u, \sigma_\mu)}{\partial p_i} + \frac{\partial R(q, p)}{\partial p_i} \right) dt, \\ dp_i &= B_{ij}[q^i(t), t] dW^j(t) + \\ &\quad \left( \bar{F}_i - \frac{\partial H_\gamma(q, p, u, \sigma_\mu)}{\partial q^i} + \frac{\partial R(q, p)}{\partial q^i} \right) dt, \\ d\bar{\sigma}^i &= -\frac{\partial H_\gamma(q, p, u, \sigma_\mu)}{\partial u_i} dt, \quad (i = 1, \dots, N) \\ q^i(0) &= \bar{q}_0^i, \quad p_i(0) = \bar{p}_i^0.\end{aligned}$$

If we have the case that not all of the configuration joints on the configuration manifold  $M$  are active in the specified robot task, we can introduce the coupling Hamiltonians  $H^j = H^j(q, p)$ ,  $j = 1, \dots, M \leq N$ , corresponding to the system's active joints, and we come to *affine Hamiltonian function*  $H_a : T^*M \rightarrow \mathbb{R}$ , in local canonical coordinates on  $T^*M$  given as [NS90]

$$H_a(q, p, u) = H_0(q, p) - H^j(q, p) u_j. \quad (5.50)$$

Using  $\delta$ -Hamiltonian biomechanical system (5.39–5.41) and the affine Hamiltonian function (5.50), affine  $a_\delta$ -Hamiltonian FC-system can be defined as

$$\dot{q}^i = \frac{\partial H_0(q, p)}{\partial p_i} - \frac{\partial H^j(q, p)}{\partial p_i} u_j + \frac{\partial R}{\partial p_i}, \quad (5.51)$$

$$\dot{p}_i = F_i - \frac{\partial H_0(q, p)}{\partial q^i} + \frac{\partial H^j(q, p)}{\partial q^i} u_j + \frac{\partial R}{\partial q^i}, \quad (5.52)$$

$$\dot{o}^i = -\frac{\partial H_a(q, p, u)}{\partial u_i} = H^j(q, p), \quad (5.53)$$

$$q^i(0) = q_0^i, \quad p_i(0) = p_i^0, \quad (5.54)$$

$$(i = 1, \dots, N; \quad j = 1, \dots, M \leq N).$$

Using the Lie-derivative exact feedback linearization (see (5.2.1) above), and applying the *constant relative degree*  $r$  (see [Isi89, SI89]) to all  $N$  joints of the affine  $a_\delta$ -Hamiltonian FC-system (5.51–5.54), the control law for asymptotic tracking the reference outputs  $\sigma_R^j$  could be formulated as

$$u_j = \frac{\dot{\sigma}_R^{(r)j} - \mathcal{L}_f^{(r)} H^j + \sum_{s=1}^r \gamma_{s-1} (\sigma_R^{(s-1)j} - \mathcal{L}_f^{(s-1)} H^j)}{\mathcal{L}_g \mathcal{L}_f^{(r-1)} H^j},$$

where standard MIMO-vector-fields  $f$  and  $g$  are given by

$$f = \left( \frac{\partial H_0}{\partial p_i}, -\frac{\partial H_0}{\partial q^i} \right), \quad g = \left( -\frac{\partial H^j}{\partial p_i}, \frac{\partial H^j}{\partial q^i} \right)$$

and  $\gamma_{s-1}$  are the coefficients of linear differential equation of order  $r$  for the error function  $e(t) = \sigma^j - \sigma_R^j$

$$e^{(r)} + \gamma_{r-1} e^{(r-1)} + \dots + \gamma_1 e^{(1)} + \gamma_0 e = 0.$$

Using the fuzzified  $\mu$ -Hamiltonian biomechanical system (5.44–5.46) and the affine Hamiltonian function (5.50), affine  $a_\mu$ -Hamiltonian FC-system can be defined as

$$\dot{q}^i = \frac{\partial H_0(q, p, \sigma_\mu)}{\partial p_i} - \frac{\partial H^j(q, p, \sigma_\mu)}{\partial p_i} u_j + \frac{\partial R(q, p)}{\partial p_i},$$

$$\dot{p}_i = \bar{F}_i - \frac{\partial H_0(q, p, \sigma_\mu)}{\partial q^i} + \frac{\partial H^j(q, p, \sigma_\mu)}{\partial q^i} u_j + \frac{\partial R(q, p)}{\partial q^i},$$

$$\dot{\sigma}^i = -\frac{\partial H_a(q, p, u, \sigma_\mu)}{\partial u_i} = H^j(q, p, \sigma_\mu),$$

$$q^i(0) = \bar{q}_0^i, \quad p_i(0) = \bar{p}_i^0, \quad (i = 1, \dots, N; \quad j = 1, \dots, M \leq N).$$

Using the fuzzy-stochastic  $[\mu\sigma]$ -Hamiltonian biomechanical system (5.47–5.49) and the affine Hamiltonian function (5.50), affine  $a_{\mu\sigma}$ -Hamiltonian FC-system can be defined as

$$\begin{aligned}
dq^i &= \left( \frac{\partial H_0(q, p, \sigma_\mu)}{\partial p_i} - \frac{\partial H^j(q, p, \sigma_\mu)}{\partial p_i} u_j + \frac{\partial R(q, p)}{\partial p_i} \right) dt, \\
dp_i &= B_{ij}[q^i(t), t] dW^j(t) + \\
&\quad \left( \bar{F}_i - \frac{\partial H_0(q, p, \sigma_\mu)}{\partial q^i} + \frac{\partial H^j(q, p, \sigma_\mu)}{\partial q^i} u_j + \frac{\partial R(q, p)}{\partial q^i} \right) dt, \\
d\bar{o}^i &= -\frac{\partial H_a(q, p, u, \sigma_\mu)}{\partial u_i} dt = H^j(q, p, \sigma_\mu) dt, \\
q^i(0) &= \bar{q}_0^i, \quad p_i(0) = \bar{p}_i^0, \quad (i = 1, \dots, N; j = 1, \dots, M \leq N).
\end{aligned}$$

Being high-degree and highly nonlinear, all of these affine control systems are extremely sensitive upon the variation of parameters, inputs, and initial conditions. The sensitivity function  $S$  of the affine Hamiltonian  $H_a(q, p, u)$  upon the parameters  $\beta_i$  (representing segment lengths  $L_i$ , masses  $m_i$ , moments of inertia  $J_i$  and joint dampings  $b_i$ , see [IS01, Iva91]), is in the case of  $a_\delta$ -Hamiltonian FC-system defined as

$$S(H, \beta) = \frac{\beta_i}{H_a(q, p, u)} \frac{\partial H_a(q, p, u)}{\partial \beta_i},$$

and similarly in other two  $a_\mu$ - and  $a_{\mu\sigma}$ - cases.

The three affine FC-level systems  $a_\delta$ ,  $a_\mu$  and  $a_{\mu\sigma}$ , resemble (in a fuzzy-stochastic-Hamiltonian form), Houk's autogenetic motor servo of muscle spindle and Golgi tendon proprioceptors [Hou79], correcting the covariant driving torques  $F_i = F_i(t, q, p)$  by local 'reflex controls'  $u_i(t, q, p)$ . They form the nonlinear loop functor  $L = \Xi[\mathcal{L}] : \mathcal{E}\mathcal{X} \Rightarrow \mathcal{E}\mathcal{X}^*$ .

### Cerebellar Control Level

Our second task is to establish the nonlinear loop functor  $L = \Xi[\mathcal{L}] : \mathcal{T}\mathcal{A} \Rightarrow \mathcal{T}\mathcal{A}^*$  on the category  $\mathcal{T}\mathcal{A}$  of the cerebellar FC-level. Here we propose an oscillatory neurodynamical  $(x, y, \omega)$ -system (adapted from [IJB99a]), a bidirectional, self-organized, associative-memory machine, resembling the function of a set of excitatory granule cells and inhibitory Purkinje cells in the middle layer of the cerebellum (see [EIS67, HBB96]). The neurodynamical  $(x, y, \omega)$ -system acts on *neural-image manifold*  $M_{im}^N$  of the configuration manifold  $M^N$  as a pair of smooth, '1-1' and 'onto' maps  $(\Psi, \Psi^{-1})$ , where  $\Psi : M^N \rightarrow M_{im}^N$  represents the feedforward map, and  $\Psi^{-1} : M_{im}^N \rightarrow M^N$  represents the feedback map. Locally, it is defined in Riemannian neural coordinates  $x^i, y_i \in V_y$  on  $M_{im}^N$ , which are in bijective correspondence with symplectic joint coordinates  $q^i, p_i \in U_p$  on  $T^*M$ .

The  $(x, y, \omega)$ -system is formed out of two distinct, yet nonlinearly-coupled neural subsystems, with  $A^i(q)$  (A.37) and  $B_i(p)$  (5.58) as system inputs, and the feedback-control 1-forms  $u_i$  (5.63) as system outputs:

1. Granule cells excitatory (contravariant) and Purkinje cells inhibitory (covariant) activation  $(x, y)$ -dynamics (A.35–5.58), defined respectively by a vector-field  $x^i = x^i(t) : M \rightarrow TM$ , representing a cross-section of the tangent bundle  $TM$ , and a 1-form  $y_i = y_i(t) : M \rightarrow T^*M$ , representing a cross-section of the cotangent bundle  $T^*M$ ; and
2. Excitatory and inhibitory unsupervised learning  $(\omega)$ -dynamics (5.58–5.60) generated by random differential Hebbian learning process (5.61–5.63), defined respectively by contravariant synaptic tensor-field  $\omega^{ij} = \omega^{ij}(t) : M \rightarrow TTM_{im}^N$  and covariant synaptic tensor-field  $\omega_{ij} = \omega_{ij}(t) : M \rightarrow T^*T^*M$ , representing cross-sections of contravariant and covariant tensor bundles, respectively.

The system equations are defined as

$$\dot{x}^i = A^i(q) + \omega^{ij} f_j(y) - x^i, \quad (5.55)$$

$$\dot{y}_i = B_i(p) + \omega_{ij} f^j(x) - y_i, \quad (5.56)$$

$$A^i(q) = K_q(q^i - q_R^i), \quad (5.57)$$

$$B_i(p) = K_p(p_i^R - p_i), \quad (5.58)$$

$$\dot{\omega}^{ij} = -\omega^{ij} + I^{ij}(x, y), \quad (5.59)$$

$$\dot{\omega}_{ij} = -\omega_{ij} + I_{ij}(x, y), \quad (5.60)$$

$$I^{ij} = f^i(x) f^j(y) + \dot{f}^i(x) \dot{f}^j(y) + \sigma^{ij}, \quad (5.61)$$

$$I_{ij} = f_i(x) f_j(y) + \dot{f}_i(x) \dot{f}_j(y) + \sigma_{ij}, \quad (5.62)$$

$$u_i = \frac{1}{2}(\delta_{ij} x^i + y_i), \quad (i, j = 1, \dots, N). \quad (5.63)$$

Here  $\omega$  is a symmetric 2nd order synaptic tensor-field;  $I^{ij} = I^{ij}(x, y, \sigma)$  and  $I_{ij} = I_{ij}(x, y, \sigma)$  respectively denote contravariant-excitatory and covariant-inhibitory random differential Hebbian innovation-functions with tensorial Gaussian noise  $\sigma$  (in both variances);  $f$ s and  $\dot{f}$ s denote sigmoid activation functions ( $f = \tanh(\cdot)$ ) and corresponding signal velocities ( $\dot{f} = 1 - f^2$ ), respectively in both variances;

$A^i(q)$  and  $B_i(p)$  are contravariant-excitatory and covariant-inhibitory neural inputs to granule and Purkinje cells, respectively;  $u_i$  are the corrections to the feedback-control 1-forms on the cerebellar FC-level.

Nonlinear activation  $(x, y)$ -dynamics (A.35–5.58), describes a two-phase biological neural oscillator field, in which excitatory neural field excites inhibitory neural field, which itself reciprocally inhibits the excitatory one.  $(x, y)$ -dynamics represents a nonlinear extension of a linear, Lyapunov-stable, conservative, gradient system, defined in local neural coordinates  $x^i, y_i \in V_y$  on  $T^*M$  as

$$\dot{x}^i = -\frac{\partial \Phi}{\partial y_i} = \omega^{ij} y_j - x^i, \quad \dot{y}_i = -\frac{\partial \Phi}{\partial x^i} = \omega_{ij} x^j - y_i. \quad (5.64)$$

The gradient system (5.64) is derived from scalar, neuro-synaptic action potential  $\Phi : T^*M \rightarrow \mathbb{R}$ , given by a negative, smooth bilinear form in  $x^i, y_i \in V_y$  on  $T^*M$  as

$$-2\Phi = \omega_{ij}x^ix^j + \omega^{ij}y_iy_j - 2x^iy_i, \quad (i, j = 1, \dots, N), \quad (5.65)$$

which itself represents a  $\Psi$ -image of the Riemannian metrics  $g : TM \rightarrow \mathbb{R}$  on the configuration manifold  $M$ .

The nonlinear oscillatory activation  $(x, y)$ -dynamics (A.35–5.58) is obtained from the linear conservative dynamics (5.64) by adding configuration-dependent inputs  $A^i$  and  $B_i$ , as well as sigmoid activation functions  $f_j$  and  $f^j$ , respectively. It represents an interconnected pair of excitatory and inhibitory neural fields.

Both variant-forms of learning  $(\omega)$ -dynamics (5.59–5.60) are given by generalized unsupervised (self-organizing) Hebbian learning scheme (see [Kos92]) in which  $\dot{\omega}_{ij}$  (resp.  $\dot{\omega}^{ij}$ ) denotes the new-update value,  $-\omega_{ij}$  (resp.  $-\omega^{ij}$ ) corresponds to the old value and  $I_{ij}(x^i, y_j)$  (resp.  $I^{ij}(x^i, y_j)$ ) is the innovation function of the symmetric 2nd order synaptic tensor-field  $\omega$ . The nonlinear innovation functions  $I_{ij}$  and  $I^{ij}$  are defined by random differential Hebbian learning process (5.61–5.62). As  $\omega$  is symmetric and zero-trace coupling synaptic tensor, the conservative linear activation dynamics (5.64) is equivalent to the rule that the state of each neuron (in both neural fields) is changed in time iff the scalar action potential  $\Phi$  (5.65), is lowered. Therefore, the scalar action potential  $\Phi$  represents the monotonically decreasing Lyapunov function (such that  $\dot{\Phi} \leq 0$ ) for the conservative linear dynamics (5.64), which converges to a local minimum or ground state of  $\Phi$ . That is to say, the system (5.64) moves in the direction of decreasing the scalar action potential  $\Phi$ , and when both  $\dot{x}^i = 0$  and  $\dot{y}_i = 0$  for all  $i = 1, \dots, N$ , the steady state is reached.

In this way, the neurodynamical  $(x, y, \omega)$ -system acts as tensor-invariant self-organizing (excitatory / inhibitory) associative memory machine, resembling the set of granule and Purkinje cells of cerebellum [HBB96].

The feedforward map  $\Psi : M \rightarrow M$  is realized by the inputs  $A^i(q)$  and  $B_i(p)$  to the  $(x, y, \omega)$ -system, while the feedback map  $\Psi^{-1} : M \rightarrow M$  is realized by the system output, i.e., the feedback-control 1-forms  $u_i(x, y)$ . These represent the cerebellar FC-level corrections to the covariant torques  $F_i = F_i(t, q, p)$ .

The tensor-invariant form of the oscillatory neurodynamical  $(x, y, \omega)$ -system (A.35–5.63) resembles the associative action of the granule and Purkinje cells in the tuning of the limb cortico-rubro-cerebellar recurrent network [HBB96], giving the cerebellar correction  $u_i(x, y)$  to the covariant driving torques  $F_i = F_i(t, q, p)$ . In this way  $(x, y, \omega)$ -system forms the nonlinear loop functor  $L = \Xi[\mathcal{L}] : \mathcal{TA} \Rightarrow \mathcal{TA}^*$ .

**Cortical Control Level**

Our third task is to establish the nonlinear loop functor  $L = \Xi[\mathcal{L}] : \mathcal{ST} \Rightarrow \mathcal{ST}^*$  on the category  $\mathcal{ST}$  of the cortical FC-level.

Recall that for the purpose of cortical control, the purely rotational biomechanical manifold  $M$  could be firstly reduced to  $N$ -torus and subsequently transformed to  $N$ -cube ('hyper-joystick'), using the following geometric techniques (see (2.4.4) above).

Denote by  $S^1$  the constrained unit circle in the complex plane. This is an Abelian Lie group. We have two reduction homeomorphisms

$$SO(3) \gtrsim SO(2) \triangleright SO(2) \triangleright SO(2), \quad \text{and} \quad SO(2) \approx S^1,$$

where ' $\triangleright$ ' denotes the noncommutative semidirect product.

Next, let  $I^N$  be the unit cube  $[0, 1]^N$  in  $\mathbb{R}^N$  and ' $\sim$ ' an equivalence relation on  $\mathbb{R}^N$  obtained by 'gluing' together the opposite sides of  $I^N$ , preserving their orientation. Therefore,  $M$  can be represented as the quotient space of  $\mathbb{R}^N$  by the space of the integral lattice points in  $\mathbb{R}^N$ , that is a constrained torus  $T^N$ :

$$\mathbb{R}^N / Z^N = I^N / \sim \cong \prod_{i=1}^N S_i^1 \equiv \{(q^i, i = 1, \dots, N) : \text{mod } 2\pi\} = T^N.$$

In the same way, the momentum phase-space manifold  $T^*M$  can be represented by  $T^*T^N$ .

Conversely by 'ungluing' the configuration space we get the primary unit cube. Let ' $\sim^*$ ' denote an equivalent decomposition or 'ungluing' relation. By the *Tychonoff product-topology theorem*, for every such quotient space there exists a 'selector' such that their quotient models are homeomorphic, that is,  $T^N / \sim^* \approx A^N / \sim^*$ . Therefore  $I_q^N$  represents a 'selector' for the configuration torus  $T^N$  and can be used as an  $N$ -directional ' $\hat{q}$ -command-space' for FC. Any subset of DOF on the configuration torus  $T^N$  representing the joints included in the general biomechanics has its simple, rectangular image in the rectified  $\hat{q}$ -command space – selector  $I_q^N$ , and any joint angle  $q^i$  has its rectified image  $\hat{q}^i$ .

In the case of an end-effector,  $\hat{q}^i$  reduces to the position vector in external-Cartesian coordinates  $z^r$  ( $r = 1, \dots, 3$ ). If orientation of the end-effector can be neglected, this gives a topological solution to the standard inverse kinematics problem.

Analogously, all momenta  $\hat{p}_i$  have their images as rectified momenta  $\hat{p}_i$  in the  $\hat{p}$ -command space – selector  $I_p^N$ . Therefore, the total momentum phase-space manifold  $T^*T^N$  obtains its 'cortical image' as the  $(\widehat{q, p})$ -command space, a trivial 2ND bundle  $I_q^N \times I_p^N$ .

Now, the simplest way to perform the feedback FC on the cortical  $(\widehat{q, p})$ -command space  $I_q^N \times I_p^N$ , and also to mimic the cortical-like behavior [1,2],

is to use the 2ND fuzzy-logic controller, in pretty much the same way as in popular ‘inverted pendulum’ examples [Kos92, Kos96].

We propose the fuzzy feedback-control map  $\Xi$  that maps all the rectified joint angles and momenta into the feedback-control 1-forms

$$\Xi : (\hat{q}^i(t), \hat{p}_i(t)) \mapsto u_i(t, q, p), \quad (5.66)$$

so that their corresponding universes of discourse,  $\hat{M}^i = (\hat{q}_{max}^i - \hat{q}_{min}^i)$ ,  $\hat{P}_i = (\hat{p}_i^{max} - \hat{p}_i^{min})$  and  $U_i = (u_i^{max} - u_i^{min})$ , respectively, are mapped as

$$\Xi : \prod_{i=1}^N \hat{M}^i \times \prod_{i=1}^N \hat{P}_i \rightarrow \prod_{i=1}^N U_i. \quad (5.67)$$

The 2N-D map  $\Xi$  (5.66–5.67) represents a *fuzzy inference system*, defined by (adapted from [IJB99b]):

1. *Fuzzification* of the crisp *rectified* and *discretized* angles, momenta and controls using Gaussian-bell membership functions

$$\mu_k(\chi) = \exp\left[-\frac{(\chi - m_k)^2}{2\sigma_k}\right], \quad (k = 1, 2, \dots, 9),$$

where  $\chi \in D$  is the common symbol for  $\hat{q}^i$ ,  $\hat{p}_i$  and  $u_i(q, p)$  and  $D$  is the common symbol for  $M^i$ ,  $\hat{P}_i$  and  $U_i$ ; the mean values  $m_k$  of the seven partitions of each universe of discourse  $D$  are defined as  $m_k = \lambda_k D + \chi_{min}$ , with partition coefficients  $\lambda_k$  uniformly spanning the range of  $D$ , corresponding to the set of nine linguistic variables  $L = \{NL, NB, NM, NS, ZE, PS, PM, PB, PL\}$ ; standard deviations are kept constant  $\sigma_k = D/9$ . Using the linguistic vector  $L$ , the  $9 \times 9$  FAM (fuzzy associative memory) matrix (a ‘linguistic phase-plane’), is heuristically defined for each human joint, in a symmetrical weighted form

$$\mu_{kl} = \varpi_{kl} \exp\{-50[\lambda_k + u(q, p)]^2\}, \quad (k, l = 1, 2, \dots, 9)$$

with weights  $\varpi_{kl} \in \{0.6, 0.6, 0.7, 0.7, 0.8, 0.8, 0.9, 0.9, 1.0\}$ .

2. *Mamdani inference* is used on each FAM-matrix  $\mu_{kl}$  for all human joints:
  - (i)  $\mu(\hat{q}^i)$  and  $\mu(\hat{p}_i)$  are combined inside the fuzzy IF-THEN rules using AND (Intersection, or Minimum) operator,

$$\mu_k[\bar{u}_i(q, p)] = \min\{\mu_{kl}(\hat{q}^i), \mu_{kl}(\hat{p}_i)\}.$$

(ii) the output sets from different IF-THEN rules are then combined using OR (Union, or Maximum) operator, to get the final output, fuzzy-covariant torques,

$$\mu[u_i(q, p)] = \max_k\{\mu_k[\bar{u}_i(q, p)]\}.$$

3. Defuzzification of the fuzzy controls  $\mu[u_i(q, p)]$  with the ‘center of gravity’ method

$$u_i(q, p) = \frac{\int \mu[u_i(q, p)] du_i}{\int du_i},$$

to update the crisp feedback-control 1-forms  $u_i = u_i(t, q, p)$ . These represent the cortical FC-level corrections to the covariant torques  $F_i = F_i(t, q, p)$ .

Operationally, the construction of the cortical  $(\widehat{q, p})$ -command space  $I_q^N \times I_p^N$  and the 2ND feedback map  $\Xi$  (5.66–5.67), mimic the regulation of locomotor conditioned reflexes by the motor cortex [HBB96], giving the cortical correction to the covariant driving torques  $F_i$ . Together they form the nonlinear loop functor  $\mathcal{NL} = \Xi[\mathcal{L}] : \mathcal{ST} \Rightarrow \mathcal{ST}^*$ .

A sample output from the leading human-motion simulator, *Human Biodynamics Engine* (developed by the authors in Defence Science & Technology Organisation, Australia), is given in Figure 5.5, giving the sophisticated 264 DOF analysis of adult male running with the speed of 5 m/s.

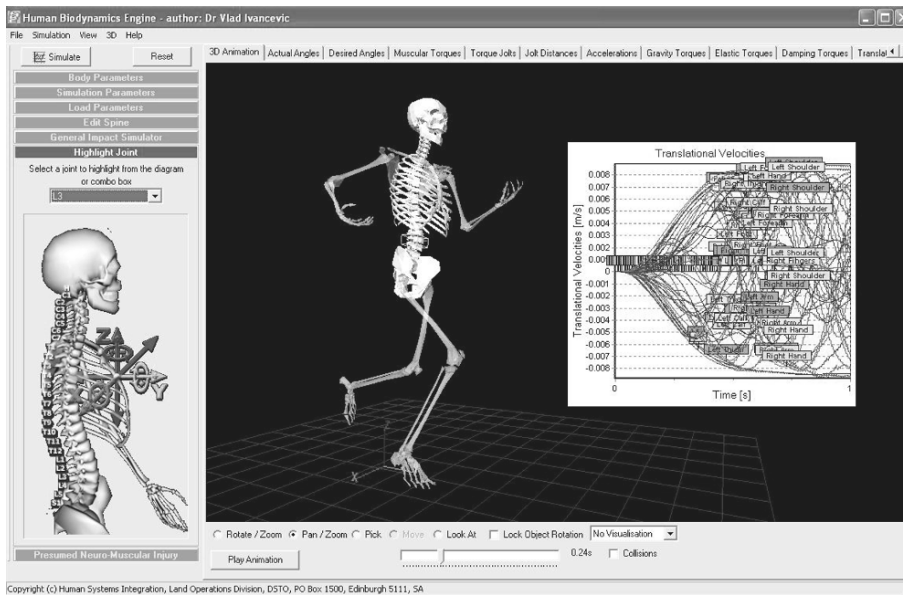


Fig. 5.11. Sample output from the Human Biodynamics Engine: running with the speed of 5 m/s.

## Covariant Biophysics of Electro–Muscular Stimulation

In this Chapter we develop covariant biophysics of electro–muscular stimulation, as an externally induced generator of our *covariant muscular forces*,  $F_i = mg_{ij}a^j$ . The so-called *functional electrical stimulation* (FES) of human skeletal muscles is used in rehabilitation and in medical orthotics to externally stimulate the muscles with damaged neural control (see, e.g., [VHI87]). However, the repetitive use of electro–muscular stimulation, besides functional, causes also structural changes in the stimulated muscles, giving the physiological effect of muscular training.

### 6.1 Basics of Electrical Muscular Stimulation

The use of low and very low frequency impulses in the body, delivered through electrodes, is known as transcutaneous stimulation of the nerves, electro–acupuncture and electro–stimulation. Here, an electromagnetic field accompanies the passage of the electric current through the conductive wire. This is generally known as the term ‘electromagnetic therapy’.

In the original sense acupuncture meant the inserting of needles in specific regions of the body. Electro–acupuncture supplies the body with low–volt impulses through the medium of surface electrodes to specific body regions or by non specific electrodes. Transcutaneous electric stimulation of the nerves (TENS) has for years been a well known procedure in conventional medicine. The impulses that are produced with this type of stimulation, are almost identical with those of electro–stimulation, yet many doctors still assume, that they are two different therapies. This has resulted in TENS being considered as a daily therapy, while electro–acupuncture or electro–stimulation were treated as ‘alternative therapy’. Apart from the fact, that electro–acupuncture electro–impulses are delivered through needles, both therapies should be considered identical. Patients, who have reservations about the use of needles, can by the use of electric impulses over surface electrodes on the skin, have a satisfactory alternative (see Figure 6.1). We choose the term electro–stimulation,

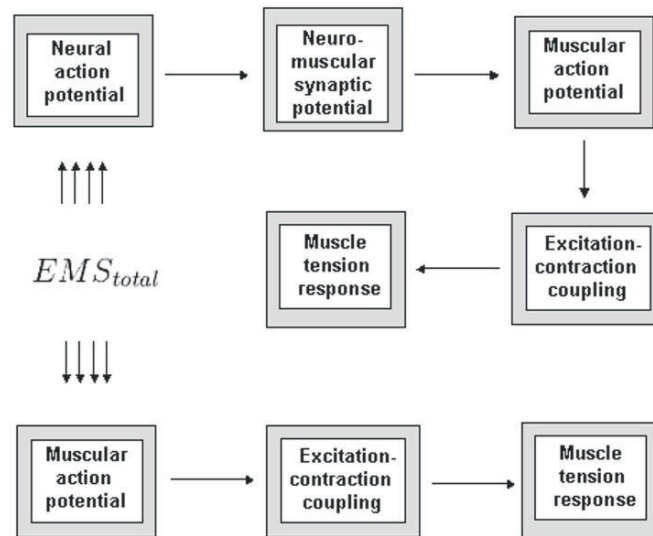


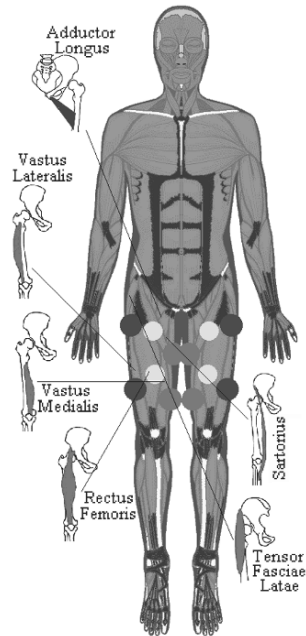
Fig. 6.1. Schematic of electrical muscular stimulation  $EMS$ .

because the acupuncture system is not included in all therapies. Clinical tests have showed that there are two specific types of reactions:

- The first reaction is spontaneous and dependent on the choice of body region. The stimulation of this part of the body results in an unloading, that can be compared with that of a battery. Normally this goes hand in hand with an immediate improvement in the patient. This effect of unloading may also be reached by non-specific electric stimulation.
- The second normal reaction is of a delayed nature, that results in relaxation and control of pain. Moreover two other important effects follow, that begin between 10 and 20 minutes after the start of the treatment. This reaction is associated (combined) with different chemicals, such as beta-endorphins and 5-hydroxytryptamins. When using low and very low frequency stimulations, the second effect is obtained by the utilization of specific frequencies on the body. This is independent of the choice of a specific part of the body, because the connected electromagnet makes the induction of secondary electric current in the whole body possible.

Now, when cosmetic surgeons perform *electrical muscular stimulation* ( $EMS$ , for short) on the human face or body (as schematically depicted on Figure 6.1), they usually take for granted half-a-dozen biophysical processes that are actually involved in this apparently simple *stimulus-response-type* action.

When the surface electrical muscular stimulation  $EMS$  pads are applied to the certain place of the human face or body, the first considerable tissue reaction is depolarization of sarcolemma, close to the electrodes. Muscular ability



**Fig. 6.2.** Surface *EMS* performed on the human leg, together with anatomy of the stimulated leg muscles.

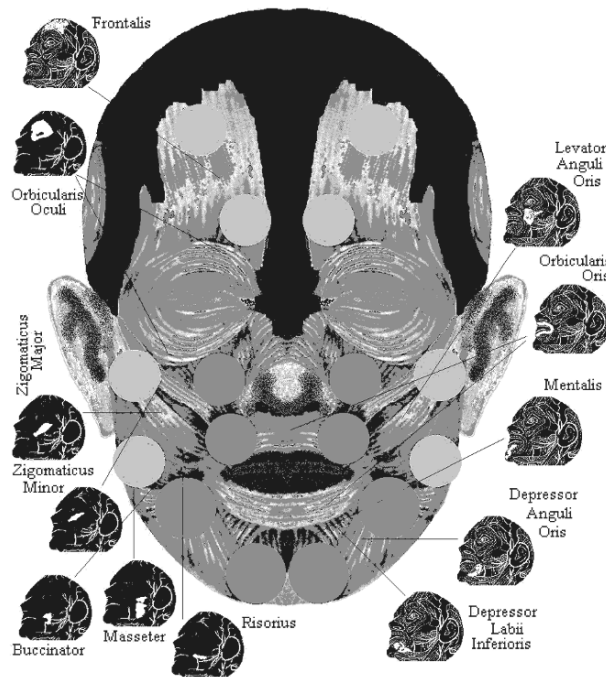
(similar to the neural one, but about ten times slower) to produce an action potential as a response to the stimulation, is termed ‘excitability’. By means of the *EMS*, current is passed across a membrane to produce a transient depolarization of the resting potential of sarcolemma, which, if it is of sufficient duration and magnitude, can initiate the train of events that produces muscular action potential (see Figure 6.1). The minimum necessary intensity of stimulus is called the threshold stimulus. The term ‘threshold’ is commonly used to refer either to the absolute magnitude of the muscle–cell membrane potential at which an action potential is initiated or to the magnitude of depolarization from resting potential (in which the membrane naturally polarizes sodium and potassium ions) required to initiate an action potential. A stimulus of less than threshold intensity is referred to as subthreshold, one of greater than threshold intensity as super–threshold. The threshold potential for excitation is not a fixed parameter. The thresholds of different muscle–membranes may vary considerably. Furthermore, the threshold of a single cell can change, either rapidly, as after a train of impulses produced by the  $EMS_{total}$ , or more slowly, in response to metabolic or hormonal influences.

On the other hand, in view of modern biophysics, there are *six distinctive phases of electrical muscular stimulation*, as usually performed using the surface pads (like those on Figures 6.1 and 6.1):

1. *Electrodynamic stimulation fields*, consisting of:
  - a) External Maxwell electrodynamics (smooth, causal, unique and fully predictive); and
  - b) Internal cellular bio–quantum electrodynamics (rapidly fluctuating, uncertain and stochastic, allowing only probabilistic approach).
2. *Muscular contraction paths*, consisting of:
  - a) Anatomical external muscular mechanics; and
  - b) Myofibrillar internal cellular bio–quantum mechanics.
3. *Geometric face & body shapes and curvatures*, consisting of:
  - a) Smooth 2D external skin geometry; and
  - b) Coarse–grained and fractal, internal  $n$ D cellular muscle–fat geometry.

Combined together, these six electro–mechano–geometric faces of electro–muscular stimulation generate the three–link *EMS–transition functor*:

$$\text{ELECTRICAL STIMUL} \Rightarrow \text{MUSCULAR CONTRACT} \Rightarrow \text{FACE or BODY SHAPE}$$



**Fig. 6.3.** Surface *EMS* performed on the human face, together with anatomy of the stimulated facial muscles (elaborated further in Table 6.5.1).

The *EMS* transition functor is based on Feynman–like experimental approach to electrical muscular stimulation (see Figure 6.2): the flow of elec-

tric current from the negative surface pad  $A^\ominus$  to the positive pad  $B^\oplus$  can be approximated by the vector sum of complex vectors  $\sum_k \rho_k e^{i\theta_k} = \rho_k(\cos \theta_k + i \sin \theta_k)$ , (in the complex plane), where  $\theta_k$  are proportional to the time taken by each vector  $\rho_k$ . This vector sum will be developed into the proper Feynman path integral (see [Fey98]).

The purpose of this Chapter is a modern and rigorous description of the above transition map, by elaboration of the six electro–mechano–geometric facets of the surface electro–muscular stimulation. All relevant classical biophysical theories are given in Appendix.

## 6.2 EMS Functor

Biophysically, electrical muscular stimulation represents a union of external electrical stimulation fields, internal myofibrillar excitation–contraction paths, and dissipative skin & fat geometries, formally written as

$$EMS_{total} = EMS_{fields} \cup EMS_{paths} \cup EMS_{geom}. \quad (6.1)$$

Following the current trends of the XXI century biophysics, corresponding to each of the three  $EMS$ –phases in (6.1) we formulate:

1. The *least action principle* (see section 3.3 above), to model a unique, external–anatomical, predictive and smooth, macroscopic  $EMS$  field–path–geometry; and
2. Associated *Feynman path integral* (see subsection 3.3.7 above), to model an ensemble of rapidly and stochastically fluctuating, internal, microscopic, fields–paths–geometries of the cellular  $EMS$ , to which the external–anatomical macro–level represents both time and ensemble *average*.<sup>1</sup>

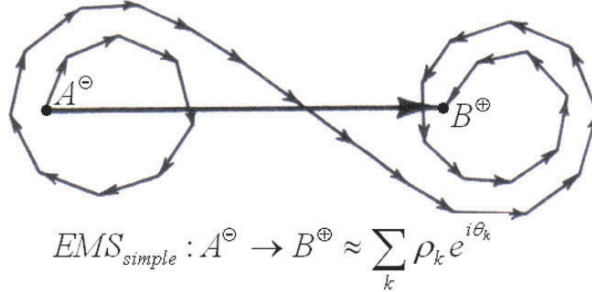
In the proposed formalism, muscular excitation–contraction paths  $x^i(t)$  are caused by electrodynamic stimulation fields  $F^k(t)$ , while they are both affected by dissipative and noisy skin & fat shapes and curvatures, defined by the local *Riemannian metric tensor*  $g_{ij}$ .

In the following text, we first formulate the global model for the  $EMS_{total}$ , to set up the general formalism to be specialized subsequently for each of the three  $EMS$ –phases.

### 6.2.1 Global macro–level of $EMS_{total}$

In general, at the *macroscopic*  $EMS$ –level we first formulate the *total action*  $S[\mathcal{P}]$ , our central quantity, which can be described through physical dimensions of *Energy*  $\times$  *Time* = *Effort* (which is also the dimension of the *Planck constant*  $\hbar$  (= 1 in normal units) (see, e.g., [DEF99]). This total action quantity

<sup>1</sup> Recall that *ergodic hypothesis* equates *time average* with *ensemble average*.



**Fig. 6.4.** Simplified Feynman–like experimental approach to electrical muscular stimulation: the flow of electric current from the negative surface pad  $A^\ominus$  to the positive pad  $B^\oplus$  can be approximated by the vector sum of complex vectors  $\rho_k e^{i\theta_k}$ , where  $\theta_k$  are proportional to the time taken by each vector  $\rho_k$ ; this vector sum will be further developed into Feynman integral (see [Fey98]).

has immediate biophysical ramifications: *the greater the action – the higher the stimulation effect on the new shape*. The action  $S[\Phi]$  depends on macroscopic fields, paths and geometries, commonly denoted by an abstract field symbol  $\Phi^i$ . The action  $S[\Phi]$  is formally defined as a temporal integral from the *initial* time instant  $t_{ini}$  to the *final* time instant  $t_{fin}$ ,

$$S[\Phi] = \int_{t_{ini}}^{t_{fin}} \mathfrak{L}[\Phi] dt, \quad (6.2)$$

with *Lagrangian density*, given by

$$\mathfrak{L}[\Phi] = \int d^n x \mathcal{L}(\Phi^i, \partial_{x^j} \Phi^i),$$

where the integral is taken over all  $n$  coordinates  $x^j = x^j(t)$  of the *EMS*, and  $\partial_{x^j} \Phi^i$  are time and space partial derivatives of the  $\Phi^i$ –variables over coordinates.

Second, we formulate the *least action principle* as a minimal variation  $\delta$  of the action  $S[\Phi]$

$$\delta S[\Phi] = 0, \quad (6.3)$$

which, using variational *Euler–Lagrangian equations* (see section 3.3 above), derives field–motion–geometry of the unique and smooth *EMS*–transition functor

$$\mathcal{T} : \text{STIMUL}_{t_{ini}} \Rightarrow \text{CONTRACT}_{t_{mid}} \Rightarrow \text{SHAPE}_{t_{fin}},$$

acting at a macro–level from some initial time  $t_{ini}$  to the final time  $t_{fin}$  (via the intermediate time  $t_{mid}$ ).

Here, we have in place *n*–categorical *Lagrangian–field structure* on the *muscular Riemannian configuration manifold*  $M$ ,

$$\Phi^i : [0, 1] \rightarrow M, \Phi^i : \Phi_0^i \mapsto \Phi_1^i,$$

generalized from the recursive homotopy dynamics (3.5.1) above, using

$$\frac{d}{dt} f_{\dot{x}^i} = f_{x^i} \longrightarrow \partial_\mu \left( \frac{\partial \mathcal{L}}{\partial_\mu \Phi^i} \right) = \frac{\partial \mathcal{L}}{\partial \Phi^i},$$

with

$$[x_0, x_1] \mapsto [\Phi_0^i, \Phi_1^i].$$

In this way, we get macro-objects in the global *EMS*: a single electrodynamic stimulation field described by Maxwell field equations, a single muscular excitation-contraction path described by Lagrangian equation of motion, and a single Riemannian skin & fat geometry.

### 6.2.2 Local Micro-Level of $EMS_{total}$

After having properly defined macro-level  $EMS_{total}$ , with a unique and globally-smooth *EMS*-transition functor  $\mathcal{T}$ , we move down to the *microscopic cellular EMS*-level of rapidly fluctuating electrodynamic fields, sarcomere-contraction paths and coarse-grained, fractal muscle-fat geometry, where we cannot define a unique and smooth field-path-geometry. The most we can do at this level of *fluctuating noisy uncertainty*, is to formulate an adaptive path integral and calculate overall probability amplitudes for ensembles of local transitions from negative *EMS*-pad  $A^\ominus$  to the positive pad  $B^\oplus$  (see Figure 6.2). This *probabilistic transition micro-dynamics* is given by a multi field-path-geometry, defining the microscopic *transition amplitude* corresponding to the macroscopic *EMS*-transition functor  $\mathcal{T}$ . So, what is externally the transition functor, internally is the transition amplitude. The absolute square of the transition amplitude is the *transition probability*.

Now, the total *EMS*-transition amplitude, from the initial state *STIMUL*, to the final state *SHAPE*, is defined on  $EMS_{total}^2$

$$\langle SHAPE | STIMUL \rangle_{total} \equiv \mathcal{F} : STIMUL_{t_0} \Rightarrow SHAPE_{t_1}, \quad (6.4)$$

given by *modern adaptive generalization* of the classical *Feynman path integral*, see [FH65, Fey72, Fey98, DEF99]). The transition map (6.4) calculates *overall probability amplitude* along a multitude of wildly fluctuating fields, paths and geometries, performing the *microscopic* transition from the micro-state  $STIMUL_{t_0}$  occurring at initial micro-time instant  $t_0$  to the micro-state  $SHAPE_{t_1}$  at some later micro-time instant  $t_1$ , such that all micro-time instants fit inside the global transition interval  $t_0, t_1, \dots, t_s \in [t_{ini}, t_{fin}]$ . It is symbolically written as

<sup>2</sup> We use the famous Dirac symbol  $\mathcal{F}$  to denote summation over ‘discrete spectrum’ and integration over ‘continuous spectrum’ of fields, paths and geometries in the micro-*EMS*.

$$\langle SHAPE|STIMUL \rangle_{total} = \int \mathcal{D}[w\Phi] e^{iS[\Phi]}, \quad (6.5)$$

where the Lebesgue integration is performed over all continuous  $\Phi_{con}^i = \text{fields} + \text{paths} + \text{geometries}$ , while summation is performed over all discrete processes and regional topologies  $\Phi_{dis}^j$ . The symbolic differential  $\mathcal{D}[w\Phi]$  in the general path integral (6.5), represents an *adaptive path measure*, defined as a weighted product

$$\mathcal{D}[w\Phi] = \lim_{N \rightarrow \infty} \prod_{s=1}^N w_s d\Phi_s^i, \quad (i = 1, \dots, n = con + dis), \quad (6.6)$$

which is in practice satisfied with a large  $N$ .

In the exponent of the path integral (6.5) we have the action  $S[\Phi]$  and the imaginary unit  $i = \sqrt{-1}$  ( $i$  can be converted into the real number  $-1$  using the so-called *Wick rotation*). Feynman path integrals are usually computed by the use of *perturbative expansion methods* (see Appendix, section A.3; for other non-standard applications of Feynman path integrals see [Ing97, Ing98]).

In this way, we get a range of micro-objects in the local  $EMS_{total}$  at the short time-level: ensembles of rapidly fluctuating, noisy and crossing electrical stimulation fields, myofibrillar contraction paths and local skin & fat shape-geometries. However, by averaging process, both in time and along ensembles of fields, paths and geometries, we can recover the corresponding global, smooth and fully predictive, external  $EMS_{total}$  transition-dynamics  $\mathcal{T}$ .

### 6.2.3 Micro-Level Adaptation and Muscular Training

The adaptive path integral (6.5–6.6) incorporates the local muscular training process (see Appendix) according to the basic learning formula (see e.g., [Gro82, IJB99a])

$$NEW\ VALUE = OLD\ VALUE + INNOVATION,$$

where the term *VALUE* represents respectively *biological images* of the *STIMUL*, *CONTRACT* and *SHAPE*.

The general *synaptic weights*  $w_s = w_s(t)$  in (6.6) are updated by the *homeostatic neuro-muscular feedbacks* during the transition process  $\mathcal{T}$ , according to one of the two standard neural training schemes, in which the micro-time level is traversed in discrete steps, i.e., if  $t = t_0, t_1, \dots, t_s$  then  $t + 1 = t_1, t_2, \dots, t_{s+1}$ :

1. A *self-organized, unsupervised*, e.g., Hebbian-like training rule [Heb49]:

$$w_s(t + 1) = w_s(t) + \frac{\sigma}{\eta} (w_s^d(t) - w_s^a(t)), \quad (6.7)$$

where  $\sigma = \sigma(t)$ ,  $\eta = \eta(t)$  denote *signal* and *noise*, respectively, while superscripts  $d$  and  $a$  denote *desired* and *achieved* muscular micro-states, respectively; or

2. A certain form of a *supervised gradient descent training*:

$$w_s(t+1) = w_s(t) - \eta \nabla J(t), \quad (6.8)$$

where  $\eta$  is a small constant, called the *step size*, or the *training rate*, and  $\nabla J(n)$  denotes the gradient of the ‘performance hyper-surface’ at the  $t$ -th iteration.

### 6.3 Electrical Stimulation Fields: $EMS_{fields}$

#### 6.3.1 External Smooth Maxwell Electrodynamics

On the macro-level in the phase  $EMS_{fields}$  we formulate the *electrodynamic field action principle* (see, e.g. [DEF99])

$$\delta S[F] = 0, \quad (6.9)$$

with the action  $S[F]$  dependent on  $N$  electrodynamic stimulation fields  $F^i = F^i(x)$ , defined as a temporal integral

$$S[F] = \int_{t_{ini}}^{t_{fin}} \mathfrak{L}[F] dt, \quad (6.10)$$

with Lagrangian density given by

$$\mathfrak{L}[F] = \int d^n x \mathcal{L}(F_i, \partial_{x^j} F^i),$$

where the integral is taken over all  $n$  coordinates  $x^j = x^j(t)$  of the EMS, and  $\partial_{x^j} F^i$  are partial derivatives of the electrodynamic field variables over coordinates.

The action principle (6.9) implies the following *Maxwell electrodynamics*, presented here in vector, tensor and modern exterior differential form.

Given the following 3D vector-fields: the *electrical field*  $\mathbf{E}$ , the *magnetic field*  $\mathbf{B}$  and the *electrical current*  $\mathbf{J}$ , as well as the *scalar electrical potential*  $\rho$ , the Maxwell electrical vector equations read<sup>3</sup> (see, e.g., [MTW73]):

1. *Electrostatics*:

$$\nabla \cdot \mathbf{E} \equiv \operatorname{div} \mathbf{E} = 4\pi\rho, \quad \text{and}$$

2. *Electrodynamics*:

$$\partial_t \mathbf{E} - \nabla \times \mathbf{B} \equiv \partial_t \mathbf{E} - \operatorname{curl} \mathbf{B} = -4\pi\mathbf{J}.$$

<sup>3</sup> Only electrodynamic half of the Maxwell electro-magnetic field is elaborated here, as the other, magnetodynamic part has a minor role in physiology of electro-muscular stimulation.

Otherwise, given the 4D electromagnetic tensor–field *Faraday*,

$$F^{\alpha\beta} = \begin{pmatrix} 0 & E_x & E_y & E_z \\ -E_x & 0 & B_z & -B_y \\ -E_y & -B_z & 0 & B_x \\ -E_z & B_y & -B_x & 0 \end{pmatrix},$$

together with the 4D *electric current* vector–field  $J^\alpha = (\mathbf{J}, -\rho)$ , the tensor Maxwell equation reads (with *electrostatics and electrodynamics combined*):

$$F^{\alpha\beta}{}_{;\beta} = 4\pi J^\alpha.$$

Finally, given the two–form *Maxwell*  $*F \equiv F_{\alpha\beta}$ , which is a dual of the *Faraday* tensor, (also calculated as  $F = dA$ , where  $A$  is the one–form of *electrical potential*), and the three–form *charge*  $*J$  (which is the dual one–form), the *exterior Maxwell equation* reads:

$$d*F = 4\pi *J.$$

The two–form *Maxwell*  $*F \equiv F_{\alpha\beta}$ , defines the *Lorentz force* one–form of the electro–muscular stimulation field,

$$Q_\alpha \equiv \dot{p}_\alpha \propto e F_{\alpha\beta} v^\beta,$$

where  $e$  is total electric charge and  $v^\beta$  is the velocity vector–field of the stimulation flow. This equation says that the muscular force  $Q_\alpha$  generated by the simulation is proportional to the stimulation field strength  $F_{\alpha\beta}$ , velocity of the stimulation flow  $v^\beta$  through the skin–fat–muscle tissue, as well as the total stimulation charge  $e$ .

Now, let  $M$  be a smooth  $n$ D closed manifold with a Riemannian metric  $g_{ij}$  (see Chapter 2) and also with an exact two–form  $F = dA$ . Consider the problem of existence of closed extremals of the functional

$$S(\gamma) = \int_\gamma (\sqrt{g_{ij} \dot{x}^i \dot{x}^j} + A_i \dot{x}^i) dt,$$

on the space of closed curves  $\gamma \in M$ . This functional is a natural generalization of the usual functional of length, and its closed extremals correspond to periodic trajectories of the motion of particles on the Riemannian manifold  $M$  when the kinetic energy is defined by the metric tensor  $g_{ij}$ . When the Lagrangian function

$$L = \sqrt{g_{ij} \dot{x}^i \dot{x}^j} + A_i \dot{x}^i$$

is everywhere positive, we obtain the *Finsler metric* [Bah88], and the periodic problem can be studied by the methods of Morse theory (section 4.2.1 above).

### 6.3.2 Internal Cellular Bio–Quantum Electrodynamics

At the same time, on the micro–level in the phase  $EMS_{fields}$  we have the Feynman–type *sum over fields*  $F^i$  ( $i = 1, \dots, N$ ) given by the adaptive path integral (see, e.g. [DEF99])

$$STIMUL_{fields} = \int \mathcal{D}[wF] e^{iS[F]} \quad \underline{Wick} \quad \int \mathcal{D}[wF] e^{-S[F]}, \quad (6.11)$$

with action  $S[F]$  given by the temporal integral (6.10), while  $\underline{Wick}$  denotes the so–called Wick–rotation of the time variable  $t$  to imaginary values  $t \mapsto \tau = it$ . The resulting bio–quantum field represents the *bundle of cellular electrodynamic flux tubes*.

Now, during the XX century, the *electrodynamic flux tubes* were described by the Dirac–Schwinger–Tomonaga equations of *quantum electrodynamics*<sup>4</sup>. Today, the similar kind of *flux tubes* is in a more sophisticated way described by the *conformal Landau–Ginzburg model* (see, e.g., [DEF99]).

Technical details of these advanced physical theories are beyond the scope of the present article. In simplified terms, we can say that they all describe *field–generated solitons*<sup>5</sup> (see the next section for a *solitary model of muscular excitation–contraction*). The main point of all these quantum field theories and their biophysical applications is that their *macro–level averaging lift* (either in time or across the ensemble of cellular tubes) produces the classical Maxwell electrodynamics (6.3.1) above. On their own, they describe *rapidly fluctuating, fractal and noisy, electrodynamic fields flowing from the source* (–) *electrode to the sink* (+) *electrode* – as described in the *Schwinger formalism* (see, e.g., his lecture in the Nobel e–Museum).

<sup>4</sup> Mathematically, quantum electrodynamics has the structure of an Abelian *gauge theory* with a  $U(1)$  gauge group. The gauge field which mediates the interaction between the charged spin 1/2 fields is the electromagnetic field. Physically, this translates to the picture of charged particles interacting with each other by the exchange of photons.

<sup>5</sup> In classical mathematical physics, by a *soliton* one usually means a “travelling wave” solution of a nonlinear partial differential equation  $u_t = F(u, u_x, \dots)$ , i.e., a solution of the form  $u(x, t) = f(x - vt)$ . Solitons play a very important role in the theory of *integrable mechanical systems*, where any solution can be approximated by a superposition of solitons moving at different velocities, as we have in the next section where we develop a *solitary model of muscular excitation–contraction*. As a result, the theory of integrable systems is sometimes called soliton theory. In this section, however, we are interested in solitons arising in electrical field theory (as travelling wave solutions of the classical field equations) and primarily in the role they play in quantization of electrical field theories, which is a different point of view from the one in classical soliton theory.

## 6.4 Stimulated Muscular Contraction Paths: $EMS_{paths}$

### 6.4.1 External Anatomical Muscular Mechanics

On the macro–level in the phase  $EMS_{paths}$  we have the *muscular contraction action principle*

$$\delta S[x] = 0,$$

with the *mechanical action*  $S[x]$  given by

$$S[x] = \int_{t_{ini}}^{t_{fin}} dt \left[ \frac{m}{2} \dot{x}_i^2 + F(x) \right], \quad (6.12)$$

where overdot denotes time derivative, so that  $\dot{x}^i$  represents the external (anatomical) muscular contraction speed, while  $m$  denotes the total estimated mass of the stimulated muscle. The corresponding Euler–Lagrangian equation, with the *kinetic energy of muscular contraction*

$$E_{kin} = \frac{1}{2} g_{ij} \dot{x}^i \dot{x}^j,$$

generated by *muscular Riemannian metrics*  $g_{ij}$  (see the next section on anatomical geometry), gives the *Newtonian equation of motion* (see e.g., [Arn89])

$$\frac{d}{dt} \frac{\partial E_{kin}}{\partial \dot{x}^i} - \frac{\partial E_{kin}}{\partial x^i} \equiv m \ddot{x}^i = -\partial_x F(x), \quad (6.13)$$

where  $\partial_s$  denotes the partial derivative with respect to the variable  $s$  (which is either space coordinate  $x$  or time  $t$ ).

### 6.4.2 Internal Myofibrillar Bio–Quantum Mechanics

At the same time, on the micro–level in the phase  $EMS_{paths}$ , instead of a single path defined by the Newtonian equation of motion for the whole muscle (6.13), we have an ensemble of fluctuating and crossing, fractal paths with weighted probabilities (of the unit total sum). This ensemble of micro–paths is defined by the simplest instance of our adaptive path integral (6.5), similar to the Feynman’s original *sum over histories*,

$$CONTRACT_{paths} = \int \mathcal{D}[wx] e^{iS[x]}, \quad (6.14)$$

where  $\mathcal{D}[wx]$  is a functional measure on the *space of all weighted paths*, and the exponential depends on the action  $S[x]$  given by (6.12). In the language of transition–propagators, the integral over histories (6.14) can be decomposed into the product of *myofibrillar action propagators*.<sup>6</sup> This procedure can be

<sup>6</sup> *Feynman propagators* are otherwise called *Fredholm kernels* or *Green’s functions*.

redefined in a mathematically cleaner way if we Wick-rotate the time variable  $t$  to imaginary values  $t \mapsto \tau = it$ , thereby making all integrals real:

$$\int \mathcal{D}[wx] e^{iS[x]} \xrightarrow{\text{Wick}} \int \mathcal{D}[wx] e^{-S[x]}. \quad (6.15)$$

Discretization of (6.15) gives the standard *thermodynamic partition function*

$$Z = \sum_j e^{-w_j E^j / T}, \quad (6.16)$$

where  $E^j$  is the motion energy eigenvalue (reflecting each possible motivational energetic state),  $T$  is the temperature environmental control parameter, and the sum runs over all motion energy eigenstates (labelled by the index  $j$ ). From (6.16), we can further calculate all thermodynamical and statistical  $EMS$ -properties (see [Fey72]), as for example, *transition entropy*  $S = k_B \ln Z$ , etc.

Now, both the action integral (6.12) and the path integral (6.14) are closely related to the *molecular soliton model of muscular contraction*, as described by the *Kortevæg-De Vries equation* (3.32) and *nonlinear Schrödinger equation* (3.30) (see subsection 3.2.3 above). It is clear that these two solitary equations have a *quantum-mechanical* origin.<sup>7</sup> Recall, that by the use of the first quantization method (instead of the Feynman integral), every classical biodynamic observable  $F$  is represented in the Hilbert space  $L^2(\psi)$  of square-integrable complex  $\psi$ -functions by a Hermitian (self-adjoint) linear operator  $\hat{F}$  with real eigenvalues. The classical Poisson bracket  $\{F, G\} = K$  corresponds to the *Dirac quantum commutator*  $[\hat{F}, \hat{G}] = i\hat{K}$  (where, as always we have used normal units in which  $\hbar = 1$ ). Therefore the classical evolution equation (3.28) corresponds, in the *Heisenberg picture*, to the *quantum evolution equation* (see, e.g., [Dir30])

$$i\hat{F} = [\hat{F}, \hat{H}],$$

for any representative operator  $\hat{F}$  and *quantum Hamiltonian operator*  $\hat{H}$ . By Ehrenfest's theorem (see, e.g., [Fey72]), this equation is also valid for expectation values  $\langle \cdot \rangle$  of observables, that is,

$$i \langle \hat{F} \rangle = \langle [\hat{F}, \hat{H}] \rangle.$$

For technical details on *classical muscular mechanics*, including the celebrated work of Nobel Laureates:

1. the *microscopic sliding filament model* of A.F. Huxley;

<sup>7</sup> As Richard Feynman says in *The Feynman Lectures on Physics*: “Where did we get that [Schrödinger equation] from? It's not possible to derive it from anything you know. It came out of the mind of Schrödinger.” Yet, Schrödinger equation can be (and usually is) derived from the Feynman path integral.

2. the *macroscopic force–velocity model* of A.V. Hill;
3. the celebrated *Hodgkin–Huxley neural* (and subsequently muscular) *excitation model* (A.L. Hodgkin and A.F. Huxley); and
4. the *Eccles model of synaptic activation*;

– see Appendix.

## 6.5 Anatomical Geometry of the Face & Body Shape: *EMS<sub>geom</sub>*

### 6.5.1 External Face & Body Geometry

On the macro–level in the phase *EMS<sub>geom</sub>* representing a smooth skin 2D manifold–patch  $M_2$  with the Riemannian metric tensor  $g_{ij} = g_{ij}(M_2)$  defined at each local face or body point, we formulate the *geometric action principle*

$$\delta S[g_{ij}] = 0,$$

where  $S = S[g_{ij}]$  is the 2D *geodesic action* on the surface  $M$ ,

$$S[g_{ij}] = \int d^n x \sqrt{g_{ij} dx^i dx^j}, \quad (6.17)$$

(Einstein’s summation convention over repeated indices is assumed).

The corresponding Euler–Lagrangian equation gives the *geodesic equation* of the *shortest path* on the manifold  $M_2$ ,

$$\ddot{x}^i + \Gamma_{jk}^i \dot{x}^j \dot{x}^k = 0, \quad (6.18)$$

where the symbol  $\Gamma_{jk}^i$  denotes the so–called *affine connection* which is the source of *curvature*, which is geometric description for *noise* (see [Ing97, Ing98]). The higher the local curvatures of the skin manifold–patch  $M_2$ , the greater the internal *EMS*–noise. This noise is the source of our micro–level fat–related fluctuations.

Assuming that the electro–physiological principles of the *EMS*–based body–shaping are identical (only less subtle) to the principles of the *EMS*–based face–shaping, in the following subsections, we will focus on the facial anatomical geometry.

### Local Facial Curvatures and Their Deviations

In this subsection we consider human face, with its distinguished local anatomical features, as a 2D Riemannian manifold (i.e, a smooth skin manifold–patch  $M_2$ ), determined by muscular structural and functional anatomy (see Figure 6.5). Here we demonstrate that this anatomical geometry is not static, but

Facial Musculature				
Muscle	Origin	Insertion	Action	Innervation
depressor anguli oris	oblique line of mandible	angle of mouth	pulls the corner of the mouth downward	marginal mandibular & buccal branches of facial nerve (VII)
levator labii superioris	inferior margin of orbit	skin of upper lip	elevates upper lip	buccal branch of facial nerve (VII)
zygomaticus major	zygomatic bone, upper lateral surface	skin of angle of mouth	elevates and draws the corner of mouth laterally	zygomatic and buccal branches of facial nerve (VII)
orbicularis oris	skin and fascia of lips and area surrounding lips	skin and fascia of lips	purses the lips	buccal branch of facial nerve (VII)
buccinator	pterygomandibular raphe, mandible, and maxilla lateral to molar teeth	angle of mouth & lateral portion of upper and lower lips	pulls corner of mouth laterally; pulls cheek against teeth	buccal branches of facial nerve (VII)
platysma	fascia overlying the pectoralis major and deltoid muscles	inferior border of mandible and skin of lower face	draws corners of mouth down; aids in depression of the mandible	facial nerve (VII), cervical branch

**Table 6.1.** Functional anatomy of the facial musculature (for whole body anatomy, see any anatomical textbook, e.g., [Mar98].)

rather dynamic in an extremely complex way, which can be controlled by a proper  $EMS$ .

Recall from Chapter 2, that Riemannian *metric* on any smooth  $n$ D Riemannian manifold  $M$  is a positive-definite quadratic form  $g : M \rightarrow \mathbb{R}$ , which is in local coordinates  $(x^1(s), \dots, x^n(s))$ , dependent on the affine line parameter  $s$  at a point  $m \in M$ , defined as a symmetric  $(0, 2)$  tensor-field  $g_{ij}(m) = g\left(\frac{\partial}{\partial x^i}, \frac{\partial}{\partial x^j}\right)(m)$ , (see also [Boo86, Iva04, Iva02, IP01b, Iva05]).

An infinitesimal distance between the two nearby local points  $m$  and  $n$  on  $M$  is defined by the *line element*

$$ds^2 = g_{ij} dx^i dx^j,$$



**Fig. 6.5.** Structural anatomy of the facial musculature (together with superficial branches of the facial nerve), showing local geometric features: distances (metrics), curvatures and directions for muscular contractions (see Table 6.1), modelled here as geodesic deviations. Here we show only facial EMS, assuming that all biophysical and geometric principles are the same (only less subtle) for body EMS.

and realized by the geodesics  $x^i(s)$  (see Chapter 2). In local coordinates  $(x^1(s), \dots, x^n(s))$  at a point  $m \in M$ , the geodesic defining equation (6.18), derived from the *geometric action principle* (6.17), is a second order ordinary differential equation with the *Christoffel symbols*  $\Gamma_{jk}^i = \Gamma_{jk}^i(m)$  of the *affine* (Levi–Civita) *connection*  $\nabla_{\dot{x}^i}$  are calculated at the point  $m \in M$  with local coordinates  $(x^1(s), \dots, x^n(s))$ .

If  $\Gamma_{jk}^i(m) = 0$ , the manifold  $M$  is *flat* at the point  $m$ . This means that the *Riemann curvature tensor*, a symmetric (1, 3) tensor field  $R_{jkl}^i = R_{jkl}^i(m)$ , locally defined at a point  $m \in M$  as

$$R_{jkl}^i = \partial_{x^k} \Gamma_{jl}^i - \partial_{x^l} \Gamma_{jk}^i + \Gamma_{\mu k}^i \Gamma_{jl}^\mu - \Gamma_{\mu l}^i \Gamma_{jk}^\mu,$$

also vanishes at a point  $m \in M$ , i.e.,  $R_{jkl}^i(m) = 0$ .

Elliptic manifolds have positive curvature, i.e.,  $R_{jkl}^i(m) > 0$  and nearby geodesics are converging on it (see Figure 6.5), while hyperbolic ones have negative curvature, i.e.,  $R_{jkl}^i(m) < 0$  and nearby geodesics are diverging on it (see Figure 6.6). In case of a surface, which is a 2D manifold, the metric tensor is reduced to the scalar curvature  $R$ . An example of elliptic (convex)

surfaces is the sphere with the curvature  $R = +\rho^{-2}$  (where  $\rho$  is the radius), while an example of hyperbolic (concave) surfaces is the Lobachevsky plane with the curvature  $R = -1$ .

Now, recall from section 2.5 above, that the rate of change of a vector field  $A^k$  on the manifold  $M$  along the curve  $x^i(s)$  is properly defined by the *covariant derivative*:

$$\frac{D}{ds}A^k = \dot{x}^i \nabla_{\dot{x}^i} A^k = \dot{x}^i (\partial_{x^i} A^k + \Gamma_{ij}^k A^j) = \dot{A}^k + \Gamma^k_{ij} \dot{x}^i A^j,$$

which defines the parallel transport along the curve  $x^i(s)$  at a point  $m \in M$  as  $\frac{D}{ds}A^k(m) = 0$ .

By applying the previous result to itself, we can obtain an expression for the second covariant derivative of the vector field  $A^k$  along the curve  $x^i(s)$ :

$$\frac{D^2}{ds^2}A^k = \frac{d}{ds} \left( \dot{A}^k + \Gamma^k_{ij} \dot{x}^i A^j \right) + \Gamma^k_{ij} \dot{x}^i \left( \dot{A}^j + \Gamma^j_{mn} \dot{x}^m A^n \right).$$

In the same local coordinates  $(x^1(s), \dots, x^n(s))$  at a point  $m \in M$ , let  $\delta x^i = \delta x^i(s)$  denote the vector-field of *geodesic deviation*, i.e., the infinitesimal vector-field describing both *normal* and *tangential* separation between the two neighboring geodesics, then the *Jacobi equation* of the geodesic deviation on the manifold  $M$  holds ([Arn89]):

$$\frac{D^2 \delta x^i}{ds^2} + R^i_{jkl} \dot{x}^j \delta x^k \dot{x}^l = 0. \quad (6.19)$$

This equation describes the *relative acceleration* between two infinitesimally close facial geodesics, which is proportional both to the facial curvature (measured by the Riemann tensor  $R^i_{jkl}$  at a point  $m \in M$ ), and to the geodesic deviation  $\delta x^i$ . Solutions of the Jacobi equation (6.19) are called *Jacobi fields*, or *Jacobi flows*.

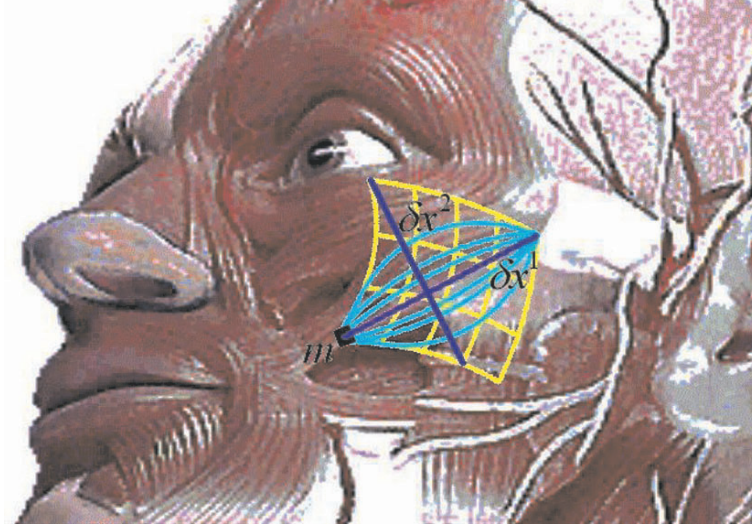
### Human Face as a Riemannian Patch-Manifold

Local anatomical features of the human face can be considered as a collection of local 2D Riemannian manifold-patches  $M_2^i$ , i.e., Riemannian patches, determined by skeletal and muscular anatomy. Each of these local patches  $M_2^i$  is represented by its own local coordinates  $(x^1(s), x^2(s))_i$ , defined at a distinguished point  $m$ . We propose here a 2D Jacobi fields  $\delta x^1, \delta x^2$  (see Figures 6.5 and 6.6) to model respectively normal and tangential components of contractions of the facial muscles.

In 2D, the Riemann curvature tensor simplifies into:

$$R^i_{jmn} = \frac{1}{2} R g^{ik} (g_{km} g_{jn} - g_{kn} g_{jm}),$$

where  $R$  denotes the *scalar curvature*. Consequently the equation of geodesic deviation (6.19) also simplifies into



**Fig. 6.6.** Local coordinate chart defined in a neighborhood of a point  $m$  on the *convex–ecliptic* patch–manifold  $M_2$  of the facial musculature, together with the converging geodesic deviation: its tangent component  $\delta x^1$  and its normal component  $\delta x^2$ .

$$\frac{D^2}{ds^2}\delta x^i + \frac{R}{2}\delta x^i - \frac{R}{2}\dot{x}^i(g_{jk}\dot{x}^j\delta x^k) = 0. \quad (6.20)$$

Now, if we work in a local Cartesian coordinate system, defined at the tangent plane  $T_m M_2$  at a point  $m$  by an orthogonal projection imaging, the covariant derivative  $\frac{D^2}{ds^2}$  reduces to the ordinary derivative  $\frac{d^2}{ds^2}$  (as the Christoffel symbols  $\Gamma_{jk}^i$  vanish) and the metric tensor  $g_{ij}$  reduces to identity matrix  $I_{ij}$ , so our  $2D$  equation of geodesic deviation (6.20) reduces into a simple second order ordinary differential equation in just two coordinates  $x^i$  ( $i = 1, 2$ )

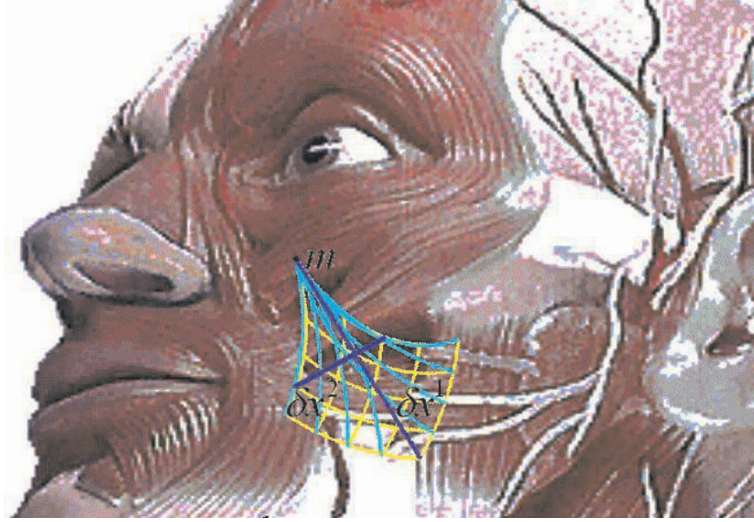
$$\frac{d^2}{ds^2}\delta x^i + \frac{R}{2}\delta x^i - \frac{R}{2}\dot{x}^i(I_{jk}\dot{x}^j\delta x^k) = 0.$$

Also, if we require that the two nearby geodesics be nearly parallel, the last term in (6.20) vanishes, and we are left with

$$\frac{D^2}{ds^2}\delta x^i + \frac{R}{2}\delta x^i = 0. \quad (6.21)$$

Again, if we work in a locally Cartesian coordinate system, our *flat 2D equation of geodesic deviation* simplifies into *harmonic oscillator* in which the scalar curvature  $R/2$  plays the role of the *spring constant*:

$$\frac{d^2}{ds^2}\delta x^i + \frac{R}{2}\delta x^i = 0. \quad (6.22)$$



**Fig. 6.7.** Local coordinate chart defined in a neighborhood of a point  $m$  on the *concave-hyperbolic* patch-manifold  $M_2$  of the facial musculature, together with the diverging geodesic deviation: its tangent component  $\delta x^1$  and its normal component  $\delta x^2$ .

Therefore, equations (6.21) and (6.20) could be respectively regarded as the first-order and second-order perturbations of the linear oscillator equation (6.22). These three equations represent the three levels of detail in our modelling of the facial muscular movements. The oscillator equation (6.22) has a simple family of sinus functions (with certain amplitudes, frequencies and phases) as a solution, while the two nonlinear equations (6.21) and (6.20) could be numerically integrated for zero initial deviation and its velocity, using any explicit Runge-Kutta-like integrator (see, e.g. [IS01]). Each of them describes the facial movement caused by muscular contraction dependent on its local curvature, i.e., anatomical shape. Also, all three geometric oscillators have kinetic and potential energies respectively defined as quadratic forms:

$$E_{kin} = \frac{1}{2}g_{ij}\delta\dot{x}^i\delta\dot{x}^j, \quad U = \frac{1}{4}Rg_{ij}\delta x^i\delta x^j,$$

and derived from the muscular action principle (6.12–6.13) above.

### 6.5.2 Cellular Muscle–Fat Geometry

On the micro-level in the phase  $EMS_{geom}$ , we have an adaptive *sum over fractal geometries*, represented by the path integral over all regional Riemannian metrics  $g_{ij} = g_{ij}(x)$  varying from point to point inside an  $n$ -dimensional *muscle-fat manifold*  $M$ , underlying the external skin surface,

$$SHAPE_{geom} = \int \mathcal{D}[wg_{ij}] e^{iS[g_{ij}]} \xrightarrow{\text{Wick}} \int \mathcal{D}[wg_{ij}] e^{-S[g_{ij}]}, \quad (6.23)$$

where  $\mathcal{D}[g_{ij}]$  denotes diffeomorphism equivalence classes of metrics  $g_{ij}(x)$  of *Skin*.

To include the severe change of topological structure (e.g., a change in a number of holes) in the manifold  $M$ , equation (6.23) can be extended as

$$SHAPE_{geom/top} = \sum_{\text{topol.}} \int \mathcal{D}[wg_{ij}] e^{iS[g_{ij}]}, \quad (6.24)$$

where the topological sum is taken over all components of connectedness of the manifold  $M$  determined by its *Euler characteristics* [Iva02]. This type of integral defines the *theory of fluctuating geometries*, a propagator between  $(n - 1)$ –dimensional boundaries of the  $n$ –dimensional manifold  $M$ . One has to contribute a meaning to the integration over geometries. A key ingredient in doing so is to approximate in a natural way the smooth structures of the manifold  $M$  by piecewise linear structures (mostly using topological simplices  $\Delta$ <sup>8</sup>). In this way, after the Wick–rotation (6.15), the integral (6.23–6.24) becomes a *simple statistical system*, given by partition function

$$Z = \sum_{\Delta} \frac{1}{C_{\Delta}} e^{-S_{\Delta}},$$

where the summation is over all triangulations  $\Delta$  of the manifold  $M$ , while the number  $C_T$  is the order of the automorphism group of the performed triangulation.

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<sup>8</sup> This is called the *simplicial approximation*.

# A

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## Appendix

### A.1 Basic Formulas from Tensor Analysis

Biomechanical laws must be independent of any particular coordinate systems used in describing them mathematically, if they are to be valid. In other words, all biomechanical equations need to be tensorial or *covariant*. Therefore, for the reference purpose, in this subsection, we give the basic formulas from the standard tensor calculus, which is used throughout the text. The basic notational convention used in tensor calculus is Einstein's summation convention over repeated indices. More on this subject can be found in any standard textbook on mathematical methods for scientists and engineers, or mathematical physics (we recommend [MTW73]).

#### A.1.1 Transformation of Coordinates and Elementary Tensors

To introduce tensors, consider a standard linear  $nD$  matrix system,  $\mathbf{Ax} = \mathbf{b}$ . It can be rewritten in the so-called *covariant form* as

$$a_{ij}x^j = b_i, \quad (i, j = 1, \dots, n). \quad (\text{A.1})$$

Here,  $i$  is a *free index* and  $j$  is a *dummy index* to be summed upon, so the expansion of (A.1) gives

$$\begin{aligned} a_{11}x^1 + a_{12}x^2 + \dots + a_{1n}x^n &= b_1, \\ a_{21}x^1 + a_{22}x^2 + \dots + a_{2n}x^n &= b_2, \\ &\dots \\ a_{n1}x^1 + a_{n2}x^2 + \dots + a_{nn}x^n &= b_n, \end{aligned}$$

as expected from the original matrix form  $\mathbf{Ax} = \mathbf{b}$ . This indicial notation can be more useful than the matrix one, like e.g., in computer science, where indices would represent loop variables. However, the full potential of tensor analysis is to deal with nonlinear multivariate systems, which are untractable by linear matrix algebra and analysis. The core of this *nonlinear multivariate analysis* is *general functional transformation*.

### Transformation of Coordinates

Suppose that we have two sets of curvilinear coordinates that are single-valued, continuous and smooth functions of time,  $x^j = x^j(t)$ , ( $j = 1, \dots, m$ ) and  $\bar{x}^i = \bar{x}^i(t)$ , ( $i = 1, \dots, n$ ), respectively, representing trajectories of motion of some biomechanical system. Then a general ( $m \times n$ )D transformation (i.e., a nonlinear map)  $x^j \mapsto \bar{x}^i$  is defined by the set of transformation equations

$$\bar{x}^i = \bar{x}^i(x^j), \quad (i = 1, \dots, n; j = 1, \dots, m). \quad (\text{A.2})$$

In case of the square transformation,  $m = n$ , we can freely exchange the indices, like e.g., in general relativity theory. On the other hand, in the general case of rectangular transformation,  $m \neq n$ , like e.g., in robotics, and we need to take care of these ‘free’ indices.

Now, if the *Jacobian determinant* of this *coordinate transformation* is different from zero,

$$\left| \frac{\partial \bar{x}^i}{\partial x^j} \right| \neq 0,$$

then the transformation (A.2) is reversible and the inverse transformation,

$$x^j = x^j(\bar{x}^i),$$

exists as well. Finding the inverse transformation is the problem of matrix inverse: in case of the square matrix it is well defined, although the inverse might not exist if the matrix is singular. However, in case of the square matrix, its proper inverse does not exist, and the only tool that we are left with is the so-called *Moore–Penrose pseudoinverse*, which gives an optimal solution (in the least-squares sense) of an overdetermined system of equations. Every (overdetermined) rectangular coordinate transformation gives rise to a *redundant system*.

For example, in Euclidean 3D space  $\mathbb{R}^3$ , transformation from Cartesian coordinates  $y^k = \{x, y, z\}$  into spherical coordinates  $x^i = \{\rho, \theta, \varphi\}$  is given by

$$y^1 = x^1 \cos x^2 \cos x^3, \quad y^2 = x^1 \sin x^2 \cos x^3, \quad y^3 = x^1 \sin x^3, \quad (\text{A.3})$$

with the Jacobian matrix given by

$$\left( \frac{\partial y^k}{\partial x^i} \right) = \begin{pmatrix} \cos x^2 \cos x^3 & -x^1 \sin x^2 \cos x^3 & -x^1 \cos x^2 \sin x^3 \\ \sin x^2 \cos x^3 & x^1 \cos x^2 \cos x^3 & -x^1 \sin x^2 \sin x^3 \\ \sin x^3 & 0 & x^1 \cos x^3 \end{pmatrix} \quad (\text{A.4})$$

and the corresponding Jacobian determinant,  $\left| \frac{\partial y^k}{\partial x^i} \right| = (x^1)^2 \cos x^3$ .

An inverse transform is given by

$$x^1 = \sqrt{(y^1)^2 + (y^2)^2 + (y^3)^2}, \quad x^2 = \arctan \left( \frac{y^2}{y^1} \right), \\ x^3 = \arctan \left( \frac{y^3}{\sqrt{(y^1)^2 + (y^2)^2}} \right), \quad \text{with} \quad \left| \frac{\partial x^i}{\partial y^k} \right| = \frac{1}{(x^1)^2 \cos x^3}.$$

As a main biomechanical example, we have a rectangular transformation from 6 DOF external, end-effector (e.g., hand) coordinates, into  $n$  DOF internal, joint-angle coordinates. In most cases this is a redundant manipulator system, with infinite number of possible joint trajectories.

### Scalar Invariants

A *scalar invariant* (or, a zeroth order tensor) with respect to the transformation (A.2) is the quantity  $\varphi = \varphi(t)$  defined as

$$\varphi(x^i) = \bar{\varphi}(\bar{x}^i),$$

which does not change at all under the coordinate transformation. In other words,  $\varphi$  is *invariant* under (A.2). Biodynamic examples of scalar invariants include various energies (kinetic, potential, biochemical, mental) with the corresponding kinds of work, as well as related thermodynamic quantities (free energy, temperature, entropy, etc.).

### Vectors and Covectors

Any geometric object  $v^i = v^i(t)$  that under the coordinate transformation (A.2) transforms as

$$\bar{v}^i = v^j \frac{\partial \bar{x}^i}{\partial x^j}, \quad (\text{remember, summing upon } j\text{-index}),$$

represents a *vector*, traditionally called a *contravariant vector*, or, a first-order contravariant tensor. Standard biomechanical examples include both translational and rotational velocities and accelerations.

On the other hand, any geometric object  $v_i = v_i(t)$  that under the coordinate transformation (A.2) transforms as

$$\bar{v}_i = v_j \frac{\partial x^j}{\partial \bar{x}^i},$$

represents a *one-form* or *covector*, traditionally called a *covariant vector*, or, a first order covariant tensor. Standard biomechanical examples include both translational and rotational momenta, forces and torques.

### Second-Order Tensors

Any geometric object  $t^{ik} = t^{ik}(t)$  that under the coordinate transformation (A.2) transforms as

$$\bar{t}^{ik} = t^{jl} \frac{\partial \bar{x}^i}{\partial x^j} \frac{\partial \bar{x}^k}{\partial x^l}, \quad (i, k = 1, \dots, n; j, l = 1, \dots, m),$$

represents a *second-order contravariant tensor*. It can be obtained as an *outer product* of two contravariant vectors,  $t^{ik} = u^i v^k$ .

Any geometric object  $t_{ik} = t_{ik}(t)$  that under the coordinate transformation (A.2) transforms as

$$\bar{t}_{ik} = t_{jl} \frac{\partial x^j}{\partial \bar{x}^i} \frac{\partial x^l}{\partial \bar{x}^k},$$

represents a *second-order covariant tensor*. It can be obtained as an outer product of two covariant vectors,  $t_{ik} = u_i v_k$ .

Any geometric object  $t_k^i = t_k^i(t)$  that under the coordinate transformation (A.2) transforms as

$$\bar{t}_k^i = t_l^j \frac{\partial \bar{x}^i}{\partial x^j} \frac{\partial x^l}{\partial \bar{x}^k},$$

represents a *second-order mixed tensor*. It can be obtained as an outer product of a covariant vector and a contravariant vector,  $t_k^i = u^i v_k$ .

Standard biomechanical examples include:

1. The fundamental (material) covariant metric tensor  $\mathbf{g} \equiv g_{ik}$ , i.e., inertia matrix, given usually by the transformation from Cartesian coordinates  $y^j$  to curvilinear coordinates  $x^i$ ,

$$g_{ik} = \frac{\partial y^j}{\partial x^i} \frac{\partial y^j}{\partial x^k}, \quad (\text{summing over } j).$$

It is used in the quadratic metric form  $ds^2$  of the space in consideration (e.g., a certain biomechanical configuration space)

$$ds^2 \equiv dy^j dy^j = g_{ik} dx^i dx^k,$$

where the first term on the r.h.s denotes the *Euclidean metrics*, while the second term is the *Riemannian metric* of the space, respectively.

2. Its inverse  $\mathbf{g}^{-1} \equiv g^{ik}$ , given by

$$g^{ik} = (g_{ik})^{-1} = \frac{G_{ik}}{|g_{ik}|}, \quad G_{ik} \text{ is the cofactor of the matrix } (g_{ik});$$

3. The *Kronecker-delta* symbol  $\delta_k^i$ , given by

$$\delta_k^i = \begin{cases} 1 & \text{if } i = k \\ 0 & \text{if } i \neq k \end{cases},$$

used to denote the metric tensor in Cartesian orthogonal coordinates.  $\delta_k^i$  is a discrete version of the *Dirac  $\delta$ -function*. The *generalized Kronecker-delta symbol*  $\delta_{lmn}^{ijk}$  (in 3D) is the product of *Ricci antisymmetric tensors*  $\varepsilon^{ijk}$  and  $\varepsilon_{lmn}$ ,

$$\delta_{lmn}^{ijk} = \varepsilon^{ijk} \varepsilon_{lmn} = \begin{cases} 0 & \text{if at least two indices are equal} \\ +1 & \text{if both } ijk \text{ and } lmn \text{ are either even or odd} \\ -1 & \text{if one of } ijk, lmn \text{ is even and the other is odd} \end{cases}.$$

For example, to derive components of the metric tensor  $\mathbf{g} \equiv g_{ij}$  in standard spherical coordinates, we use the relations (A.3–A.4) between the spherical coordinates  $x^i = \{\rho, \theta, \varphi\}$  and the Cartesian coordinates  $y^k = \{x, y, z\}$ , and the definition,  $g_{ij} = \frac{\partial y^k}{\partial x^i} \frac{\partial y^k}{\partial x^j}$ , to get the metric tensor (in matrix form)

$$(g_{ij}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & (x^1)^2 \cos^2 \varphi & 0 \\ 0 & 0 & (x^1)^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \rho^2 \cos^2 \varphi & 0 \\ 0 & 0 & \rho^2 \end{pmatrix}, \quad (\text{A.5})$$

and the inverse metric tensor

$$(g^{ij}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{(x^1)^2 \cos^2 \varphi} & 0 \\ 0 & 0 & \frac{1}{(x^1)^2} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\rho^2 \cos^2 \varphi} & 0 \\ 0 & 0 & \frac{1}{\rho^2} \end{pmatrix}. \quad (\text{A.6})$$

Given a tensor, we can derive other tensors by raising and lowering its indices, by their multiplication with covariant and contravariant metric tensors. In this way, the so-called *associated tensors* to the given tensor are formed. For example,  $v^i$  and  $v_i$  are associated tensors, related by

$$v_i = g_{ik} v^k \quad \text{and} \quad v^i = g^{ik} v_k.$$

Given two vectors,  $\mathbf{u} \equiv u^i$  and  $\mathbf{v} \equiv v^i$ , their inner (dot, or scalar) product is given by

$$\mathbf{u} \cdot \mathbf{v} \equiv g_{ij} u^i v^j,$$

while their vector (cross) product (in 3D) is given by

$$\mathbf{u} \times \mathbf{v} \equiv \varepsilon_{ijk} u^j v^k.$$

### Higher-Order Tensors

As a generalization of above tensors, consider a geometric object  $R_{kps}^i = R_{kps}^i(t)$  that under the coordinate transformation (A.2) transforms as

$$\bar{R}_{kps}^i = R_{lqt}^j \frac{\partial \bar{x}^i}{\partial x^j} \frac{\partial x^l}{\partial \bar{x}^k} \frac{\partial x^q}{\partial \bar{x}^p} \frac{\partial x^t}{\partial \bar{x}^s}, \quad (\text{all indices} = 1, \dots, n). \quad (\text{A.7})$$

Clearly,  $R_{kjl}^i = R_{kjl}^i(x, t)$  is a fourth order tensor, once contravariant and three times covariant, representing the central tensor in Riemannian geometry, called the *Riemann curvature tensor*. As all biomechanical configuration spaces are Riemannian manifolds, they are all characterized by curvature tensors. In case  $R_{kjl}^i = 0$ , the corresponding Riemannian manifold reduces to the Euclidean space of the same dimension, in which  $g_{ik} = \delta_k^i$ .

If one contravariant and one covariant index of a tensor are set equal, the resulting sum is a tensor of rank two less than that of the original tensor. This process is called *tensor contraction*.

If to each point of a region in an  $nD$  space there corresponds a definite tensor, we say that a *tensor-field* has been defined. In particular, this is a *vector-field* or a *scalar-field* according as the tensor is of rank one or zero. It should be noted that a tensor or tensor field is not just the set of its components in one special coordinate system, but all the possible sets of components under any transformation of coordinates.

### Tensor Symmetry

A tensor is called *symmetric* with respect to two indices of the same variance if its components remain unaltered upon interchange of the indices; e.g.,  $a_{ij} = a_{ji}$ , or  $a^{ij} = a^{ji}$ . A tensor is called *skew-symmetric* (or, *antisymmetric*) with respect to two indices of the same variance if its components change sign upon interchange of the indices; e.g.,  $a_{ij} = -a_{ji}$ , or  $a^{ij} = -a^{ji}$ . Regarding tensor symmetry, in the following we will prove several useful propositions.

(i) *Every second-order tensor can be expressed as the sum of two tensors, one of which is symmetric and the other is skew-symmetric.* For example, a second order tensor  $a_{ij}$ , which is for  $i, j = 1, \dots, n$  given by the  $n \times n$ -matrix

$$a_{ij} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{n2} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix},$$

can be rewritten as

$$\begin{aligned} a_{ij} &= \frac{1}{2}a_{ij} + \frac{1}{2}a_{ij} + \frac{1}{2}a_{ji} - \frac{1}{2}a_{ji}, & \text{that can be rearranged as} \\ &= \frac{1}{2}a_{ij} + \frac{1}{2}a_{ji} + \frac{1}{2}a_{ij} - \frac{1}{2}a_{ji}, & \text{which can be regrouped as} \\ &= \frac{1}{2}(a_{ij} + a_{ji}) + \frac{1}{2}(a_{ij} - a_{ji}), & \text{which can be written as} \\ &= a_{(ij)} + a_{[ij]}, \end{aligned}$$

where  $a_{(ij)}$  denotes its symmetric part, while  $a_{[ij]}$  denotes its skew-symmetric part, as required.

(ii) *Every quadratic form can be made symmetric.* For example, a quadratic form  $a_{ij}x^i x^j$ , that (for  $i, j = 1, \dots, n$ ) expands as

$$\begin{aligned} a_{ij}x^i x^j &= a_{11}x^1 x^1 + a_{12}x^1 x^2 + \dots + a_{1n}x^1 x^n + \\ &+ a_{21}x^2 x^1 + a_{22}x^2 x^2 + \dots + a_{2n}x^2 x^n + \\ &\dots \\ &+ a_{n1}x^n x^1 + a_{n2}x^n x^2 + \dots + a_{nn}x^n x^n, \end{aligned}$$

with a non-symmetric second order tensor  $a_{ij}$ , can be made symmetric in the following way.

$$a_{ij}x^i x^j = \frac{1}{2}a_{ij}x^i x^j + \frac{1}{2}a_{ij}x^i x^j.$$

If we swap indices in the second term, we get

$$\begin{aligned} &= \frac{1}{2}a_{ij}x^i x^j + \frac{1}{2}a_{ji}x^j x^i, \quad \text{which is equal to} \\ &= \frac{1}{2}(a_{ij} + a_{ji})x^i x^j. \end{aligned}$$

If we now use a substitution,

$$\begin{aligned} \frac{1}{2}(a_{ij} + a_{ji}) &\equiv b_{ij} = b_{ji}, \quad \text{we get} \\ a_{ij}x^i x^j &= b_{ij}x^i x^j, \end{aligned}$$

where  $a_{ij}$  is non-symmetric and  $b_{ij}$  is symmetric, as required.

(iii) *Every second order tensor that is the sum  $a^{ij} = u^i v^j + u^j v^i$ , or,  $a_{ij} = u_i v_j + u_j v_i$  is symmetric.* In both cases, if we swap the indices  $i$  and  $j$ , we get  $a^{ji} = u^j v^i + u^i v^j$ , (resp.  $a_{ji} = u_j v_i + u_i v_j$ ), which implies that the tensor  $a^{ij}$  (resp.  $a_{ij}$ ) is symmetric.

(iv) *Every second order tensor that is the difference  $b^{ij} = u^i v^j - u^j v^i$ , or,  $b_{ij} = u_i v_j - u_j v_i$  is skew-symmetric.* In both cases, if we swap the indices  $i$  and  $j$ , we get  $b^{ji} = -(u^j v^i - u^i v^j)$ , (resp.  $b_{ji} = -(u_j v_i - u_i v_j)$ ), which implies that the tensor  $b^{ij}$  (resp.  $b_{ij}$ ) is skew-symmetric.

### A.1.2 Euclidean Tensors

#### Basis Vectors and the Metric Tensor in $\mathbb{R}^n$

The natural *Cartesian coordinate basis* in an  $n$ D Euclidean space  $\mathbb{R}^n$  is defined as a set of  $n$ D unit vectors  $e^i$  given by

$$e^1 = \{1, 0, 0, \dots\}^t, \quad e^2 = \{0, 1, 0, \dots\}^t, \quad e^3 = \{0, 0, 1, \dots\}^t, \dots, \quad e^n = \{0, 0, \dots, 1\}^t,$$

(where index  $t$  denotes transpose) while its dual basis  $e_i$  is given by:

$$e_1 = \{1, 0, 0, \dots\}, \quad e_2 = \{0, 1, 0, \dots\}, \quad e_3 = \{0, 0, 1, \dots\}, \dots, \quad e_n = \{0, 0, \dots, 1\},$$

(no transpose) where the definition of the dual basis is given by the Kronecker's  $\delta$ -symbol, i.e., the  $n \times n$  identity matrix:

$$e^i \cdot e_j = \delta_j^i = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix},$$

that is the metric tensor in Cartesian coordinates equals  $\mathbf{g} = \delta_j^i$ . In general, (i.e., curvilinear) coordinate system, the metric tensor  $\mathbf{g} = g_{ij}$  is defined as the scalar product of the dual basis vectors, i.e., the  $n \times n$  matrix:

$$g_{ij} = e_i \cdot e_j = \begin{bmatrix} g_{11} & g_{12} & g_{13} & \dots & g_{1n} \\ g_{21} & g_{22} & g_{23} & \dots & g_{2n} \\ g_{31} & g_{32} & g_{33} & \dots & g_{3n} \\ \dots & \dots & \dots & \dots & \dots \\ g_{n1} & g_{n2} & g_{n3} & \dots & g_{nn} \end{bmatrix}.$$

### Tensor Products in $\mathbb{R}^n$

Let  $\mathbf{u}$  and  $\mathbf{v}$  denote two vectors in  $\mathbb{R}^n$ , with their components given by

$$u^i = u \cdot e^i, \quad \text{and} \quad v^j = v \cdot e^j,$$

where  $u = |\mathbf{u}|$  and  $v = |\mathbf{v}|$  are their respective norms (or, lengths). Then their inner product (i.e., scalar, or dot product)  $\mathbf{u} \cdot \mathbf{v}$  is a scalar invariant  $S$ , defined as

$$S = u^i \cdot v^j = g_{ij} u^i v^j.$$

Besides the dot product of two vectors  $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$ , there is also their tensor product (i.e., generalized vector, or cross product), which is a second order tensor

$$\mathbf{T} = \mathbf{u} \otimes \mathbf{v}, \quad \text{in components, } T^{ij} = u^i \otimes v^j.$$

In the natural basis  $e_i$  this tensor is expanded as

$$\mathbf{T} = T^{ij} e_i \otimes e_j,$$

while its components in the dual basis read:

$$T^{ij} = T(e^i, e^j),$$

where  $T = |\mathbf{T}|$  is its norm. To get its components in curvilinear coordinates, we need first to substitute it in Cartesian basis:

$$T^{ij} = T^{mn} (e_m \otimes e_n)(e^i, e^j),$$

then to evaluate it on the slots:

$$T^{ij} = T^{mn} e_m \cdot e^i e_n \cdot e^j,$$

and finally to calculate the other index configurations by lowering indices, by means of the metric tensor:

$$T_j^i = g_{jm} T^{im}, \quad T_{ij} = g_{im} g_{jn} T^{mn}.$$

#### A.1.3 Tensor Derivatives on Riemannian Manifolds

Consider now some  $n$ D Riemannian manifold  $M$  with the metric form (i.e., line element)  $ds^2 = g_{ik} dx^i dx^k$ , as a configuration space for a certain biomechanical system (e.g., human spine, or arm-shoulder complex).

### Christoffel's Symbols

Partial derivatives of the metric tensor  $g_{ik}$  form themselves special symbols that do not transform as tensors (with respect to the coordinate transformation (A.2)), but nevertheless represent important quantities in tensor analysis. They are called *Christoffel symbols of the first kind*, defined by

$$\Gamma_{ijk} = \frac{1}{2}(\partial_{x^i}g_{jk} - \partial_{x^j}g_{ki} + \partial_{x^k}g_{ij}), \quad \left( \text{remember, } \partial_{x^i} \equiv \frac{\partial}{\partial x^i} \right)$$

and *Christoffel symbols of the second kind*, defined by

$$\Gamma_{ij}^k = g^{kl}\Gamma_{ijl}.$$

The Riemann curvature tensor  $R_{ijk}^l$  (A.7) of the manifold  $M$ , can be expressed in terms of the later as

$$R_{ijk}^l = \partial_{x^j}\Gamma_{ik}^l - \partial_{x^k}\Gamma_{ij}^l + \Gamma_{rj}^l\Gamma_{ik}^r - \Gamma_{rk}^l\Gamma_{ij}^r.$$

For example, in 3D spherical coordinates,  $x^i = \{\rho, \theta, \varphi\}$ , with the metric tensor and its inverse given by (A.5, A.6), it can be shown that the only nonzero Christoffel's symbols are:

$$\begin{aligned} \Gamma_{12}^2 = \Gamma_{21}^2 = \Gamma_{13}^3 = \Gamma_{31}^3 = \frac{1}{\rho}, \quad \Gamma_{23}^3 = \Gamma_{32}^2 = -\tan \theta, \quad (\text{A.8}) \\ \Gamma_{22}^1 = -\rho, \quad \Gamma_{33}^1 = -\rho \cos^2 \theta, \quad \Gamma_{33}^2 = \sin \theta \cos \theta. \end{aligned}$$

### Geodesics

From the Riemannian metric form  $ds^2 = g_{ik}dx^i dx^k$  it follows that the distance between two points  $t_1$  and  $t_2$  on a curve  $x^i = x^i(t)$  in  $M$  is given by

$$s = \int_{t_1}^{t_2} \sqrt{g_{ik}\dot{x}^i \dot{x}^k} dt.$$

That curve  $x^i = x^i(t)$  in  $M$  which makes the distance  $s$  a minimum is called a *geodesic* of the space  $M$  (e.g., in a sphere, the geodesics are arcs of great circles). Using the calculus of variations, the geodesics are found from the differential *geodesic equation*,

$$\ddot{x}^i + \Gamma_{jk}^i \dot{x}^j \dot{x}^k = 0, \quad (\text{A.9})$$

where overdot means derivative upon the line parameter  $s$ .

For example, in 3D spherical coordinates  $x^i = \{\rho, \theta, \varphi\}$ , using (A.8), geodesic equation (A.9) becomes a system of three scalar ODEs,

$$\begin{aligned} \ddot{\rho} - \rho \dot{\theta}^2 - \rho \cos^2 \theta \dot{\varphi}^2 = 0, \quad \ddot{\theta} + \frac{2}{\rho} \dot{\rho} \dot{\theta} + \sin \theta \cos \theta \dot{\varphi}^2 = 0, \\ \ddot{\varphi} + \frac{2}{\rho} \dot{\rho} \dot{\varphi} - 2 \tan \theta \dot{\theta} \dot{\varphi} = 0. \end{aligned} \quad (\text{A.10})$$

### The Covariant Derivative

Ordinary total and partial derivatives of vectors (covectors) *do not transform as vectors* (covectors) with respect to the coordinate transformation (A.2). For example, let  $y^k$  be Cartesian coordinates and  $x^i$  be general curvilinear coordinates of a dynamical system (with  $i, k = 1, \dots, n$ ). We have:  $x^i(t) = x^i[y^k(t)]$ , which implies that

$$\frac{dx^i}{dt} = \frac{\partial x^i}{\partial y^k} \frac{dy^k}{dt}, \quad \text{or equivalently,} \quad \dot{x}^i = \frac{\partial x^i}{\partial y^k} \dot{y}^k,$$

that is a transformation law for the contravariant vector, which means that the velocity  $v^i \equiv \dot{x}^i \equiv \frac{dx^i}{dt}$  is a proper contravariant vector. However, if we perform another time differentiation, we get

$$\frac{d^2x^i}{dt^2} = \frac{\partial x^i}{\partial y^k} \frac{d^2y^k}{dt^2} + \frac{\partial^2 x^i}{\partial y^k \partial y^m} \frac{dy^k}{dt} \frac{dy^m}{dt},$$

which means that  $\frac{d^2x^i}{dt^2}$  is *not* a proper vector.

$\frac{d^2x^i}{dt^2}$  is an acceleration vector only in a special case when  $x^i$  are another Cartesian coordinates; then  $\frac{\partial^2 x^i}{\partial y^k \partial y^m} = 0$ , and therefore the original coordinate transformation is linear,  $x^i = a_k^i y^k + b^i$  (where  $a_k^i$  and  $b^i$  are constant).

Therefore,  $\frac{d^2x^i}{dt^2}$  represents an acceleration vector only in terms of Newtonian mechanics in a Euclidean space  $\mathbb{R}^n$ , while it is not a proper acceleration vector in terms of Lagrangian or Hamiltonian mechanics in general curvilinear coordinates on a smooth manifold  $M^n$ . And we know that Newtonian mechanics in  $\mathbb{R}^n$  is sufficient only for fairly simple mechanical systems.

The above is true for any tensors. So we need to find another derivative operator to be able to preserve their tensor character. The solution to this problem is called the *covariant derivative*.

The covariant derivative  $v^i_{;k}$  of a contravariant vector  $v^i$  is defined as

$$v^i_{;k} = \partial_{x^k} v^i + \Gamma^i_{jk} v^j.$$

Similarly, the covariant derivative  $v_{i;k}$  of a covariant vector  $v_i$  is defined as

$$v_{i;k} = \partial_{x^k} v_i - \Gamma^j_{ik} v_j.$$

Generalization for the higher order tensors is straightforward; e.g., the covariant derivative  $t^j_{kl;q}$  of the third order tensor  $t^j_{kl}$  is given by

$$t^j_{kl;q} = \partial_{x^q} t^j_{kl} + \Gamma^j_{qs} t^s_{kl} - \Gamma^s_{kq} t^j_{sl} - \Gamma^s_{lq} t^j_{ks}.$$

The covariant derivative is the most important tensor operator in general relativity (its zero defines *parallel transport*) as well as the basis for defining other differential operators in mechanics and physics.

### Covariant Form of Gradient, Divergence, Curl and Laplacian

**Gradient.** If  $\varphi = \varphi(x^i, t)$  is a scalar field, the gradient one-form  $\text{grad}(\varphi)$  is defined by

$$\text{grad}(\varphi) = \nabla\varphi = \varphi_{;i} = \partial_{x^i}\varphi.$$

**Divergence.** The divergence  $\text{div}(v^i)$  of a vector-field  $v^i = v^i(x^i, t)$  is defined by contraction of its covariant derivative with respect to the coordinates  $x^i = x^i(t)$ , i.e., the contraction of  $v^i_{;k}$ , namely

$$\text{div}(v^i) = v^i_{;i} = \frac{1}{\sqrt{g}}\partial_{x^i}(\sqrt{g}v^i).$$

**Curl.** The curl  $\text{curl}(\theta_i)$  of a one-form  $\theta_i = \theta_i(x^i, t)$  is a second order covariant tensor defined as

$$\text{curl}(\theta_i) = \theta_{i;k} - \theta_{k;i} = \partial_{x^k}\theta_i - \partial_{x^i}\theta_k.$$

**Laplacian.** The Laplacian  $\Delta\varphi$  of a scalar invariant  $\varphi = \varphi(x^i, t)$  is the divergence of  $\text{grad}(\varphi)$ , or

$$\Delta\varphi = \nabla^2\varphi = \text{div}(\text{grad}(\varphi)) = \text{div}(\varphi_{;i}) = \frac{1}{\sqrt{g}}\partial_{x^i}(\sqrt{g}g^{ik}\partial_{x^k}\varphi).$$

### The Absolute Derivative

The *absolute derivative* (or *intrinsic*, or *Bianchi's derivative*) of a contravariant vector  $v^i$  along a curve  $x^k = x^k(t)$  is denoted by  $\dot{v}^i \equiv Dv^i/dt$  and defined as the inner product of the covariant derivative of  $v^i$  and  $\dot{x}^k \equiv dx^k/dt$ , i.e.,  $v^i_{;k}\dot{x}^k$ , and is given by

$$\dot{v}^i = v^i + \Gamma^i_{jk}v^j\dot{x}^k.$$

Similarly, the absolute derivative  $\dot{v}_i$  of a covariant vector  $v_i$  is defined as

$$\dot{v}_i = v_i - \Gamma^j_{ik}v_j\dot{x}^k.$$

Generalization for the higher order tensors is straightforward; e.g., the absolute derivative  $\dot{t}^j_{kl}$  of the third order tensor  $t^j_{kl}$  is given by

$$\dot{t}^j_{kl} = t^j_{kl} + \Gamma^j_{qs}t^s_{kl}\dot{x}^q - \Gamma^s_{kq}t^j_{sl}\dot{x}^q - \Gamma^s_{lq}t^j_{ks}\dot{x}^q.$$

*The absolute derivative is the most important operator in biomechanics, as it is the basis for the covariant form of both Lagrangian and Hamiltonian equations of motion of many biomechanical systems.*

*Application to Curve Geometry*

Given three unit vectors: *tangent*  $\tau^i$ , *principal normal*  $\beta^i$ , and *binormal*  $\nu^i$ , as well as two scalar invariants: curvature  $K$  and torsion  $T$ , of a curve  $\gamma(s) = \gamma[x^i(s)]$ , the so-called *Frenet–Serret formulae* are valid<sup>1</sup>

$$\begin{aligned}\dot{\tau}^i &\equiv \dot{\tau}^i + \Gamma_{jk}^i \tau^j \dot{x}^k = K\beta^i, \\ \dot{\beta}^i &\equiv \dot{\beta}^i + \Gamma_{jk}^i \beta^j \dot{x}^k = -(K\tau^i + T\nu^i), \\ \dot{\nu}^i &\equiv \dot{\nu}^i + \Gamma_{jk}^i \nu^j \dot{x}^k = T\beta^i.\end{aligned}$$

*Application to Mechanical Definitions of Acceleration and Force*

In modern analytical mechanics, the two fundamental notions of *acceleration* and *force* in general curvilinear coordinates are substantially different from the corresponding terms in Cartesian coordinates as commonly used in engineering mechanics. Namely, the acceleration vector *is not* an ordinary time derivative of the velocity vector; ‘even worse’, the force, which is a paradigm of a vector in statics and engineering vector mechanics, *is not* a vector at all. Proper mathematical definition of the acceleration vector is the absolute time derivative of the velocity vector, while the force is a differential one–form.

To give a brief look at these ‘weird mathematical beasts’, consider a material dynamical system described by  $n$  curvilinear coordinates  $x^i = x^i(t)$ . First, recall from subsection A.1.3 above, that an ordinary time derivative of the velocity vector  $v^i(t) = \dot{x}^i(t)$  *does not transform as a vector* with respect to the general coordinate transformation (A.2). Therefore,  $a^i \neq \dot{v}^i$ . So, we need to use its absolute time derivative to define the acceleration vector (with  $i, j, k = 1, \dots, n$ ),

$$a^i = \dot{v}^i \equiv \frac{Dv^i}{dt} = v_{;k}^i \dot{x}^k \equiv \dot{v}^i + \Gamma_{jk}^i v^j \dot{x}^k \equiv \ddot{x}^i + \Gamma_{jk}^i \dot{x}^j \dot{x}^k, \quad (\text{A.11})$$

which is equivalent to the l.h.s of the geodesic equation (A.9). Only in the particular case of Cartesian coordinates, the general acceleration vector (A.11) reduces to the familiar engineering form of the Euclidean acceleration vector<sup>2</sup>,  $\mathbf{a} = \dot{\mathbf{v}}$ .

For example, in standard spherical coordinates  $x^i = \{\rho, \theta, \varphi\}$ , we have the components of the acceleration vector given by (A.10), if we now reinterpret overdot as the time derivative,

<sup>1</sup> In this paragraph, the overdot denotes the total derivative with respect to the line parameter  $s$  (instead of time  $t$ ).

<sup>2</sup> Any Euclidean space can be defined as a set of Cartesian coordinates, while any Riemannian manifold can be defined as a set of curvilinear coordinates. Christoffel’s symbols  $\Gamma_{jk}^i$  vanish in Euclidean spaces defined by Cartesian coordinates; however, they are nonzero in Riemannian manifolds defined by curvilinear coordinates (see Chapter 2 for geometric details).

$$a^\rho = \ddot{\rho} - \rho \dot{\theta}^2 - \rho \cos^2 \theta \dot{\varphi}^2, \quad a^\theta = \ddot{\theta} + \frac{2}{\rho} \dot{\rho} \dot{\varphi} + \sin \theta \cos \theta \dot{\varphi}^2,$$

$$a^\varphi = \ddot{\varphi} + \frac{2}{\rho} \dot{\rho} \dot{\varphi} - 2 \tan \theta \dot{\theta} \dot{\varphi}.$$

Now, using (A.11), the *Newton’s fundamental equation of motion, that is the basis of all science*,  $\mathbf{F} = m \mathbf{a}$ , gets the following tensorial form

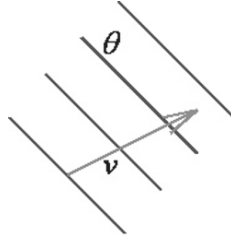
$$F^i = m a^i = m \dot{v}^i = m(v^i_{;k} \dot{x}^k) \equiv m(\dot{v}^i + \Gamma^i_{jk} v^j v^k) = m(\ddot{x}^i + \Gamma^i_{jk} \dot{x}^j \dot{x}^k), \quad (\text{A.12})$$

which defines Newtonian force as a contravariant vector.

However, modern Hamiltonian dynamics reminds us that: (i) Newton’s own force definition was not really  $\mathbf{F} = m \mathbf{a}$ , but rather  $\mathbf{F} = \dot{\mathbf{p}}$ , where  $\mathbf{p}$  is the system’s momentum, and (ii) the momentum  $\mathbf{p}$  is not really a vector, but rather a dual quantity, a differential one–form<sup>3</sup> (see Chapter 2 for details). Consequently, the force, as its time derivative, is also a one–form (see Figure A.1). This new force definition includes the precise definition of the mass distribution within the system, by means of its Riemannian metric tensor  $g_{ij}$ . Thus, (A.12) has to be modified as

$$F_i = m g_{ij} a^j \equiv m g_{ij} (v^j_{;k} \dot{x}^k) \equiv m g_{ij} (\dot{v}^j + \Gamma^j_{ik} v^i v^k) = m g_{ij} (\ddot{x}^j + \Gamma^j_{ik} \dot{x}^i \dot{x}^k), \quad (\text{A.13})$$

where the quantity  $m g_{ij}$  is called the *material metric tensor*, or *inertia matrix*. Equation (A.13) generalizes the notion of the Newtonian force  $\mathbf{F}$ , from Euclidean space  $\mathbb{R}^n$  to the Riemannian manifold  $M$  (see Chapter 2).



**Fig. A.1.** A one–form  $\theta$  (which is a family of parallel (hyper)surfaces, the so–called *Grassmann planes*) pierced by the vector  $v$  to give a scalar product  $\theta(v) \equiv \langle \theta, v \rangle = 2.6$  (see [MTW73] for technical details).

*Application to Fluid Mechanics: Continuity Equation*

The most important equation in continuum mechanics, in particular in fluid mechanics, is the celebrated *equation of continuity*,

<sup>3</sup> For example, in Dirac’s  $\langle bra|ket \rangle$  formalism, *kets* are vectors, while *bras* are one–forms; in matrix notation, columns are vectors, while rows are one–forms.

$$\partial_t \rho + \operatorname{div}(\rho \dot{\mathbf{x}}) = 0. \quad (\text{A.14})$$

Here we derive the continuity equation (A.14), using the absolute time derivative and starting from the *mass conservation principle*,

$$\overline{\dot{dm}} = 0, \quad (\text{A.15})$$

where  $dm$  denotes an infinitesimal mass of a fluid (continuum) particle. If we introduce the fluid density  $\rho = dm/dv$ , where  $v$  is the infinitesimal volume of a fluid particle, then the mass conservation principle (A.15) can be written as

$$\overline{\dot{\rho} dv} = 0,$$

which is the absolute derivative of a product, and therefore expands into

$$\dot{\rho} dv + \overline{\dot{dv}} = 0. \quad (\text{A.16})$$

Now, as the fluid density is a function of both time  $t$  and spatial coordinates  $x^k$ , i.e., a scalar-field,  $\rho = \rho(x^k, t)$ , its total time derivative  $\dot{\rho}$ , figuring in (A.16), is defined by

$$\dot{\rho} = \partial_t \rho + \partial_{x^k} \rho \partial_t x^k \equiv \partial_t \rho + \rho_{;k} \dot{x}^k \equiv \partial_t \rho + \operatorname{grad}(\rho) \cdot \dot{\mathbf{x}}. \quad (\text{A.17})$$

Regarding  $\overline{\dot{dv}}$ , the other term figuring in (A.16), we start by expanding an elementary volume  $dv$  along the sides  $\{dx_{(p)}^i, dx_{(q)}^j, dx_{(r)}^k\}$  of an elementary parallelepiped,

$$dv = \frac{1}{3!} \delta_{ijk}^{pqr} dx_{(p)}^i dx_{(q)}^j dx_{(r)}^k, \quad (i, j, k, p, q, r = 1, 2, 3)$$

so that its absolute derivative becomes

$$\begin{aligned} \overline{\dot{dv}} &= \frac{1}{2!} \delta_{ijk}^{pqr} \overline{\dot{dx}_{(p)}^i} dx_{(q)}^j dx_{(r)}^k \\ &= \frac{1}{2!} \dot{x}_{;l}^i \delta_{ijk}^{pqr} dx_{(p)}^l dx_{(q)}^j dx_{(r)}^k \quad (\text{using } \overline{\dot{dx}_{(p)}^i} = \dot{x}_{;l}^i dx_{(p)}^l), \end{aligned}$$

which finally simplifies into

$$\overline{\dot{dv}} = \dot{x}_{;k}^k dv \equiv \operatorname{div}(\dot{\mathbf{x}}) dv. \quad (\text{A.18})$$

Substituting (A.17) and (A.18) into (A.16) gives

$$\overline{\dot{\rho} dv} \equiv (\partial_t \rho + \rho_{;k} \dot{x}^k) dv + \rho \dot{x}_{;k}^k dv = 0. \quad (\text{A.19})$$

As we are dealing with arbitrary fluid particles,  $dv \neq 0$ , so from (A.19) follows

$$\partial_t \rho + \rho_{;k} \dot{x}^k + \rho \dot{x}_{;k}^k \equiv \partial_t \rho + (\rho \dot{x}^k)_{;k} = 0. \quad (\text{A.20})$$

Equation (A.20) is the covariant form of the continuity equation, which in standard vector notation becomes (A.14).

In classical biomechanics, the continuity equation (A.14) forms the basis of *hemodynamics*, or blood flow dynamics.

#### A.1.4 The Covariant Force Law in Human-Like Biomechanics

Objective of this final tensor subsection is to generalize the fundamental Newtonian 3D equation,  $\mathbf{F} = m\mathbf{a}$ , for the generic biomechanical system, consisting of a number of flexibly-coupled rigid segments (see Figures 2.2–2.3 above), and thus to formulate the fundamental biomechanical law: *the covariant force law*.

To be able to apply the covariant formalism, we need to start with the suitable coordinate transformation (A.2), in this case as a relation between the 6 *external*  $SE(3)$  rigid-body coordinates,  $y^e = y^e(t)$  ( $e = 1, \dots, 6$ ), and  $2n$  *internal joint coordinates*,  $x^i = x^i(t)$  ( $i = 1, \dots, 2n$ ) ( $n$  angles, forming the constrained  $n$ -torus  $T^n$ , plus  $n$  very restricted translational coordinates, forming the hypercube  $I^n \subset \mathbb{R}^n$ ). Once we have these two sets of coordinates, external- $y^e$  and internal- $x^i$ , we can perform the general functional transformation (A.2) between them,

$$x^i = x^i(y^e). \quad (\text{A.21})$$

Now, although the coordinate transformation (A.21) is nonlinear and even unknown at this stage, there is something known and simple about it: the corresponding transformation of differentials is *linear and homogenous*,

$$dx^i = \frac{\partial x^i}{\partial y^e} dy^e,$$

which implies the *linear and homogenous transformation of velocities*,

$$\dot{x}^i = \frac{\partial x^i}{\partial y^e} \dot{y}^e. \quad (\text{A.22})$$

Our *internal velocity vector-field* is defined by the set of ODEs (A.22), at each *representative point*  $x^i = x^i(t)$  of the biomechanical configuration manifold  $M = T^n \times I^n$ , as  $v^i \equiv v^i(x^i, t) := \dot{x}^i(x^i, t)$ .

Note that in general, a *vector-field* represents a field of vectors defined at every point  $x^i$  within some region  $U$  (e.g., movable segments/joints only) of the total configuration manifold  $M$  (consisting of all the segments/joints). Analytically, vector-field is defined as a set of autonomous ODEs (in our case, the set (A.22)). Its solution gives the *flow*, consisting of *integral curves* of the vector-field, such that all the vectors from the vector-field are tangent to integral curves at different representative points  $x^i \in U$ . In this way, through every representative point  $x^i \in U$  passes both a curve from the flow and its tangent vector from the vector-field. Geometrically, vector-field is defined as a cross-section of the tangent bundle  $TM$ , the so-called *velocity phase-space*. Its *geometrical dual* is the *1-form-field*, which represents a field of one-forms (see Figure A.1), defined at the same representative points  $x^i \in U$ . Analytically, 1-form-field is defined as an *exterior differential system*, an algebraic dual to the autonomous set of ODEs. Geometrically, it is defined as a cross-section of the

cotangent bundle  $T^*M$ , the so-called *momentum phase-space*. Together, the vector-field and its corresponding 1-form-field define the *scalar potential field* (e.g., kinetic and/or potential energy) at the same movable region  $U \subset M$ . See Chapter 2 for technical details.

Now, we are on the half-way to covariant biomechanics. We need to formulate the internal acceleration vector-field,  $a^i \equiv a^i(x^i, \dot{x}^i, t)$ , acting in all movable joints, and at the same time generalizing the Newtonian 3D acceleration vector  $\mathbf{a}$ .

According to Newton, acceleration is a rate-of-change of velocity. But, from the previous subsections, we know that  $a^i \neq \dot{v}^i$ . However,

$$a^i := \dot{v}^i = \dot{v}^i + \Gamma_{jk}^i v^j v^k = \ddot{x}^i + \Gamma_{jk}^i \dot{x}^j \dot{x}^k. \quad (\text{A.23})$$

Once we have the *internal acceleration vector-field*  $a^i = a^i(x^i, \dot{x}^i, t)$ , defined by the set of ODEs (A.23) (including *Levi-Civita connections*  $\Gamma_{jk}^i$  of the Riemannian configuration manifold  $M$ ), we can finally define the *internal force 1-form field*,  $F_i = F_i(x^i, \dot{x}^i, t)$ , as a family of force one-forms, half of them rotational and half translational, acting in all movable joints,

$$F_i := mg_{ij} a^j = mg_{ij} (\dot{v}^j + \Gamma_{ik}^j v^i v^k) = mg_{ij} (\ddot{x}^j + \Gamma_{ik}^j \dot{x}^i \dot{x}^k), \quad (\text{A.24})$$

where we have used the simplified *material metric tensor*,  $mg_{ij}$ , for the biomechanical system (considering, for simplicity, all segments to have equal mass  $m$ ), defined by its *Riemannian kinetic energy form*

$$T = \frac{1}{2} mg_{ij} v^i v^j.$$

Equation  $F_i = mg_{ij} a^j$ , defined properly by (A.24) at every representative point  $x^i$  of the biomechanical configuration manifold  $M$ , formulates the sought for *covariant force law*, that generalizes the fundamental Newtonian equation,  $\mathbf{F} = m\mathbf{a}$ , for the generic biomechanical system. Its meaning is:

**Force 1-form-field = Mass distribution  $\times$  Acceleration vector-field**

In other words, *the field (or, family) of force one-forms  $F_i$ , acting in all movable joints (with constrained rotations on  $T^n$  and very restricted translations on  $I^n$ ), causes both rotational and translational accelerations of all body segments, within the mass distribution  $mg_{ij}$ <sup>4</sup>, along the flow-lines of the vector-field  $a^j$ .*

<sup>4</sup> More realistically, instead of the simplified metric  $mg_{ij}$  we have the *material metric tensor*  $G_{ij}$  (1.9), including all  $k$  segmental masses  $m_\chi$ , as well as the corresponding moments and products of inertia,

$$G_{ij}(x, m) = \sum_{\chi=1}^k m_\chi \delta_{rs} \frac{\partial y^r}{\partial x^i} \frac{\partial y^s}{\partial x^j}, \quad (r, s = 1, \dots, 6; i, j = 1, \dots, 2n),$$

as defined in Figures 2.2–2.3 above.

From the control theory perspective, a vector-field is a dynamical system, a set of differential equations (A.23) that has a set of force one-forms  $F_i$  as its inputs (see Chapter 5).

The purpose of Chapter 2 is to put this *core biomechanical law* into rigorous settings of smooth manifolds and their (co)tangent bundles.

### A.1.5 The Essence of Hamiltonian Biomechanics

The *covariant force law*,  $F_i = mg_{ij}a^j$ , defined by (A.24) above, has the following Hamiltonian reformulation. We start with the *conservative Hamiltonian biomechanics* on the *cotangent bundle*  $T^*M$  of the system's *configuration manifold*  $M$  (see Figures 2.2–2.3 above), given by (see Chapter 3)

$$\dot{q}^\alpha = \partial_{p_\alpha} H(q^\alpha, p_\alpha), \quad \dot{p}_\alpha = -\partial_{q^\alpha} H(q^\alpha, p_\alpha), \quad (\alpha = 1, \dots, n).$$

The *forced Hamiltonian biomechanics* on  $T^*M$  is given by

$$\dot{q}^\alpha = \partial_{p_\alpha} H(q^\alpha, p_\alpha), \quad \dot{p}_\alpha = F_\alpha(t, q^\alpha, p_\alpha) - \partial_{q^\alpha} H(q^\alpha, p_\alpha),$$

where  $F_\alpha$  are muscular torques. The *generalized Hamiltonian biomechanics* (forced & dissipative) on  $T^*M$  is now given by

$$\begin{aligned} \dot{q}^\alpha &= \partial_{p_\alpha} H(q^\alpha, p_\alpha) - \partial_{p_\alpha} R(q^\alpha, p_\alpha), \\ \dot{p}_\alpha &= F_\alpha(t, q^\alpha, p_\alpha) - \partial_{q^\alpha} H(q^\alpha, p_\alpha) - \partial_{q^\alpha} R(q^\alpha, p_\alpha). \end{aligned} \quad (\text{A.25})$$

The generalized Hamiltonian system (A.25) covers several types of classical dynamical systems (see Chapter 3):

- (i) in case  $F_\alpha = 0$ ,  $R = 0$  and  $H \neq 0$  – conservative Hamiltonian system;
- (ii) in case  $F_\alpha = 0$ ,  $R \neq 0$  and  $H \neq 0$  – dissipative Hamiltonian system;
- (iii) in case  $F_\alpha = 0$ ,  $R \neq 0$  and  $H = 0$  – bidirectional gradient system;
- (iv) in case  $F_\alpha \neq 0$ ,  $R = 0$  and  $H = 0$  – simple Newtonian system;
- (v) in case  $F_\alpha \neq 0$ ,  $R = 0$  and  $H \neq 0$  – generalized Newtonian system.

The *generalized Hamiltonian control system* on  $T^*M$  is obtained from (A.25) in the following way. First we introduce the *control Hamiltonian function*,  $H_C : T^*M \times R \rightarrow R$ . In the local coordinates  $q^\alpha, p_\alpha \in U_p \subset T^*M$ , the control Hamiltonian is given by

$$H_C(q, p, u) = H_0(q, p) - q^\alpha u_\alpha, \quad (\alpha = 1, \dots, n)$$

where  $u_\alpha = u_\alpha(t, q, p)$  are *neural control inputs*, and the physical Hamiltonian  $H_0(q, p)$  represents the system's *total energy function*  $H_0 : T^*M \times \mathbb{R} \rightarrow \mathbb{R}$ . The natural input-output control system is now defined as

$$\begin{aligned} \dot{q}^\alpha &= \partial_{p_\alpha} H_C(q, p, u) + \partial_{p_\alpha} R(q, p), & \dot{p}_\alpha &= F_\alpha - \partial_{q^\alpha} H_C(q, p, u) + \partial_{q^\alpha} R(q, p), \\ & & y^\alpha &= -\partial_{u_\alpha} H_C(q, p, u), \end{aligned}$$

where  $y^\alpha$  are *control outputs* (see Chapter 5).

## A.2 Muscular System

### A.2.1 Muscular Histology

*Human skeletal and face muscles*, accounting for more than 40% of the body weight in man, consist of bundles of elongated, cylindric cells called *muscle fibers*, 50 to 200  $\mu$  in diameter and often many centimeters long. Bundles of muscle fibers, each called *fasciculus*, are surrounded by a connective tissue covering, the *endomysium* (see, e.g., [Mou80, Mar98]).

A muscle consists of a number of fasciculi encased in a thick outer layer of connective tissue, the *perimysium*. At both ends of a muscle the connective tissue melds into a tendon by which the muscle is attached to the face or bony skeleton. In some muscles (*fusiform*), the muscle fibers run the whole length of muscle between the tendons, which form at opposite ends. In most muscles (*pennate*), one of the tendons penetrates through the center of the muscle; muscle fibers run at an angle to the axis of the whole muscle from the central tendon to the perimysium.

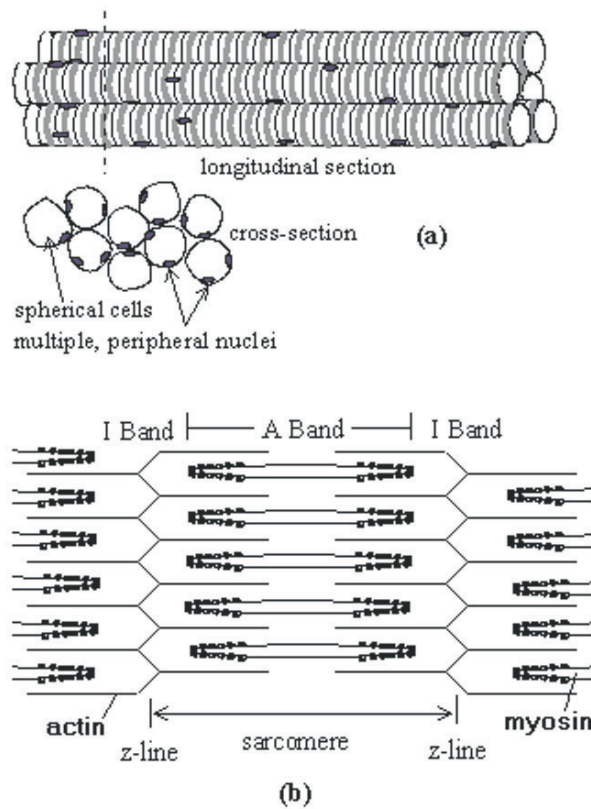
Like other cells, muscle cells are surrounded by a cell membrane, the *sarcolemma*. *Myofibrils*, the *contractile elements*, are numerous parallel, lengthwise threads 1 to 3 in diameter that fill most of the muscle fiber. The *cross striations*, seen in the skeletal and face muscles with electron microscope, are located in the myofibrils. Squeezed between the myofibrils and the sarcolemma is a small amount of cytoplasm, the *sarcoplasm*, in which are suspended multiple nuclei, numerous mitochondria, lysosomes, lipid droplets, glycogen granules, and other intracellular inclusions. The sarcoplasm contains glycogen, glycolytic enzymes, nucleotides, creatine phosphate, amino acids, and peptides.

Sarcoplasm also contains a well-developed endoplasmic reticulum, which in muscle is called *sarcoplasmic reticulum*. The sarcoplasmic reticulum forms an extensive hollow membranous system within the cytoplasm surrounding the myofibrils. Periodically, there are branching invaginations of the sarcolemma called *T tubules* or transverse tubules. The sarcoplasmic reticulum bulges out on either side of the T tubules to form large *lateral cisternae*. The T tubule and two sets of lateral cisternae constitute a *triad*. The triads play an important role in muscle excitation-contraction coupling (by release of  $Ca^{++}$  ions).

Two types of muscle fibers are found in human skeletal and face muscles: *red* and *white muscle fibers*, being histochemically and functionally distinctive. Many muscles are mixed, containing both types of fibers, which can be distinguished by various histochemical stains. In addition to muscle cells and fibroblasts in the connective tissue, a whole muscle contains fat cells and histiocytes.

Each muscle fiber contains numerous contractile elements - *myofibrils* (1–3  $\mu$  in diameter) which are biological machines that utilize chemical energy from metabolism of food in the form of *adenosine triphosphate*, *ATP* hydrolysis to produce mechanical work. An understanding of contractility and muscle function requires, thus, both histo-mechanical and bio-energetic insight.

Contractile machinery unit of the myofibril, *sarcomere* (1.5–3.5  $\mu$  long; on electron microscope it is seen as bounded by two *Z* lines, with *H* zone in the middle of the *A* band) is constituted of a great number of longitudinal protein filaments of two kinds: thick, *myosin* filaments (about 120  $\text{\AA}$  in diameter and about 1.8  $\mu$  long; they are located in the center of the sarcomere arranged in a hexagonal array about 450  $\text{\AA}$  apart) and thin, *actin* filaments (about 80  $\text{\AA}$  in diameter and about 1.0  $\mu$  long; they are anchored into the transverse filaments forming the *Z* line) (see Figure A.2). Each myosin filament is surrounded by six actin filaments. Each myosin filament has two heads and two projections from opposite sides at about 143  $\text{\AA}$  intervals along its length.



**Fig. A.2.** Cellular structure of the voluntary (skeletal) human muscle: (a) Muscular fibers with their cross-sections; (b) Sarcomere with overlapping myofilaments.

### A.2.2 Classical Theories of Muscular Contraction

#### Huxley's Sliding Filament Theory

Essential for the contraction process are *cross bridges* (see Figure A.2). They extend from myosin filaments to touch one of the adjacent actin filaments. Each thin filament receives cross bridges from the three adjacent thick filaments. During shortening the two sets of interdigitating filaments slide with respect to each other, cross and finally overlap each other. This process of muscle shortening involving progressive interdigitation of the two sets of protein filaments represents the *sliding filament mechanism*, discovered and mathematically formulated as a *microscopic theory of muscular contraction* in 1954–57 by A.F. Huxley [HN54, Hux57].

According to Huxley, the myosin heads and cross bridges are elastic elements with a mechanism for attaching themselves transiently to specific sites on the thin filaments. The following cyclic events take place during muscular contraction:

1. The cross bridges extend from myosin filaments and attach themselves to specific sites on actin filaments. The probability that attachment will occur is  $f(x)$ , where  $x$  is the instantaneous distance between the equilibrium position (0) and the maximum distance for attachment  $h$  along the myofibrillar axis.
2. The cross bridges detach with probability  $g(x)$ .

If we let  $N$  equal the density of cross bridges and  $n$  the fraction of cross bridges that are attached, then  $nN$  equals the density of attached cross bridges. Huxley's rate equation for cross-bridge attachment-detachment, i.e. the *sliding filament model* of muscular contraction is now given by:

$$\dot{n} = f(x)[1 - n(x, t)] - g(x)n(x, t) = f(x) - [f(x) + g(x)]n(x, t). \quad (\text{A.26})$$

Huxley's model (A.26) leads to expressions for the force developed by the cross bridges. For an *isometric steady-state contraction* the *contraction tension* or *contraction force* is given by:

$$F_0 = 0.5 N h^2 \frac{kf}{f + g}, \quad (\text{A.27})$$

where  $k = k(x)$  is the stiffness of the cross-bridge spring. For *isotonic* steady states it recovers the classical *Hill's force-velocity* relation (A.28). The *static force* expression says that the force (or tension) generated in the muscle is the function of the interfilamentar overlap, and its maximum is about the middle of the shortening, where the acto-myosin overlap is maximal. This is the so-called *parabolic length-tension curve* of muscular contraction.

### Hill's Force–Velocity Muscular Dynamics

The *dynamic force–velocity relation* of muscular contraction is firstly discovered in 1938, by A.V. Hill [Hil38], in his thermodynamic studies of muscular work, and put into the basis of *macroscopic muscle–load dynamics*. Hill's famous *hyperbolic force–velocity curve* has the equation:

$$(F + a)v = (F_0 + F)b, \quad (\text{A.28})$$

and says that the muscle force is greatest in isometric conditions (without motion), while the velocity of shortening is maximal without external load; in other words, muscle is either 'strong' or 'fast', but no both. Constants  $a$  and  $b$  correspond respectively to the energy dissipated during the contraction and the velocity of the mechano–chemical processes.

Hill showed that energy change in muscle during contraction can be described by the following *thermodynamic relation*:

$$U = A + W + M, \quad (\text{A.29})$$

where  $U$  is the total energy change associated with contraction,  $A$  is the *activation heat* (i.e., the heat production associated with the activation of the contractile elements),  $W$  is the mechanical work performed by the muscle by lifting a load,  $\alpha\Delta x$  is the *shortening heat*, and  $M$  is the *maintenance heat* of contraction.

The activation heat begins and is almost completely liberated before any tension is developed, i.e. it is predominantly connected with the excitation–contraction coupling process, and corresponds in time to the *latency relaxation* of muscle. It is associated with the internal work required to transform the contractile elements from the resting to the active state. Part of the activation heat probably is associated with a change in the elastic properties of muscle, but about two thirds of it is associated with the release of  $Ca^{++}$  ions from the triads, its binding by troponin and the subsequent rearrangement of the thin filament proteins. The activation heat is greatest for the first twitch after a period rest and becomes smaller with succeeding twitches.

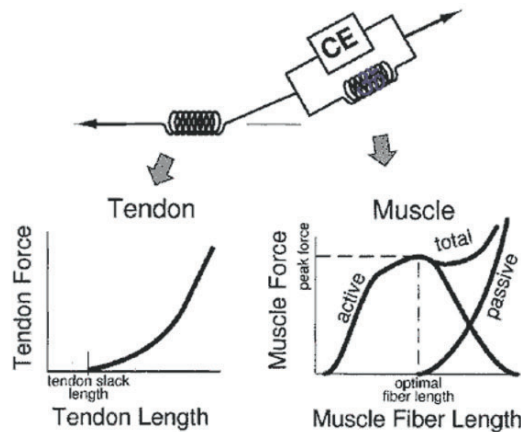
The maintenance heat begins at about the time tension begins and can be divided into two parts: the labile maintenance heat and the stable maintenance heat. For isometric contractions at shorter than rest length, both the labile and the stable heats diminish. For stretched muscle, the labile heat is approximately constant, whereas the stable heat diminishes with stretching and is roughly proportional to the degree of interfilamentar overlap. The stable heat has quite different values in functionally different muscles; it is low when the muscle maintains tension efficiently and vice versa.

The shortening heat is proportional mainly to the distance of shortening and does not depend greatly on the load, the speed of shortening, or the amount of work performed. Since mechanical work is  $W = P\Delta x$ , substituting this in the above thermodynamic relation (A.29) gives the *heat equation*:

$$U = A + (P + \alpha) \Delta x + M. \quad (\text{A.30})$$

From the analogy of the term  $(P + \alpha)$  in the heat equation (A.30) and the term  $(P + a)$  in the force-velocity equation (A.28), Hill was able to show a rough equivalence between the coefficient of the shortening heat  $\alpha$  and the force-velocity constant  $a$ . The shortening heat is greatest for the first twitch after a period of rest and is less for subsequent twitches.

Last, note should be made of *thermoelastic heat*. Generally speaking, resting muscle has rubberlike thermoelastic properties, whereas actively contracting muscle has springlike thermoelastic properties. During the development of tension the change in elastic properties is accompanied by an absorption of heat by the muscle. As tension falls during relaxation, an equivalent amount of heat is released by the muscle owing to its elastic properties. The various kinds of muscle heat must be corrected for the thermoelastic heat. However, for a complete cycle of contraction and relaxation, the net heat produced by thermoelastic mechanisms is zero.



**Fig. A.3.** Hill's model of the skeletal muscle–tendon complex.

In the same seminal paper [Hil38], Hill also proposed a three-element rheological model of the skeletal muscle–tendon complex (see Figure A.3). In this model the length–tension property of muscle is represented by an active contractile element (CE) in parallel with a passive elastic element. Total isometric muscle force is assumed to be the sum of muscle force when it is inactive (passive) and when it is maximally excited (active). The muscle is in series with tendon, which is represented by a nonlinear spring. Pennation angle ( $\alpha$ ) is the angle between tendon and muscle fibers. Tendon slack length is the length of tendon at which force initially develops during tendon stretch. The model was scaled to represent each muscle by specifying the muscle's

peak force, optimal fiber length, tendon slack length, and pennation angle based on data collected in anatomical experiments.

Hill's muscle-tendon model has been widely applied in biomechanical musculo-skeletal modelling.

### Hatze's Myocybernetics

Dynamics of human skeletal and face muscles is in the most sophisticated form described in the series of papers of Hatze (see [Hat78]). His muscle-control model involves excitation dynamics of neuro-muscular inputs (motor units) and contraction dynamics based on Huxley's sliding-filament theory of muscle contraction. In brief, Hatze's *myocybernetics* can be divided into *excitation dynamics* and *contraction dynamics*. The excitation dynamics of a single muscle fibre stimulated by trains of normalized nerve impulses  $\alpha(t)$  is represented by the system

$$\ddot{\beta} + c_4\dot{\beta} + c_5\beta = c_6V_N\alpha(t), \beta(0) = \dot{\beta}(0) = 0, \quad (\text{A.31})$$

$$\ddot{\gamma} + (c_1\dot{\gamma} + c_2\gamma)/\rho^*(\xi) = c_3V_T\beta(t), \gamma(0) = \dot{\gamma}(0) = 0,$$

$$\delta\dot{q} = d_1\{d_2[1 - k^2(\xi)][h(\dot{x}i) - 1/(1 - q_0)] - \delta q\} \delta q(t_s) = 0,$$

where  $\rho^*(\xi)$  is *normalized Ca density function*,  $k(\xi)$  is *filamentary-overlap function*,  $h(\dot{x}i)$  is *velocity-dependence function*;

$c_1, \dots, c_6, d_1, d_2, V_N, V_T, q_0$  are defined constants;  $V_T\beta(t)$  is *action potential* as appearing in the interior of the  $T$ -system of the fibre, while  $\gamma(t)$  denotes the *free Ca-ion concentration* in the interfilamentary space; the variable  $\delta q$  expresses the *stretch potentiation* induced by an elongation of the tetanized fibre.

The variable  $\xi$  designates the *normalized length of the contractile element* of the fibre, and is defined by the contraction dynamics,

$$\dot{\xi} = a_1[1/a_2 \arcsin h a_3 \ln(\frac{q^*k(\xi)}{b_2[f^{SE}/\bar{f} + b_1k_1(\xi)]} - a_4)] - \frac{1}{2},$$

$$\xi(0) = \xi_0, \quad (\text{A.32})$$

where  $a_1, \dots, a_4, b_1, b_2$  are defined constants,  $f^{SE}/\bar{f}$  is the *normalized force across the series elastic element*,  $b_1k_1(\xi)$  is the *passive sarcomere tension*, and  $q^*$  is the *active state*.

### Hodgkin-Huxley Theory of Neural Action Potential

The celebrated *Hodgkin-Huxley HH-neuron model* is described by the nonlinear coupled differential equations for the four variables,  $V$  for the membrane potential, and  $m, h$  and  $n$  for the gating variables of Na and K channels, and it is given by [HH52, Hod64]

$$\begin{aligned}
C\dot{V} &= -g_{\text{Na}}m^3h(V - V_{\text{Na}}) - g_{\text{K}}n^4(V - V_{\text{K}}) - g_{\text{L}}(V - V_{\text{L}}) + I_j^{\text{ext}}, \\
\dot{m} &= -(a_m + b_m)m + a_m, & \dot{h} &= -(a_h + b_h)h + a_h, \\
\dot{n} &= -(a_n + b_n)n + a_n, & \text{where} & \\
a_m &= 0.1(V + 40)/[1 - e^{-(V+40)/10}], & b_m &= 4e^{-(V+65)/18}, \\
a_n &= 0.01(V + 55)/[1 - e^{-(V+55)/10}], & b_n &= 0.125e^{-(V+65)/80}, \\
a_n &= 0.07e^{-(V+65)/20}, & b_n &= 1/[1 + e^{-(V+35)/10}].
\end{aligned} \tag{A.33}$$

Here the reversal potentials of Na, K channels and leakage are  $V_{\text{Na}} = 50$  mV,  $V_{\text{K}} = -77$  mV and  $V_{\text{L}} = -54.5$  mV; the maximum values of corresponding conductivities are  $g_{\text{Na}} = 120$  mS/cm<sup>2</sup>,  $g_{\text{K}} = 36$  mS/cm<sup>2</sup> and  $g_{\text{L}} = 0.3$  mS/cm<sup>2</sup>; the capacity of the membrane is  $C = 1$   $\mu\text{F}/\text{cm}^2$ . The external, input current is given by

$$I_j^{\text{ext}} = g_{\text{syn}}(V_a - V_c) \sum_n \alpha(t - t_{in}), \tag{A.34}$$

which is induced by the pre-synaptic spike-train input applied to the neuron  $i$ , given by

$$U_i(t) = V_a \sum_n \delta(t - t_{in}).$$

In equation (A.34),  $t_{in}$  is the  $n$ th firing time of the spike-train inputs,  $g_{\text{syn}}$  and  $V_c$  denote the conductance and the reversal potential, respectively, of the synapse,  $\tau_s$  is the time constant relevant to the synapse conduction, and  $\alpha(t)$  is the alpha function given by

$$\alpha(t) = (t/\tau_s) e^{-t/\tau_s} \Theta(t).$$

where  $\Theta(t)$  is the Heaviside function. The HH model was originally proposed to account for the property of squid giant axons [HH52, Hod64] and it has been generalized with modifications of ion conductances. The HH-type models have been widely adopted for a study on activities of *transducer neurons* such as motor and thalamus relay neurons, which transform the amplitude-modulated input to spike-train outputs.

### Muscular Action Potential

Hodgkin-Huxley theory of neural action potential was adapted by Noble [Nob62] as a model of muscular action potential. Noble model has the same form as the HH-neuron model (A.33), with changed the values of constants, so that the whole signal is about 10 times slower. Noble's model was later modified by Hatze's muscular excitation dynamics (A.31) and complemented by his contraction dynamics (A.32).

Now, to simplify Hatze's myocybernetics, and yet to retain all the necessary excitation-contraction dynamics, as well as to establish the neuro-muscular inter-connection, we propose herein approach of recurrent diffusion

physics. The EFS–response mapping  $\mathcal{F}$  of a skeletal or face muscle, i.e., the response of the muscle system  $\mathcal{M}$  to the efferent functional stimulation from the neural network system  $\mathcal{N}$  – can be stated in the form of the *force generator* time behavior,  $\mathcal{F} : \mathbb{R} \rightarrow \text{Hom}_t(\mathcal{N}, \mathcal{M})$ , where:  $t$  denotes stimulation time,  $\mathcal{N}$  and  $\mathcal{M}$  correspond to the left  $\mathbb{R}$ –moduli of neural and muscular systems. The mapping  $\mathcal{F}$  can be considered as an effect of a *fifth–order transmission cascade* ( $\mathcal{F}_1 \mapsto \mathcal{F}_2 \mapsto \mathcal{F}_3 \mapsto \mathcal{F}_4 \mapsto \mathcal{F}_5$ ), where  $\mathcal{F}_i$  ( $i = 1, \dots, 5$ ) represent *neural action potential, synaptic potential, muscular action potential, excitation–contraction coupling and muscle tension generating*, respectively (see [Iva91]).

According to [Nob62, Hak93, Hak02], all transmission components of the system ( $\mathcal{F}_1 \mapsto \mathcal{F}_2 \mapsto \mathcal{F}_3 \mapsto \mathcal{F}_4 \mapsto \mathcal{F}_5$ ), where  $\mathcal{F}_i$  ( $i = 1, \dots, 5$ ) can be considered as being some kind of *diffusion processes*, forming the fifth–order transmission *flux* cascade.

Mapping  $\mathcal{F}$  (for all included motor units in the particular muscle contraction) can be described by fifth order *recurrent, distributed parameter* diffusion system [Iva91]

$$\begin{aligned} C_k \frac{\partial V_k}{\partial t} &= \frac{1}{R_k} \frac{\partial^2 V_{k-1}}{\partial z^2} - J_k(V_k), & \text{with boundary condition at } z = 0, \\ V_k(0, t) &= V_0 \sin(2\pi f t) = S(t), & (k = 1, \dots, 5). \end{aligned}$$

The single element  $\mathcal{F}_4$ , ( $k = 1, \dots, 5$ ) behavior is now given by

$$\begin{aligned} V_k(z, t) &= V_0 \exp(-z_k/m) \sin(2\pi f(t - z_k/n)), \\ m &= \frac{1}{R_k C_k f}, & n &= \frac{4\pi f}{R_k C_k}. \end{aligned}$$

For muscle–mechanical purpose, the presented distributed map  $\mathcal{F}$  can be first mathematically approximated with the corresponding lumped parameter  $R_k C_k$  electric circuit (where the second circuit represents the *Eccles model of synaptic activation* (see [Ecc64, EIS67]) and the last one corresponds to the low-pass filter representing the contraction process itself), at  $x = \textit{tendon}$

$$\begin{aligned} \dot{z}_k &= \frac{1}{T_k} (b_k z_{k-1} - z_k), & (k = 1, \dots, 5), \\ z_k(0) &= 0, & z_0 &= S(t), & z_5 &= F(t), \end{aligned}$$

where  $T_k = R_k C_k$  are time characteristics of the circuits in cascade, and  $b_k$  are corresponding input gains (conversion factors).

The single muscle behavior in the lumped approximation form is given by the recurrent sum of its transient and weighting terms (with time legs  $\tau_k$ )

$$z_k(t) = b_k z_{k-1} (1 - \exp(-t/T_k)) + z_k \exp(-(t - \tau_k)/T_k).$$

The presented distributed mapping  $\mathcal{F}$  can be further physically approximated with a second order forced–dumped linear oscillator in a Cauchy form

$$T\ddot{z} + 2aT\dot{z} + cz = bS, \quad z(0) = \dot{z}(0) = 0,$$

where  $a$  (having dimension of force) corresponds to energy dissipated during the contraction,  $b$  (having dimension of velocity) is the phosphagenic energy transducing rate, while  $c$  corresponds to the second derivative of the stress-strain curve of the series viscoelastic element [Wil56] of the muscular actuator (assumed in exponential three-parameter form).

The complete efferent face and body neuro-muscular system  $(\mathcal{N}, \mathcal{M})$  is now given by the set of equations

$$\begin{aligned} \dot{x}^i &= -D_j^i x^i + T_j^i g^i(x^i) + S^i, & (i, j = 1, \dots, n), \\ C_k \frac{\partial V_k}{\partial t} &= \frac{1}{R_k} \frac{\partial^2 V_{k-1}}{\partial z^2} - J_k(V_k), & (k = 1, \dots, 5); \end{aligned}$$

or, its discrete form

$$\dot{x}^i = (b - y^i)x^i, \quad \dot{y}^i = -vy^i + g(x^i + T_j^i y^j), \quad (\text{A.35})$$

$$\dot{z}_k = \frac{1}{T_k}(b_k z_{k-1} - z_k), \quad (k = 1, \dots, 5), \quad (\text{A.36})$$

$$z_k(0) = 0, \quad z_0 = S(t), \quad z_5 = F(t). \quad (\text{A.37})$$

Equations (A.35,A.37) constitute a  $3n$ -dimensional phase-space (for  $n = 5$  or  $k = i$ ) being a *hiper-cube*  $\equiv$  *neuro-muscular control space*. The feedback control  $\mathcal{F}^{-1}$  of the mapping  $\mathcal{F}$  is performed by muscular *autogenetic motor servo*.

### Houk's Autogenetic Motor Servo

It is now well-known (see [Hou79, HBB96]) that voluntary contraction force  $\mathcal{F}$  of a skeletal or face muscle system  $\mathcal{M}$  is reflexly excited (positive reflex feedback  $+\mathcal{F}^{-1}$  by responses of its *spindle receptors* to stretch and is reflexly inhibited (negative reflex feedback  $-\mathcal{F}^{-1}$  by responses of its *Golgi tendon organs* to contraction. Stretch and unloading reflexes are mediated by combined actions of several autogenetic neural pathways.

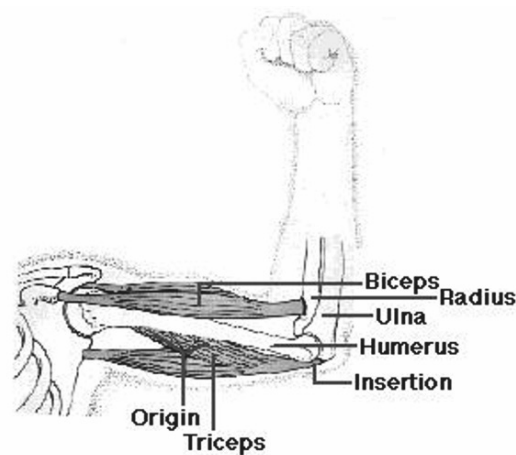
James Houk's term '*autogenetic*' means that the stimulus excites receptors located in the same face or body muscle that is the target of the reflex response. The most important of these muscle receptors are the primary and secondary endings in muscle-spindles, sensitive to length change - positive length feedback  $+\mathcal{F}^{-1}$ , and the Golgi tendon organs, sensitive to contractile force - negative force feedback  $-\mathcal{F}^{-1}$ .

The gain  $G$  of the length feedback  $+\mathcal{F}^{-1}$  can be expressed as the *positional stiffness* (the ratio  $G \approx S = dF/dx$  of the force  $\mathcal{F}$ -change to the length  $x$ -change) of the muscle system  $\mathcal{M}$ . The greater the stiffness  $S$ , the less will the muscle be disturbed by a change in load and the more reliable will be the performance of the muscle system  $\mathcal{M}$  in executing controlled changes in length  $+\mathcal{F}^{-1}$ .

The autogenetic circuits ( $+\mathcal{F}^{-1}$ ) and ( $-\mathcal{F}^{-1}$ ) appear to function as *servoregulatory loops* that convey continuously graded amounts of excitation and inhibition to the large (*alpha*) skeletomotor neurons. Small (*gamma*) fusimotor neurons innervate the contractile poles of muscle spindles and function to modulate spindle–receptor discharge.

### A.2.3 The Equivalent Muscular Actuator

A single skeletal muscle, (e.g., the triceps brachii muscle, see Figure A.4), is attached at its *origin* to a large area of bone (the humerus in case of the triceps). At its other end, the *insertion*, it tapers into a glistening white *tendon* which, (in case of the triceps is attached to the ulna). As the triceps contracts, the insertion is pulled toward the origin and the arm is straightened or extended at the elbow. Thus the triceps is an *extensor*. Because skeletal muscle exerts force only when it contracts, a second muscle – a *flexor* – is needed to flex or bend the joint (e.g., the biceps brachii muscle is the flexor of the forearm). Together, they (the biceps and triceps) make up an antagonistic pair of muscles, which we will call forming the *equivalent muscular actuator*. Similar pairs, i.e., equivalent muscular actuators, working antagonistically across other joints, provide for almost all the movement of the skeleton. The equivalent muscular actuator has the role of ‘driver’ in biodynamics. It generates the equivalent muscular torque, which is the *primary cause* of human–like motion [Iva91, IS01].



**Fig. A.4.** An antagonistic pair of human skeletal muscles, one flexor and the other extensor (in the case of the forearm, biceps brachii and triceps brachii, respectively), forming the *equivalent muscular actuator* – the primary cause of the human–like motion.

### A.2.4 Biochemistry of Muscular Contraction

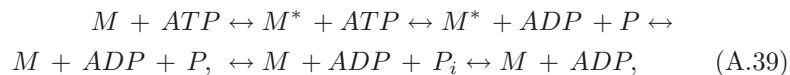
The immediate energy source for contraction in human muscles is adenosine triphosphate ATP (see [Mou80, Mar98, IS00]). Muscle contains about  $2 \mu\text{mole}$  ATP/gram wet weight. The myosin head is the only site of the major ATP hydrolysis in active muscle. At the concentrations of ATP, ADP (*adenosine diphosphate*), and  $P_i$  (*inorganic phosphate*) present in the sarcoplasm, ATP hydrolysis yields about  $11.5 \text{ kcal/mole}$ . About  $0.3 \mu\text{mole}$  of ATP/gram muscle is hydrolyzed by a single muscle twitch. The ATP hydrolysis overall scheme:



represents actually the complex six-step chain-reaction  $\{k_i\}$ , ( $i = 1, \dots, 5$ ), which can be summarized as follows:

1. Myosin reacts rapidly with ATP to form a complex; the myosin is from its resting (low-energy) form converted to an energy-rich form.
2. While complexed to the myosin, ATP is hydrolyzed to ADP and  $P_i$ . Reaction 2 is much more rapid than reaction 1. (This step is extremely temperature sensitive).
3. In reaction 3, while the ADP and  $P_i$  are still attached to the myosin, the latter is converted to a low-energy form. This step is slow, rate limiting in the sequence of reactions, and insensitive to temperature changes.
4. Reactions 4 and 5 are rapid.

Therefore, the reaction sequence proceeds as follows:



where  $M$  is miosin in low-energy form,  $M^*$  is miosin in energy-rich form, and symbol  $\leftrightarrow$  actually represents a pair of reversible reactions  $\{k_i, k_{i-1}\}$ , ( $i = 1, \dots, 5$ ).

Muscles also contain about  $20 \mu\text{mole}$  CP/gram (*creatine phosphate*). Creatine phosphate can phosphorylate ADP to form ATP in a reversible reaction catalyzed by the enzyme *creatine kinase*.

Muscle contains large amounts of creatine kinase; it amounts to more than 25 percent of the soluble cytoplasmic protein. As soon as ATP is hydrolyzed, the ADP formed is very rapidly rephosphorylated by CP and the ATP is regenerated. Thus CP forms a reservoir of energy-rich phosphate bonds to quickly replenish the sarcoplasmic ATP.

Ultimately, ATP is produced by *glycolysis* and respiration [Mou80]. In glycolysis (the so called *Embden-Meyerhoff pathway*), glucose is degraded to pyruvate, or to lactic acid in the absence of  $O_2$ , yielding 2 moles ATP/mole glucose metabolized. Intracellular glycogen granules provide a very readily available source of glucose. Muscles normally contain 9 to 16 gm/kg glycogen or, for a well-fed man of average height and weight, the total glycogen

stores in muscle amount to 300 – 500 *gram*, with another 55 – 90 *gram* in the liver. Glycogen breakdown in muscle begins immediately on stimulation, and the amount of muscle glycogen depleted is proportional to the mechanical work done. Glycogen is hydrolyzed by the enzyme phosphorylase to *glucose-1-phosphate*, which then enters the glycolytic pathway.

*Red muscle fibers* respond to a stimulus with a relatively slow twitch (maximum shortening velocity about 17 mm/sec) and therefore are also called *slow fibers*, whereas *white muscle fibers* react to a stimulus with a rapid twitch (maximum shortening velocity about 42mm/sec) and therefore are also called fast fibers. Red muscle has a more extensive blood supply than white muscle. Red muscle fibers are able to sustain activity for long periods of time whereas white muscle fibers characteristically produce short bursts of great tension followed by the rapid onset of fatigue.

Whole red and white muscles differ in *ATPase* activity, and, indeed, the purified contractile protein myosin extracted from red and white muscle differs in *ATPase* activity, a finding associated with different myosin light chains. White muscle and white muscle actomyosin show the greater *ATPase* activity. The innervation of red and white muscle differs, and, indeed, whether a given muscle is red or white results from trophic influences of the motor nerve.

Slow muscle fibers are generally thinner and possess many sarcosomes (mitochondria) containing large amounts of respiratory enzymes, as well as copious quantities of the  $O_2$ -carrying protein *myoglobin* in the sarcoplasm and man lipid droplets. The numerous sarcosomes and high level of myoglobin give slow fibers their red color. Fast (or white) muscle fibers, on the other hand, are generally of larger diameter and contain large amounts of phosphorylase and glycolytic enzymes and large deposits of glycogen. Slow muscles derive energy predominantly from respiration, whereas in fast muscle fibers, glycolysis and lactate production are more prominent.

## A.3 Path Integral Methods

In this section we review Feynman path integral methods, from both historical and modern perspective (see also subsection 1.1.3).

### A.3.1 Historical Remarks

#### Extract from Feynman's Nobel Lecture

In his Nobel Lecture, December 11, 1965, Richard (Dick) Feynman said that he and his PhD supervisor, John Wheeler, had found the *action*  $A = A[x; t_i, t_j]$ , directly involving the *motions of the charges only*,<sup>5</sup>

<sup>5</sup> *Wheeler-Feynman Idea* [WF49] "The energy tensor can be regarded only as a provisional means of representing matter. In reality, *matter consists of electrically charged particles.*"

$$\begin{aligned}
A[x; t_i, t_j] &= m_i \int (\dot{x}_\mu^i \dot{x}_\mu^i)^{\frac{1}{2}} dt_i + \frac{1}{2} e_i e_j \int \int \delta(I_{ij}^2) \dot{x}_\mu^i(t_i) \dot{x}_\mu^j(t_j) dt_i dt_j \\
&\quad \text{with } (i \neq j) \\
I_{ij}^2 &= [x_\mu^i(t_i) - x_\mu^j(t_j)] [x_\mu^i(t_i) - x_\mu^j(t_j)],
\end{aligned} \tag{A.40}$$

where  $x_\mu^i = x_\mu^i(t_i)$  is the four-vector *position* of the  $i$ th particle as a function of the proper time  $t_i$ , while  $\dot{x}_\mu^i(t_i) = dx_\mu^i(t_i)/dt_i$  is the *velocity* four-vector.

The first term in the action  $A[x; t_i, t_j]$  (A.40) is the integral of the proper time  $t_i$ , the *ordinary action of relativistic mechanics of free particles of mass  $m_i$*  (summation over  $\mu$ ). The second term in the action  $A[x; t_i, t_j]$  (A.40) represents the *electrical interaction of the charges*. It is summed over each pair of charges (the factor  $\frac{1}{2}$  is to count each pair once, the term  $i = j$  is omitted to avoid self-action). The *interaction is a double integral over a delta function of the square of space-time interval  $I^2$  between two points on the paths*. Thus, interaction occurs only when this interval vanishes, that is, *along light cones* (see [WF45, WF49]).

Feynman comments here: “The fact that the interaction is exactly one-half advanced and half-retarded meant that we could write such a principle of least action, whereas interaction via retarded waves alone cannot be written in such a way. So, all of classical electrodynamics was contained in this very simple form.”

“...The problem is only to make a quantum theory, which has as its classical analog, this expression (A.40). Now, there is no unique way to make a quantum theory from classical mechanics, although all the textbooks make believe there is. What they would tell you to do, was find the momentum variables and replace them by  $(\hbar/i)(\partial/\partial x)$ , but I couldn't find a momentum variable, as there wasn't any.”

“The character of quantum mechanics of the day was to write things in the famous *Hamiltonian way* (in the form of Schrödinger equation), which described how the wave function changes from instant to instant, and in terms of the Hamiltonian operator  $H$ . If the classical physics could be reduced to a Hamiltonian form, everything was all right. Now, least action does not imply a Hamiltonian form if the action is a function of anything more than positions and velocities at the same moment. If the action is of the form of the integral of the Lagrangian  $L = L(\dot{x}, x)$ , a function of the velocities and positions at the same time  $t$ ,

$$S[x] = \int L(\dot{x}, x) dt, \tag{A.41}$$

then you can start with the Lagrangian  $L$  and then create a Hamiltonian  $H$  and work out the quantum mechanics, more or less uniquely. But the action  $A[x; t_i, t_j]$  (A.40) involves the key variables, positions (and velocities), at two different times  $t_i$  and  $t_j$  and therefore, it was not obvious what to do to make the quantum-mechanical analogue...”

So, Feynman was looking for the action integral in quantum mechanics. He says: “...I simply turned to Professor Jehle and said, “Listen, do you know

any way of doing quantum mechanics, starting with action – where the action integral comes into the quantum mechanics?” “No”, he said, “but Dirac has a paper in which the Lagrangian, at least, comes into quantum mechanics.” What Dirac said was the following: There is in quantum mechanics a very important quantity which carries the wave function from one time to another, besides the differential equation but equivalent to it, a kind of a kernel, which we might call  $K(x', x)$ , which carries the wave function  $\psi(x)$  known at time  $t$ , to the wave function  $\psi(x')$  at time  $t + \varepsilon$ ,

$$\psi(x', t + \varepsilon) = \int K(x', x) \psi(x, t) dx.$$

Dirac points out that this function  $K$  was analogous to the quantity in classical mechanics that you would calculate if you took the exponential of  $[i\varepsilon$  multiplied by the Lagrangian  $L(\dot{x}, x)]$ , imagining that these two positions  $x, x'$  corresponded to  $t$  and  $t + \varepsilon$ . In other words,

$$K(x', x) \quad \text{is analogous to} \quad e^{i\varepsilon L(\frac{x' - x}{\varepsilon}, x)/\hbar}.$$

So, Feynman continues: “What does he mean, they are analogous; what does that mean, *analogous*? What is the use of that?” Professor Jehle said, “You Americans! You always want to find a use for everything!” I said that I thought that Dirac must mean that they were *equal*. “No”, he explained, “he doesn’t mean they are equal.” “Well”, I said, “Let’s see what happens if we make them equal.”

“So, I simply put them equal, taking the simplest example where the Lagrangian is

$$L = \frac{1}{2}M\dot{x}^2 - V(x),$$

but soon found I had to put a constant of proportionality  $N$  in, suitably adjusted. When I substituted for  $K$  to get

$$\psi(x', t + \varepsilon) = \int N \exp \left[ \frac{i\varepsilon}{\hbar} L\left(\frac{x' - x}{\varepsilon}, x\right) \right] \psi(x, t) dx \quad (\text{A.42})$$

and just calculated things out by Taylor series expansion, *out came the Schrödinger equation*. So, I turned to Professor Jehle, not really understanding, and said, “Well, you see, Dirac meant that they were proportional.” Professor Jehle’s eyes were bugging out – he had taken out a little notebook and was rapidly copying it down from the blackboard, and said, “No, no, this is an important discovery. You Americans are always trying to find out how something can be used. That’s a good way to discover things!” So, I thought I was finding out what Dirac meant, but, as a matter of fact, had made the discovery that what Dirac thought was analogous, was, in fact, equal. I had then, at least, the connection between the Lagrangian and quantum mechanics, but still with wave functions and infinitesimal times.”

“It must have been a day or so later when I was lying in bed thinking about these things, that I imagined what would happen if I wanted to calculate the wave function at a finite interval later. I would put one of these factors  $e^{i\varepsilon L}$  in here, and that would give me the wave functions the next moment,  $t + \varepsilon$ , and then I could substitute that back into (A.42) to get another factor of  $e^{i\varepsilon L}$  and give me the wave function the next moment,  $t + 2\varepsilon$ , and so on and so on. In that way I found myself thinking of a large number of integrals, one after the other in sequence. In the integrand was the product of the exponentials, which, of course, was the exponential of the sum of terms like  $\varepsilon L$ . Now,  $L$  is the Lagrangian and  $\varepsilon$  is like the time interval  $dt$ , so that if you took a sum of such terms, that’s exactly like an integral. That’s like Riemann’s formula for the integral  $\int L dt$ , you just take the value at each point and add them together. We are to take the limit as  $\varepsilon \rightarrow 0$ , of course. Therefore, the connection between the wave function of one instant and the wave function of another instant a finite time later could be obtained by an infinite number of integrals (because  $\varepsilon$  goes to zero, of course), of exponential where  $S$  is the action expression (A.41). At last, I had succeeded in representing quantum mechanics directly in terms of the action  $S[x]$ .”

Fully satisfied, Feynman comments: “This led later on to the idea of the **transition amplitude** for a path: that for each possible way that the particle can go from one point to another in space–time, there’s an amplitude. That amplitude is  $\mathbf{e}$  to the power of  $[i/\hbar$  times the action  $S[x]$  for the path], i.e.,  $e^{iS[x]/\hbar}$ . Amplitudes from various paths superpose by addition. This then is another, a third way, of describing quantum mechanics, which looks quite different from that of Schrödinger or Heisenberg, but which is equivalent to them.”

“...Now immediately after making a few checks on this thing, what I wanted to do, of course, was to substitute the action  $A[x; t_i, t_j]$  (A.40) for the other  $S[x]$  (A.41). The first trouble was that I could not get the thing to work with the relativistic case of spin one–half. However, although I could deal with the matter only nonrelativistically, I could deal with the light or the photon interactions perfectly well by just putting the interaction terms of (A.40) into any action, replacing the mass terms by the non–relativistic  $L dt = \frac{1}{2} M \dot{x}^2 dt$ ,

$$A[x; t_i, t_j] = \frac{1}{2} \sum_i m_i \int (\dot{x}_\mu^i)^2 dt_i + \frac{1}{2} \sum_{i,j(i \neq j)} e_i e_j \int \int \delta(I_{ij}^2) \dot{x}_\mu^i(t_i) \dot{x}_\mu^j(t_j) dt_i dt_j.$$

When the action has a delay, as it now had, and involved more than one time, I had to lose the idea of a wave function. That is, I could no longer describe the program as: given the amplitude for all positions at a certain time to compute the amplitude at another time. However, that didn’t cause very much trouble. It just meant developing a new idea. *Instead of wave functions we could talk about this: that if a source of a certain kind emits a particle, and a detector is there to receive it, we can give the amplitude that the source will emit and the*

*detector receive*,  $e^{iA[x;t_i,t_j]/\hbar}$ . We do this without specifying the exact instant that the *source* emits or the exact instant that any *detector* receives, without trying to specify the state of anything at any particular time in between, but by just finding the *amplitude for the complete experiment*. And, then we could discuss how that amplitude would change if you had a scattering sample in between, as you rotated and changed angles, and so on, without really having any wave functions...It was also possible to discover what the old concepts of energy and momentum would mean with this generalized action. And, so I believed that I had a quantum theory of classical electrodynamics – or rather of this new classical electrodynamics described by the action  $A[x; t_i, t_j]$  (A.40)...”

### Configuration (Lagrangian) Path Integral

Dirac and Feynman first developed the lagrangian approach to functional integration. To review this approach, we start with the *time-dependent Schrödinger equation*

$$i\hbar \partial_t \psi(x, t) = -\partial_{x^2} \psi(x, t) + V(x) \psi(x, t)$$

appropriate to a particle of mass  $m$  moving in a potential  $V(x)$ ,  $x \in \mathbb{R}$ . A solution to this equation can be written as an integral (see e.g., [Kla97, Kla00]),

$$\psi(x'', t'') = \int K(x'', t''; x', t') \psi(x', t') dx' ,$$

which represents the wave function  $\psi(x'', t'')$  at time  $t''$  as a linear superposition over the wave function  $\psi(x', t')$  at the initial time  $t'$ ,  $t' < t''$ . The integral kernel  $K(x'', t''; x', t')$  is known as the *propagator*, and according to Feynman [Fey48] it may be given by

$$K(x'', t''; x', t') = \mathcal{N} \int \mathcal{D}[x] e^{(i/\hbar) \int [(m/2) \dot{x}^2(t) - V(x(t))] dt} ,$$

which is a formal expression symbolizing an integral over a suitable set of paths. This integral is supposed to run over all continuous paths  $x(t)$ ,  $t' \leq t \leq t''$ , where  $x(t'') = x''$  and  $x(t') = x'$  are fixed end points for all paths. Note that the integrand involves the *classical Lagrangian* for the system.

To overcome the convergence problems, Feynman adopted a *lattice regularization* as a procedure to yield well-defined integrals which was then followed by a limit as the lattice spacing goes to zero called the continuum limit. With  $\varepsilon > 0$  denoting the lattice spacing, the details regarding the lattice regularization procedure are given by

$$\begin{aligned} K(x'', t''; x', t') &= \lim_{\varepsilon \rightarrow 0} (m/2\pi i\hbar\varepsilon)^{(N+1)/2} \int \dots \\ &\dots \int \exp\left\{ (i/\hbar) \sum_{l=0}^N [(m/2\varepsilon)(x_{l+1} - x_l)^2 - \varepsilon V(x_l)] \right\} \prod_{l=1}^N dx_l , \end{aligned}$$

where  $x_{N+1} = x''$ ,  $x_0 = x'$ , and  $\varepsilon \equiv (t'' - t')/(N+1)$ ,  $N \in \{1, 2, 3, \dots\}$ . In this version, at least, we have an expression that has a reasonable chance of being well defined, provided, of course, that one interprets the conditionally convergent integrals involved in an appropriate manner. One common and fully acceptable interpretation adds a convergence factor to the exponent of the preceding integral in the form  $-(\varepsilon^2/2\hbar) \sum_{i=1}^N x_i^2$ , which is a term that formally makes no contribution to the final result in the continuum limit save for ensuring that the integrals involved are now rendered absolutely convergent.

### Phase-Space (Hamiltonian) Path Integral

It is necessary to retrace history at this point to recall the introduction of the *phase-space path integral* by Feynman [Fey51]. In Appendix B to this article, Feynman introduced a formal expression for the configuration or  $q$ -space propagator given by (see e.g., [Kla97, Kla00])

$$K(q'', t''; q', t') = \mathcal{M} \int \mathcal{D}[p] \mathcal{D}[q] \exp\{(i/\hbar) \int [p\dot{q} - H(p, q)] dt\}.$$

In this equation one is instructed to integrate over all paths  $q(t)$ ,  $t' \leq t \leq t''$ , with  $q(t'') \equiv q''$  and  $q(t') \equiv q'$  held fixed, as well as to integrate over all paths  $p(t)$ ,  $t' \leq t \leq t''$ , without restriction.

It is widely appreciated that the phase space path integral is more generally applicable than the original, Lagrangian, version of the path integral. For instance, the original configuration space path integral is satisfactory for Lagrangians of the general form

$$L(x) = \frac{1}{2} m\dot{x}^2 + A(x)\dot{x} - V(x),$$

but it is unsuitable, for example, for the case of a relativistic particle with the Lagrangian

$$L(x) = -m\sqrt{c^2 - \dot{x}^2}$$

expressed in units where the speed of light is unity. For such a system – as well as many more general expressions – the phase space form of the path integral is to be preferred. In particular, for the relativistic free particle, the phase space path integral

$$\mathcal{M} \int \mathcal{D}[p] \mathcal{D}[q] \exp\{(i/\hbar) \int [p\dot{q} - qrt\dot{p}^2 + m^2] dt\},$$

is readily evaluated and yields the correct propagator.

### Feynman-Kac Formula

Through his own research, M. Kac was fully aware of *Wiener's theory of Brownian motion* and the *associated diffusion equation* that describes the

corresponding *distribution function*. Therefore, it is not surprising that he was well prepared to give a path integral expression in the sense of Feynman for an equation similar to the time-dependent Schrödinger equation save for a rotation of the time variable by  $-\pi/2$  in the complex plane, namely, by the change  $t \rightarrow -it$  (see e.g., [Kla97, Kla00]). In particular, Kac [Kac51] considered the equation

$$\partial_t \rho(x, t) = \partial_{x^2} \rho(x, t) - V(x) \rho(x, t). \quad (\text{A.43})$$

This equation is analogous to Schrödinger equation but of course differs from it in certain details. Besides certain constants which are different, and the change  $t \rightarrow -it$ , the nature of the dependent variable function  $\rho(x, t)$  is quite different from the normal quantum mechanical wave function. For one thing, if the function  $\rho$  is initially real it will remain real as time proceeds. Less obvious is the fact that if  $\rho(x, t) \geq 0$  for all  $x$  at some time  $t$ , then the function will continue to be nonnegative for all time  $t$ . Thus we can interpret  $\rho(x, t)$  more like a probability density; in fact in the special case that  $V(x) = 0$ , then  $\rho(x, t)$  is the probability density for a Brownian particle which underlies the *Wiener measure*. In this regard,  $\nu$  is called the diffusion constant.

The fundamental solution of (A.43) with  $V(x) = 0$  is readily given as

$$W(x, T; y, 0) = \frac{1}{\sqrt{2\nu T}} \exp\left(-\frac{(x-y)^2}{2\nu T}\right),$$

which describes the solution to the diffusion equation subject to the initial condition

$$\lim_{T \rightarrow 0^+} W(x, T; y, 0) = \delta(x - y).$$

Moreover, it follows that the solution of the diffusion equation for a general initial condition is given by

$$\rho(x'', t'') = \int W(x'', t''; x', t') \rho(x', t') dx'.$$

Iteration of this equation  $N$  times, with  $\epsilon = (t'' - t')/(N + 1)$ , leads to the equation

$$\rho(x'', t'') = N' \int \dots \int e^{-(1/2\nu\epsilon) \sum_{i=0}^N (x_{i+1} - x_i)^2} \prod_{l=1}^N dx_l \rho(x', t') dx',$$

where  $x_{N+1} \equiv x''$  and  $x_0 \equiv x'$ . This equation features the imaginary time propagator for a free particle of unit mass as given formally as

$$W(x'', t''; x', t') = \mathcal{N} \int \mathcal{D}[x] e^{-(1/2\nu) \int \dot{x}^2 dt},$$

where  $\mathcal{N}$  denotes a formal normalization factor.

The similarity of this expression with the Feynman path integral [for  $V(x) = 0$ ] is clear, but there is a profound difference between these equations. In the former (Feynman) case the underlying measure is only *finitely additive*, while in the latter (Wiener) case the continuum limit actually defines a genuine measure, i.e., a *countably additive measure* on paths, which is a version of the famous *Wiener measure*. In particular,

$$W(x'', t''; x', t') = \int d\mu_W^\nu(x),$$

where  $\mu_W^\nu$  denotes a measure on continuous paths  $x(t)$ ,  $t' \leq t \leq t''$ , for which  $x(t'') \equiv x''$  and  $x(t') \equiv x'$ . Such a measure is said to be a *pinned Wiener measure*, since it specifies its path values at two time points, i.e., at  $t = t'$  and at  $t = t'' > t'$ .

We note that Brownian motion paths have the property that with probability one they are concentrated on continuous paths. However, it is also true that the time derivative of a Brownian path is almost nowhere defined, which means that, with probability one,  $\dot{x}(t) = \pm\infty$  for all  $t$ .

When the potential  $V(x) \neq 0$  the propagator associated with (A.43) is formally given by

$$W(x'', t''; x', t') = \mathcal{N} \int \mathcal{D}[x] e^{-(1/2\nu) \int \dot{x}^2 dt - \int V(x) dt},$$

an expression which is well defined if  $V(x) \geq c$ ,  $-\infty < c < \infty$ . A mathematically improved expression makes use of the Wiener measure and is given by

$$W(x'', t''; x', t') = \int e^{-\int V(x(t)) dt} d\mu_W^\nu(x).$$

This is an elegant relation in that it represents a solution to the differential equation (A.43) in the form of an integral over Brownian motion paths suitably weighted by the potential  $V$ . Incidentally, since the propagator is evidently a strictly positive function, it follows that the solution of the differential equation (A.43) is nonnegative for all time  $t$  provided it is nonnegative for any particular time value.

### Itô Formula

Itô [Ito60] proposed another version of a *continuous-time regularization* that resolved some of the troublesome issues. In essence, the proposal of Itô takes the form given by

$$\lim_{\nu \rightarrow \infty} \mathcal{N}_\nu \int \mathcal{D}[x] \exp\left\{\frac{i}{\hbar} \int \left[\frac{1}{2} m \dot{x}^2 - V(x)\right] dt\right\} \exp\left\{-(1/2\nu) \int [\ddot{x}^2 + \dot{x}^2] dt\right\}.$$

Note well the alternative form of the auxiliary factor introduced as a regulator. The additional term  $\ddot{x}^2$ , the square of the second derivative of  $x$ , acts to smooth

out the paths sufficiently well so that in the case of (21) both  $x(t)$  and  $\dot{x}(t)$  are continuous functions, leaving  $\ddot{x}(t)$  as the term which does not exist. However, since only  $x$  and  $\dot{x}$  appear in the rest of the integrand, the indicated path integral can be well defined; this is already a positive contribution all by itself (see e.g., [Kla97, Kla00]).

### A.3.2 Standard Path Integral Quantization

#### Canonical versus Path Integral Quantization

Recall that in the usual, *canonical formulation* of quantum mechanics, the system's phase-space coordinates,  $q$ , and momenta,  $p$ , are replaced by the corresponding Hermitian operators in the Hilbert space, with real measurable eigenvalues, which obey *Heisenberg commutation relations*.

The *path integral quantization* is instead based directly on the notion of a propagator  $K(q_f, t_f; q_i, t_i)$  which is defined such that (see [Ryd96, CL84, Gun03])

$$\psi(q_f, t_f) = \int K(q_f, t_f; q_i, t_i) \psi(q_i, t_i) dq_i, \quad (\text{A.44})$$

i.e., the wave function  $\psi(q_f, t_f)$  at final time  $t_f$  is given by a Huygens principle in terms of the wave function  $\psi(q_i, t_i)$  at an initial time  $t_i$ , where we have to integrate over all the points  $q_i$  since all can, in principle, send out little wavelets that would influence the value of the wave function at  $q_f$  at the later time  $t_f$ . This equation is very general and is simply an expression of causality. We use the normal units with  $\hbar = 1$ .

According to the usual interpretation of quantum mechanics,  $\psi(q_f, t_f)$  is the *probability amplitude* that the particle is at the point  $q_f$  and the time  $t_f$ , which means that  $K(q_f, t_f; q_i, t_i)$  is the probability amplitude for a transition from  $q_i$  and  $t_i$  to  $q_f$  and  $t_f$ . The probability that the particle is observed at  $q_f$  at time  $t_f$  if it began at  $q_i$  at time  $t_i$  is

$$P(q_f, t_f; q_i, t_i) = |K(q_f, t_f; q_i, t_i)|^2.$$

Let us now divide the time interval between  $t_i$  and  $t_f$  into two, with  $t$  as the intermediate time, and  $q$  the intermediate point in space. Repeated application of (A.44) gives

$$\psi(q_f, t_f) = \int \int K(q_f, t_f; q, t) dq K(q, t; q_i, t_i) \psi(q_i, t_i) dq_i,$$

from which it follows that

$$K(q_f, t_f; q_i, t_i) = \int dq K(q_f, t_f; q, t) K(q, t; q_i, t_i).$$

This equation says that the transition from  $(q_i, t_i)$  to  $(q_f, t_f)$  may be regarded as the result of the transition from  $(q_i, t_i)$  to all available intermediate points

$q$  followed by a transition from  $(q, t)$  to  $(q_f, t_f)$ . This notion of *all possible paths* is crucial in the path integral formulation of quantum mechanics.

Now, recall that the *state vector*  $|\psi, t\rangle_S$  in the *Schrödinger picture* is related to that in the *Heisenberg picture*  $|\psi\rangle_H$  by

$$|\psi, t\rangle_S = e^{-iHt} |\psi\rangle_H,$$

or, equivalently,

$$|\psi\rangle_H = e^{iHt} |\psi, t\rangle_S.$$

We also define the vector

$$|q, t\rangle_H = e^{iHt} |q\rangle_S,$$

which is the Heisenberg version of the Schrödinger state  $|q\rangle$ . Then, we can equally well write

$$\psi(q, t) = \langle q, t | \psi \rangle_H. \quad (\text{A.45})$$

By completeness of states we can now write

$$\langle q_f, t_f | \psi \rangle_H = \int \langle q_f, t_f | q_i, t_i \rangle_H \langle q_i, t_i | \psi \rangle_H dq_i,$$

which with the definition of (A.45) becomes

$$\psi(q_f, t_f) = \int \langle q_f, t_f | q_i, t_i \rangle_H \psi(q_i, t_i) dq_i.$$

Comparing with (A.44), we get

$$K(q_f, t_f; q_i, t_i) = \langle q_f, t_f | q_i, t_i \rangle_H.$$

Now, let us compute the *quantum-mechanics propagator*

$$\langle q', t' | q, t \rangle_H = \langle q' | e^{-iH(t-t')} | q \rangle$$

using the path integral formalism that will incorporate the direct quantization of the coordinates, without Hilbert space and Hermitian operators.

The first step is to divide up the time interval into  $n + 1$  tiny pieces:  $t_l = l\varepsilon + t$  with  $t' = (n + 1)\varepsilon + t$ . Then, by completeness, we can write (dropping the Heisenberg picture index  $H$  from now on)

$$\begin{aligned} \langle q', t' | q, t \rangle &= \int dq_1(t_1) \dots \int dq_n(t_n) \langle q', t' | q_n, t_n \rangle \times \\ &\quad \times \langle q_n, t_n | q_{n-1}, t_{n-1} \rangle \dots \langle q_1, t_1 | q, t \rangle. \end{aligned} \quad (\text{A.46})$$

The integral  $\int dq_1(t_1) \dots dq_n(t_n)$  is an *integral over all possible paths*, which are not trajectories in the normal sense, since there is no requirement of continuity, but rather *Markov chains*.

Now, for small  $\varepsilon$  we can write

$$\langle q', \varepsilon | q, 0 \rangle = \langle q' | e^{-i\varepsilon H(P, Q)} | q \rangle = \delta(q' - q) - i\varepsilon \langle q' | H(P, Q) | q \rangle,$$

where  $H(P, Q)$  is the Hamiltonian (e.g.,  $H(P, Q) = \frac{1}{2}P^2 + V(Q)$ , where  $P, Q$  are the momentum and coordinate operators). Then we have (see [Ryd96, CL84, Gun03])

$$\langle q' | H(P, Q) | q \rangle = \int \frac{dp}{2\pi} e^{ip(q'-q)} H\left(p, \frac{1}{2}(q' + q)\right).$$

Putting this into our earlier form we get

$$\langle q', \varepsilon | q, 0 \rangle \simeq \int \frac{dp}{2\pi} \exp\left[i\left\{p(q' - q) - \varepsilon H\left(p, \frac{1}{2}(q' + q)\right)\right\}\right],$$

where the 0th order in  $\varepsilon \rightarrow \delta(q' - q)$  and the 1st order in  $\varepsilon \rightarrow -i\varepsilon \langle q' | H(P, Q) | q \rangle$ . If we now substitute many such forms into (A.46) we finally get

$$\begin{aligned} \langle q', t' | q, t \rangle &= \lim_{n \rightarrow \infty} \int \prod_{i=1}^n dq_i \prod_{k=1}^{n+1} \frac{dp_k}{2\pi} \times \\ &\times \exp\left\{i \sum_{j=1}^{n+1} [p_j(q_j - q_{j-1})] - H\left(p_j, \frac{1}{2}(q_j + q_{j+1})\right) (t_j - t_{j-1})\right\}, \end{aligned} \quad (\text{A.47})$$

with  $q_0 = q$  and  $q_{n+1} = q'$ . Roughly, the above formula says to *integrate over all possible momenta and coordinate values associated with a small interval*, weighted by something that is going to turn into the *exponential of the action*  $e^{iS}$  in the limit where  $\varepsilon \rightarrow 0$ . It should be stressed that the different  $q_i$  and  $p_k$  integrals are independent, which implies that  $p_k$  for one interval can be completely different from the  $p_{k'}$  for some other interval (including the neighboring intervals). In principle, the integral (A.47) should be defined by *analytic continuation into the complex plane* of, for example, the  $p_k$  integrals.

Now, if we go to the differential limit where we call  $t_j - t_{j-1} \equiv d\tau$  and write  $\frac{(q_j - q_{j-1})}{(t_j - t_{j-1})} \equiv \dot{q}$ , then the above formula takes the form

$$\langle q', t' | q, t \rangle = \int \mathcal{D}[p] \mathcal{D}[q] \exp\left\{i \int_t^{t'} [p\dot{q} - H(p, q)] d\tau\right\},$$

where we have used the shorthand notation

$$\int \mathcal{D}[p] \mathcal{D}[q] \equiv \int \prod_{\tau} \frac{dq(\tau) dp(\tau)}{2\pi}.$$

Note that the above integration is an integration over the  $p$  and  $q$  values at every time  $\tau$ . This is what we call a *functional integral*. We can think of a

given set of choices for all the  $p(\tau)$  and  $q(\tau)$  as defining a *path in the 6D phase-space*. The most important point of the above result is that we have obtained an expression for a *quantum-mechanical transition amplitude* in terms of an integral involving only pure complex numbers, without operators.

We can actually perform the above integral for Hamiltonians of the type  $H = H(P, Q)$ . We use square completion in the exponential for this, defining the integral in the complex  $p$  plane and continuing to the physical situation. In particular, we have

$$\int_{-\infty}^{\infty} \frac{dp}{2\pi} \exp \left\{ i\varepsilon \left( p\dot{q} - \frac{1}{2}p^2 \right) \right\} = \frac{1}{\sqrt{2\pi i\varepsilon}} \exp \left[ \frac{1}{2}i\varepsilon\dot{q}^2 \right],$$

(see [Ryd96, CL84, Gun03]) which, substituting into (A.47) gives

$$\langle q', t' | q, t \rangle = \lim_{n \rightarrow \infty} \int \prod_i \frac{dq_i}{\sqrt{2\pi i\varepsilon}} \exp \left\{ i\varepsilon \sum_{j=1}^{n+1} \left[ \frac{1}{2} \left( \frac{q_j - q_{j-1}}{\varepsilon} \right)^2 - V \left( \frac{q_j + q_{j-1}}{2} \right) \right] \right\}.$$

This can be formally written as

$$\langle q', t' | q, t \rangle = \int \mathcal{D}[q] e^{iS[q]},$$

where

$$\int \mathcal{D}[q] \equiv \int \prod_i \frac{dq_i}{\sqrt{2\pi i\varepsilon}},$$

while

$$S[q] = \int_t^{t'} L(q, \dot{q}) d\tau$$

is the *standard action* with the *Lagrangian*

$$L = \frac{1}{2}\dot{q}^2 - V(q).$$

Generalization to many degrees of freedom is straightforward:

$$\langle q'_1 \dots q'_N, t' | q_1 \dots q_N, t \rangle = \int \mathcal{D}[p] \mathcal{D}[q] \exp \left\{ i \int_t^{t'} \left[ \sum_{n=1}^N p_n \dot{q}_n - H(p_n, q_n) \right] d\tau \right\},$$

$$\text{with } \int \mathcal{D}[p] \mathcal{D}[q] = \int \prod_{n=1}^N \frac{dq_n dp_n}{2\pi}.$$

Here,  $q_n(t) = q_n$  and  $q_n(t') = q'_n$  for all  $n = 1, \dots, N$ , and we are allowing for the full Hamiltonian of the system to depend upon all the  $N$  momenta and coordinates collectively.

### Elementary Applications

(i) Consider first

$$\begin{aligned} & \langle q', t' | Q(t_0) | q, t \rangle \\ &= \int \prod dq_i(t_i) \langle q', t' | q_n, t_n \rangle \dots \langle q_{i_0}, t_{i_0} | Q(t_0) | q_{i-1}, t_{i-1} \rangle \dots \langle q_1, t_1 | q, t \rangle, \end{aligned}$$

where we choose one of the time interval ends to coincide with  $t_0$ , i.e.,  $t_{i_0} = t_0$ . If we operate  $Q(t_0)$  to the left, then it is replaced by its eigenvalue  $q_{i_0} = q(t_0)$ . Aside from this one addition, everything else is evaluated just as before and we will obviously obtain

$$\langle q', t' | Q(t_0) | q, t \rangle = \int \mathcal{D}[p] \mathcal{D}[q] q(t_0) \exp \left\{ i \int_t^{t'} [p\dot{q} - H(p, q)] d\tau \right\}.$$

(ii) Next, suppose we want a path integral expression for  $\langle q', t' | Q(t_1) Q(t_2) | q, t \rangle$  in the case where  $t_1 > t_2$ . For this, we have to insert as intermediate states  $|q_{i_1}, t_{i_1}\rangle \langle q_{i_1}, t_{i_1}|$  with  $t_{i_1} = t_1$  and  $|q_{i_2}, t_{i_2}\rangle \langle q_{i_2}, t_{i_2}|$  with  $t_{i_2} = t_2$  and since we have ordered the times at which we do the insertions we must have the first insertion to the left of the 2nd insertion when  $t_1 > t_2$ . Once these insertions are done, we evaluate  $\langle q_{i_1}, t_{i_1} | Q(t_1) = \langle q_{i_1}, t_{i_1} | q(t_1)$  and  $\langle q_{i_2}, t_{i_2} | Q(t_2) = \langle q_{i_2}, t_{i_2} | q(t_2)$  and then proceed as before and get

$$\langle q', t' | Q(t_1) Q(t_2) | q, t \rangle = \int \mathcal{D}[p] \mathcal{D}[q] q(t_1) q(t_2) \exp \left\{ i \int_t^{t'} [p\dot{q} - H(p, q)] d\tau \right\}.$$

Now, let us ask what the above integral is equal to if  $t_2 > t_1$ ? It is obvious that what we get for the above integral is  $\langle q', t' | Q(t_2) Q(t_1) | q, t \rangle$ . Clearly, this generalizes to an arbitrary number of  $Q$  operators.

(iii) When we enter into quantum field theory, the  $Q$ 's will be replaced by fields, since it is the fields that play the role of coordinates in the 2nd quantization conditions.

### Sources

The *source* is represented by modifying the Lagrangian:

$$L \rightarrow L + J(t)q(t).$$

Let us define  $|0, t\rangle^J$  as the ground state (vacuum) vector (in the moving frame, i.e. with the  $e^{iHt}$  included) in the presence of the source. The required *transition amplitude* is

$$Z[J] \propto \langle 0, +\infty | 0, -\infty \rangle^J,$$

where the source  $J = J(t)$  plays a role analogous to that of an electromagnetic current, which acts as a source of the electromagnetic field. In other words, we

can think of the scalar product  $J_\mu A^\mu$ , where  $J_\mu$  is the current from a scalar (or Dirac) field acting as a source of the potential  $A^\mu$ . In the same way, we can always define a current  $J$  that acts as the source for some arbitrary field  $\phi$ .  $Z[J]$  (otherwise denoted by  $W[J]$ ) is a functional of the current  $J$ , defined as (see [Ryd96, CL84, Gun03])

$$Z[J] \propto \int \mathcal{D}[p]\mathcal{D}[q] \exp \left\{ i \int_t^{t'} [p(\tau)\dot{q}(\tau) - H(p, q) + J(\tau)q(\tau)] d\tau \right\},$$

with the *normalization condition*  $Z[J = 0] = 1$ . Here, the argument of the exponential depends upon the functions  $q(\tau)$  and  $p(\tau)$  and we then integrate over all possible forms of these two functions. So the exponential is a functional that maps a choice for these two functions into a number. For example, for a quadratically completable  $H(p, q)$ , the  $p$  integral can be performed as a  $q$  integral

$$Z[J] \propto \int \mathcal{D}[q] \exp \left\{ i \int_{-\infty}^{+\infty} \left( L + Jq + \frac{1}{2}i\varepsilon q^2 \right) d\tau \right\},$$

where the addition to  $H$  was chosen in the form of a *convergence factor*  $-\frac{1}{2}i\varepsilon q^2$ .

## Fields

Let us now treat the *abstract scalar field*  $\phi(x)$  as a coordinate in the sense that we imagine dividing space up into many little cubes and the average value of the field  $\phi(x)$  in that cube is treated as a coordinate for that little cube. Then, we go through the multi-coordinate analogue of the procedure we just considered above and take the continuum limit. The final result is

$$Z[J] \propto \int \mathcal{D}[\phi] \exp \left\{ i \int d^4x \left( \mathcal{L}(\phi(x)) + J(x)\phi(x) + \frac{1}{2}i\varepsilon\phi^2 \right) \right\},$$

where for  $\mathcal{L}$  we would employ the Klein Gordon Lagrangian form. In the above, the  $dx_0$  integral is the same as  $d\tau$ , while the  $d^3\mathbf{x}$  integral is simply summing over the sub-Lagrangians of all the different little cubes of space and then taking the continuum limit.  $\mathcal{L}$  is the Lagrangian density describing the Lagrangian for each little cube after taking the many-cube limit (see [Ryd96, CL84, Gun03]) for the full derivation).

We can now introduce *interactions*,  $\mathcal{L}_I$ . Assuming the simple form of the Hamiltonian, we have

$$Z[J] \propto \int \mathcal{D}[\phi] \exp \left\{ i \int d^4x \left( \mathcal{L}(\phi(x)) + \mathcal{L}_I(\phi(x)) + J(x)\phi(x) \right) \right\},$$

again using the normalization factor required for  $Z[J = 0] = 1$ .

For example of Klein Gordon theory, we would use

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_I, \quad \mathcal{L}_0 = \frac{1}{2}[\partial_\mu \phi \partial^\mu \phi - \mu^2 \phi^2], \quad \mathcal{L}_I = \mathcal{L}_I(\phi),$$

where  $\partial_\mu \equiv \partial_{x^\mu}$  and we can freely manipulate indices, as we are working in Euclidean space  $\mathbb{R}^3$ . In order to define the above  $Z[J]$ , we have to include a convergence factor  $i\varepsilon\phi^2$ ,

$$\mathcal{L}_0 \rightarrow \frac{1}{2}[\partial_\mu \phi \partial^\mu \phi - \mu^2 \phi^2 + i\varepsilon\phi^2],$$

so that

$$Z[J] \propto \int \mathcal{D}[\phi] \exp \left\{ i \int d^4x \left( \frac{1}{2}[\partial_\mu \phi \partial^\mu \phi - \mu^2 \phi^2 + i\varepsilon\phi^2] + \mathcal{L}_I(\phi(x)) + J(x)\phi(x) \right) \right\}$$

is the appropriate *generating function* in the free field theory case.

### Gauges

In the path integral approach to quantization of the *gauge theory*, we implement *gauge fixing* by restricting in some manner or other the path integral over gauge fields  $\int \mathcal{D}[A_\mu]$ . In other words we will write instead

$$Z[J] \propto \int \mathcal{D}[A_\mu] \delta(\text{some gauge fixing condition}) \exp \left\{ i \int d^4x \mathcal{L}(A_\mu) \right\}.$$

A common approach would be to start with the *gauge condition*

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \frac{1}{2}(\partial^\mu A_\mu)^2$$

where the electrodynamic field tensor is given by  $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ , and compute

$$Z[J] \propto \int \mathcal{D}[A_\mu] \exp \left\{ i \int d^4x [\mathcal{L}(A_\mu(x)) + J_\mu(x)A^\mu(x)] \right\}$$

as the *generating function* for the *vacuum expectation* values of *time ordered products* of the  $A_\mu$  fields. Note that  $J_\mu$  should be conserved ( $\partial^\mu J_\mu = 0$ ) in order for the full expression  $\mathcal{L}(A_\mu) + J_\mu A^\mu$  to be *gauge invariant* under the integral sign when  $A_\mu \rightarrow A_\mu + \partial^\mu \Lambda$ . For a proper approach, see [Ryd96, CL84, Gun03].

### Geometries

In this subsection, following [SK98], we describe path integral quantization on Riemannian–symplectic manifolds. Let  $\hat{q}^j$  be a set of Cartesian coordinate canonical operators satisfying the Heisenberg commutation relations  $[\hat{q}^j, \hat{q}^k] = i\omega^{jk}$ . Here  $\omega^{jk} = -\omega^{kj}$  is the canonical symplectic structure (see section 2.6.2 above). We introduce the canonical coherent states as  $|q\rangle \equiv e^{iq^j \omega_{jk} \hat{q}^k} |0\rangle$ , where

$\omega_{jn}\omega^{nk} = \delta_j^k$ , and  $|0\rangle$  is the ground state of a harmonic oscillator with unit angular frequency. Any state  $|\psi\rangle$  is given as a function on phase space in this representation by  $\langle q|\psi\rangle = \psi(q)$ . A general operator  $\hat{A}$  can be represented in the form  $\hat{A} = \int dq a(q)|q\rangle\langle q|$ , where  $a(q)$  is the lower symbol of the operator and  $dq$  is a properly normalized form of the Liouville measure. The function  $A(q, q') = \langle q|\hat{A}|q'\rangle$  is the *kernel of the operator*.

The main object of the path integral formalism is the integral kernel of the evolution operator

$$K_t(q, q') = \langle q|e^{-it\hat{H}}|q'\rangle = \int_{q(0)=q'}^{q(t)=q} \mathcal{D}[q] e^{i \int_0^t d\tau (\frac{1}{2} q^j \omega_{jk} q^k - h)} . \quad (\text{A.48})$$

Here  $\hat{H}$  is the Hamiltonian, and  $h(q)$  its symbol. The measure formally implies a sum over all phase-space paths pinned at the initial and final points, and a Wiener measure regularization implies the following replacement

$$\mathcal{D}[q] \rightarrow \mathcal{D}[\mu_\nu(q)] = \mathcal{D}[q] e^{-\frac{1}{2\nu} \int_0^t d\tau q^2} = N_\nu(t) d\mu_W^\nu(q) . \quad (\text{A.49})$$

The factor  $N_\nu(t)$  equals  $2\pi e^{\nu t/2}$  for every degree of freedom,  $d\mu_W^\nu(q)$  stands for the Wiener measure, and  $\nu$  denotes the diffusion constant. We denote by  $K_t^\nu(q, q')$  the integral kernel of the evolution operator for a finite  $\nu$ . The Wiener measure determines a stochastic process on the *flat* phase space. The integral of the symplectic one-form  $\int q\omega dq$  is a stochastic integral that is interpreted in the Stratonovich sense. Under general coordinate transformations  $q = q(\bar{q})$ , the Wiener measure describes *the same* stochastic process on *flat* space in the curvilinear coordinates  $dq^2 = d\sigma(\bar{q})^2$ , so that the value of the integral is not changed apart from a possible phase term. After the calculation of the integral, the evolution operator kernel is obtained by taking the limit  $\nu \rightarrow \infty$ . The existence of this limit, and also the covariance under general phase-space coordinate transformations, can be most easily proved through the *operator formalism* for the regularized kernel  $K_t^\nu(q, q')$ .

Note that the integral (A.48) with the Wiener measure inserted can be regarded as an ordinary Lagrangian path integral with a complex action, where the configuration space is the original phase space and the Hamiltonian  $h(q)$  serves as a potential. Making use of this observation it is not hard to derive the corresponding Schrödinger-like equation

$$\partial_t K_t^\nu(q, q') = \left[ \frac{\nu}{2} \left( \partial_{q^j} + \frac{i}{2} \omega_{jk} q^k \right)^2 - ih(q) \right] K_t^\nu(q, q') , \quad (\text{A.50})$$

subject to the initial condition  $K_{t=0}^\nu(q, q') = \delta(q-q')$ ,  $0 < \nu < \infty$ . One can easily show that  $\hat{K}_t^\nu \rightarrow \hat{K}_t$  as  $\nu \rightarrow \infty$  for all  $t > 0$ . The covariance under general coordinate transformations follows from the covariance of the “kinetic” energy of the Schrödinger operator in (A.50): The Laplace operator is replaced by the

Laplace-Beltrami operator in the new curvilinear coordinates  $q = q(\bar{q})$ , so the solution is not changed, but written in the new coordinates. This is similar to the covariance of the ordinary Schrödinger equation and the corresponding *Lagrangian* path integral relative to general coordinate transformations on the configuration space: The kinetic energy operator (the Laplace operator) in the ordinary Schrödinger equation provides a term *quadratic* in time derivatives in the path integral measure which is sufficient for the general coordinate covariance. We remark that the regularization procedure based on the modified Schrödinger equation (A.50) applies to far more general Hamiltonians than those quadratic in canonical momenta and leading to the conventional *Lagrangian* path integral.

### A.3.3 Modern String Actions and Transition Amplitudes

For the sake of completeness, in this subsection we give a brief review of modern path integral methods in quantum fields and string theory (mainly following [DEF99]). Recall that the fundamental quantities in quantum field theory (QFT) are the transition amplitudes,  $IN \implies OUT$ , for processes in which a number of *IN* incoming particles scatter to produce a number of *OUT* outgoing particles. The square modulus of the transition amplitude yields the *probability* for this process to take place.

The only way we have today to define string theory is by giving a *rule* for the evaluation of transition amplitudes, order by order in the loop expansion, i.e., genus by genus. The rule is to assign a relative weight to a given configuration and then to sum over all configurations. To make this more precise, we first describe the system's configuration manifold  $M$ .

We assume that  $\Sigma$  and  $M$  are smooth manifolds, of dimensions 2 and  $n$  respectively, and that  $x$  is a continuous map from  $\Sigma$  to  $M$ . If  $\xi^m$ ,  $m = 1, 2$ , are local coordinates on  $\Sigma$  and  $x^\mu$ ,  $\mu = 1, \dots, n$ , are local coordinates on  $M$  then the map  $x$  may be described by functions  $x^\mu(\xi^m)$  which are continuous.

To each system configuration we can associate a weight  $e^{-S[x, \Sigma, M]}$ , ( $S \in \mathbb{C}$ ) and the *transition amplitude*, *Amp*, for specified external strings (incoming and outgoing) is obtained by summing over all surfaces  $\Sigma$  and all possible maps  $x$ .

$$Amp = \sum_{\text{surfaces } \Sigma} \sum_x e^{-S[x, \Sigma, M]}.$$

We now need to specify each of these ingredients:

- 1) We assume  $M$  to be an  $nD$  Riemannian manifold, with metric  $g$ . A special case is flat Euclidean space-time  $\mathbb{R}^n$ . The space-time metric is assumed *fixed*.

$$ds^2 = (dx, dx)_g = g_{\mu\nu}(x) dx^\mu \otimes dx^\nu.$$

- 2) The metric  $g$  on  $M$  induces a metric on  $\Sigma$ :  $\gamma = x^*(g)$ ,

$$\gamma = \gamma_{mn} d\xi^m \otimes d\xi^n, \quad \gamma_{mn} = g_{\mu\nu} \frac{\partial x^\mu}{\partial \xi^m} \frac{\partial x^\nu}{\partial \xi^n}.$$

This metric is non-negative, but depends upon  $x$ . It is advantageous to introduce an intrinsic Riemannian metric  $g$  on  $\Sigma$ , independently of  $x$ ; in local coordinates, we have

$$g = g_{mn}(\xi)d\xi^m \otimes d\xi^n.$$

A natural intrinsic candidate for  $S$  is the area of  $x(\Sigma)$ , which gives the *Nambu-Goto action*

$$\text{Area}(x(\Sigma)) = \int_{\Sigma} d\mu_{\gamma} = \int_{\Sigma} n^2 \xi \sqrt{\det \gamma_{mn}},$$

which depends only upon  $g$  and  $x$ , but not on  $g$ . However, the transition amplitudes derived from the Nambu-Goto action are *not well-defined* quantum-mechanically.

Otherwise, we can take as starting point the *Polyakov action*

$$S[x, g] = \kappa \int_{\Sigma} (dx, *dx)_g = \kappa \int_{\Sigma} d\mu_g g^{mn} \partial_m x^{\mu} \partial_n x^{\nu} g_{\mu\nu}(x),$$

where  $\kappa$  is the *string tension* (a positive constant with dimension of inverse length square). The stationary points of  $S$  with respect to  $g$  are at  $g^0 = e^{\phi} \gamma$  for some function  $\phi$  on  $\Sigma$ , and thus  $S[x, g^0] \sim \text{Area}(x(\Sigma))$ .

The Polyakov action leads to *well-defined* transition amplitudes, obtained by integration over the space  $\text{Met}(\Sigma)$  of all positive metrics on  $\Sigma$  for a given topology, as well as over the space of all maps  $\text{Map}(\Sigma, M)$ . We can define the path integral

$$\text{Amp} = \sum_{\substack{\text{topologies} \\ \Sigma}} \int_{\text{Met}(\Sigma)} \frac{1}{N(g)} \int_{\text{Map}(\Sigma, M)} \mathcal{D}[x] e^{-S[x, g, g]},$$

where  $N$  is a normalization factor, while the measures  $\mathcal{D}[g]$  and  $\mathcal{D}[x]$  are constructed from  $\text{Diff}^+(\Sigma)$  and  $\text{Diff}(M)$  invariant  $L^2$  norms on  $\Sigma$  and  $M$ . For fixed metric  $g$ , the action  $S$  is well-known: its stationary points are the harmonic maps  $x: \Sigma \rightarrow M$ . Here, however,  $g$  varies and in fact is to be integrated over. For a general metric  $g$ , the action  $S$  defines a *nonlinear sigma model*, which is renormalizable because the dimension of  $\Sigma$  is 2. It would not in general be renormalizable in dimension higher than 2, which is usually regarded as an argument against the existence of fundamental membrane theories (see [DEF99]).

### Transition Amplitude for a Single Point Particle

The transition amplitude for a single point particle could in fact be obtained in a way analogous to how we prescribed string amplitudes. Let space-time be again a Riemannian manifold  $M$ , with metric  $g$ . The prescription for the transition amplitude of a particle travelling from a point  $y \in M$  to a point  $y'$

to  $M$  is expressible in terms of a sum over all (continuous) paths connecting  $y$  to  $y'$ :

$$Amp(y, y') = \sum_{\substack{\text{paths} \\ \text{joining } y \text{ and } y'}} e^{-S[\text{path}]}.$$

Paths may be parametrized by maps from  $C = [0, 1]$  into  $M$  with  $x(0) = y$ ,  $x(1) = y'$ . A simple worldline action for a massless particle is obtained by introducing a metric  $g$  on  $[0, 1]$

$$S[x, g] = \frac{1}{2} \int_C d\tau g(\tau)^{-1} \dot{x}^\mu \dot{x}^\nu g_{\mu\nu}(x),$$

which is invariant under  $\text{Diff}^+(C)$  and  $\text{Diff}(M)$ .

Recall that the analogous prescription for the point particle transition amplitude is the path integral

$$Amp(y, y') = \int_{\text{Met}(C)} \mathcal{D}[g] \frac{1}{N} \int_{\text{Map}(C, M)} \mathcal{D}[x] e^{-S[x, g]}.$$

Note that for string theory, we had a prescription for transition amplitudes valid for all topologies of the worldsheet. For point particles, there is only the topology of the interval  $C$ , and we can only describe a single point particle, but not interactions with other point particles. To put those in, we would have to supply additional information.

Finally, it is very instructive to work out the amplitude  $Amp$  by carrying out the integrations. The only  $\text{Diff}^+(C)$  invariant of  $g$  is the length  $L = \int_0^1 d\tau g(\tau)$ ; all else is generated by  $\text{Diff}^+(C)$ . Defining the normalization factor to be the volume of  $\text{Diff}(C)$ :  $N = \text{Vol}(\text{Diff}(C))$  we have  $\mathcal{D}[g] = \mathcal{D}[v] dL$  and the transition amplitude becomes

$$Amp(y, y') = \int_0^\infty dL \int \mathcal{D}[x] e^{-\frac{1}{2L} \int_0^1 d\tau (\dot{x}, \dot{x})_g} = \int_0^\infty dL \langle y' | e^{-L\Delta} | y \rangle = \left\langle y' \left| \frac{1}{\Delta} \right| y \right\rangle.$$

Thus, the amplitude is just the Green function at  $(y, y')$  for the Laplacian  $\Delta$  and corresponds to the propagation of a massless particle (see [DEF99]).

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## Index

- 1-form-field, 405
- Abelian category, 60
- Abelian group, 39
- absolute covariant derivative, 158, 164
- absolute derivative, 401
- abstract functor machine, 279
- abstract scalar field, 432
- acceleration, 83, 158, 294, 402
- achieved, 378
- actin, 409
- action, 419
- action functional, 19
- action potential, 413
- action principle, 18, 19, 21
- action principle – path integral, 19
- action-angle system of canonical coordinates, 226
- action-angle variables, 202
- activated, 353
- activation heat, 411
- active joints, 354
- active state, 413
- actually are, 30
- adaptive control, 316
- adaptive neural measure, 353
- adaptive path measure, 378
- adaptive sensory-motor transition amplitude, 353
- adaptive signal tracking, 349
- additive functor, 61
- adenosine diphosphate, 418
- adenosine triphosphate, 408
- adjoint group action, 123
- adjoint map, 114
- adjunction, 52
- adjustable pattern generator, 355
- admissible controls, 333
- admissible variation, 275
- affine, 340, 386
- affine connection, 160, 196, 384
- affine control system, 340
- affine Hamiltonian control action, 356
- affine Hamiltonian control function, 354
- affine Hamiltonian servo-system, 354
- affine Levi-Civita connection, 219
- algebra, 109
- algebra homomorphism, 109
- algebra of classical observables, 197
- almost complex structure, 179
- alpha, 30, 417
- Ambrose-Singer theorem, 155
- amplitude, 353
- analogous, 421
- antagonistic muscle-pairs, 28
- anthropomorphic product-tree, 134
- anti-holomorphic, 178
- antiderivation, 93
- approximate feedback linearization, 330
- arc, 13
- arc-element, 160
- area functional, 242
- arrows, 43
- associated tensors, 395
- associative composition, 42
- associativity of morphisms, 43
- asymptotically stable, 199, 323

- atlas, 64
- ATPase, 419
- attracting set, 200
- autogenetic, 30, 416
- autogenetic motor servo, 30, 416
- autogenetic–reflex action, 353
- autonomous dynamical systems, 11
  
- back adjunction, 52
- ball-and-socket joints, 119
- Banach manifold, 65
- Banach space, 65
- base space, 72
- basic formula of feedback control, 313
- basin of attraction, 200
- Bendixon’s criterion, 201
- Betti, 46
- Betti numbers, 46, 98, 292
- bi-invariant differential forms, 116
- Bianchi covariant derivative, 194, 219
- Bianchi symmetry condition, 163
- biholomorphism, 176
- bijection, 44
- bijective, 33
- bilinear map, 185
- binormal, 402
- biological images, 378
- biomechanical action, 235
- biomechanical bundles, 66
- biomechanics functor machine, 279
- biomechanics homology group, 311
- body-fixed frame, 211
- bone fractures, 286
- Bott periodicity, 73
- boundary, 15, 62
- boundary operator, 298
- brain-like control functor, 357
- brain–motor–controller, 136
- Brouwer degree, 168
- Brownian dynamics, 278
- bundle of cellular electrodynamic flux tubes, 381
- Burgers dynamical system, 155
  
- calculus of variations, 18
- Campbell–Baker–Hausdorff, 105
- canonical coordinates, 196
- canonical formulation, 427
- canonical transformation, 186
  
- Cartan magic formula, 107
- Cartan theorem, 152
- Cartesian axes, 8
- Cartesian coordinate basis, 397
- Cartesian product, 33, 38
- Casimir form, 228
- Casimir functions, 260
- categorification, 55
- category, 43, 276
- category of Lie groups, 66, 306
- category of smooth manifolds, 309
- category of vector bundles, 309
- Cauchy’s theorem, 208
- Cauchy–Riemann equations, 176
- cerebellar electrical potential, 357
- cerebellar level, 352
- cerebellar models, 358
- cerebellar sensory–motor amplitude, 356
- cerebellar sensory–motor transition probability, 356
- cerebellum, 136, 352, 354
- chain complex, 61
- chain rule, 32, 68, 95
- Chapman–Kolmogorov law, 79, 86
- characteristic distribution, 330
- charge, 380
- Chern–Simons quantum mechanics, 259
- Christoffel symbols, 160, 219, 386, 399
- class of objects, 43
- classical biomechanical action, 235
- classical muscular mechanics, 383
- closed, 15
- closed form, 62, 95
- closed path, 36
- closed-loop nonlinear system, 327
- coadjoint group action, 123
- cobasis, 90
- coboundary, 62
- coboundary operators, 289
- cochain complex, 62
- cocomplete category, 52
- cocycle, 62
- cocycle condition, 70
- codifferential, 101
- codomain, 33, 43
- coframing, 90
- cofunctor, 46
- cohomologous, 70

- cohomology class, 18
- cohomology exact sequence, 290
- cohomology object, 62
- coimage, 60
- cokernel, 60
- colimit, 51, 52
- collision detection, 151
- commensurate, 202
- commutative diagram, 43
- commutative diagrams of arrows, 37
- commutative flow, 38
- commutator, 220
- compact, 35
- compactness, 35
- complete subcategory, 44
- completely integrable Hamiltonian system, 151
- complex, 95
- complex manifold, 176
- complex phase–space manifold, 205
- complex structure, 176
- complex vector bundle, 178
- complexified tangent space, 177
- components, 36
- composition, 32
- conatural projection, 68
- concave–hyperbolic, 389
- configuration manifold, 9, 63, 407
- configuration space, 191
- conflict resolution manoeuvres, 126
- conformal Killing forms, 182
- conformal Killing tensor–fields, 183
- conformal Killing vector–fields, 181
- conformal Killing–Riemannian geometry, 181
- conformal Landau–Ginzburg model, 381
- conformal symmetry of the manifold, 181
- conformal twistor, 181
- conformal vector, 183
- conformal vector–field, 182
- conformal vector–fields, 182
- conformally covariant twistor equation, 181
- Conley’s continuation principle, 298
- connected, 36
- connectedness, 35
- connection, 158, 159, 386
- connection homotopy, 163
- conservation law, 22, 243
- conservation of angular momentum, 22
- conservation of electric charge, 24
- conservation of energy, 22
- conservation of linear momentum, 22
- conservative Hamiltonian biomechanics, 407
- conservative particle, 7
- constant of motion, 198
- constrained Hamilton–d’Alembert equations, 253
- constrained variational calculus, 257
- constrained variational principle, 251
- contact
  - form, 244
  - manifold, 245, 246
- contact manifold, 244
- contact transformations, 243
- continual time systems, 318
- continual–sequential state equation, 279
- continuity, 34
- continuous deformation, 34
- continuous–time regularization, 426
- contractile elements, 408
- contraction, 5, 28, 89
- contraction dynamics, 413
- contravariant acceleration functor, 189
- contravariant functor, 46
- contravariant Hom–functor, 48
- contravariant Lagrangian dynamics, 276
- contravariant vector, 393
- control, 128
- control Hamiltonian function, 29, 407
- control outputs, 407
- control strategies, 128
- controlled Van der Pol oscillator, 329
- convergence factor, 432
- convex–ecliptic, 388
- cooperating, 133
- coordinate chart, 64
- coordinate transformation, 392
- cost of a trajectory, 129
- cotangent bundle, 68, 135, 407
- cotangent Lie algebra, 122
- cotangent map, 68
- cotangent space, 68
- counit natural transformation, 52
- coupling Hamiltonians, 354
- covariant, 391

- covariant components, 8
- covariant derivative, 387, 400
- covariant differentiation, 157
- covariant Euler–Lagrange equations, 275
- covariant force equation, 239
- covariant force functor, 188, 272, 313
- covariant force functor , 357
- covariant force law, 5, 63, 188, 191, 272, 286, 289, 313, 357, 406
- covariant form, 391, 401
- covariant functor, 46
- covariant Hom–functor, 48
- covariant inertia tensor, 10
- covariant Lagrangian equations, 12
- covariant muscular forces, 371
- covariant vector, 393
- covector, 393
- covector–field, 87
- cover, 35
- covering, 35, 66
- creatine kinase, 418
- creatine phosphate, 418
- critical path, 294
- critical point, 297
- critical points, 172
- cross bridges, 410
- cross striations, 408
- curl, 14
- curvature, 384
- curvature operator, 157, 163
- curve, 7, 63
- curve on a manifold, 66
- cycle, 62
  
- D’Alambert–Lagrange principle, 91
- D’Alembert’s Principle of virtual displacement, 11
- De Rham cohomology group, 18, 97, 291
- De Rham complex, 95
- De Rham differential complexes, 290
- De Rham theorem, 96, 97, 100, 291
- decomposable system, 280
- defuzzification, 369
- degree of symmetry, 182
- derivation, 14, 74
- derivative map, 85
- desired, 378
- desired response, 328
- deterministic biomechanical jerk function, 287
- deterministic chaos, 278
- diagonal functor, 48
- diffeomorphism, 44, 66
- difference, 329
- differential, 102
- differential algebraic equation, 265
- diffusion processes, 415
- dimensional neural network, 353
- dinatural transformations, 50
- Dirac bracket, 259
- Dirac equation, 182
- Dirac matrices, 109
- Dirac operator, 182
- Dirac quantum commutator, 383
- direct system, 42
- directional derivative, 102
- discrete time systems, 318
- dissipation function, 269
- dissipative Hamiltonian biomechanics, 28
- dissipative structures, 27
- distribution, 91, 336
- disturbance, 128
- divergence, 14
- domain, 31, 33, 43
- driving torque one–forms, 25, 27
- dual, 68, 87
- dual  $(n - p)$ –forms, 17
- dual picture, 46
- dummy index, 391
- dynamic force–velocity relation, 411
- dynamics of the relative configuration, 127
  
- Eccles model of synaptic activation, 384, 415
- effective action, 114
- Einstein’s summation convention, 1
- electric current, 380
- electrical current, 379
- electrical field, 379
- electrical muscular stimulation, 372
- electrical potential, 380
- electrodynamics field action principle, 379
- electrodynamics flux tubes, 381

- element, 13
- ellipsoid of inertia, 10
- Embden–Meyerhoff pathway, 418
- endomysium, 408
- endpoint conditions, 275
- energy conservation, 24
- ensemble average, 375
- epic, 61
- epimorphism, 44
- epimorphisms, 33
- equal, 421
- equation of continuity, 403
- equation of geodesic deviation, 388
- equilibrium point, 322
- equilibrium solution, 199
- equivalence relation, 33
- equivalent muscular actuator, 417
- equivalent muscular actuators, 28, 352
- ergodic hypothesis, 375
- error function, 29
- essence of feedback control, 321
- Euclidean 3D metric tensor, 10
- Euclidean 3D space, 7, 8
- Euclidean metrics, 394
- Euler, 46
- Euler characteristics, 390
- Euler’s vector equation, 222
- Euler–Lagrange equation, 162, 192, 242, 243, 302
- Euler–Lagrange functional derivative, 148
- Euler–Lagrangian equations, 19, 21, 376
- Euler–Poincaré characteristics, 98, 292
- Euler–Poincaré equations, 195
- evolution operator, 79
- exact, 16, 60
- exact form, 62, 95
- excitation, 5, 28
- excitation dynamics, 413
- excitation model, 384
- excitation–contraction dynamics, 352
- existence of identity morphism, 43
- exponential map, 112, 120, 139
- exponentially stable, 323
- exponentially stable in the large, 323
- exponentiation, 138
- extended Hamiltonian, 261
- extended Pfaffian system, 274
- extension principle, 284
- exterior algebra, 88
- exterior derivative, 14, 93, 128
- exterior differential forms, 13
- exterior differential system, 243, 405
- exterior differential systems, 90
- exterior Maxwell equation, 380
- exterior product, 17
- external coordinates, 134
- faithful functor, 48
- Faraday, 380
- fasciculus, 408
- feedback torque one-forms, 354
- Feynman path integral, 18, 248, 375, 377
- Feynman propagator, 248
- fiber derivative, 252
- fiber-derivative, 149
- fibrations, 71
- fibre, 68, 72
- fibre bundle, 71
- fibre derivative, 306
- field, 41
- field theory, 20
- field-generated solitons, 381
- fifth-order transmission cascade, 415
- filamentary-overlap function, 413
- final object, 43
- Finsler metric, 380
- first integral, 198
- first variation, 243, 294
- first variation formula, 162, 294
- fisherman’s derivative, 102
- fixed, 435
- fixed point, 199
- flag, 91
- flow, 85, 405
- flow line, 82, 86
- flow property, 85
- fluctuating noisy uncertainty, 377
- flux, 415
- flux tubes, 381
- foliation, 337
- force, 402
- force equation, 219
- force generator, 415
- force plates, 7
- forced dissipative Hamiltonian biomechanics, 29

- forced Hamiltonian biomechanics, 407
- forced Lagrangian equation, 91
- forced transition amplitude, 21
- forgetful, 48
- form commutator, 17
- formal exponential, 86
- forward dynamics, 7
- forward kinematics, 134
- Fréchet derivative, 220
- Fredholm kernels, 382
- free  $Ca$ -ion concentration, 413
- free action, 114
- free index, 391
- Frenet–Serret formulae, 402
- Frobenius–Cartan criterion, 152
- front adjunction, 52
- full embedding, 48
- full functor, 48
- fully nonlinear control system, 321
- function, 31
- function space, 36
- functional, 242, 243, 245
- functional derivative, 19, 21, 220
- functional electrical stimulation, 371
- functional integral, 429
- functional manifold, 155
- functional of the path, 19
- functor, 46
- functor category, 49
- functor machine, 280
- functor morphism, 48
- fundamental group, 47
- fundamental groupoid, 45
- fusiform, 408
- fuzzy differential equation, 283
- fuzzy inference system, 368
- fuzzy numbers, 283
- fuzzy region of uncertainty, 284
- fuzzy set, 284
- fuzzy–stochastic biomechanical jerk function, 287
- fuzzy–stochastic transformation, 285
  
- Galilei group, 117
- gamma, 30, 417
- gauge fixing, 433
- gauge invariant, 433
- gauge symmetries, 259
- gauge symmetry, 24
  
- gauge theory, 381, 433
- Gauss map, 168
- Gauss–Bonnet formula, 157
- Gauss–Bonnet theorem, 98
- Gaussian curvature, 13, 157
- general functional transformation, 391
- general linear Lie algebra, 105
- general theory of systems, 279
- generalized chain complexes, 290
- generalized cochain complexes, 289
- generalized coordinates, 11, 63
- generalized force vector, 12
- generalized Hamiltonian biomechanics, 407
- generalized Hamiltonian control system, 407
- generalized infinitesimal symmetry, 148
- generalized Kronecker–delta symbol, 394
- generalized momenta, 22
- generalized vector–field, 147
- generalized velocity vector, 11
- generating function, 433
- geodesic, 83, 160, 162, 399
- geodesic action, 384
- geodesic deviation, 165, 387
- geodesic equation, 163, 384, 399
- geodesic flow, 194, 219, 308
- geodesic separation vector, 13
- geodesic spray, 84, 194, 219, 308
- geodesically generated distribution, 345
- geodesically invariant, 345
- geometric action principle, 384, 386
- geometric isomorphism, 71
- geometrical dual, 405
- geometroynamics, 6, 9
- global complex analysis, 205
- global geodesics problems, 292
- global solution, 86
- glucose–1–phosphate, 419
- glycolysis, 418
- goal of a control system, 315
- Godement product, 49
- Golgi tendon organs, 30, 354, 416
- gradient, 14, 85, 161
- gradient conformal Killing tensor, 183
- gradient flow, 297
- gradient force 1–forms, 276
- gradient force vector–fields, 276

- Grassmann algebra, 88  
 Grassmann planes, 403  
 Green's functions, 382  
 Green's operator, 304  
 Green's theorem, 243  
 group, 39, 45  
 group action, 40, 119  
 group conjugation, 123  
 group homomorphism, 40  
 group monomorphism, 40  
 groupoid, 45  
 growth condition, 283  
  
 Haar measure, 114  
 Hamel equations, 195  
 Hamilton's equations, 196  
 Hamilton's principle, 18, 192  
 Hamilton–Dirac equations, 260  
 Hamilton–Poisson biomechanical system, 221  
 Hamiltonian, 130  
 Hamiltonian action, 187  
 Hamiltonian biomechanics, 69  
 Hamiltonian energy function, 196  
 Hamiltonian flow, 199  
 Hamiltonian function, 218  
 Hamiltonian mechanical system, 196  
 Hamiltonian phase–flow, 308  
 Hamiltonian vector–field, 196, 217  
 Hamiltonian way, 420  
 harmonic, 101  
 harmonic exterior differential form, 301  
 harmonic oscillator, 388  
 harmonic projection, 304  
 harmonic representative, 304  
 Hartman–Grobman theorem, 263  
 heat bath, 278  
 heat equation, 140, 146, 169, 303, 411  
 Hebbian–like learning, 353  
 Heisenberg commutation relations, 427  
 Heisenberg picture, 383, 428  
 hemodynamics, 404  
 Hermitian metric, 178  
 Hermitian position operator, 21  
 Hessian, 149, 161  
 hidden symmetries, 233  
 Hilbert, 41  
 Hilbert 19th problem, 234  
 Hilbert 23rd problem, 234  
  
 Hilbert 4th problem, 160  
 Hilbert manifold, 65  
 Hilbert space, 65  
 hinge joints, 119  
 hiper–cube  $\equiv$  neuro–muscular control space, 416  
 Hodge Laplacian, 302  
 Hodge star, 17, 89, 100  
 Hodge theory, 302  
 Hodge's theorem, 181  
 Hodge–De Rham decomposition, 302  
 Hodge–De Rham Laplacian, 298  
 Hodgkin–Huxley HH–neuron model, 413  
 Hodgkin–Huxley neural, 384  
 holomorphic cotangent space, 178  
 holomorphic tangent space, 178  
 holonomic atlas, 74  
 holonomic coframes, 75  
 holonomic frames, 74  
 holonomous frame field, 74  
 Hom–bifunctor, 48  
 homeomorphism, 44  
 homeostatic neuro–muscular feedbacks, 378  
 homoclinic orbits, 201  
 homogenous quadratic form, 11  
 homological algebra, 46  
 homologous in, 208  
 homology group, 46, 47  
 homology object, 61  
 homothetic Killing tensor, 183  
 homotopic, 35  
 homotopies of homotopies, 58  
 homotopy, 34, 35  
 homotopy axiom, 292  
 homotopy classes, 36  
 homotopy lifting property, 71  
 homotopy of loops, 37  
 homotopy operators, 96, 332  
 Human Biodynamics Engine, 369  
 hybrid dynamics, 278  
 hyperbolic force–velocity, 29  
 hyperbolic force–velocity curve, 411  
 hyperbolic force–velocity relation, 270  
 hyperbolic point, 199  
  
 ideal, 41  
     differential, 245

- identity, 42
- identity functor, 48
- image, 16, 60
- imprecision of measurement, or estimation, 278
- impulse torque–time relation, 270
- inclusion functor, 48
- incommensurate, 202
- independence condition, 245
- index, 90, 172
- index theorem, 296
- indirect adaptive control, 317
- inertia matrix, 403
- inertia tensor, 10
- infinite prolongation, 148
- infinitesimal generator, 120
- initial object, 43, 44
- injection, 33, 44
- inorganic phosphate, 418
- input map, 280
- input process, 280
- insertion operator, 89
- integrability, 233
- integrable mechanical systems, 381
- integrable systems, 188
- integral curve, 82, 86
- integral curves, 405
- integral element, 90
- integral manifold, 244, 245, 275, 336
- integral over all possible paths, 428
- integrand, 14
- interactions, , 432
- interior product, 89
- internal acceleration vector–field, 406
- internal force 1–form field, 406
- internal joint coordinates, 134, 405
- internal velocity vector–field, 405
- intervertebral disclinations, 286
- intervertebral dislocations, 286
- invariant, 393
- invariant tori, 201
- invariants of the dynamical system, 22
- inverse kinematics, 134
- inverse kinematics problem, 319
- inverse loop, 37
- inverse system, 42
- inverted pendulum, 313
- involution, 71, 138
- involution closure, 336
- irreversible processes, 27
- iso–energetic paths, 240
- isolated equilibrium point, 322
- isometric steady–state contraction, 410
- isometry group, 182
- isomorphism, 44
- isotropy group, 115
- Ito quadratic cotangent bundle, 283
- Ito quadratic tangent bundle, 282
- Jacobi equation, 387
- Jacobi equation of geodesic deviation, 13, 165
- Jacobi fields, 165, 295, 387
- Jacobi flows, 387
- Jacobi identity, 109, 220
- Jacobi operator, 243
- Jacobian, 32
- Jacobian determinant, 392
- jet bifunctor, 78
- jet prolongation, 78
- jet space, 141
- jets, 244
- Kähler condition, 303
- Kähler form, 179
- Kähler manifold, 302
- Kähler metric, 179
- Kähler potential, 180
- Kähler structure, 179
- Kalman filter, 318
- Kalman regulator, 318
- kernel, 15, 60
- kernel of the operator, 434
- Killing equation, 181
- Killing form, 211
- Killing spinor–field, 182
- Killing tensor–field, 183, 233
- Killing vector–field, 232
- Killing–Yano equation, 182
- kinematic constraint distribution, 256
- kinematic singularities, 134
- kinetic energy, 11
- kinetic energy of muscular contraction, 382
- Kortevæg–De Vries equation, 147, 223, 383
- Kronecker–delta, 394
- lack of memory, 278

- Lagrange multipliers, 251, 346
- Lagrange stability, 324
- Lagrange–d’Alembert principle, 251
- Lagrange–Poincaré equations, 196
- Lagrangian, 193, 242, 243, 430
- Lagrangian action formalism, 19
- Lagrangian biomechanics, 68
- Lagrangian density, 20, 376
- Lagrangian equations, 22
- Lagrangian flow, 308
- Lagrangian function, 13, 18, 19, 162
- Lagrangian–field structure, 376
- Langevin rate equations, 278
- Laplace equation, 142
- Laplace transform, 320
- Laplace–Beltrami operator, 161
- Laplacian, 18, 161
- Laplacian symmetry, 184
- latency relaxation, 411
- lateral cisternae, 408
- lattice regularization, 423
- laws of motion, 80
- Lax type representation, 151
- leaf space, 337
- least action principle, 375, 376
- Lefschetz theorem, 181
- left adjoint, 52
- left cancellable, 44
- left exact, 61
- left extension, 112
- left ideal, 109
- left invariant vector–field, 111
- left inverse, 44
- left–invariant Lagrangian, 195
- left–invariant Riemannian metric, 211
- Legendre map, 149, 230
- Legendre submanifold, 245, 246
  - transverse, 245, 246
- Legendre transformation, 252, 253, 306
- level curves, 201
- level set, 81
- Levi–Civita connection, 159
- Levi–Civita connections, 406
- Lie algebra, 105, 109, 127, 220
- Lie algebra homomorphism, 109
- Lie bracket, 104, 109
- Lie bracket property, 145
- Lie derivative, 76, 102, 131, 197
- Lie functor, 112
- Lie group, 110, 127
- Lie subalgebra, 109
- Lie–invariant geometric objects, 151
- Lie–Lagrangian biomechanics functor, 272
- Lie–Poisson bracket, 124, 220
- limit, 51, 52
- limit set, 199
- line, 13
- line bundle, 72
- line element, 385
- line integral, 14
- linear controllability, 330
- linear system, 329
- linearization, 199
- Liouville equation, 282
- Liouville measure, 269
- Liouville theorem, 224
- Liouville–Arnold theorem, 227
- Lipschitz condition, 84, 283
- local geodesic, 292
- locally accessible system, 340
- locally configuration accessible, 343
- locally configuration controllable, 343
- locally exact, 95
- loop, 36
- Lorentz force, 380
- Lorentzian spin geometry, 183
- Lyapunov criterion, 349
- Lyapunov exponent, 217
- Lyapunov function, 324
- Lyapunov function candidate, 316
- Möbius bundle, 72
- machine learning, 348
- macro–level averaging lift, 381
- macroscopic force–velocity model, 384
- macroscopic muscle–load dynamics, 411
- magnetic field, 379
- maintenance heat, 411
- Mamdani inference, 368
- manifold, 63
- manifold with boundary, 97
- manipulability measure, 134
- Markov chain, 278, 428
- Markov process, 278
- mass conservation principle, 404
- material covariant metric tensor, 238
- material metric tensor, 11, 403, 406

- matrix commutator, 105
- Maupertius action principle, 162
- Maurer–Cartan equations, 152
- maximal geodesic, 83
- maximal integral curve, 82
- maximal integral manifold, 336
- Maxwell, 380
- Maxwell electrodynamics, 379
- mean curvature, 242
- mechanical action, 382
- mechanical metric, 162
- Melnikov function, 205
- metric, 385
- metric tensor, 8, 158, 219
- microscopic sliding filament model, 383
- microscopic theory of muscular contraction, 410
- model space, 65
- module, 41
- molecular soliton model of muscular contraction, 383
- moment of inertia, 10
- momentum functions, 130
- momentum map, 120, 187, 211
- momentum map , 232
- momentum phase–space, 26, 135, 217, 406
- monic, 61
- monomorphism, 33, 44
- Moore–Penrose pseudoinverse, 392
- morphism of vector–fields, 86
- morphisms, 42
- Morse function, 172
- Morse index, 297
- Morse theory, 172
- motion capture, 7
- motion planning, 151
- motor servo, 353, 354
- multiindex, 88
- muscle fibers, 408
- muscle–fat manifold, 389
- muscular active–state element equation, 28
- muscular contraction action principle, 382
- muscular level, 352
- muscular Riemannian configuration manifold, 376
- muscular Riemannian metrics, 382
- myocybernetics, 413
- myofibrillar action propagators, 382
- myofibrils, 408
- myoglobin, 419
- myosin, 409
- n–categories, 53
- Nambu–Goto action, 436
- Nash strategies, 127
- natural equivalence, 49
- natural inclusion, 49
- natural isomorphism, 49
- natural projection, 67
- natural transformation, 48
- natural vector bundle, 75
- neural control inputs, 407
- neural path integral, 353
- neural pathways, 353
- neural phase–space path integral, 356
- neural–image coordinates, 358
- neural–image manifold, 364
- Newton’s second law, 7
- Newtonian equation of motion, 7, 382
- Noether, 46
- Noether Lagrangian symmetry, 148
- Noether symmetries, 148
- Noether theorem, 22, 243
- Noetherian module, 42
- Noetherian ring, 41
- noise, 378, 384
- non–anticipating solution, 283
- non–cooperative case, 133
- non–cooperative Nash equilibrium, 133
- non–degenerate 1–form, 244
- nondegenerate, 185
- nonholonomic rolling constraints, 254
- nonlinear affine control system, 321
- nonlinear control design, 316
- nonlinear controllability criterion, 336
- nonlinear decomposable system, 280
- nonlinear multivariate analysis, 391
- nonlinear process–functor, 280
- nonlinear Schrödinger equation, 222, 383
- nonlinear sigma model, 436
- nonlinear system behavior, 280
- nonwandering set, 200
- normal, 387
- normal bundle, 73

- normal subgroup, 40
- normal vector-field, 81
- normalization condition, 432
- normalized force across the series elastic element, 413
- normalized length of the contractile element, 413
- null object, 44
- nullity, 296
- number of degrees of freedom, 9
- numerical invariants of spaces, 46
  
- objects, 42
- observability map, 279
- one parameter subgroup, 112
- one-form, 14, 393
- one-to-one, 33, 44
- onto, 33, 44
- open cover, 35
- optimal cost, 130
- optimal Hamiltonian, 130
- orbit, 40, 115
- orbit space, 115
- orbitally stable, 263
- orientation, 97
- outer product, 394
- output map, 280
- output process, 280
- overall probability amplitude, 377
- overdetermined, 233
  
- parabolic Einstein equation, 169
- parabolic length-tension curve, 410
- parallel transport, 194, 308
- parameter update law, 349
- parameter variation, 294
- parking theorem, 335
- partial order, 33
- partially ordered set, 33
- partition functions, 357
- passive sarcomere tension, 413
- path, 36
- path components, 36
- path connected, 36
- path integral quantization, 427
- pennate, 408
- performance, 313
- perimysium, 408
- period, 98
  
- perturbation theory, 203
- perturbative expansion methods, 378
- Pfaff theorem, 244
- Pfaffian exterior differential system, 274
- Pfaffian system, 243
- phase space, 7
- phase trajectory, 199
- phase-space path integral, 424
- phase-space spreading effect, 269
- Philip Hall basis, 338
- piecewise smooth paths, 293
- planar rigid body, 341
- Planck constant, 375
- Poincaré, 46
- Poincaré lemma, 14, 95, 96, 291
- Poincaré-Cartan form, 246
- Poincaré-Hopf theorem, 98
- point particle, 19
- pointed set, 36
- pointed topological space, 36
- Poisson bracket, 131, 151, 197, 257
- Poisson evolution equation, 220
- Poisson manifold, 219
- Poisson tensor-field, 229
- Polyakov action, 436
- position, 420
- positional stiffness, 30, 416
- possibility distribution, 284
- potential, 7, 162
- potential energy, 12
- potential field, 19
- predecessor, 129
- principal axes of inertia, 10
- principal normal, 402
- principal planes of inertia, 10
- probabilistic transition micro-dynamics, 377
- probability, 435
- probability amplitude, 427
- prolongation, 141
- prolonged generalized vector-field, 147
- prolonged group action, 144
- pseudo-inverse, 134
- pull-back, 76
- pull-back diagram, 37
- pull-back vector bundle, 70
- push-forward, 76
  
- quantization, 19

- quantum biomechanical action, 235
- quantum electrodynamics, 381
- quantum evolution equation, 383
- quantum Hamiltonian operator, 383
- quantum-like adaptive control, 356
- quantum-mechanical transition
  - amplitude, 430
- quantum-mechanics propagator, 428
- quotient space, 136
  
- radius of a circular protected zone, 128
- range, 31, 43
- rank condition, 333
- Rayleigh – Van der Pol’s dissipation
  - function, 27
- reachability map, 279
- reachable set, 340
- reaction, 352
- realization problem, 280
- reciprocal activation, 354
- reciprocal inhibition, 354
- reciprocal innervation of agonists and
  - inhibition of antagonists, 352
- recurrent, distributed parameter, 415
- recursive homotopy dynamics, 276
- red, 408
- reduced curvature 1-form, 156
- reduced phase-space, 188
- reduction equivalence relation, 136
- redundancy, 134
- redundant manipulator, 271
- redundant system, 392
- related vector-fields, 77
- relation, 33
- relative acceleration, 165, 387
- relative degree, 328
- relative order, 328
- representation of a category, 48
- representation of a group, 48
- representative point, 63, 405
- retraction, 44
- Ricci antisymmetric tensors, 394
- Ricci curvature, 158
- Ricci flow, 169
- Ricci tensor, 158, 163
- Riemann curvature tensor, 13, 157, 163, 386, 395
- Riemannian kinetic energy form, 406
- Riemannian manifold, 8, 13, 89, 191
  
- Riemannian metric, 157, 219, 238, 394
- Riemannian metric tensor, 375
- right adjoint, 52
- right cancellable, 44
- right exact, 61
- right ideal, 109
- right inverse, 44
- rigid body, 211
- rigid body with a fixed point, 211
- ring, 40
- robotic leg, 340
- robust control, 316
- robustness, 313
- Rodrigues relation, 122
- rolling disk, 346
- rotational Hill’s parameters, 29
- rotational symplectic geometry/mechanics, 25
  
- saddle, 127
- saddle solution, 129, 130
- safe operation, 128
- sarcolemma, 408
- sarcomere, 409
- sarcoplasm, 408
- sarcoplasmic reticulum, 408
- scalar curvature, 158, 165, 387
- scalar electrical potential, 379
- scalar function, 14
- scalar invariant, 393
- scalar potential field, 406
- scalar product, 8
- scalar-field, 396
- Schrödinger picture, 428
- Schwinger formalism, 381
- second tangent bundle, 71
- second variation, 243, 294
- second variation formula, 166, 295
- second vector bundle, 71
- second-order contravariant tensor, 394
- second-order covariant tensor, 394
- second-order mixed tensor, 394
- section, 44
- sectional curvature, 164
- sections of biomechanical bundles, 79
- self-organized, 378
- semidirect product, 125, 136
- sensory-motor integration, 352
- separatrix, 201

- servoregulatory loops, 30, 417
- set of morphisms, 43
- short exact sequence, 60
- shortening heat, 411
- shortest path, 384
- signal, 378
- similar in all animals, 355
- simple mechanical control systems, 338
- simple mechanical systems, 192
- simple statistical system, 390
- simplicial approximation, 390
- singularity, 199
- skew-symmetric, 185
- sliding filament mechanism, 410
- sliding filament model, 410
- slow fibers, 419
- small time locally controllable, 333
- small-time local controllability, 340
- smooth, 64
- smooth homomorphism, 110
- smooth manifold, 14
- smooth map, 65
- solitary model of muscular excitation-contraction, 381
- soliton, 222, 381
- source, 46, 356, 431
- space of all weighted paths, 382
- special Euclidean group in 3D space, 123
- special Euclidean group in the plane, 122
- special Euclidean group of motions, 271
- speed, 83
- spinal control level, 352
- spinal level, 352
- spindle receptors, 30, 354, 416
- spinor, 109
- spinor-fields, 181
- spray, 87
- spring constant, 388
- stability, 313
- stable, 199
- stable in the sense of Lyapunov, 322
- standard action, 430
- star-shaped, 96
- state feedback, 339
- state vector, 428
- state-space approach, 315
- stationary, 242, 243
- step size, 379
- stiffness-servo, 29
- stimulus-response-type, 372
- stochastic forces, 278
- stochastic influence, 278
- stochastic Taylor expansion, 283
- stochastic tensor bundle, 282
- stochastic transformation, 282
- Stokes formula, 14, 97
- stretch potentiation, 413
- string tension, 436
- structure equations, 171
- subgroup, 40
- submanifold immersion, 244
- sum over fields, 381
- sum over fractal geometries, 389
- sum over histories, 382
- sum-over-histories, 18
- supervising, 353
- surface integral, 14
- surjection, 33, 44
- swept volume, 151
- symmetric, 161
- symmetric affine connection, 159
- symmetric product, 344
- symmetrical load-lifting, 266
- symmetry, 243
- symmetry group, 140
- symplectic form, 185, 186
- symplectic group, 185
- symplectic Lie algebra, 125
- symplectic Lie group, 125
- symplectic manifold, 186, 196
- symplectic map, 186
- symplectic matrix, 125
- symplectomorphism, 185
- synaptic weights, 353, 378
- system dynamics, 279
- system's center of mass, 10
- T tubules, 408
- tangent, 402
- tangent bundle, 67, 72, 134
- tangent functor, 79
- tangent Lie algebra, 121
- tangent map, 66, 67
- tangent space, 66
- tangent vector, 9
- tangent vector-field, 81

- tangential, 387
- target, 46
- target set, 128
- tensor bundles, 75
- tensor contraction, 395
- tensor-field, 74, 396
- terminal object, 44
- the sectional curvature, 157
- theory of fluctuating geometries, 390
- thermodynamic partition function, 383
- thermodynamic relation, 411
- thermoelastic heat, 412
- three-form, 14
- time average, 375
- time ordered products, 433
- time-dependent flow, 80
- time-dependent Schrödinger equation, 423
- time-dependent vector-field, 86
- topological group, 111
- topological manifold, 63
- topological space, 34
- topologically dual functors, 309
- torque-jerk, 286
- torque-time, 28
- torsion, 160
- torsion free, 161
- total action, 375
- total derivative, 145
- total energy function, 407
- total space, 72
- total system's response, 279
- trajectory, 84, 128
- transducer neurons, 414
- transformation
  - contact, 242
  - point, 242
- transformation classical, 242
- transformation gauge, 242
- transition amplitude, 19, 247, 377, 431, 435
- transition amplitude, 21
- transition entropy, 357, 383
- transition functor, 374
- transition maps, 64
- transition probability, 377
- transitive action, 114
- translational biomechanics, 7
- translational Hamiltonian equations of motion, 7
- translational vector geometry, 5
- trapping region, 200
- triad, 408
- triangular identities, 60
- trivial fibration, 72
- twistor forms, 182
- twistor operator, 182
- two-form, 14
- two-sided ideal, 109
- two-sided inverse, 44
- Tychonoff product-topology theorem, 367
- uniaxial rotational joint, 198
- uniformly asymptotically stable, 323
- uniformly bounded, 324
- uniformly stable, 323
- uniformly ultimately bounded, 324
- unique functorial relation, 304
- unique minimal geodesic, 293
- unit natural transformation, 52
- universal properties, 38, 51
- unsupervised, 378
- vacuum expectation, 433
- variation vector-field, 162
- vector bundle, 69
- vector bundle functor, 75
- vector bundle homomorphism, 69
- vector-field, 80, 396, 405
- velocity, 83, 158, 294, 420
- velocity phase-space, 26, 135, 193, 405
- vertical lift, 71, 343
- virtual displacement, 12
- virtual work, 12
- volume form, 101, 219
- volume integral, 14
- weak functorial inverse, 52
- wedge product, 88, 89
- well-posed variational problem, 274
- white muscle fibers, 408, 419
- Wick rotation, 378
- Wiener measure, 425, 426
- winding number, 207
- zero morphism, 44
- zero-sum dynamical game, 128

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