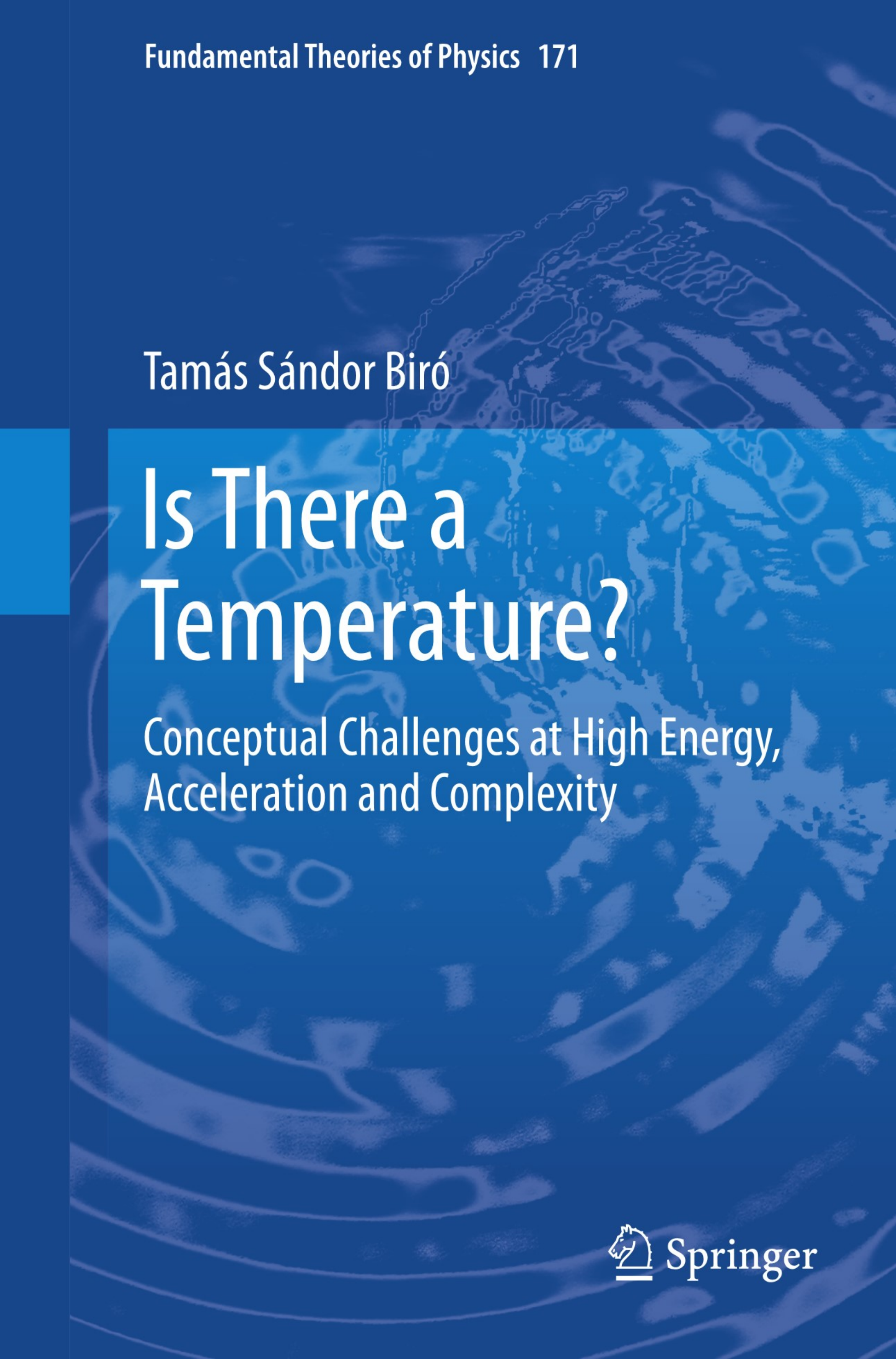

Fundamental Theories of Physics 171

Tamás Sándor Biró

Is There a Temperature?

Conceptual Challenges at High Energy, Acceleration and Complexity

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To Tünde, Szilvia, Réka, Gábor and Kati.

Preface

Yet another book about thermodynamics? Wherefore? This almost 200-year-old physics subject is being discussed in depth and presented in a plethora of textbooks extensively. It is not my intention to add one to this number. It is the experience in modern research problems dealing with matter under extreme conditions which challenges me to write a book about this topic. Physical matter at high energy, velocity and momenta, under extreme acceleration or deceleration, or by another particular circumstance, such as unusual complexity, does behave strangely. Talking about extremely high or low, by the familiar thermometer not measurable temperatures, leads us not only to the question, what is the temperature of such matter, but also to the question, whether the very concept of absolute temperature is applicable: Is there a temperature at all?

The more important this question becomes since the “social” disciplines of physics, like biological physics, econophysics, sociological models started to apply mathematical models and concepts originally devised for the study of “ordinary,” i.e. atomic matter. These generalized statistical and stochastic models apply quantities analogous to the physical energy, to the entropic measure of order and disorder, and to the associated concept of absolute temperature. By such applications of physics, however, the exception seems to be the rule: most studied distribution properties are peculiar from the classical thermodynamics viewpoint. To give an example, the Black–Sholes model, describing pricing strategies for derivative financial transactions,[1] is mathematically a classical diffusion model, like the Fokker–Planck equation. Meanwhile, it turned out that more realistic models describing the price fluctuations do show a fat tail, namely a non-Gaussian distribution. Such tails, frequently occurring as power-law tails, can be described as a result of anomalous diffusion. The general theory dealing with such distributions, as classical thermodynamics does with the canonical exponential energy distribution, is in its making currently. One of her tentative names is *non-extensive thermodynamics*.

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[1] The Bank of Sweden Prize in Economic Sciences in Memory of Alfred Nobel was awarded to Robert C. Merton and Myron S. Sholes in 1997, who worked out this model in close collaboration with Fisher Black.

However, this book is not another introduction into non-extensive thermodynamics either. There are good books devoted to this task. The intention here is to present basic concepts at the very heart of statistical physics as they are challenged in high energy nuclear and particle physics by phenomena like energy distribution of particles irradiated from a fireball mimicking the Big Bang in little, like a quite formal use of absolute temperature as a parameter of higher than four-dimensional objects or like the particular behavior of colored noise in the dynamics of elementary fields. By doing so we particularly concentrate to the recurring question whether all the "anomalous" thermodynamics behavior is just a finite-size finite-time effect, or it survives the (in several cases only theoretical) limit of a large number of degree of freedom, commonly called the "thermodynamical limit." This question can presently be answered in the mathematical framework; the answers in physical experiments seem to be delegated to the future. Notably, also the question: Is there a temperature? in these exotic, highly energetic physical phenomena.

Budapest and Piliscsaba *Tamás Sándor Bíró*
August 2009–September 2010

Acknowledgments

There are due acknowledgments for a number of persons. The most important catalyzing event to start writing this book was a general question on the $\Sigma\Phi$ (Statistics in Physics) Conference, in Kolymbari, Crete, in 2008 from an Editor of Springer Verlag to the participants: whether anyone had an idea to write a good, interesting physics book. I attended that conference and subconsciously began thinking about how to confront some uncleared usage of statistical physics methods in the area of high-energy physics, more closely heavy-ion collisions, with challenging questions of contemporary statistical physics – which the conference was partially organized about. I responded to the inquiry that I possibly would have an idea.

One year later there came an e-mail from Jeanine Burke, of Springer Verlag, enquiring if I still had the idea to write a book about challenges at the merge of high-energy and statistical physics. In fact, I was already occupied with the writing of another book, about variational principles in the basic laws of physics, at that time. Nevertheless, I responded positively and sent an outline of the contents, a quickly written introduction, and filled out a detailed questionnaire to the Editors. They then selected this idea to be a project, we signed a contract, and so I began work on it. I have to thank the Springer Verlag for motivating me to really work on this project, and to Rebecca Nison for escorting my authorship.

From my colleagues in Physics I thank first of all Prof. Constantino Tsallis, who – besides being a well-known promoter of the new view on the possible extension of thermodynamics and statistical physics beyond the classical grounds – also personally supported my efforts to understand and generalize the classical concepts in my own way and to present part of the problems from my particular corner of view in several discussions. Dr. Giorgio Torrieri from the Frankfurt University helped me a lot on getting into contact with works on classical and string-theory induced higher-dimensional gravity and this way to put the perspective on really far-stretched theoretical challenges on the concepts of temperature and entropy. Furthermore, I thank Prof. Miklós Gyulassy from Columbia University for his patient conversations with me and for his critical remarks about this topic. I have learned a lot about which questions would be important to answer.

There are more colleagues with whom I had the privilege to co-author scientific publications, whose results are in one or the other way now involved in the material discussed in this book. I thank them for their inspiration and help. With Prof. Rogerio Rosenfeld I had my adventure on the field of financial models and learned the importance of coupled stochastic dynamics in challenging the classical models. Prof. Berndt Müller from the Duke University involved me in the research on the role of chaotic dynamics in non-Abelian field theory and – developing from this study – on possible spontaneous mechanisms for an emerging quantum theory from a higher-dimensional, two-time variable background. This settled the fundamentals of my interest in questioning beyond the "textbook wisdom". With Prof. Carsten Greiner (now at Frankfurt University, that time at Duke University and at Giessen University) I have started studies on stochastic dynamics in field theory in connection with the – there common – graph-language of Feynman and Keldysh. This paved my way to become interested in the role of noise on the most elementary level in physics.

Important parts of this book are rooted in common research with the following colleagues. The study with Dr. Jakovác on multiplicative noise and the production of power-law tailed energy distributions in stochastic field theory applied to elementary particle plasmas was induced by the challenge of non-extensive behavior in systems with long range micro-dynamical effects. In the thermodynamical interpretation and in selecting out far-reaching consequences of observations on power-law tailed particle spectra in heavy-ion collisions, Prof. Géza Györgyi from the Eötvös University in Budapest was an excellent discussion partner and a wealthy source of original ideas. The study and computer modeling of those spectra was (and to some extent is) carried out in collaboration with my younger colleagues Gábor Purcsel, Dr. Gergely Barnaföldi, and Károly Ürmössy at my own institute, the KFKI RMKI, Budapest. Last but not the least, Dr. Péter Ván himself having a long history of personal interest in fundamental questions of thermodynamics, worked with me on deepening and refining our understanding about relativistic thermodynamics, in particular on its possible connections to theoretical practices in contemporary applications of relativistic hydrodynamics to the description of high-energy particle systems.

Finally, I would like to thank especially my colleagues Dr. Antal Jakovác from the Budapest Technical University, Dr. István Rácz, Dr. Etele Molnár, and Dr. Péter Ván from KFKI RMKI research institute in Budapest for their countless discussions and active support during the preparation of this book – including manuscript reading.

Contents

Acronyms

BG	Boltzmann–Gibbs
BGS	Boltzmann–Gibbs–Shannon
BH	Black hole
CERN	European Organization for Nuclear Research (original French name: Centre Europeénne pour la Recherche Nucléaires)
FAIR	Facility for Antiproton and Ion Research
QCD	Quantum chromodynamics
EoS	Equation of state
HIC	Heavy ion collision
KMS	Kubo–Martin–Schwinger
LHC	Large Hadron Collider (at CERN)
MB	Maxwell–Boltzmann
PDF	Probability density function
RHIC	Relativistic Heavy Ion Collider (at Brookhaven, NY, US)
RN	Reissner–Nordstrøm
SPS	Superconducting Proton Synchrotron (at CERN)
SI	Système International d'Unités (International System for Measuring Units)

Chapter 1
Introduction

Energy, entropy and temperature are key concepts both in classical and modern physics. It is, however, challenging to understand their meaning in phenomena involving matter under extreme conditions, such as high velocity, acceleration or complexity. The historical path of the evolution of these concepts roots in the seventeenth century mechanics and nineteenth century thermodynamics. Quests for a mathematical and microscopical foundation for these key concepts brought life to studies of ergodicity, chaos, kinetic theory and physical chemistry in the turn of the nineteenth and twentieth centuries. In fact, emotionally loaded disputes between Poincaré's concept of recurrence in phase space and Boltzmann's model about the emergence of irreversibility by following reversible microrules made it difficult to generally accept either view. Physical measurement and interpretation, theoretical construction of the quantity called *absolute temperature* are the topics in Chaps. 2 and 3.

Modern microphysics, first of all quantum mechanics, has been triggered by this need for understanding the natural laws of motions on the level of atoms: a traditional field of chemistry became a central research topic in physics. The Boltzmannian (and Gibbsean) views of entropy and temperature, however, are not challenged by non-relativistic quantum mechanics, since it is founded on reversible equations. Nevertheless, due to the operator formalism, the use of which is forced upon us by the phenomenon of quantum uncertainty, the interpretation of temperature becomes more delicate than in the classical setting. Also, the mechanisms by which the microscopical motion is concluded in macroscopic trends, in particular the notion of *noise* and the mathematical tool of stochastic differential equations, are extending thermodynamics. One has to be, however, sober about distinguishing between finite size and finite time (transient) effects and variations of basic concepts due to violation of assumptions like short range interaction and statistical independence. Some effects due to a finite phase space are demonstrated in Chap. 4.

High complexity challenges the classical concepts of thermodynamics at its very roots. Starting with generalized formulas for the relation between entropy and the probability distribution of microstates, (i.e. generalizing Boltzmann's famous

T.S. Biró, *Is There a Temperature? Conceptual Challenges at High Energy, Acceleration and Complexity*, Fundamental Theories of Physics 171,
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logarithmic formula), through the interpretation of certain, energy-shell dependent, colored noise effects in terms of generalized canonical energy distributions (often with power-law tails), till the general features of infinite repetition of abstract composition rules (and its possible relevance to high energy physics phenomenology) there are contemporary challenges of a special nature, related to fundamental statistical physics concepts. Chapter 5 of this book deals with such questions.

Twentieth century and contemporary physics research challenges the classical concepts in several further ways. The theory of special relativity, dealing with high velocity motions, has changed basic features of our view about *motion* in general: on the one hand there is a maximal speed by which any material body may move, and on the other hand for a moving observer energy is inevitably mixed with momentum, so the description of thermodynamics as *energetics* relativistically becomes an entangled, complex problem. Furthermore, the demand of causality requires local description, and makes it a complicated task to synchronize the measurements of time in an extended space. Due to this, the classical concept of an extended *thermodynamical body* appears less useful. Although a homogenized, density based description emerges, the fingerprints of the concept of volume and mechanical work (also important to identify *internal* energy and heat relativistically) remain, e.g. in the occurrence of a local expansion rate, the Hubble constant. A discussion about the question, how should temperature transform by relativistic motion, has been started by Planck and Einstein. Their views has been challenged in the 1960s, and was confronted with the fact that boxes filled with radiation transform differently (i.e. showing a Doppler-effect) than ordinary, massive bodies, in the 1990s. Actual measurements on particle energy spectra with masses are obtained in high energy accelerator experiments from the late 1980s. Experiences with these spectra challenge Einstein's formula and a more complex formula should be used today. Also the number of degrees of freedom involved in forming such energy spectra are much less than for ordinary bodies, just a few thousand instead of Avogadro's number (6×10^{23}). This causes observable mesoscopic features, deviations from the so called *canonical* distribution. These challenges to the classical concept of temperature are discussed in Chap. 6.

Modern developments in the theory of gravity, initiated by Einstein in 1916, have the *equivalence principle* at their heart: acceleration and gravitational fields are physically equivalent. This theory of general relativity allows for surprising mathematical solutions in certain cosmological or high-gravity setups: the physically extremely exciting but experimentally only indirectly observable *black holes* are wrapped into a *horizon*, the limit of no return, from where even light is to heavy to take off. Hawking and Bekenstein observed in 1975 that the merge of two black holes follow rules similar to those by the entropy in thermodynamics: there is an asymmetry between fusion and fission of horizons. They suggested, at the beginning absolutely just as a mathematical analogy, to associate a temperature to this kind of entropy for counting for the total – by construction internal – energy change of black holes. This quantity, the gravitational acceleration on the horizon surface, corrected by the red-shift factor, behaves like the absolute temperature.

On the other hand, due to the equivalence principle, strong acceleration, as it occurs by stopping accelerated particles, and strong gravitational fields, as it occurs near a black hole, are physically equivalent. This gave rise to the idea to interpret the emergence of thermally looking particle spectra in accelerator experiments as an effect mimicking strong gravitational fields. In theory, the vacuum itself occurs as a thermal ensemble for an accelerated observer and therefore the temperature fitted to the energy slope of observed particle spectra may be related to a – constant – deceleration factor (this is called the Unruh effect).

Moreover, contemporary theoretical models, partially motivated by string theory, describe the thermodynamics of strongly interacting elementary matter, briefly called *quark matter*, in an imagined ten dimensional spacetime as being on the four-dimensional horizon of a five-dimensional black hole. Here again, the surface gravity serves as a temperature, and this concept works astonishingly well when comparing with results of involved numerical calculations (lattice QCD) done in models in ordinary four-dimensional spacetime. It is still not completely understood why and in what depth consorts this temperature with the original thermodynamical concept. These challenges are presented in Chap. 7.

Field theory, the basic theoretical tool in elementary particle physics, discovers again a mathematical analogy between canonical partition sums and quantum path integrals. This analogy supported the idea of a quantization method based on thermal noise in a second time dimension, the idea of *stochastic quantization* (Parisi). Speculations about a quantum theory emerging from a sub-quantum physics motivated the notion *chaotic quantization*, where the "normal" quantum behavior in four-dimensional spacetime would emerge as a "holographic shadow" of a higher-dimensional ergodic motion on a lattice. However, even disregarding these speculations, there are enough challenges for formulating and understanding *thermal field theory* from the scratch: the quantity temperature should not be used as a parameter, but rather has to be described by the solution of microscopic field dynamics. This leads us to the problem of describing noisy dynamics and to understand leading order quantum effects on it in the framework of quantum field theory. The most widely known of them being the interpretation of the inverse absolute temperature as a periodicity in imaginary time. This challenge is outlined in Chap. 8.

This book is devoted to the concept of temperature, its evolution from the classical beginnings to a modern everyday tool in research. Its primary purpose is to raise and partially discuss questions which are challenging the classical knowledge laid down in textbooks. Many (but of course not all) of these challenges can be understood already by simple means, without following involved mathematical derivations in professional depth. The author hopes therefore that this book will be useful for physics students at the major and doctorate level as well as for active researchers, and for everyone who is interested to take an intellectual challenge by following the use and misuse, the acceptance and debate, the evolution and revolution of core concepts in contemporary physics.

Chapter 2
How to Measure the Temperature

The three main methods for measuring the temperature: by direct contact with a thermometer, by analyzing radiation spectra stemming from a thermal source, and by conjecturing from the observed chemical composition.

2.1 Thermoscopes and Thermometers

In order to develop or understand relevant mathematical models used to describe the laws of nature in theoretical physics it is of help to enlist first what the intuition says about the issue. Several of our concepts in science, in particular the basic thermodynamical quantities, like heat, energy, temperature, are also rooted in our perception – as a first, naturally given device to form our feelings and thoughts through our senses. Based on this, and following the push towards objectivity, man-constructed devices enlarge our sensory field and make different personal experiences more comparable at the same time. Finally, quantification and introduction of a standardized scale leads to the mature state of being a scientific (and technical) concept. Such concepts can be parts and actors of a scientific theory then, aiming at a logical system of explanations for phenomena which is free from the smallest contradiction.

This process takes its time. Historically, physics developed through several centuries to the science it is today. This is, in particular, true for the concepts related to thermal phenomena. In this section we deal with devices constructed and used for measurements of heat. Thermoscopes just react to the presence or transfer of heat, thermometers translate this process into a temperature scale. The very question of the arbitrariness of such scales has been answered in classical thermodynamics by pointing out the physical sense behind a universal, so called absolute temperature scale. This existence and constructibility statement is part of the problematics connected to the zeroth theorem, alias the zeroth law of thermodynamics.

T.S. Biró, *Is There a Temperature? Conceptual Challenges at High Energy, Acceleration and Complexity*, Fundamental Theories of Physics 171,
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2.1.1 Heat Perception

Human beings (and many others) do show sensitivity to heat, to this special form of energy change. Mostly – and most safely – radiated heat can be sensed; the best by hands or by the face. Since this happens without mechanical contact seen by our eyes or felt by our pressure sensitive cells – heat is considered to be something more mystical than the mechanical concepts, like force or energy. In fact, the interpretation of heat as a substance, the "caloricum," was the predecessor theory to the "kinetic" one, interpreting heat as internal motion. Joseph Black worked out several important concepts of thermionic physics based on this – in retrospective abandoned – view. Among others he introduced quantities like specific heat, latent heat, melting and evaporation heat, and heat capacity [1].

Experiments have been designed to demonstrate and measure the heat substance. Benjamin Thompson (Lord Rumford) concluded from his experiments at the end of eighteenth century that the weight of heat, the change in weight by 1° temperature rise, has to be less than one to a million (10^{-6}). The final victory for the kinetic over the substantial interpretation of heat was brought by the formulation of the principle of equipartition, explaining not only the nature of heat, but interpreting both the principle of energy conservation and the irreversibility trend by dissipative phenomena in a unified framework. It is a remarkable irony of history that today we consider a mass equivalent to all type of energy, including the kinetic energy of microscopic (atomic) motion. This effect is, however, very small in the everyday life of SI units, $k_{\mathrm{B}}T/mc^2$ being in the order of magnitude of 10^{-40} for 1° temperature difference in a body with a mass of one kilogram (about 2 pounds). The situation is quite different in particle physics, where this ratio approaches one in some situations.[1] For the latter it is unavoidable to work out a relativistic theory of heat and thermal phenomena.

Radiated heat is frequently accompanied by visible light; and from the modern physics we know that both light and heat radiation are in fact mediated by photons – just a little different in energy. This issue touches the question about the very nature of light: is it an electromagnetic wave or a corpuscle called photon? In fact both views led to predictions of radiation spectra of so called absolute black bodies – bodies that emit the same spectra of radiation they absorb. Max Planck has established his formula for the black body radiation spectrum by interpolating the entropy-energy relation, $S(E)$, between these complementary views [2,3].

Also by touching we can sense whether a body is warm or cold; whether it is warmer or colder than oneself. Being in water cold and hot streams can be sensed quite sharply. In this case we meet with the flow nature of heat: it circumvents our sensory device (the skin), it flows from warmer to colder places. This flow is sometimes steady, sometimes turbulent. Already in the Middle Ages became clear that

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[1] For example, pions have $mc^2 = 140$ MeV and experience in heavy ion collisions carried out in modern accelerators a temperature around $k_{\mathrm{B}}T = 120 - 160$ MeV.

heat-related, or shortly thermal phenomena are associated to two main properties: one is more like an intensity (modern physics names the temperature as an intensive variable), the other is more like a quantity, increasing with the extension of the hot body (so called extensive quantity). The favorite example is flame: its thermal intensity is greater than that of a piece of hot iron, while the latter carries more substance of heat (and causes more damage to us than a flame at the same temperature).

And finally heat conduction, the third form of heat transfer, can be detected by our senses: the far better conductivity of metals is responsible for the fact that by touching them they appear appreciably colder than an insulator, like wool or wood or human skin, at the same temperature. This process leads much faster to thermal equilibrium than the previous ones, especially by radiative contact we never expect to be equilibrated to the temperature of the source (e.g. the Sun) in our lifetime.[2] And still, thermodynamics states that the thermal equilibrium is universal in the sense, that this state is independent of the way, of the material consistence and of the speed of changes by which we arrive at it. Furthermore, once equilibrium is achieved, it will also be maintained – at least in lack of serious disturbances.

Such a behavior really can only be understood on the basis of coupling our macroscopic, from the world of senses and human made human size devices stemming information to assumptions and models about the microscopical behavior of matter: the kinetic theory of heat and the concept of entropy as information about microscopical order and disorder are rooted very much in the above universality and maintenance properties of a thermal equilibrium state.

2.1.2 The First Thermometers

The first devices were just sensitive to the change of heat without actually measuring it, the so called thermoscopes. Thermometers connect this sensitivity to a scale; to a quantitative measurement between two fixed physical points [4].

Most devices make use of a physical sensitivity to heat, such as dilation (the common thermometers using mercury or alcohol), or change in the electric properties (digital thermometers). Phenomena related to dilation of air and vapor reacting to heat were already known in ancient civilizations. There are notes about Héron of Alexandria, who experimented with devices making use of the force of heat. Huge and heavy temple gates were secretly opened by the use of the work exerted by heat.

The use of dilation for the measurement of heat intensity – the temperature – had a long technical evolution. Reproducibility requires that such devices become robust, but still delicate enough to react fast to changes and delicate enough not to influence the measured object unduly. Instead of air water, later alcohol became the favorite signal material, just to give room at the end to mercury. First, thermoscopes

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[2] Actually, one leaves the sunny spot before his/her own temperature becomes uncomfortable.

constructed in the renaissance Italy were open systems reacting to air pressure as well as to temperature. Such *baro-thermoscopes* were also constructed by Galilei and Toricelli, later by the Bernoullis – just to mention a few famous names.

The device known nowadays as “Galilei thermometer” was invented by Ferdinand II, Grand Duke of Tuscany. In a closed glass tube, filled with a mixture of water and alcohol, small, colored vesicles of different density swim. Depending on the temperature more of them float at the top and some of them sink to the bottom. The temperature is calibrated to the middle one. This device is already a thermometer, since numbers, measures of temperature, are associated to each floating sphericle. This device usually measures temperatures with a resolution of 2°C (cf. Fig. 2.1).

Fig. 2.1 So called Galilei Thermometer – actually invented by Ferdinand II Grand Duke of Tuscany

It is not clear who was the first constructor of a thermometer. Tradition names Galilei as well as Santorio, Avicenna, Cornelius Drebbel or Robert Fludd. Fludd's thermometer, introduced in 1638, uses a vertical tube with a bulb at the top, the other end immersed into water. The basic design with a bulb and a tube remained til the modern times; it separates the "reaction zone" in the bulb from the "read-out zone" in the tube. The first who put a scale besides the tube could have been Francesco Sagredo or Santorio.

The standardization of the temperature scale also has a long history. Christian Huygens suggested to use the melting and boiling of water as two characteristic points to fix the scale in 1665. In 1701, Isaac Newton proposed to use 12° between the melting of ice and the body temperature. The sexagesimal and the decimal system fought long. In the continent the decimal metric system has been established after the French revolution, while in England the dozen- and sixty-based counting remained more common. Regarding the temperature scales this evolution peaked in the Celsius (also called centigrade) and the Fahrenheit scales.

2.1.3 Réaumur, Fahrenheit and Celsius

Thermometers using the physical phenomenon dilation (of alcohol or mercury) attach a scale to the tube. The points on this scale has to be fixed. Assuming linearity – what is behind almost all scales in use – actually two points would suffice. Two dramatic and easily reproducible physical events can serve well to fix a temperature scale. More points may serve to control the linearity of the dilation subsequently. The number of subdivisions are absolutely arbitrary, different suggestions were made, thought to be "natural" for the contemporaries.

René Antoine Ferchault de Réaumur (1683–1757) suggested in 1731 a temperature scale using an octogesimal division between the freezing point of water (zero point, 0^oR) and its boiling at normal atmospheric pressure (80^oR). The grads were designed to belong to one thousandth change of the volume contained in the bulb and in the tube up to the zero mark. The choice of 80 was quite natural for the French, especially before the Revolution, when they introduced the decimal metric system. Eighty has several divisors among whole numbers: $80 = 2\times 40$, 4×20, 5×16 and 8×10. This helps for fast calculations and rapid perception.

Daniel Gabriel Fahrenheit proposed in 1724 his 96-based system. By using mercury filling, a finer grading was demanded. He fixed the scale to the melting point of salty ice at -18°C centigrades and to the human body temperature at $+36$°C centigrades. These are the zero point, 0°F and the upper end, 96°F. Again these numbers are easily divided by a number of divisors: $96 = 2\times 48$, 3×32, 4×24, 6×16 and 8×12.

The scale suggested by Anders Celsius in 1742 takes one hundred subdivisions between the freezing and boiling point of water at normal atmospheric pressure. This became part of the metric system during the French revolution in 1790, and is in use all over the world today. Owing to the different fixing points and numbers of subdivisions, there are linear formulas for transforming temperatures between these scales. Obtaining Fahrenheit temperature from the Celsius one, the linear equation

$$F = aC + b \tag{2.1}$$

has to be fixed at two points. Zero Fahrenheit belongs to -18 centigrades, while 96°F to 36 centigrades:

$$\begin{aligned} 0 &= -18a + b \\ 96 &= 36a + b. \end{aligned} \tag{2.2}$$

Subtracting from the second line the first one we get $96 = 54a$, so the proportionality coefficient becomes $a = 96/54 = 16/9$. This value is often approximated by $a \approx 9/5$ intending to facilitate fast computation by heart ($16 \times 5 = 80$ while $9 \times 9 = 81$, it makes an error faintly larger than 1%). Substituting the result for a into the first line, the parameter b can be obtained as being $b = 18 \times 16/9 = 2 \times 16 = 32$. Finally the transformation formula is given by

$$F = \frac{16}{9}C + 32 \approx \frac{9}{5}C + 32. \tag{2.3}$$

Perhaps it is easier to remember a few special values at centigrades divisible by nine. They are collected in the following table (Table 2.1).

F	0	16	32	48	64	80	96
C	−18	−9	0	9	18	27	36

Table 2.1 Easy to remember values in the Fahrenheit and Celsius temperature scales

This table is very simple if the Fahrenheit values are written in hexadecimal (16-based) number system and the Celsius values in a nonal (9-based) system (cf. Table 2.2). The fast computation can be based on a special form (2.3) emphasizing that Fahrenheit degrees are at best grouped into sixteens while Celsius degrees into groups of nines:

$$\frac{F}{16} = \frac{C}{9} + 2 \tag{2.4}$$

As a consequence in both the nonal and the hexadecimal system the shift is two times the base, “20” (meaning $2 \times 16 = 32$ or $2 \times 9 = 18$ respectively).

$_{16}$F	0	10	20	30	40	50	60
$_{9}$C	−20	−10	0	10	20	30	40

Table 2.2 Hexadecimal and nonal number system values in the Fahrenheit and Celsius temperature scales

Since then the technology of thermometers undergone a process of refinement and diversion. The handy size clinical thermometer we know today was introduced in 1866. It delivers a result in five minutes with a precision of 0.1°C. There can be several sources for a thermometer being imprecise. The calibration has to be done with great care, since pressure influences the value of temperature. Distilled water at ice melting and boiling is regarded at standard atmospheric pressure according to the actually valid international standard. The linear interpolation between the calibrated points also may depend on the material used for dilation. The mercury in a glass tube may show the maximal deviance from the value measured by the electric resistance of platinum in the middle of the scale, at 50°C. Due to glass-technology a variation in the diameter of capillaries also cannot be excluded.

Modern electric thermometers, like the platinum resistance thermometer, has a resolution of $\Delta T = 0.1°\mathrm{C}$ and is calibrated at five points at $-18, 0, 40, 70$ and 100 centigrades. At the interpolation points it reaches an accuracy of ±0.2°C. For scientific purposes and in the industry several other thermometers are in use. Infrared thermometers are very good at telemetry: they measure spot temperatures at a distance. They are particularly useful for measuring high temperatures (like in metal industry) or temperatures of moving objects. Their scale is based on the black body radiation formula; for shiny or gray surfaces corrections have to be made (usually included in the software). It is also of theoretical interest, the temperature of moving bodies is related to the relativity principle and will be discussed in some detail in Chap. 6.

Bi-metallic stemmed thermometers (so called thermocouples) are used in food-industry, thermistors (electronic devices with temperature sensitive resistance) by cooking and baking. Modern electronics and solid state physics also have developed a number of smart thermometers. Liquid crystal thermometers are in clinical and household use. Temperature measurement based on radiance is the principle behind phosphor thermometry. This plethora of methods and technologies is rather overwhelming than reassuring. Which is the correct temperature? Must physics depend on so many circumstances? Melting and boiling of one, dilation or electric conductivity of another material? One would very much welcome a universal temperature.

2.1.4 The Absolute Temperature

The above wish did not remain without fulfillment. Although the temperature scale is still arbitrary, there is an exclusive zero point on physical grounds. In order to explain this fact a correspondence between the energy, as contained in internal microscopic motion, and the temperature, as an intensity property of this motion, had to be established. Furthermore also the heat, describing the substantial component in thermal phenomena had to be understood.

Studies about the nature of heat led to the formulation of energy conservation. The absolute temperature scale is zero when the internal motion is at its minimum: in the classical physics this energy is zero, in the quantum mechanics (established later than the introduction of the absolute temperature scale) a small zero point motion is present. In this stage the order is maximal, the number of ways of realizing this macrostate are minimal. The absolute zero point turned out to be at about $-273°$C. The absolute scale is in centigrades, just the starting point, the "absolute zero" differs from the Celsius scale. This temperature is named after Lord Kelvin (Thomson) and is denoted by "K". Since the state of thermal equilibrium is universal, the "absolute" temperature is also universal in the sense of being independent of the material consistence [5].

According to present international agreement the Kelvin scale is fixed to two points: the absolute zero 0K is at $-273.15°$C and the value 273.16K at the triple point of standard water with a specific mixture of hydrogen and oxygen isotopes. This triple point, where ice is melting, is at 0.01°C. Practically this definition fixes the absolute temperature to be measured by the same scale as the Celsius one, just shifted by a constant amount of 273.15.

In physics, the absolute Kelvin-temperature is the only sensible temperature to talk about. It is often cited in the equivalent energy units using the Boltzmann constant:[3] $k_{\mathrm{B}} \approx 1.38 \times 10^{-23} \mathrm{m}^2\ \mathrm{kg}\ \mathrm{s}^{-2}\ \mathrm{K}^{-1}$. In particle physics, often "temperature" is written but the energy $k_{\mathrm{B}}T$ is meant.

2.2 Spectral Temperature

The classical concept of temperature rests on the concept of thermal equilibrium. The first thermometers and the first problems discussed in thermodynamics – stemming from demands to solve problems in everyday life and industry – were based on direct contact between large bodies; under such circumstances thermal equilibration happens fast. While a perfect reservoir has an infinite ability to give or absorb energy and heat (it has an infinite heat capacity) and therefore it keeps its own temperature during a thermal contact with other objects, a perfect thermometer on the other hand reacts immediately to changes in temperature and its own temperature equals to the temperature of the attached body (it has zero heat capacity). Building on these ideal properties, thermodynamical theories assume large objects to be investigated. So large that they themselves can serve as a perfect reservoir for their smaller parts. Whenever this approximation becomes physically meaningful, we consider the so called *thermodynamical limit*. Please note, that this definition of

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[3] This name was actually given by Max Planck.

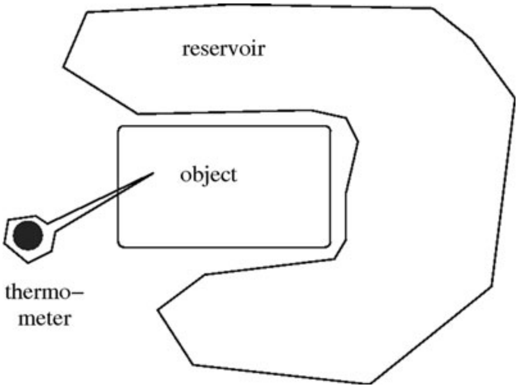

Fig. 2.2 Size relations between thermometer, object and heat reservoir. In the thermodynamical limit, all are realized in the same system

the thermodynamical limit is not restricted to large volume or large particle number only; if the behavior as its own heat reservoir is established by any means, this limit is considerable. As the revers of this coin, a small part of a large enough object may serve as a thermometer. In ideal thermal equilibrium, it must have the same temperature as the rest of extended body, signals received from such a local spot in principle reflect information about the whole equilibrated object (cf. Fig. 2.2).

The direct and stationary contact between object and thermometer is a sufficient but not a necessary condition for a temperature measurement. Measuring the temperature from a distance is based on radiation. In this case, one assumes that the spectrum (energy distribution) of the radiation is characteristic to the emitting source and essentially was not distorted in its way to the detecting device. In the most common cases of astronomical spectroscopy this assumption is quite natural, since the outer space is very rarely polluted by objects. Yet, sometimes, it happens that some cloud, plasma or strong magnetic field shields the observed object from us and then the radiation can become distorted from its original shape. Fortunately, detecting and measuring a large enough part of the energy distribution in a radiation itself reveals whether it stems from an ideal object, called black body, at one fixed temperature, or not.

In order to rely on temperature measurements by spectral analysis, one utilizes a background knowledge established during the past two centuries. It includes a number of “laws” associated to different facets of thermal electromagnetic radiation, converging to the (quantum-)statistical theory of photons. In the next subsection, we follow this path and gradually introduce the most important concepts underlying the black body radiation. Then, analog to the statistical model of photons, we consider other particles. The main question to be discussed is how their spectral distribution reflects the temperature of the emitting source (provided no disturbance between emission and detection).

2.2.1 Black Body Radiation

Measuring temperature by radiation has the enormous advantage that it can be done from a distance. The theory behind radiation, however, also had to be developed first. An object, emitting radiation, first of all has to be in thermal equilibrium for the applicability of thermodynamics, otherwise we would already fail at the level of the zeroth law. The thermal equilibrium state of a radiating object is defined by Kirchhoff's law, formulated by Gustav Kirchhoff in 1859: the emitted and absorbed energy by the radiation must be equal. And not only as a total amount, but in detail: at each energy of the photons. Since the concept of photons was not yet established that time; the experience of equality was formulated in terms of wavelength. In each small interval around a selected wavelength, emission and absorption are equally efficient by a body in thermal equilibrium. The wavelength, λ and the (circular) frequency, ω are related by $\omega = 2\pi c/\lambda$ and $d\omega = -2\pi c d\lambda/\lambda^2$. A brief formulation of Kirchhoff's law is given as

$$\text{emissivity}(\omega) = \text{constant} \times \text{absorptivity}(\omega)$$

This is the *detailed balance* principle applied to radiation. The fraction of incident power (energy rate in time) may also depend on the angle; for the sake of simplicity it is often left out from the physical discussion. The laws of thermodynamics must be valid in general, therefore it is frequently enough to consider only the isotropic case.

An object fulfilling Kirchhoff's law is an absolute *black body*, it is an ideal, theoretical object. But reality is surprisingly close to this ideal. As a corollary to Kirchhoff's law, the emissivity of a real body cannot be higher than that of a black body: in thermal equilibrium the entropy is maximal. Kirchoff's law can be interpreted as a detailed balance between a box with an emitting and absorbing wall filled with electromagnetic radiation. Denoting the frequency distribution of the black body radiation inside the box at (absolute) temperature, T, by $B(\omega,T)$, the energy incident to the wall defines the absorptivity coefficient, $A(\omega)$:

$$E_{\text{in}} = A(\omega)B(\omega,T). \tag{2.5}$$

Similarly, the emitted energy defines the emissivity coefficient, $\varepsilon(\omega)$:

$$E_{\text{out}} = \varepsilon(\omega)B(\omega,T). \tag{2.6}$$

The not absorbed power (energy per unit time) is called reflectivity, $R(\omega) = 1 - A(\omega)$. How big these frequency-dependent coefficients are, depends on the material quality of the wall; the ratio between emissivity and absorptivity is, however, a general statement about the thermal equilibrium of radiation. So is the *spectral distribution* of energy in the radiation, $B(\omega,T)$: It is determined by the temperature and the detailed balance principle only. As we shall see later, it contains two constants of nature: Boltzmann's constant relating the absolute temperature to energy units and Planck's constant describing the relation between frequency and energy units.

Now we turn to the determination of the black body radiation spectrum, $B(\omega,T)$. At first global characteristica of the radiation power became known. The current density of emitted energy in thermal black body radiation of temperature T was discovered to be proportional to the fourth power, $J_e = \sigma T^4$, around the mid of nineteenth century. Based on experiments John Tyndall had found out that a body radiates at $1{,}473\,\mathrm{K}$ about 11.7 times more energy than at $798\,\mathrm{K}$.[4] Jozef Stefan realized in 1879 that $11.7 \approx (1{,}473/798)^4$. Stefan also determined the coefficient to be $\sigma = 5.67\times 10^{-8}\,\mathrm{J\,sm^{-2}K^{4}}$. Finally, Ludwig Boltzmann gave a thermodynamical explanation assuming ideal heat equipartition between matter and light in 1884. The coefficient σ is called "Stefan–Boltzmann constant." Another global description of the black body radiation is given by Wien's law, presented in 1893. It establishes a scaling relation between the frequency (wavelength) and temperature dependence and hence makes a prediction about the frequency of maximal intensity at a given temperature. According to Wien's law $\lambda_{\max}T$ is constant. Equivalently, $\omega_{\max}/T$ is also constant.

Approximate descriptions of the spectrum $B(\omega,T)$ of black body radiation were given by Wien, Raleigh, and Jeans. A radiation spectrum fulfilling Wien's law is emerging if the dependence is given as

$$B(\omega,T) = \omega^3 f(\omega/T), \tag{2.7}$$

i.e. the temperature dependence occurs only via the ratio ω/T. The prefactor ω^3 is set by the requirement that total (frequency integrated) energy current density (which is simply related to the total energy density by the velocity of light) stays in accordance with the Stefan–Boltzmann law:

$$\int \omega^3 f(\omega/T)\,\mathrm{d}\omega \;=\; \sigma T^4, \tag{2.8}$$

which is easy to prove by using $x = \omega/T$ as the integration variable. The position of maximum is determined by setting the derivative $\frac{\partial B}{\partial \omega}$ to zero:

$$\frac{\partial}{\partial \omega} B(\omega,T) = 3\omega^2 f(\omega/T) + \frac{1}{T}\,\omega^3 f'(\omega/T) = 0. \tag{2.9}$$

Dividing this equation by T^2 we gain a condition purely in terms of ω/T:

$$3\frac{\omega^2}{T^2} f\left(\frac{\omega}{T}\right) + \frac{\omega^3}{T^3} f'\left(\frac{\omega}{T}\right) = 0. \tag{2.10}$$

Its solution reveals the frequency of maximal intensity at a given temperature and reproduces Wien's law: $\omega_{\max}/T$ is constant.

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[4] Allegedly, Tyndall had not measured really a black body and the precise value should have been a factor of 18.6. But the $\sim T^4$ law was already established by the time of more precise measurements.

Based on this expectation Wien undertook a determination of the function $f(\omega/T)$ in 1896. He assumed that (1) the radiation law $B(\omega,T)$ can be connected to the Maxwell–Boltzmann distribution of the kinetic energy of particles in an ideal gas, and (2) this energy has to be replaced by an expression depending solely on the frequency of radiation. Choosing the simplest, i.e. a linear correspondence, he had guessed the following spectral law

$$B(\omega,T) = b\omega^3 \mathrm{e}^{-a\omega/T}. \tag{2.11}$$

Max Planck had tried to establish this formula. He knew that the black body radiation is independent of material quality of the wall enclosing the radiation, it has to be determined by general principles valid in thermal equilibrium. Therefore he choose a simple model for the matter part: harmonic oscillators. These oscillators have eigenfrequency ω and the negative and positive charges, bound by these oscillators, are the source for the electromagnetic radiation in the box. The energy density of the radiation in the box and the average energy of oscillators become then in equilibrium:

$$B(\omega,T) = \frac{2\omega^2}{\pi c^3} E(\omega,T). \tag{2.12}$$

According to the classical equipartition theorem the average energy per degree of freedom is $k_{\mathrm{B}}T/2$. Counting two independent polarization states of electromagnetic waves one considers $E(\omega,T) = k_{\mathrm{B}}T$. This way

$$B(\omega,T) = \frac{2\omega^2}{\pi c^3} k_{\mathrm{B}}T, \tag{2.13}$$

not having a maximum. This result is the Raleigh–Jeans radiation law, established in 1900. Raleigh obtained this result by counting standing waves around the frequency ω in a cavity.

Planck [2, 3] had found a way from the relation (2.12) to the Wien spectrum (2.11) from the following assumption about the entropy carried by the oscillators:

$$S(E) = \frac{E}{a\omega} \ln \frac{E}{be\omega}, \tag{2.14}$$

with e being Euler's number. Applying now the definition $1/T = \partial S/\partial E$ one obtains Wien's spectral law. Naturally, Planck had chosen the entropy formula for the oscillators just to arrive at the given spectral law. He was not satisfied with this result. Later, in 1900, he obtained his famous interpolating formula between the Raleigh–Jeans and the Wien spectra. Seeking for an entropy maximum, he inspected the second derivatives:

$$\begin{aligned} \frac{\partial^2 S}{\partial E^2} &= \frac{\text{const}}{E}, \\ \frac{\partial^2 S}{\partial E^2} &= \frac{\text{const}}{E^2}, \end{aligned} \tag{2.15}$$

for the Wien–Planck and Raleigh–Jeans distributions, respectively. Planck took the interpolating formula

$$\frac{\partial^2 S}{\partial E^2} = -\frac{a}{E(E+b)}. \tag{2.16}$$

This formula reconstructs Wien's result for low average oscillator energy, $E \ll b$, at a fixed frequency. Likewise for high energy the Raleigh–Jeans result is obtained. For the general case Planck's interpolating formula leads to

$$\frac{1}{T} = \frac{\partial S}{\partial E} = -\int \frac{a}{E(E+b)}\,\mathrm{d}E \;=\; -\frac{a}{b}\ln\frac{E}{E+b}. \tag{2.17}$$

Inverting this result we obtain the average oscillator energy as a function of temperature

$$E = \frac{b}{\mathrm{e}^{b/aT} - 1}. \tag{2.18}$$

Using Wien's scaling form one obtains $E = \omega f(\omega/T)$, and due to this $b \propto \omega$ and $b/a \propto \omega$. Finally, relying on the equipartition formula, (and counting for the $\mathrm{d}^3k \sim \omega^2 \mathrm{d}\omega$ elementary phase space cells) Planck's law for radiative energy density distribution is given as

$$B(\omega,T) = b' \frac{\omega^3}{\mathrm{e}^{a'\omega/T} - 1}. \tag{2.19}$$

Here, a' and b' are frequency independent constants. Comparing the Planck law with the Stefan–Boltzmann law and Wien's "maximum shift" formula a new constant of nature can be derived, today called Planck's constant: $h = 6.55 \times 10^{-27}$ erg sec. Denoting by $\hbar = h/2\pi$, the constant a' is identified as being $a' = \hbar/k_{\mathrm{B}}$. The scaling variable in electromagnetic radiation spectra is given by $x = \hbar\omega/k_{\mathrm{B}}T$. Finally, Planck re-derived his formula based on permuting partitions of energy quanta of $E = \hbar\omega$ among oscillators. We introduce a similar derivation in the next chapter discussing the statistical foundations of thermodynamics.

Below we give a short summary of formulas related to these classical thermodynamical theories of black body radiation:

Stefan – Boltzmann	$cE/V = \sigma T^4$	global property	
Raleigh – Jeans	$\frac{\partial^2 S}{\partial E^2} = -\frac{1}{E^2},$	$\frac{1}{T} = \frac{\partial S}{\partial E} = \frac{1}{E},$	$E = k_{\mathrm{B}}T$
Wien	$\frac{\partial^2 S}{\partial E^2} = \frac{a}{E},$	$\frac{1}{T} = \frac{\partial S}{\partial E} = a\ln E,$	$E = b\omega \mathrm{e}^{-\omega/aT}$
Planck	$\frac{\partial^2 S}{\partial E^2} = \frac{a}{E} - \frac{a}{E+b},$	$\frac{1}{T} = \frac{\partial S}{\partial E} = a\ln\frac{E}{E+b},$	$E = \frac{\hbar\omega}{\mathrm{e}^{\hbar\omega/k_{\mathrm{B}}T} - 1}$

2.2.2 Particle Spectra

Following the advent of quantum theory by Planck's formula in 1900, it soon became interpreted as an ideal gas of photons by Einstein and Bose. The Planck constant, $\hbar$ is the proportionality constant between the energy of a quantum, thought to be a particle, and the frequency of the radiation wave: $E = \hbar\omega$. Soon the wave – particle duality was extended to known elementary particles, first to the electron by de Broglie. Niels Bohr, in order to explain the stability of atoms inspite the fact that elementary charges, the electrons, seemed to move on curved (circular) trajectories around the nucleus and therefore should have lost their energy by electromagnetic radiation, as "normal" accelerating charges do, invented the quantization principle: the electrons may change their energy only by packets representing a finite value, which is related to the frequency of emitted or absorbed photon by the Planckian conjecture, $E = \hbar\omega$. De Broglie discovered that interpreting the electrons bound in atoms as standing particle waves with wave number, k (and a wavelength, $\lambda = 2\pi/k$), corresponding to their momenta as $p = \hbar k$, Bohr's quantization principle follows. This way there can be a general correspondence between particles and waves, relating energy and momenta to frequency and wave number. In particular a statistical counting of states of particles freely moving in a large volume, V, is equivalent to a counting of possible standing waves in a large cavity. This is the origin of the habit, that by analyzing modern accelerator experiments [6], the energy distributions of detected particles is called *particle spectra*.

Free particles in a large box constitute an ideal gas. The possible states are characterized by possible values of momenta, in a finite box it is a discrete spectrum related to standing sine waves. In the large volume limit, however, the sum over discrete momentum states is well approximated by integrals over continuous (often quoted as "classical") momenta. As a reminiscent to the quantum theory the integral measure, the elementary cell in phase space, is normalized by the original Planck constant, $h = 2\pi\hbar$. This way particles freely moving in an "infinite" volume in all three spatial directions represent continuously distributed states with the following elementary measure (cell) in phase space:

$$d\Gamma = \frac{d^3p \, d^3x}{(2\pi\hbar)^3}. \tag{2.20}$$

Ignoring the Planck constant, this coincides with the classical phase space for the mechanical motion of mass points. In fact, particles in an ideal gas are treated as non-interacting ones; and they do so – most of the time. This peaceful existence is, however, interrupted by very short dramatic events, the collisions. Collisions play one important role: they ensure equipartition by exchanging individual particle momenta. For the macroscopic view this occurs as randomizing the momenta. This way they come close to the Gibbsean ideal: long term repeated observations of a macroscopic system pick up images of a randomized statistical ensemble.

The simplest, so called *thermal models* of particle spectra stemming from energetic collisions, consider an ideal gas of particles or particle mixtures at a given temperature [6–11]. This simple idea leads to predictions for the energy and momentum distributions of detected and identified particles in modern accelerator experiments. Slow particles, moving with velocities of negligible magnitude compared to the speed of light, can be considered as non-relativistic; their kinetic energy practically satisfies the $E=\mathbf{p}^2/2m$ relation. The distribution of energies, momenta and velocities resemble that of ordinary atomic gases at room temperature. Regarding the velocity distribution it is called Maxwell-distribution; as a distribution of energy the Gibbs distribution. Obtaining them from equal probabilities for phase space cells is due to Boltzmann; therefore, it is also called Maxwell–Boltzmann and Boltzmann–Gibbs distribution. In particle physics it is shortly called Boltzmann-distribution.

A particle with mass m, three-momentum $\mathbf{p}$ and kinetic energy $E=\mathbf{p}^2/2m$ is distributed according to the Gibbs factor $\mathrm{e}^{-E/k_{\mathrm{B}}T}$ in a large volume at absolute temperature T. Using $k_{\mathrm{B}}=1$ units the differential probability to find a particle around the momentum $\mathbf{p}$ (and anywhere in the coordinate space) is given by a Gaussian formula

$$f(\mathbf{p},\mathbf{x})=C\mathrm{e}^{-\mathbf{p}^2/2mT}\,\mathrm{d}\Gamma. \tag{2.21}$$

Here, C is a normalization constant related to the total particle number, $N=\int f\mathrm{d}\Gamma$ in the large volume $V=\int 1\,\mathrm{d}^3x$. The above distribution, f, is the one-particle distribution giving the differential probability to find a representative particle near to a point in the phase space. This probability is solely a function of the energy of particle – such systems have a chance to be thermodynamic systems.

This distribution leads to a temperature dependent average particle density

$$n=\frac{N}{V}=C\mathrm{d}^3p\,\mathrm{e}^{-\mathbf{p}^2/2mT}. \tag{2.22}$$

From here on we use the $\hbar=1$ convention, counting frequencies in energy units. The above integral can be factorized into Gauss-integrals over the momentum components $\mathbf{p}=(p_x,p_y,p_z)$ and results in

$$n=C\left(\frac{mT}{2\pi}\right)^{3/2}. \tag{2.23}$$

The energy density can be obtained similarly by evaluating the integral

$$e=\frac{E}{V}=C\mathrm{d}^3p\,\frac{\mathbf{p}^2}{2m}\,\mathrm{e}^{-\mathbf{p}^2/2mT}. \tag{2.24}$$

Instead of carrying out more complicated Gauss integrals it is enough to observe that

$$\frac{\partial}{\partial T}\,\mathrm{e}^{-\mathbf{p}^2/2mT}=\frac{1}{T^2}\,\frac{\mathbf{p}^2}{2m}\,\mathrm{e}^{-\mathbf{p}^2/2mT}. \tag{2.25}$$

This way we obtain

$$e = T^2 \frac{\partial n}{\partial T} = T^2 C \frac{3}{2} \left(\frac{mT}{2\pi} \right)^{1/2} \frac{m}{2\pi}. \tag{2.26}$$

This result simplifies to $e = 3nT/2$ revealing the formula for the average kinetic energy per particle

$$\frac{E}{N} = \frac{e}{n} = \frac{3}{2} T. \tag{2.27}$$

Since the particles move in three independent directions, this result conforms with the more general statement that due to the equipartition of energy in an ideal system to each degree of freedom of motion there is an average energy of $k_B T/2$.

> The average energy per kinetic degree of freedom, $k_B T/2$ is a *measure of temperature* in ideal systems.

Finally, the pressure of an ideal gas can be obtained by using a relation derived from gas heating and expansion experiments: the Boyle–Mariotte law,

$$pV = NT \tag{2.28}$$

in $k_B = 1$ units. From here, using the general thermodynamical definition for the chemical potential μ as a variable associated to particle number, we get

$$n := \frac{\partial p}{\partial \mu} = \frac{p}{T}. \tag{2.29}$$

This means that the pressure must have the following form:

$$p(\mu, T) = e^{\mu/T} g(T). \tag{2.30}$$

Comparison with the result (2.23) leads to the conclusion that the normalization constant C also contains the factor $e^{\mu/T}$, and this is its only dependence on the temperature. All this, of course, is true only as long as the classical filling pattern of the phase space is assumed; the formula (2.30) is not valid when quantum statistics is considered. In particular it is not valid for radiation, for a quantum gas of photons.

In practical accelerator experiments the particle velocities are relativistic, they achieve a large portion of the speed of light. The Maxwell–Boltzmann statistics therefore cannot be applied for analyzing momentum spectra. Nor the Planck law is valid, since the particle mass and the characteristic temperature are also in the same order, $k_B T \sim mc^2$, especially for pions in high energy experiments. The hadronization temperature is around $k_B T = 170$ MeV, and the hadronic fireball does not cool down much before disintegrating into a non-interacting system of newly produced hadrons. Realistic estimates consider $k_B T = 120 - 140$ MeV for this "break up" temperature. The pion mass on the other hand is around $m_\pi c^2 \approx 140$ MeV, too.

As in the case of radiation, a temperature may be conjectured upon studying the whole spectrum of different momenta stemming from such events. This, however, requires a huge amount of exclusive data: Energy and all momentum components, for each particle from each elementary collision in the accelerated beam, have to be separately stored and analyzed. A fast estimate of the temperature can be obtained instead by inspecting global features of particle spectra. In analogy to Wien's law, the position of maxima might be studied, but this also requires some detailed data, albeit only near to the spectral maxima. In order to gain fast information, one rather utilizes the concept of average energy per particle as a measure of temperature.

More precisely, the average of momentum components squared are used for first estimates. In the non-relativistic Maxwell–Boltzmann distribution, one determines

$$\left\langle p_x^2 \right\rangle = \left\langle p_y^2 \right\rangle = \left\langle p_z^2 \right\rangle = mT. \tag{2.31}$$

Since the source of particles, the hadronic fireball may not be spherically symmetric but rather distributed alongside the beam axis, and – to begin with – it is hard to measure particles close to the beam direction, quite often the momentum components transverse to this direction are collected and averaged. This leads to the following expectation value, assuming a non-relativistic ideal gas:

$$\left\langle p_T^2 \right\rangle = 2mT. \tag{2.32}$$

Plotting the average transverse momentum squared of identified hadrons against their respective masses, the slope of the linear approximation delivers the temperature (cf. Fig. 2.3).

This estimate is improved in the framework of a relativistic thermal model. The single particle kinetic energy depends on the momentum according to the relativistic kinematic formula

$$E = \sqrt{\mathbf{p}^2 + m^2} - m \tag{2.33}$$

in $c = 1$ units.[5] This energy formula does not contain the rest mass energy $E_0 = m$, its low-momentum approximation is given by $E = \mathbf{p}^2/2m + \cdots$ The velocity vector of a relativistic particle is given by $\mathbf{v} = \mathbf{p}/E$ and its magnitude never exceeds one, the speed of light. The high-energy (as well as high-momentum and high-velocity) approximation of this formula coincides with the low-mass expansion, $E = |\mathbf{p}| + \cdots$ These two extreme cases are realized by classical gases and by radiation at such high temperatures where the averages are well approximated by Wien's law instead of the Planck distribution.

The Boltzmann–Gibbs energy distribution factor, $\mathrm{e}^{-E/T}$, for relativistic ideal gases contains the square root formula (2.33). Splitting the momentum vector to components parallel and transverse to the beam, $\mathbf{p} = (p_L, p_T \cos\varphi, p_T \sin\varphi)$.

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[5] We have arrived at the practical unit system of high energy particle physics assuming $k_B = \hbar = c = 1$ and therefore measuring temperature, time and distance uniformly in energy units of MeV, or in its respective powers.

Introducing further the transverse mass, satisfying $m_T^2 = m^2 + p_T^2$, one arrives at the following differential density of particles in momentum space:

$$d^3n = \frac{C}{(2\pi)^3}\, e^{-\sqrt{m_T^2+p_L^2}/T+m/T}\, m_T dm_T\, dp_L\, d\varphi. \tag{2.34}$$

Here, we utilized the fact that $p_T dp_T = m_T dm_T$. Integrating over the azimuthal angle φ and selecting out those particles which have approximately zero momentum component in the beam direction, $p_L \approx 0$, one arrives at a Boltzmann–Gibbs-like exponential distribution in the transverse mass (being the total energy in this case):

$$\left.\frac{d^2n}{p_T dp_T dp_L}\right|_{p_L=0} = \frac{C}{(2\pi)^2}\, e^{(m-m_T)/T}. \tag{2.35}$$

The average of p_T^2 – or equivalently m_T^2 – can now be easily obtained weighted by these transverse spectra (almost) perpendicular to the beam. One has

$$\left\langle m_T^2 \right\rangle = \frac{\int\limits_m^\infty m_T^3\, e^{-m_T/T}\, dm_T}{\int\limits_m^\infty m_T\, e^{-m_T/T}\, dm_T} \tag{2.36}$$

and $\langle p_T^2 \rangle = \langle m_T^2 \rangle - m^2$. The factor $e^{m/T}$ occurs both in the numerator and denominator and therefore cancels out. The exponential integrals are in general incomplete Euler Gamma functions, in the above special case they contain polynomials of m/T. The final result is

$$\left\langle p_T^2 \right\rangle = 6T^2 + 2mT\frac{m}{m+T}. \tag{2.37}$$

For massive particles this result approaches the one obtained using the two-dimensional, non-relativistic Boltzmann formula, $2mT$. For very high temperatures, $T \gg m$, however, it relates the transverse momentum square to the temperature universally, independent of the particle mass: the leading term $6T^2$ reflects an ideal gas obeying Wien's law.

Inspecting Fig. 2.3 one realizes that in hadronic fireballs emerging from accelerator experiments most particles can be treated as non-relativistic with respect to their thermal distribution, but the lightest ones, like the pion. The spectral thermometer is roughly given by a linear dependence of the average momentum squared per particle on the particle rest mass.

Summarizing, elementary particle spectra give information about the temperature of their emitting source with which they had their last thermal contact. A temperature can be reflected in the spectral shape of momentum or energy distribution, but also in average values. Most prominently the momentum squared per particle is a linear function of mass at not too relativistic temperatures $k_B T < mc^2$. The average energy per particle per kinetic degree of freedom is about $k_B T/2$ in the non-relativistic, about $k_B T$ in the extreme relativistic limit.

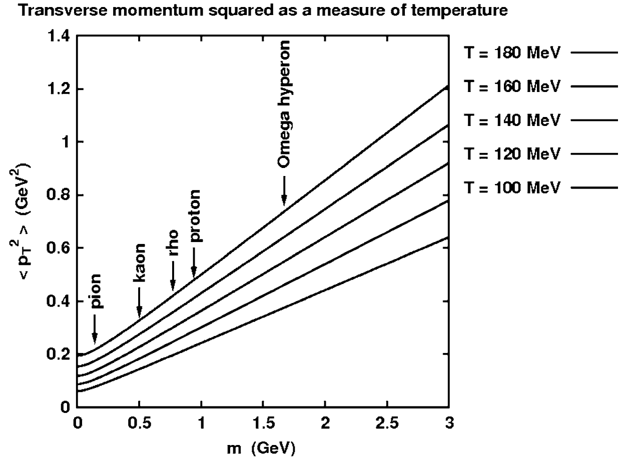

Fig. 2.3 Average transverse momentum squared, $\langle p_T^2 \rangle$, of elementary particles stemming from a hadronization in high-energy accelerator experiments according to the simplest thermal model. Characteristic temperatures, $T = 120$, 140, 160, and 180 MeV are shown in the mass range from the pion to lowest mass baryons

2.3 Chemical Temperature

Since heat and temperature do have an effect on chemical reactions, also chemical signals may be used for indicating, scaling and – with some further calculational work – to measure temperature. Most spectacular are films or liquid solutions changing their color by heating and cooling. This, in general, can be achieved by changing the concentration of some components relative to the others.

Such a method, based on comparing multiplicities (relative numbers) of different components in a (supposedly) thermalized mixture, also occurs in high energy accelerator experiments. In particular, a "chemical decoupling temperature" is conjectured, the temperature when the hadron species – detected afterward – were equilibrating with each other the last time before they have lost contact. This moment in the evolution of a hadronic fireball is called chemical decoupling [7–11]. In what follows we demonstrate this effect in simplified models of non-interacting thermal mixtures of different kinds of particles.

Ideal mixtures realize a peaceful coexistence of several different components. It means that the respective probabilities of finding one or the other component, specific particle, in a given phase space cells factorize: These are independent statistical events. Considering an ideal gas of different particles, the i-th sort having a number density n_i, the total ideal pressure is additive

$$P = \sum_i n_i T \tag{2.38}$$

in the non-relativistic Boltzmann limit (still using $k_{\mathrm{B}} = 1$ units). Each number density is determined by a common temperature, T, and the individual particle properties, most prominently by a particle rest mass, m_i and a chemical potential, μ_i. The respective ideal densities can be obtained as being

$$n_i = \mathrm{e}^{\mu_i/T}\, d_i \mathrm{d}^3 p \mathrm{e}^{-E_i(p)/T}. \tag{2.39}$$

Here, $E_i(p) = \sqrt{\mathbf{p}^2 + m_i^2}$ is the energy of a single, freely and relativistically moving particle with rest mass m_i and momentum $\mathbf{p}$. The factor d_i counts for a possible degeneracy due to internal degrees of freedom, not taking part in the particles motion but distinguishing quantum states. The best example is a polarization, with the degeneracy factor $d_s = (2s+1)$ for a particle with spin s. The chemical potential, μ_i, depends on the charges the particle carries and on the chemical potentials associated to the total density of those conserved charges:

$$\mu_i = \sum_a q_i^a \mu^a, \tag{2.40}$$

summed over all sorts of charges. In high energy accelerator experiments, the majority of hadrons is produced in a very short and energetic event governed by the elementary strong interaction; during this there are three conserved charges: the electric charge (which is strictly conserved in all interactions known to date), the baryonic charge, associated to the quark content of the hadrons, and the hypercharge, correlated with an exotic property, the so called “strangeness” of the particle. This way the chemical potential of a given particle is a linear combination of three basic chemical potentials, μ_3, μ_B, and μ_S associated to the electric charge, to the baryonic number and to the strangeness number of the particle:

$$\mu_i = q_i^{\text{electric}} \mu_3 + q_i^{\text{baryonic}} \mu_B + q_i^{\text{strangeness}} \mu_S. \tag{2.41}$$

For charge balanced hadronic fireballs these chemical potentials are negligible, but due to the incomplete detection in fluctuating events they are never exactly zero. A sizable value is expected in the first place for μ_B by using heavy nuclei for initiating the reactions. In particular, future experiments are devoted to the study of the strongly interacting hadronic and quark matter at finite total baryon density [12, 13].

By inspecting particle number ratios of identified particles, the masses m_i are known and the chemical potential and temperature dependence can be conjectured to conform with the ideal gas mixture formula (2.38). It is a natural assumption to consider that all hadrons coming from the same fireball were thermalized in about the same volume. In this case, the particle number ratios are given by the density ratios

$$\frac{N_i}{N_j} = \frac{n_i}{n_j} = \mathrm{e}^{(\mu_i - \mu_j)/T}\, \frac{f(m_i/T)}{f(m_j/T)} \frac{d_i}{d_j}, \tag{2.42}$$

if comparing two particles having the same charges with respect to electric, baryonic and strangeness degrees of freedom. The function, $f(m/T)$ can be obtained by evaluating the integral (2.39). Assuming an isotropic fireball, i.e. an equally thermalized motion in all of the three spatial directions, one has to calculate the following integral:

$$n = \mathrm{e}^{\mu/T} \frac{1}{2\pi^2} \int_m^\infty E(E^2 - m^2)^{1/2} \mathrm{e}^{-E/T} \, \mathrm{d}E. \tag{2.43}$$

The result of this integral is proportional to a special function, the modified Bessel function of second kind with index 2, denoted by $K_2(x)$. We obtain

$$n = \mathrm{e}^{\mu/T} \frac{1}{2\pi^2} m^2 T K_2(m/T). \tag{2.44}$$

At low temperatures, $T \ll m$ (in $k_\mathrm{B} = c = \hbar = 1$ units), this formula leads to the Maxwell–Boltzmann result (2.23). In the other extreme, i.e. at extreme relativistic temperatures, $T \gg m$, one obtains the following average particle density

$$n = \mathrm{e}^{\mu/T} \frac{1}{\pi^2} T^3. \tag{2.45}$$

The total energy per particle, defining the kinetic temperature for each particle mass, also can be obtained by evaluating relativistic integrals. For the sake of completeness we give here the result

$$\frac{E}{N} = \frac{e}{n} = 3T + m \frac{K_1(m/T)}{K_2(m/T)}. \tag{2.46}$$

It is particularly simple if one studies ratios of particle sorts having the same charges but different mass. This can be a comparison with a so called resonance of an elementary particle – but here the resonance decay after the chemical decoupling has to be taken into account (this happens without any interaction, too). Stable particles with all the same charge but different masses, unfortunately do not exist; in fact, the higher mass particle decays into the lower mass partner with otherwise the same properties. As an example, let us compare the ρ and π mesons in an ideal, thermal ensemble. On a very short time scale both can be treated as stable particles in thermal equilibrium. The equilibrium ratio of their numbers is given by

$$\frac{N_\rho}{N_\pi} = 3 \frac{f(m_\rho/T)}{f(m_\pi/T)}, \tag{2.47}$$

which in the non-relativistic limit becomes

$$\frac{N_\rho}{N_\pi} = 3\mathrm{e}^{(m_\pi - m_\rho)/T} \left(\frac{m_\rho}{m_\pi} \right)^{3/2}. \tag{2.48}$$

Due to the rest mass energy factor, $e^{-m/T}$, such a ratio may be used to define a chemical temperature

$$T_{\mathrm{chem}\,|\,\rho/\pi} = \frac{m_\rho - m_\pi}{\ln \frac{3N_\pi}{N_\rho} + \frac{3}{2} \ln \frac{m_\rho}{m_\pi}}. \tag{2.49}$$

Substituting the particle masses $m_\pi = 140$ MeV and $m_\rho = 770$ MeV, the chemical temperature is related to the particle ratio as

$$T_{\mathrm{chem}\,|\,\rho/\pi} = \frac{630\mathrm{MeV}}{2.557 + \ln \frac{3N_\pi}{N_\rho}}. \tag{2.50}$$

For half as much rho meson than pion this gives an estimate of $T \approx 145$ MeV.

Of course, in case of chemical and thermal equilibrium all possible ratios have to comply with the common temperature and the few chemical potentials associated to conserved charge-like quantities. In different thermal models of heavy ion reactions, further parameters, like an excluded volume of each particle sort, or fluctuating volumina can also be taken into account: the details change, but the main principle of obtaining the chemical temperature remains.

2.3.1 Challenges

In principle, the different methods for measuring the temperature, namely by direct contact, by analyzing radiation spectra and by determining from component decomposition, should deliver identical results. However, only the direct contact based measurement fulfills the requirement of the zeroth law of thermodynamics, only in this case is established the reading of the temperature value in a thermal equilibrium state between the measured object and the thermometer, also treated as a physical system. The solely idealization is the vanishing heat capacity of the thermometer; it is a task for the technology to come close to this ideal.

By conjecturing the temperature from radiation, the direct contact and hence the thermal equilibration between the thermometer, represented by the detector, and the measured object, e.g. a distant star, is not achieved during the measurement. In theory, the knowledge of the entire spectrum would reveal whether we observe a black body, – a radiation being in thermal equilibrium with its source, – but in practice only parts of a spectrum can be detected. Furthermore, both the shining surface and the motion of the observed body may distort the result of the spectral measurement. Although the latter may be disentangled by observing spectral lines, transition frequencies stemming from quantum mechanical processes between atomic states, the radiation based temperature measurement is clearly less certain than the classical one based on direct contact.

Finally, a temperature determination based on the chemical concept of analyzing component particle ratios is even less reliable. Assumptions have to be made about the statistical independence and equation of state contributions from the individual components to the mixture. Furthermore, the chemical decoupling has to happen nearly instantly (and before the kinetic decoupling), in order to trust that the detected particle sort ratios still carry information about a thermal state of the mixture. In particular by confronting with a distributed decoupling during or an instant one at the end of an evolution, which includes strong changes of temperature in space and time, the interpretation of the calculated chemical temperature has to be handled with care. The undeniable fact of a *global evolution* is unified with the theoretical concept of *local equilibrium* in such cases. For too small mesoscopic systems this concept has severe limitations. For example, there is a longstanding debate among researchers in particle physics about the question that how far can a temperature be associated to the fireball state from which observed hadronic spectra stem. While for reactions initiated by the collision of heavy atomic nuclei (lead, gold or uranium) the researchers' common sense tends to accept the thermodynamic interpretation of absolute temperature in describing experimental hadron spectra, for the reactions emerging from collisions of smaller systems (like proton on antiproton or electron–positron scattering) many indicate well argued doubts about the applicability of such a concept. But where exactly lies the borderline between these cases?

Problems

2.1. Convert by heart (and fast) the following temperature values between the Celsius and Fahrenheit scales: 36°C, 27°C, 22°C, 100°C, 32°F, 64°F, 80°F, 71°F, 451°F.

2.2. Derive Kirchhoff's law from the equality of intensities of emitted and absorbed radiation between two bodies in equilibrium.

2.3. Using Wien's law determine the wavelengths of maximal intensity for the Sun's surface, for a light bulb, for the human body, and for the cosmic microwave background.

2.4. What is the average energy carried by a photon in thermal radiation according to Planck's law, according to Wien's law and according to a Raleigh–Jeans law cut at the maximal frequency of Wien's formula?

Chapter 3
How to Interpret the Temperature

Temperature is interpreted as an intensive parameter associated to energy equilibration, as an integrating factor making the entropy change to be a total differential, as related to a Lagrange multiplier to the energy conservation condition, and as a special property of the noise.

This book is about the concept of temperature, but of course the concepts of heat and entropy also cannot escape some discussion. In fact, the theoretical background of thermodynamics rests on four pillars, on the four laws of thermodynamics. All of them make a reference to temperature, or entropy, or both. We list these postulates at the beginning of this section about thermal equilibrium, indicating the physical content of their statements, and we list them at the end again, supplemented with some easy-to-remember formulas. Here they are

0. Thermal equilibrium is universal.

1. Energy is conserved.

2. Trends irreversibly lead to equipartition of energy.

3. There is an absolute zero point of temperature.

T.S. Biró, *Is There a Temperature? Conceptual Challenges at High Energy, Acceleration and Complexity*, Fundamental Theories of Physics 171,
DOI 10.1007/978-1-4419-8041-0_3,

3.1 The Temperature as an Equilibrium Parameter

The state of thermal equilibrium is not a static state: at a finite (absolute) temperature there is internal motion and internal energy associated to this motion. The so called "macrostate" does not change appreciably. Now, if someone defines a macrostate by specifying a few variables, usually averages (or variances) of microscopical variables associated to a great number of microscopic degrees of freedom, then practically she/he fixes a few constraints on a great number of variables. Pictorially, this means to localize a very high-dimensional hypersurface in an also very high-dimensional space of possible microstates, so called configurations.

What is the correct principle behind this? The key point is that a macrostate – specified only by a few constraints or totally unspecified – can be realized by a number of microstates. And they all look the same. $\mathscr{N}$ equal agents can be arranged – without abandoning their distinguishability – in a $W = \mathscr{N}!$ ways. Now imagine that such systems are in a race: macrostate 1 can be realized by $\mathscr{N}_1$ microstates and another macrostate 2 can be made via $\mathscr{N}_2$ microstates. Observing the body for a long long time – long enough compared to the changes between microstates – one tends to see state 1 and state 2 in the proportion $\mathscr{N}_1/\mathscr{N}_2$. We infer the probability for being in a given state as

$$P_i = \frac{\mathscr{N}_i}{\sum_j \mathscr{N}_j}. \tag{3.1}$$

Thermal equilibrium between macrostates – each realized by a huge number of microstates – has to satisfy very elementary logical properties. If there is an equilibrium between body 1 and 2, then subsequently between body 2 and 3, then also between the first and third body there has to be equilibrium. This is the transitivity property. A body has to be in equilibrium with itself, otherwise its equilibrium with another body cannot be asked for (reflexivity). In an equilibrium between two bodies both are involved, so "being in equilibrium" is also a symmetric property. These three properties are best reflected in the properties of the relation "equivalence" or equity. The characteristic thermodynamic parameters, in a minimal setting the temperatures, also must be equal between bodies in equilibrium. Furthermore, if a large body is in equilibrium with itself, its parts (the subsystems) also have to be in equilibrium – and characterized by the same temperature. This way the temperature is a signal of the thermal macrostate which remains the same during (sub)division. Such a variable of state is called an *intensive* variable [5].

3.1.1 The Zeroth Law: Universal Equilibrium

The equity of temperatures describes thermal equilibrium – this is the "zeroth" law of thermodynamics. The next question is, how this quantity is related to the occurrence probability of macrostates and to the quantity of heat transferred before reaching the equilibrium. Here also some principles help.

According to the *equipartition principle* in the macro-equilibrium state all processes changing the individual occurrences of microstates become well balanced. In this state, while individual microstates still can change, giving or receiving energy packets, their overall probability stays stationary. Such processes, balancing the gain and loss terms exactly, lead to a *detailed balance* equilibrium. The micro-process can be blind against the macrostate, not knowing about trends or fashion. But simply from more realized (in a way “occupied”) microstates more can go away and also more can arrive at “vacant” microstate possibilities. The end of this process is, that the most probable state is realized in most of the time. The equilibrium principle therefore must be $W = \max$.

But where W is maximal, also its arbitrary monotonic rising function is maximal. For a quantitative formulation of the general equilibrium state we need some more specification. At this point enters the additivity property stemming from the heat-substance idea: for independent systems (or parts of one great system) the numbers of possibilities follow a multiplicative law, since the ways one and the other half can be realized are independent:

$$W_{12} = \mathcal{N}_{12}! = \mathcal{N}_1! \cdot \mathcal{N}_2! = W_1 \cdot W_2. \tag{3.2}$$

In fact, the logarithm of such a quantity is additive, and exactly this property is carried by the Boltzmannian construction of entropy

$$S = k_{\mathrm{B}} \ln W \tag{3.3}$$

with $W = \mathcal{N}!$ being the number of realizations of a macrostate by equally probable microstates.

In the usual treatment of thermodynamics there are a few macro-variables specifying the thermal (equilibrium) state: the internal energy E, the volume, V, the particle number N. There can also be more. In general, a thermal (macro)state is described by the entropy, maximal in equilibrium, and the constraint values; this relation is named as the *equation of state*:

$$S = S(E, V, N, \ldots). \tag{3.4}$$

Please note that in this form only additive, substance-like quantities are related to each other. They are called *extensive* variables. The partial derivatives of the equation of state function are denoted by

$$\frac{\partial S}{\partial E} = \frac{1}{T}, \qquad \frac{\partial S}{\partial V} = \frac{p}{T}, \qquad \frac{\partial S}{\partial N} = -\frac{\mu}{T}, \ldots \tag{3.5}$$

We show that these quantities are the "entropic intensives," exactly the quantities which become equal between bodies in equilibrium with each other.

In the state of equilibrium between two (or more) such bodies intensity like parameters should be equal. Since this very state is also the one which maximizes the entropy,[1] the equilibrium intensives and the equation of state are connected. This connection is the easiest to reveal when considering two subsystems composed into a common system with maximal entropy. One requires

$$S_{12} = S(E_{12}, V_{12}, N_{12}, \ldots) = \max. \tag{3.6}$$

while the energy, volume, particle number etc. are composed from the corresponding subsystem values

$$\begin{aligned} E_{12} &= E_1 \oplus E_2, \\ V_{12} &= V_1 \oplus V_2, \\ N_{12} &= N_1 \oplus N_2, \\ &\ldots \end{aligned} \tag{3.7}$$

For the fulfillment of having a maximal entropy state it is actually not required that the composition laws, denoted by $\oplus$ in the above equations, must coincide with the addition. But being in a maximal entropy ("maxent") state, the total derivative of $S_{12} = S(E_1, E_2, V_1, V_2, N_1, N_2, \ldots)$ must vanish:

$$\begin{aligned} \mathrm{d}S_{12} = {} & \\ & \left(\frac{\partial S}{\partial E_1}\mathrm{d}E_1 + \frac{\partial S}{\partial E_2}\mathrm{d}E_2\right) + \left(\frac{\partial S}{\partial V_1}\mathrm{d}V_1 + \frac{\partial S}{\partial V_2}\mathrm{d}V_2\right) + \left(\frac{\partial S}{\partial N_1}\mathrm{d}N_1 + \frac{\partial S}{\partial N_2}\mathrm{d}N_2\right) \\ & + \quad \cdots \quad = \quad 0. \end{aligned} \tag{3.8}$$

Besides this we fix the total energy, volume and particle number, so their total derivative is also zero

$$\begin{aligned} \mathrm{d}E_{12} &= \left(\frac{\partial E_{12}}{\partial E_1}\mathrm{d}E_1 + \frac{\partial E_{12}}{\partial E_2}\mathrm{d}E_2\right) = 0, \\ \mathrm{d}V_{12} &= \left(\frac{\partial V_{12}}{\partial V_1}\mathrm{d}V_1 + \frac{\partial V_{12}}{\partial V_2}\mathrm{d}V_2\right) = 0, \\ \mathrm{d}N_{12} &= \left(\frac{\partial N_{12}}{\partial N_1}\mathrm{d}N_1 + \frac{\partial N_{12}}{\partial N_2}\mathrm{d}N_2\right) = 0. \end{aligned} \tag{3.9}$$

---

[1] This is called Gibbs' principle.

Expressing dE_2, dV_2, and dN_2 form these equations one realizes that the entropy differential contains only three independent extensive variable of state differentials, dE_1, dV_1 and dN_1. Using the general notations for the entropy derivatives we get

$$\left(\frac{\partial S}{\partial E_1}-\frac{\frac{\partial E_{12}}{\partial E_1}}{\frac{\partial E_{12}}{\partial E_2}}\frac{\partial S}{\partial E_2}\right)dE_1+\left(\frac{\partial S}{\partial V_1}-\frac{\frac{\partial V_{12}}{\partial V_1}}{\frac{\partial V_{12}}{\partial V_2}}\frac{\partial S}{\partial V_2}\right)dV_1+\left(\frac{\partial S}{\partial N_1}-\frac{\frac{\partial N_{12}}{\partial N_1}}{\frac{\partial N_{12}}{\partial N_2}}\frac{\partial S}{\partial N_2}\right)dN_1=0. \tag{3.10}$$

The coefficients of each term must be zero separately. This way one arrives at the following general equilibrium condition

$$\begin{aligned}\frac{\partial S}{\partial E_1}\frac{1}{\frac{\partial E_{12}}{\partial E_1}}&=\frac{\partial S}{\partial E_2}\frac{1}{\frac{\partial E_{12}}{\partial E_2}}\\ \frac{\partial S}{\partial V_1}\frac{1}{\frac{\partial V_{12}}{\partial V_1}}&=\frac{\partial S}{\partial V_2}\frac{1}{\frac{\partial V_{12}}{\partial V_2}}\\ \frac{\partial S}{\partial N_1}\frac{1}{\frac{\partial N_{12}}{\partial N_1}}&=\frac{\partial S}{\partial N_2}\frac{1}{\frac{\partial N_{12}}{\partial N_2}}.\end{aligned} \tag{3.11}$$

These equations can be interpreted as equalities for the thermodynamical intensives, meaning that the zeroth law – which is a postulate – is fulfilled, if and only if the derivatives of the composition laws with respect to the individual values of the corresponding extensives are

- Only functions of the corresponding variable or can be factorized into such functions.
- The respective ratios between the subsystems can be kept constant.

Addition as a composition law satisfies both requirements with the partial derivatives of composition laws being all over 1. In this case, the equilibrium condition, the equality of intensives:

$$T_1=T_2, \qquad p_1=p_2, \qquad \mu_1=\mu_2, \tag{3.12}$$

coincides with the equality of the corresponding entropic derivatives.

In a more general situation, the "thermodynamical" temperature is not simply given by the derivative of the entropy with respect to the energy, but it is a more complicated expression. Still, equilibrium exists and it is universal, and in this universal equilibrium the temperatures (and other intensives) are equal. The composition law of extensives must, however, show the factorizing property[2]

$$\frac{\partial E_{12}}{\partial E_1}=A(E_1)B(E_2), \qquad \frac{\partial E_{12}}{\partial E_2}=A(E_2)B(E_1), \tag{3.13}$$

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[2] In fact, this can be supplemented with a further symmetric factor, $C(E_1,E_2)=C(E_2,E_1)$.

and then the equilibrium condition (3.11) for the energy exchange part becomes

$$\frac{\partial S}{\partial E_1}\frac{1}{A(E_1)B(E_2)}=\frac{\partial S}{\partial E_2}\frac{1}{A(E_2)B(E_1)}. \tag{3.14}$$

This equation can be written in a way that only quantities belonging to one or the other system are collected at the corresponding sides, pointing out that the thermodynamical temperatures are given as

$$\frac{1}{T_1}=\frac{\partial S}{\partial E_1}\frac{B(E_1)}{A(E_1)}=\frac{\partial S}{\partial E_2}\frac{B(E_2)}{A(E_2)}=\frac{1}{T_2}. \tag{3.15}$$

Another general class of composition laws is considered when constructing a big system by small steps: the result is an associative rule. Such rules satisfy

$$L(E_{12})=L(E_1)+L(E_2) \tag{3.16}$$

with $L(z)$ being a strict monotonic, rising function (see Sect. 5.3). We take the derivative of the above equation by E_1 getting

$$L'(E_{12})\frac{\partial E_{12}}{\partial E_1}=L'(E_1) \tag{3.17}$$

and do the same with respect to E_2. Expressing the partial derivatives of E_{12} by E_1 and E_2, respectively, the zeroth law leads to the following equation

$$\frac{\partial S}{\partial E_1}\frac{L'(E_{12})}{L'(E_1)}=\frac{\partial S}{\partial E_2}\frac{L'(E_{12})}{L'(E_2)}. \tag{3.18}$$

Dividing by the common factor, $L'(E_{12})$, we arrive at a form ready for defining the thermodynamical temperature:

$$\frac{1}{T_1}=\frac{\partial S}{\partial E_1}\frac{1}{L'(E_1)}=\frac{\partial S}{\partial E_2}\frac{1}{L'(E_2)}=\frac{1}{T_2}. \tag{3.19}$$

The zeroth law is fulfilled, the thermodynamical temperature exists in these more general cases, too. Only the very expression of $1/T$ is no more simply $\partial S/\partial E$.

Summarizing the essence of the zeroth law, a universal temperature definition is possible for factorizing composition formula derivatives, and it is related to the following general feature of the equilibrium state: The dependence of the total entropy on the subsystems' parameters (in the classical context they are called reservoir and body) is separable into a "$T_1 = T_2$" form statement, at least in the so called thermodynamical limit.

3.1.2 Microcanonical, Canonical and Grand Canonical

Depending on the constraints, besides the temperature further intensive quantities are equal in equilibrium between two thermodynamic bodies. All this varies as the constraint varies; different extensive quantities may be restricted by the prescription for their value or for the sum (in general case: the composition) of their values.

If the extensive quantities, $E, V, N, \ldots$, are all fixed for a subsystem under study, than such a system is called *isolated*. Physically, it means that no such contact to other subsystems (as parts of a whole) are active, which may allow for an exchange of quantities of the corresponding extensive variable. In particular, if no energy exchange is allowed, then the subsystem is thermally isolated and $E_1 = \text{const}$ itself. In this case a temperature, T_1, cannot be defined for the subsystem. Similarly, allowing or not to change the subsystem's volume, it is *mechanically* in contact or isolated, either $V_1 = \text{const}$ is constrained in itself or just $V_{12}(V_1, V_2)$ – mostly $V_1 + V_2$ – has a prescribed value. For the particle numbers, when having several components in a thermodynamic system, we talk about *chemical* contact and isolation, in general. Isolated subsystems keep the value of the corresponding extensive variable of state, contacted subsystems not; the latter tend to achieve an equilibrium with the rest. This equilibrium is characterized by the equity of the corresponding intensive variables of state.

The macro-equilibrium, the state of maximal entropy at given constraints, does not determine in which detailed microstate the system under study is. Being in (thermal, mechanical or chemical, or a further type) contact with other parts of a huge system, the *reservoir*, the corresponding extensive variable of state does not show a fixed value anymore. To the contrary, it fluctuates between different values as the system changes its microstate. The macrostate does not determine a precise value for energy, volume or particle number (or any further extensive – substance like – quantity), but it determines their probability distribution, i.e. the occurrence frequency of a given value in a long time observation.

An observed system in thermal contact with a reservoir will not have a fixed energy value. It will be characterized by a value of temperature, and this temperature will in turn characterize the distribution of the system energy. Under quite general assumptions this distribution is a falling exponential in the energy, $P(E) \sim e^{-E/T}$, a result due to Willard Gibbs [14]. According to the classical mechanics the physical microstate of a system is described by knowing the position and momenta of all of their constituents, like those of the atoms in a gas. In equilibrium all microstates, leading to the same – maximal – value of the total entropy, are equally frequent in the time evolution, are equally probable in an *ensemble* of copies of the same system. In a system in contact with a larger reservoir further constraints apply. Based on the principle of *a priori equal probability*, the probability of a macrostate is determined by counting all microstates realizing a state with the required composite properties.

An absolutely isolated system in equilibrium, having maximal entropy, S, and a given energy, E, in a volume, V, with N particles realizes a *microcanonical* ensemble. A subsystem in thermal contact with a reservoir, characterized by a temperature, T, in a volume V with N particles is an instance of a *canonical ensemble*. In each case, when a given physical contact is allowed and therefore the entropy is maximized under the knowledge of the corresponding intensive variable of state instead of the extensive one, a new type of ensemble emerges. The tableaux below gives an overview about the traditional names of ensembles belonging to the corresponding macroscopic equation of states. The latter is characterized by a suitable set of variables of state.

	Variables	*Ensemble*
•	(E,V,N)	Microcanonical
•	(T,V,N)	Canonical
•	(T,V,μ)	Grand-canonical
•	(T,p,N)	Pressure ensemble

These ensembles are interrelated. Allowing a given type of physical contact with a reservoir interchanges the role of corresponding extensive and intensive variables in the mathematical description. Since due to the zeroth law of thermodynamics the intensives are derived as partial derivatives of the microcanonical equation of state,[3] $S(E,V,N)$, replacing any of them with the appropriate derivative mathematically means a change, not only in the set of variables, but also in the quantity to be extremized. This procedure is called *Legendre transformation*.

In an isolated system, described by the microcanonical ensemble and the corresponding probability distribution of microstates, the equilibrium is determined by

$$S(E,V,N) = \max. \tag{3.20}$$

Equivalently, from the viewpoint of energetics, often the $E(S,V,N) = \min.$ condition is used in calculations. A Legendre transformation with respect to the energy leads to the following (implicit) definition of free energy, F:

$$\frac{1}{T} = \frac{\partial S}{\partial E}, \qquad S - E\frac{\partial S}{\partial E} = -\frac{F}{T} = \max. \tag{3.21}$$

While this Legendre transform of the entropy is maximal, the free energy, $F(T,V,N)$, is minimal in the canonical equilibrium. A further Legendre transformation with respect to the particle number leads to the thermodynamical potential, $G(T,V,\mu)$ of the grand-canonical ensemble:

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[3] At least for additive composition rules for the extensives!

$$\frac{\mu}{T} = -\frac{\partial S}{\partial N}, \qquad S - E\frac{\partial S}{\partial E} - N\frac{\partial S}{\partial N} = -\frac{G}{T} = \text{max.} \tag{3.22}$$

Finally, the pressure ensemble is found by minimizing $H(T,p,N)$ defined by

$$\frac{p}{T} = \frac{\partial S}{\partial V}, \qquad S - E\frac{\partial S}{\partial E} - V\frac{\partial S}{\partial V} = -\frac{H}{T} = \text{max.} \tag{3.23}$$

H is also called *enthalpy* or Helmholtz-free energy, while G was baptized to Gibbs-free energy (easy to remember from the initials of the names).

Considering not only huge reservoirs but also big subsystems under our long-time ("statistical") observation, the above used maximum or minimum principles are absolutely equivalent in all macroscopic properties, available for thermodynamical studies. This equivalence of ensembles or different sets of variables of states emerges only in the so called *thermodynamical limit*; in this limit the number of internal degrees of freedom in the observed subsystem is already large enough. While the mathematical proof of this statement can be rather involved under general circumstances, referring at the central limit theorem of statistics, its essence can be understood in simple terms. If a subsystem is large enough, then it must act for parts of itself as its own reservoir. Therefore all ensembles allowing or prohibiting given types of physical contacts with the outside world should not matter. In a sense the measure of contacts – an interface area – and the measure of internal actors in determining the distributions of important variables – the volume or particle number or just the extensive measure of all important degrees of freedom – become non-commensurable. The "volume"-terms overgrow all "surface"-terms. Unless the interface and the volumes are of fractal nature and/or the correlation range is long enough to cause – physical and statistical – entanglement even in large systems. Such "strange" physics will be partially discussed in Chap. 5.

3.1.3 Statistical Foundation

The statistical foundation for thermodynamics has been grown out of the kinetic theory of heat. Considering internal motion as the "substance" of heat, it was soon analyzed, what the distribution and number of possible states in the dynamical phase space of $6N$ dimension for N particles (atoms) placed at all different locations and moving in all different directions can be. By the advent of quantum theory the phase space based picture has been generalized, and a more abstract notion, the state of all possible micro-configurations has emerged. In this subsection, we demonstrate how the entropy formula and the corresponding thermal behavior can be descended from the simplest counting of statistical permutations among equivalent (degenerate) microstates.

We consider ideal systems. The ideal gas is a collection of atoms or molecules which do interact, but these interactions (mostly collisions) are restricted to short, albeit violent acts intermittent to long, free propagation periods. As a consequence (almost) all possible microstates, precise arrangements of atomic motion, are realized over a long enough observational time. Surprisingly many physical systems stay close to this ideal. Here, also in order to elaborate on the meaning of thermodynamical limit and different ensembles, we utilize an abstract model of ideal physical quantum systems. We free our study from "unimportant" complications and deliberately concentrate on the very essence of thermal bodies: energy distributions and temperatures.

The statistical task is to distribute energy between possible microstates. We consider energy quanta either carried by individual particles (such as electrons or photons) or just by collective excitations (such as phonons) as they were small packets. These packets can be distributed among "places," the possible energy levels. All microstates are described by an ensemble of occupied levels, in the simplest approach all levels are the same. Then only their number, say K is of interest. The question arises: how to distribute N energy quanta among K levels?

Quantum statistics arises if these quanta are indistinguishable. By fixing this, still two different possibilities arise: these quanta can either be put together to the same level (same microstate) in an arbitrary number, or not, just one of them. Figure 3.1 depicts these two different situations.

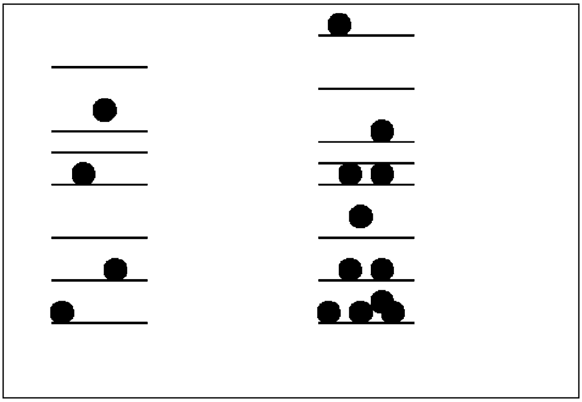

Fig. 3.1 Independent statistical distribution of indistinguishable energy quanta among energy levels. Links for excluding and rights for non-excluding quanta

Let us first investigate microstates satisfying the Pauli principle: on a given level either zero or one quantum may appear. Then the total number of micro-configurations of N indistinguishable quanta distributed among K levels can be obtained as follows. From altogether $K!$ permutations of K levels all those are equivalent where the single-occupied N ones and the unoccupied $K - N$ ones are permuted among themselves. The number of such arrangements are given by the binomial coefficient

$$W = \frac{K!}{N!(K-N)!} = \binom{K}{N}. \tag{3.24}$$

The corresponding Boltzmann-entropy, $S = k_{\mathrm{B}} \ln W$, can be approximated for large numbers of energy level and quanta, $K \to \infty$ and $N \to \infty$ while keeping the ratio $p = N/K$ constant. This means that we are seeking for the entropy maximum for a fixed average occupation ratio, p. By evaluating the expression

$$S_K = k_{\mathrm{B}} \ln \binom{K}{pK} \tag{3.25}$$

for large K, the Stirling formula,

$$\ln N! \approx N(\ln N - 1), \tag{3.26}$$

is of use. We arrive at the following entropy per level number

$$\sigma(p) := \lim_{K\to\infty} \frac{S_K}{K} = k_{\mathrm{B}} \left(-p \ln p - (1-p)\ln(1-p)\right). \tag{3.27}$$

Considering now that the total number $N = Kp$ and the total energy is $E = N\varepsilon = Kp\varepsilon$ (if each energy quantum is ε), the equilibrium probability, p maximizes the following expression:

$$-\frac{G}{T} = S - \frac{1}{T}(E - \mu N) \approx K\left(\sigma(p) - \frac{\varepsilon - \mu}{T} p\right). \tag{3.28}$$

In the limit $K \to \infty$, the approximation becomes an equality and the "best," i.e. the equilibrium distribution p is given by the vanishing derivative condition

$$\frac{\partial}{\partial p}\left(\sigma(p) - \frac{\varepsilon - \mu}{T} p\right) = 0. \tag{3.29}$$

Owing to the particular form of $\sigma(p)$ given in (3.27) we have

$$\sigma'(p) = k_{\mathrm{B}} \ln \frac{1-p}{p} = \frac{\varepsilon - \mu}{T} \tag{3.30}$$

in equilibrium states. The solution of this condition is the most probable distribution of energy quanta of ε carried each by a particle kind, from which cannot be two in the same state. This distribution describes fermions and it is named as Fermi–Dirac distribution:

$$p = \frac{1}{\mathrm{e}^{(\varepsilon-\mu)/k_{\mathrm{B}}T} + 1}. \tag{3.31}$$

These results change if the carriers of energy quanta are bosons. In this case, they can be put to the same quantum state in an unrestricted number. This situation is depicted in the right hand side of the Fig. 3.1. The main difference to the fermion case lies in the fact that now no "separator" – an energy level line – is necessary between two quanta. The K levels (places) and N quanta (particles) are freely distributed in all $(N+K)!$ permutations. Yet the indistinguishability sorts out $K!$ and $N!$ permutations of each as being the same macrostate. This way the number of possible arrangements becomes

$$W = \frac{(N+K)!}{N!K!} = \binom{N+K}{K}. \tag{3.32}$$

The corresponding entropy of a large system with $N = pK$ carriers of quanta is now given by:

$$S_K = k_\mathrm{B} \ln \binom{K+pK}{K}, \tag{3.33}$$

and for large K, using the leading terms in the Stirling formula, we arrive at the following entropy per level number

$$\sigma(p) := \lim_{K\to\infty} \frac{S_K}{K} = k_\mathrm{B}\left(-p\ln p + (1+p)\ln(1+p)\right). \tag{3.34}$$

Its derivative in a grand-canonical equilibrium state is given by:

$$\sigma'(p) = k_\mathrm{B} \ln \frac{1+p}{p} = \frac{\varepsilon - \mu}{T}, \tag{3.35}$$

whence

$$p = \frac{1}{\mathrm{e}^{(\varepsilon-\mu)/k_\mathrm{B}T} - 1}. \tag{3.36}$$

It is the equilibrium distribution of bosons, named Bose–Einstein distribution. Both the Fermi–Dirac and the Bose–Einstein distributions converge to the Boltzmann–Gibbs formula for low probability (i.e. for $N \ll K$):

$$p = \mathrm{e}^{-\frac{\varepsilon-\mu}{k_\mathrm{B}T}}. \tag{3.37}$$

In the same limit, the entropy per level value is given by the Boltzmann formula

$$\sigma(p) = k_\mathrm{B}\left(-p\ln p\right) \tag{3.38}$$

This result can straight be generalized. Let the number of all possible microstates be $\mathcal{N}$. Among them different types are specified by their indistinguishability; the number of indistinguishable states is also called degeneracy. Let these numbers be $\mathcal{N}_i$, satisfying $\mathcal{N} = \sum_i \mathcal{N}_i$. In the previous discussion, we had two kind of states only, "particles" and "holes," i.e. quanta and no quanta at a given level. For fermions we considered $\mathcal{N}_1 = N$ and $\mathcal{N}_2 = K - N$, while for bosons $\mathcal{N}_1 = N$ and $\mathcal{N}_2 = K$. In the former case, we had $\mathcal{N} = K$, in the latter $\mathcal{N} = N + K$ and K was let to grow towards infinity.

In the general discussion, we consider $\mathcal{N}_i = p_i \mathcal{N}$ and the limit $\mathcal{N} \to \infty$. The number of non-degenerate states are given by the formula for repeated permutations

$$W = \frac{\mathcal{N}!}{\prod\limits_i \mathcal{N}_i!}. \tag{3.39}$$

The Boltzmann entropy is proportional to the logarithm of this number, $S = k_\mathrm{B} \ln W$ and can be expressed in terms of $\mathcal{N}_i$ with the help of the asymptotic Stirling formula:

$$S = k_\mathrm{B} \left\{ \mathcal{N} (\ln \mathcal{N} - 1) - \sum_i \mathcal{N}_i (\ln \mathcal{N}_i - 1) \right\}. \tag{3.40}$$

Substituting $\mathcal{N}_i = p_i \mathcal{N}$ leads to

$$S = k_\mathrm{B} \left\{ \mathcal{N} (\ln \mathcal{N} - 1) - \sum_i p_i \mathcal{N} (\ln \mathcal{N} + \ln p_i - 1) \right\}. \tag{3.41}$$

Collecting terms somewhat differently, we arrive at

$$S = k_\mathrm{B} \left\{ \mathcal{N} (\ln \mathcal{N} - 1) \left[1 - \sum_i p_i \right] - \mathcal{N} \sum_i p_i \ln p_i \right\}. \tag{3.42}$$

One immediately realizes that the large $\mathcal{N}$ limit can be carried out only if

$$\sum_i p_i = 1. \tag{3.43}$$

Here is no room for "partial knowledge" or for "escort probability" (not satisfying the above normalization condition). By the fulfillment of this condition one obtains the general formula

$$\sigma(\{p_i\}) = \lim_{\mathcal{N} \to \infty} \frac{S}{\mathcal{N}} = -k_\mathrm{B} \sum_i p_i \ln p_i. \tag{3.44}$$

Although this formula is often cited as Boltzmann's entropy, in fact this is not the total entropy, but the entropy per state value. Nevertheless, a multiplicative constant can be swallowed by the unit of entropy or in the Boltzmann factor, respectively ($k'_\mathrm{B} = k_\mathrm{B} \mathcal{N}$). Such a factor does not influence the equilibrium distribution derived from the (constrained) maximum entropy principle.

In the microcanonical ensemble the entropy is maximized,

$$S = \mathcal{N} \left(\alpha \left(1 - \sum_i p_i \right) + \sigma(\{p_i\}) \right) = \max. \tag{3.45}$$

Here, we introduced the notation $\alpha = (\ln \mathcal{N} - 1)$. The variation against the p_i probabilities leads to

$$\frac{\partial \sigma}{\partial p_i} = \alpha, \tag{3.46}$$

meaning a constant probability, whatever is the precise formula for $\sigma(p)$. This is the famous microcanonical equal probability distribution. Since the sum of all p_i-s must be one, the number of different microstates, Z alone determines the microcanonical probability, $p_i = 1/Z$ and entropy:

$$S = k_{\mathrm{B}} \mathscr{N} \ln Z = k'_{\mathrm{B}} \ln Z. \tag{3.47}$$

Therewhile, $\sum_i \mathscr{N}_i = \mathscr{N}$. In the special case, when all microstates are non-degenerate, all $\mathscr{N}_i = 1$ and $Z = \mathscr{N}$. In classical statistical physics this case was considered by Boltzmann.

The canonical, grand-canonical, etc. ensembles are equilibrium realizations of the maximum entropy principle with different constraints. Here, we show the grand-canonical version, others can be derived similarly. In this case, the total energy, $E = \sum_i \mathscr{N}_i \varepsilon_i$ is fixed and a number of conserved charges, $Q^a = \sum_i \mathscr{N}_i q_i^a$. The superscript "a" denotes the kind of conserved charge: it can be electric charge or another particle charge, like baryon charge, lepton charge, hypercharge – in processes when they are conserved. It is interesting to note that classically there was a specific conserved quantity, the "matter." Retrospectively, it is related to the rest mass energy part in the more general energy conservation; classically it was treated separately and expressed in a conservation law for the number of atoms fixing atomic mass unit. In the view of modern physics, however, *the number of particles is not a conserved quantity.*

The Gibbs free energy is to be minimized in this case, the corresponding entropic potential, $-G/T = S - E/T + \sum_a \mu^a Q^a/T$ is to be maximized. This leads to the following variational principle

$$\mathscr{N} \left\{ \alpha \left(1 - \sum_i p_i \right) + \sigma(\{p_i\}) - \beta \sum_i p_i \varepsilon_i + \beta \sum_a \mu^a \sum_i p_i q_i^a \right\} = \max. \tag{3.48}$$

Here, we introduced the $\beta = 1/T$ notation. The derivative vanishes at the maximum, hence the equilibrium probabilities satisfy

$$\frac{\partial \sigma}{\partial p_i} = \alpha + \beta \left(\varepsilon_i - \sum_a \mu^a q_i^a \right). \tag{3.49}$$

The unknown parameters, α, β and μ^a, are determined by the normalization of state-probabilities and by the average energy and conserved charges:

$$\begin{aligned} \sum_i p_i &= 1, \\ \sum_i p_i \varepsilon_i &= \frac{E}{\mathscr{N}} = \bar{E}, \\ \sum_i p_i q_i^a &= \frac{Q^a}{\mathscr{N}} = \bar{Q}^a. \end{aligned} \tag{3.50}$$

3.1.4 Averages and Extremes

The zeroth law of thermodynamics is fulfilled by such microscopic (statistical and dynamical) descriptions, which achieve an equilibrium state between large parts of a total system. In this equilibrium state, deviations from the equilibrium distribution are allowed, but they have to be small compared to the system size and have to relax fast enough. While relaxation times near the equilibrium state constitute dynamical properties of the material under investigation, the "smallness" of deviations is of statistical nature.

This "smallness" means that the larger a deviation from the most probable value, the smaller its probability to occur. Moreover, its probability has to be reduced by a satisfactory rate, not influencing unduly the relations revealed in macroscopic thermodynamics. We shall discuss in the section dealing with the temperature as a property of noise the central limit theorem, stating that the effect of considering the sum of many random (i.e. wildly fluctuating) variables comes close to a *limiting distribution*, which is Gaussian in common physical systems. Here, we give a look to another aspect: in a given statistical distribution what is the probability to find cases far from the most probable one. This question is related to the study of extreme value distributions [15].

The most probable value and the average value coincide only for some simple distributions, the best example being the Gaussian function. This is the case for velocity or momentum components in a non-relativistic, ideal gas, described by the Maxwell–Boltzmann distribution. Other quantities, however, like e.g. the particle number distribution, are not symmetric; also the range for nonzero probabilities is restricted to positive values (or otherwise). Clearly, the smallness of deviations, equivalently the statistical largeness of the distribution can be quantitatively measured by the magnitude and probability of deviations. One way to restrict deviations is to require that the average value and the most probable value come close enough. With the same right one may also compare the median (the value below and above which $50-50\%$ of the distribution lie) with any of the above. A robustly single-peaked distribution will prove to be satisfactory with respect to all of these intuitive requirements.

In general, one can calculate how big portion of the probability distribution (also called probability density function, PDF) lies near to the maximum and far from it. This picture, of course, assumes having only one maximum. In case of two or several maxima, the average itself may lie far from each. The integrals of the PDF for a part of the total range, defined by thresholding the value of the differential probability, can give a measure of the concentration of probabilities in general.

There exist a number of inequalities valid for such partial integrals of the probability density function. Considering a variable, x, differentially distributed by the measure $\mathrm{d}\mu(x) = p(x)\mathrm{d}x$ (as, e.g., the number of states of a physical system between the energies E and $E+\mathrm{d}E$), the relative measure of satisfying a given constraint with a given threshold value, say $f(x) \geq t$ is formulated by the expression

$$P_f(t) := P(f(x) \geq t) = \mu\left(\{x \in X : f(x) \geq t\}\right). \tag{3.51}$$

Here, X represents the set of all possible values for x. It is clear that the above measure is between (and including) zero and one if the total (unconstrained) measure was normalized to one; it is perfect then for the probabilistic interpretation.[4]

The generalized *Markov inequality* gives an upper estimate to this quantity by using a free function, $g(t)$, which is nevertheless monotonic growing, non-negative and measurable (i.e. its integral is not divergent). Then the probability that the variable x satisfies the constraint $f(x) \geq t$ can be estimated by

$$P_f(t) \leq \frac{1}{g(t)} \int\limits_{x \in X} g\left(f(x)\right) \mathrm{d}\mu(x). \tag{3.52}$$

It is noteworthy that the upper estimate is formulated in terms of an integral over all possible values of x with the original probability density function. Interpreting the integral on the right hand side of (3.52) as an average, a so called expectation value, the inequality states that

$$P_f(t) \leq \frac{\langle g(f(x)) \rangle}{g(t)}. \tag{3.53}$$

The classical Markov inequality is a special case of this formula, valid for the probability of $x \geq t \langle x \rangle$, i.e. $f(x) = x / \langle x \rangle$, with the identity as test function, $g(t) = t$. In this case

$$P(x \geq t \langle x \rangle) \leq \frac{1}{t}, \tag{3.54}$$

the probability to exceed t times the expectation value is not greater than $1/t$. Let us demonstrate this in case of the Maxwell–Boltzmann gas. The energy distribution is Gibbsean, $P(E) \sim \exp(-E/k_{\mathrm{B}}T)$. The kinetic energy of a single particle is given as $E = \mathbf{p}^2/2m$ leading to a phase space factor of $p^2 \mathrm{d}p \propto E^{1/2} \mathrm{d}E$. The normalized PDF is of an Euler Gamma form,

$$\mathrm{d}\mu(x) = \frac{1}{\Gamma(n)} x^{n-1} \mathrm{e}^{-x} \mathrm{d}x, \tag{3.55}$$

with $x = E/k_{\mathrm{B}}T$ scaled variable and $n = 3/2$. The expectation value of x is easy to obtain

$$\langle x \rangle = \frac{\int_0^\infty x \, \mathrm{d}\mu(x)}{\int_0^\infty \mathrm{d}\mu(x)} = \frac{\Gamma(n+1)}{\Gamma(n)} = n. \tag{3.56}$$

---

[4] This measure theoretic approach to probability was pioneered by Kolmogorov in the 1940s.

The classical Markov inequality then states that $P(x \geq nt) \leq 1/t$, being restrictive only for $x > \langle x \rangle$ values. For the ideal Maxwell–Boltzmann gas $n = 3/2$, so

$$P\left(E \geq t\,\frac{3}{2}k_{\mathrm{B}}T\right) \leq \frac{1}{t}. \tag{3.57}$$

In particular, for $t = 2$ the probability to have an energy more than twice the average value must be less than $1/2$ according to the Markov inequality. Since the numerical value for this integral is $P(E \geq 3k_{\mathrm{B}}T) \approx 0.1116$, the Markov inequality is a very liberal upper limit in this case.

The Chebyshev inequality deals with the deviations from the average value. It considers $f(x) = |x - \langle x \rangle\,|$ and $g(t) = t^2$ and ensures that

$$P(|x - \langle x \rangle\,| \geq t) \leq \frac{\delta x^2}{t^2}, \tag{3.58}$$

with $\delta x^2 = \left\langle\, (x - \langle x \rangle)^2 \,\right\rangle$ being the variance of the random variable x. Since for the Euler Gamma distribution $\delta x^2 = n$, one arrives at

$$P(|x - n| \geq t) \leq \frac{n}{t^2}. \tag{3.59}$$

For the Maxwell–Boltzmann gas $n = 3/2$ and one restricts the probability of deviating from the average energy value by

$$P\left(\left|E - \frac{3}{2}k_{\mathrm{B}}T\right| \geq t\,k_{\mathrm{B}}T\right) \leq \frac{3}{2t^2}. \tag{3.60}$$

This upper limit is at 50% when $3/2t^2 = 1/2$, i.e. for $t \approx 0.577$. This means that the probability of having an energy deviating from the average value by more than $2/3 \times 0.577 \approx 0.38$ times the average energy is certainly less than 50% in the Maxwell–Boltzmann distribution.

Finally we discuss the Chernoff inequality. It is obtained by using $g(t) = \mathrm{e}^{b\langle x \rangle t}$ and $f(x) = x/\langle x \rangle$, and leads to a more stringent upper limit for large multiples of the average value:

$$P(x \geq t\,\langle x \rangle) \leq \left\langle\, \mathrm{e}^{b(x - t\langle x \rangle)} \,\right\rangle. \tag{3.61}$$

For the Euler Gamma distribution (including the Boltzmann–Gibbs energy distribution) one estimates

$$P(x \geq t\,\langle x \rangle) \leq \left(\frac{\mathrm{e}^{-bt}}{(1-b)}\right)^{\langle x \rangle} \tag{3.62}$$

with $\langle x \rangle = n$ and $n = 3/2$ for the nonrelativistic ideal gas. The parameter b between 0 and 1 can be optimized to achieve the smallest possible upper limit at a given t. The derivative of the logarithm of the upper estimate with respect to b is given by

$$\langle x \rangle\,\frac{\partial}{\partial b}\left(-\ln(1-b) - bt\right) = 0. \tag{3.63}$$

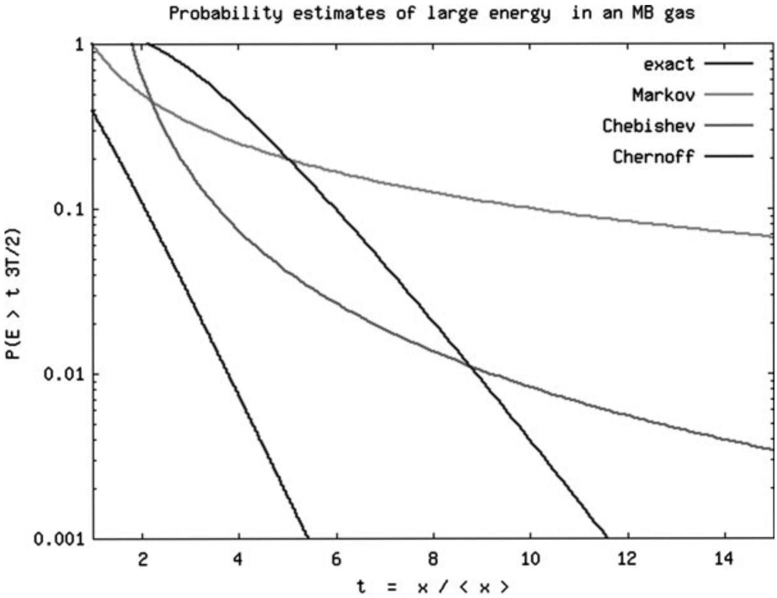

Fig. 3.2 Upper estimates from Markov, Chebyshev, and Chernoff for having t times the average energy or larger in a Maxwell–Boltzmann gas. The exact result is also shown

From this $b = 1 - 1/t$ follows, giving the best Chernoff estimate as

$$P(x \geq t\,\langle x \rangle) \;\leq\; \left(t\mathrm{e}^{1-t}\right)^{\langle x \rangle}. \tag{3.64}$$

In the Fig. 3.2, the integrated probability of having energy over a threshold value t times the average, $P(E > t\,\langle\, E\,\rangle)$, is plotted for the Maxwell–Boltzmann distribution. The classical Markov and Chebyshev estimates and the optimized Chernoff estimate are also indicated. It can be inspected that unless we speak about several multiples of the average value, these classical estimates are quite loose.

3.2 The Temperature Related to an Integrating Factor

The concept of temperature actually precedes that of heat, energy and entropy. The zeroth law – although we presented it in correspondence with the entropic maximum – holds even without taking reference to energy or entropy, or any other thermodynamic potential [5]. Its essence is, that requiring the transitivity property of the thermal equilibrium state it follows that an equation in the form $\Theta_A(A_1,A_2,\ldots) = \Theta_B(B_1,B_2,\ldots)$ exists, collecting the same function of same parameters for the bodies A and B on the respective sides of the equality. The common value is called *empirical temperature* and the very functional form of the Θ function *equation of state*. In relation with other laws of thermodynamics turns, however, out that the entropy – energy relation parametrized by an absolute temperature is the starting point of the thermodynamical description of physical systems.

In this section, we review the ideas relating heat, work and internal energy; as a corollary the efficiency of heat engines and in general all physical circular processes converting one form of energy into another, so called Carnot cycles, follow. By doing so a new facet of the concept of temperature is shown: it makes it possible that the heat, necessary to realize some repeatable (so called circular) work process, is connected to a state of the system, which is reachable in many ways and where the quantitative measure of the thermal work-potential, the entropy, has a value independently of that way. Mathematically it means that the entropy change in any small step of a thermal work process has to be an exact differential, in order its integral be independent of the integration path. Since the mechanical work, done by forces like pressure, is not a differential, but the change of internal energy is, a so called *integrating factor* is needed to construct the entropy functional. This factor proves to be identical to the reciprocal absolute temperature, $1/T$.

After this construction of the entropy, its changes, assumed to be macroscopically slothful, happening with an *adiabatic* speed, is considered. The statistical trend of its growth in lack of external driving forces is the essence of the second law of thermodynamics, albeit several formulations has been offered historically. This tendency explains why the thermal equilibrium always occurs at the entropy maximum.

Finally, since the integrating factor is $1/T$, the $T = 0$ case needs a handling with special care. In fact, classical physics cannot predict what happens at this point. The zero point of entropy at $T = 0$ had to be postulated by Nernst. As it turns out, this state is not realized by all known physical systems: glasses, being in a long term metastable state, for example are having too many nearly ground states to have really zero entropy. Another exceptional system is a gravitational black hole, discussed in Chap. 7, whose entropy actually grows by lowering the temperature.

3.2.1 First Law: Energy Conservation

In today's physics, the principle of energy conservation is central. It was not, however, so at its first suggestion. The idea was in the air in the mid of the nineteenth century [16]. Julius Robert Mayer, James Prescott Joule, and Hermann von Helmholtz are most renown of contributing to the modern development of this concept. But also others, like Justus Liebig, had elaborated on the connection between heat and chemical and life processes.

The story goes that Robert Mayer, serving as a medical doctor on a ship, had observed that the venal blood of the sailors was more red in tropical areas than far in the North. He concluded that human organisms do less oxidation in this case as usual, because the heat, necessary to keep warm blooded creatures healthy and alive, partially comes from outside. The body needs to produce less heat itself. His work, eventually published in 1842 with the title "Bemerkungen über die Kräfte der unbelebten Natur" (Notes on the Forces of inanimate Nature), was actually refused by the leading physics journal of that time, by the Annalen der Physik. Finally, Justus Liebig placed the work in a chemical journal. The problem was not Mayer's conclusion, but rather his naturphilosophical argumentation: he derived the statement of energy conservation from the principle "causa aequat effectum," i.e. that the cause were equal to its effect. Inspite of this anti-Newtonian introduction, he considers at the end a very physical question: from how high a body should fall in order to increase its temperature by 1°. By solving this problem he derives the mechanical equivalence value of heat from the heat capacity of gases at constant volume and pressure.

Joule had carried out the experiment about the mechanical work equivalence of the heat belonging to 1° change in the temperature. He also discovered and published his formula about the heat produced by electric current, I, on a resistance, R, during the time, t: $Q = I^2Rt$. His seminal work, "On the Existence of an Equivalent Relation between Heat and the Ordinary Forms of Mechanical Power," was published in 1845. He conducted his experiment, where the gravitational potential energy of a body is converted to heat by letting a small turbine to work in a fluid, several times, always refining. Finally, he obtained that 1 kcal is equivalent to 424 mkp (nowadays rather the value 427 mkp is accepted).

Helmholtz's work, with the title "Über die Erhaltung der Kraft" (On the Conservation of Force), speaks for itself.[5] The idea of energy conservation (including thermal phenomena) did not become popular at once. Its acceptance was paved also by William Thomson (Lord Kelvin), who became a young friend of Joule, and by Rudolph Clausius, who was the first establishing the connection between macroscopic observables and average properties of molecules in a gas. He derived the kinetic pressure formula, $pV = N \left\langle m\mathbf{v}^2/3 \right\rangle$, and also derived the ratio of the collective kinetic energy to the total one as $3/2$ of $(c_p - c_V)/c_V$ with c_P (c_V) being the specific heat at constant pressure (volume). Finally, Maxwell explained this heat capacity ratio by the equipartition theorem, obtaining the average kinetic energy of internal motion as $k_{\mathrm{B}}T/2$ per degree of freedom for the molecular motion: $c_p/c_V = (f+2)/f$ (in the ideal gas $f = 3$).

The first law of thermodynamics relates the total change of the internal energy (i.e. all the energy not related to a collective motion of the macroscopic body) to the work done on the system and the heat communicated to the system:

$$\mathrm{d}E = \text{Đ}Q + \text{Đ}W. \tag{3.65}$$

---

[5] In the mid-nineteenth century force, energy and momentum were not yet fixed to describe different physical quantities, they were used as synonyms.

Here, the symbol đ denotes that the infinitesimally small amount of work and heat are not differentials, they cannot be written as a sum over partial derivatives and elementary differentials of variables of state (like $\mathrm{d}E$ can). The mechanical work, originally written as $\text{đ}W = \sum_i F_i \mathrm{d}X_i$, summing over force and differential displacement coefficients, can be generalized to be a sum of similar terms: the generalized forces and displacements. In a gas, it has the form of $\text{đ}W = (-p)\mathrm{d}V$, by a chemical reaction $\text{đ}W = \mu \mathrm{d}N$, for the work done by an external magnetic field, H, the expression $\text{đ}W = H\mathrm{d}M$ suggests that the generalized force is the magnetic field and the generalized displacement coordinate is the magnetization, M. Also, surface tension and wire tension act as generalized, so called *thermodynamical* forces.

Related to the first law, a number of differential changes in macroscopic state variables can be obtained and compared. In general, such relations are called *response functions*. The *heat capacities* are obtained from the temperature change upon adding heat to the system. But heat is not a function of state, like energy or entropy, therefore also the path reaching the resulting state has to be specified. The heat capacity differs whether the warming happens at constant volume or constant pressure. Considering volume extension only (as it is characteristic to one-component gases) the mechanical work is $\text{đ}W = -p\mathrm{d}V$, so the heat capacity at constant volume becomes

$$C_V = \left.\frac{\text{đ}Q}{\mathrm{d}T}\right|_V = \left.\frac{\mathrm{d}E + p\mathrm{d}V}{\mathrm{d}T}\right|_V = \left.\frac{\partial E}{\partial T}\right|_V. \tag{3.66}$$

At constant pressure, however, the $p\mathrm{d}V$ term does not vanish and we obtain a different quantity

$$C_P = \left.\frac{\partial E}{\partial T}\right|_P + p\left.\frac{\partial V}{\partial T}\right|_P \tag{3.67}$$

For an ideal gas the energy depends only on the temperature, $E = E(T)$, so its partial derivatives with respect to T are equal either the volume, V, or the pressure, p is kept constant. Using the equation of state $pV = Nk_\mathrm{B}T$, one obtains $\partial V/\partial T = Nk_\mathrm{B}/p$ at constant p, so

$$C_P - C_V = Nk_\mathrm{B}. \tag{3.68}$$

3.2.2 Second Law: Clausius' Entropy

Accepting the first law, the conservation of energy, it was observed by Clausius that this is not enough to explain all general properties of physical phenomena by the conversion of heat, work and energy. The second law, having several phrasings, among others requires that heat spontaneously "flows" from hotter to cooler bodies only (for the opposite flow one has to invest work). Another, equivalent statement is about the impossibility of a *perpetuum mobile* of second kind: a machine which could convert heat to mechanical work with 100% efficiency. By introducing the concept of entropy, Clausius has managed in 1865 to bring both the first and the second law into a mathematical form.

Imagine a process returning at the end to the starting temperature by mild changes, at each step waiting long enough to establish thermal equilibrium. During such a *reversible* circular process heat was added to and extracted from the system, but at the end – according to Clausius' principle – there is a quantity which did not change:

$$\oint \frac{\text{Đ}Q}{T} = 0. \tag{3.69}$$

This means that no net work has been done and the final energy is equal to the initial one conforming with the first law. For such a process then the quantity $\text{Đ}Q/T$ should be a differential, $\mathrm{d}S = \text{Đ}Q/T$. The integrated quantity, S is the entropy. Its change between two arbitrary thermal states does not depend on the integration path:

$$\int\limits_A^B \frac{\text{Đ}Q}{T} = \int\limits_A^B \mathrm{d}S = S_{\mathrm{B}} - S_A. \tag{3.70}$$

With other words the entropy, S, is a variable of state; its value depends only on the state of the physical system and not on the path (history) by which this state is reached.

For *irreversible* processes there is an irrecoverable loss of energy in the form of heat production (dissipative waste of energy). This is negative for the system, so for a general process of thermodynamical nature the following inequality holds

$$\oint \frac{\text{Đ}Q}{T} < 0. \tag{3.71}$$

Let us split a circular process to a part going from A to B by an irreversible and then returning form B to A by a reversible path. Consider the case when the state B is infinitesimally close to the state A. For such processes one obtains

$$\text{Đ}Q \leq T\mathrm{d}S. \tag{3.72}$$

It implies $\mathrm{d}S \geq \text{Đ}Q/T$ for any small step in the slow process going through thermal equilibrium states (only changing its parameters, the variables of state). In particular, in an isolated big system, the subsystems, as they come to a joint equilibrium, exchange heat, but the net change of heat is altogether zero, $\text{Đ}Q = 0$. For such systems the second law of thermodynamics states that

$$\mathrm{d}S \geq 0. \tag{3.73}$$

As a consequence, in isolated total systems the joint equilibrium state belongs to the *maximal entropy*.

The absolute temperature, T, plays the role of an integrating factor in Clausius' construction: the entropy is an exact differential contrary to heat and work. Writing with generalized forces and displacements

$$dS = \frac{1}{T}\left(dE - \sum_i F_i dX_i\right) \geq 0. \tag{3.74}$$

By comparing with the discussion of the zeroth law in the previous section, one sees that for additive composition rules, the coefficients of differentials including the integrating factor, namely $1/T = \partial S/\partial E$, and $F_i/T = -\partial S/\partial X_i$, do in fact equilibrate between bodies allowing the exchange of the corresponding quantity, E and X_i, respectively.

In the case of a general, composable equilibrium, the equated entropic intensive variables may be obtained by more complex formulas. The above form of the first and second law of thermodynamics generalizes only for composition laws derivable from a function $L(E)$ – and accordingly $L_i(X_i)$. In this case one achieves

$$dS = \frac{1}{T}\left(dL(E) - \sum_i F_i dL_i(X_i)\right) \geq 0. \tag{3.75}$$

The absolute thermodynamical temperature derived from the equilibrium conditions still coincides with Clausius' integrating factor. We note, that while the form (3.74) – assuming addition as the composition rule – satisfies the homogeneity property

$$S(\lambda E, \lambda X_i) = \lambda S(E, X_i), \tag{3.76}$$

the more general composable form (3.75) is non-extensive:

$$S(\lambda E, \ldots) = \Xi(L(\lambda E), \ldots) \neq \Xi(\lambda L(E), \ldots) = \lambda S(E, \ldots). \tag{3.77}$$

3.2.3 Third Law: The Ground State

The entropy is henceforth a variable of state, its value is independent of the thermodynamic path by which the state is achieved. The differences of the entropy between two arbitrary states are computable by the Clausius integral using any reversible path. The quantity of this difference, however, is not restricted by the first and second law. Experiments at low temperatures on the other hand indicate that $dS(T, X_i)$ tends to vanish as T goes to zero – at any value of the displacement coordinates, X_i. It means that all systems must have the same – constant – entropy at zero temperature. This law was formulated by Nernst:

> At absolute zero temperature all thermodynamic systems have the same entropy; this value can be taken as zero.

In fact, even more seems to be true: there are experiments, done with certain materials, like phosphine, which exist in a number of very similar crystalline structure, in so called allotropes. At a given temperature, T_a, the equilibrium phase, A, changes to a state B or it continues being in state A, which becomes metastable. By the transition to state B a latent heat, Q_L is released. The heat capacity at $T = 0$ is zero, it cannot be else. An equilibrium state a little above T_a can be achieved by following either the stable path and then regaining the latent heat, or by following the metastable path. One obtains

$$S(T_a^+) = S_A(0) + \int_0^{T_a} C_A(T)\frac{\mathrm{d}T}{T} = S_\mathrm{B}(0) + \int_0^{T_a} C_B(T)\frac{\mathrm{d}T}{T} + \frac{Q_L}{T_a}. \tag{3.78}$$

Here, every term is measurable besides $S_A(0)$ and $S_\mathrm{B}(0)$. Such measurements verify that indeed $S_A(0) = S_\mathrm{B}(0) = 0$.

The most famous consequence of fixing the zero point of the entropy to be $S(0, X_i) = 0$ is that no physical system can be cooled to the absolute zero temperature in a finite number of adiabatic steps. The reason lies in the fact that approaching the $T = 0$, $S = 0$ point between curves of differently fixed X_i, the changes become continuously smaller and smaller. This also means that the curves for different X_i meet in this point,

$$\lim_{T\to 0} \left.\frac{\partial S}{\partial X_i}\right|_T = 0. \tag{3.79}$$

The statistical background of the third law is less obvious than that for the other laws. Utilizing Boltzmann's entropy formula, the number of states at $T = 0$ made by N degrees of freedom is only one, if it is non-degenerate, or a number g_N, called degeneracy. The third law requires that

$$S(0) = -k_\mathrm{B} \sum_i p_i \ln p_i = 0. \tag{3.80}$$

This sum of non-negative terms, $-p_i \ln p_i$, can be zero only if all contributions are zero. Any single contribution, $-p_i \ln p_i$ is only then zero if either $p_i = 0$ or $p_i = 1$. With other words for all probabilities (relative occurrences of a given state in an ensemble) the $p_i^2 = p_i$ property holds. Such states are *pure states* in the language of quantum physics. Furthermore, since by construction $\sum_i p_i = 1$, only one kind of state i may have $p_i = 1$ and all the other states have $p_i = 0$. Typically ground states of quantum systems have this property.

Very often the selected state which is realized by zero entropy is not singled out by the requirement of having the least energy, i.e. a ground state of the system. Such ground states called degenerate, and the realization of just one possibility among several degenerate ground states is a *spontaneous symmetry breaking*. A good example is a ferromagnet: in its ground state it has an infinite degeneracy due to possible rotations as a whole. But this degeneracy does not depend on the number of spins, so it does not interfere with the third law. The rotation of a ferromagnet is not a new permutation of the state of spins.

Having nonzero entropy in a system on the other hand means that more than one type of state is realized in the ensemble: since the p_i-s are not just zero and one, they can have other values in $(0,1)$ and still sum up to 1. During the time evolution of a big system several states are re-visited, and its parts configure several different states as time passes by. Nonzero entropy this way implies nonzero absolute temperature.

In summary, the classical notion of temperature is related to that of the heat (change in energy not counted for by the work of the thermodynamical forces) and to entropy, which turns out to be a measure of the internal disorder. The total change of the entropy can be obtained by taking the difference of the internal energy change and a sum of non-differentials (like mechanical work, chemical work, etc.) and then multiplying by an integrating factor $1/T$.

3.3 The Temperature Related to a Lagrange Multiplier

The equilibrium state in thermodynamics is described by maximum entropy with various extra conditions depending on the physical boundary conditions to the equilibration process. This formulation is often referred to as the *Jaynes principle*. Obtaining a thermal equilibrium state therefore is basically a variational problem. The entropy – a function of macroscopic variables in the form of an *equation of state* or a functional of microstate probabilities in the statistical approach – reaches its maximum in equilibrium. The different constraints, either due to conservation laws restricting the microscopical dynamics or just due to the arrangement of macroscopic boundaries isolating or allowing flows and work through them,[6] have to be taken into account.

A variational problem with constraints can be handled by the method of Lagrange. This is a mathematical method, applied in theoretical mechanics, in field theory, and in several other disciplines of physics, and last but not least in thermodynamics. This method is also more general than the content of the zeroth law discussed so far: by extremizing (maximizing or minimizing) a quantity (function or functional) with the parallel fulfillment of constraints is equivalent to extremizing another quantity, obtained by linearly mixing these constraints to the original quantity. Here, a very basic salient property of a maximum has to be noted: whenever a function has its maximum, at the same value of argument another function, a strict monotonic function of the previous one, also has its maximum. So the principle $S =$ maximum is virtually equivalent to $\Phi(S) =$ maximum. Such Φ functions are very numerous, more than continuously many.[7] The main word of caution, which

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[6] In the language of classical thermodynamics these boundaries are called "walls."

[7] The cardinality of their set is $\aleph_2 = 2^{\aleph_1}$.

has to be said here, is a warning: the second derivative, $S''(E)$ is already influenced by using $\Phi(S(E))$ instead of $S(E)$. This way the stability of the equilibrium may look differently by using the $S =$ maximum or $\Phi(S) =$ maximum principle.

3.3.1 Lagrange Method for Handling Constraints

Maximizing the entropy of a system by the Lagrange method leads to the form

$$S(E,X_i) - \lambda_E C_E(E) - \sum_i \lambda_i C_i(X_i) = \text{max}. \tag{3.81}$$

Here, the internal energy E plays a special role, the thermodynamical displacements X_i can be the volume, V, the particle number, N, or any further quantity of relevance in the physical problem. The factors λ_E and λ_i are the so called *Lagrange multipliers*. The partial derivatives with respect to the Lagrange multipliers lead to the constraints taken into account:

$$\begin{aligned} C_E(E) &= 0, \\ C_i(X_i) &= 0. \end{aligned} \tag{3.82}$$

The maximization with respect to the thermodynamical variables internal energy, E, and general displacement, X_i, (e.g. V, N, etc.), leads to equations reminding to the discussion of the zeroth law:

$$\begin{aligned} \frac{\partial S}{\partial E} - \lambda_E\, C_E'(E) &= 0, \\ \frac{\partial S}{\partial X_i} - \lambda_i\, C_i'(X_i) &= 0. \end{aligned} \tag{3.83}$$

Here, we restricted ourselves to unmixed constraints, C_E depended only on E, and C_i only on X_i. This restriction makes sense in the view of the zeroth law: in composable systems the total energy, $E_{12} = E_1 \oplus E_2$, – and similarly any other composed extensive quantity – satisfies an $L(E_{12}) = L(E_1) + L(E_2)$ type composition law. That such kind of composition laws can be obtained as a result of a limiting procedure by repeating the composition of small amounts will be discussed in Chap. 5. In this general case, the total entropy of a system containing several subsystems indexed by $a = A, B, \ldots$ is chosen as the quantity to be maximized in equilibrium:

$$\sum_a S(E_a, N_a, V_a, \ldots) - \lambda_E \sum_a L_{\mathrm{E}}(E_a) - \lambda_N \sum_a L_N(N_a) - \lambda_V \sum_a L_V(V_a) - \ldots = \text{max}. \tag{3.84}$$

With other words the composite values, $L_{\mathrm{E}}(E) = \sum_a L_{\mathrm{E}}(E_a)$, are fixed. For such composition laws in general and for the additive composition law in particular (replacing $L_E'(E) = 1$, etc.) we obtain from (3.83) that the Lagrange multipliers are given as

$$
\begin{aligned}
\lambda_E &= \frac{1}{L'_E(E_a)}\frac{\partial S}{\partial E_a} = \frac{1}{T},\\
\lambda_N &= \frac{1}{L'_N(N_a)}\frac{\partial S}{\partial N_a} = -\frac{\mu}{T},\\
\lambda_V &= \frac{1}{L'_V(V_a)}\frac{\partial S}{\partial V_a} = \frac{p}{T},\\
&\dots
\end{aligned}
\tag{3.85}
$$

This demonstrates that even for non-additive but associative composition laws for the macrovariables the Lagrange multipliers are related to the entropic intensives occurring due to the zeroth law of thermodynamics.

3.3.2 Statistical Picture

In the statistical picture, the above correspondence is realized by assuming a probabilistic distribution of values for subsystems. In the classical kinetic theory, such a subsystem is already microscopic, say an atom in an ideal gas or a localized spin in a magnetic crystal. The entropy of a system with $\mathscr{N}$ states, with $\mathscr{N}_i = p_i \mathscr{N}$ being the degeneracy number of a state with given microscopic properties, say an energy level of ε_i, was already given in (3.42). It was derived from the elementary permutation formula (3.39). Here, we repeat it, because of its central importance; at the same time we make room for a possible generalization of the permutation formula (for the case of non-independent states) in our notation:

$$
S = k_{\mathrm{B}}\mathscr{N}\left[(\ln\mathscr{N} - 1)\left(1 - \sum_i p_i\right) + \sum_i \sigma(p_i)\right]. \tag{3.86}
$$

In the case of independent states – and therefore permutations – from this the Boltzmann–Gibbs formula arises with

$$
\sigma(p_i) = -p_i \ln p_i. \tag{3.87}
$$

This quantity is positive for any p_i between zero and one, reaching the value zero in these two extremes only. Furthermore this expression is concave, and it ensures that the entropy is additive for taking subsets of states with independent occurrence probabilities. More about generalizing the very formula $\sigma(p_i)$ will be mentioned in Chap. 5.

Now we concentrate on the constraints by maximizing the entropy, the other basic ingredient of the Lagrange method. For the sake of simplicity we select out the energy to be constrained, discussing this way the canonical distribution, p_i.

Considering a general, *L-additive* energy composition law, in the state i with degeneracy $\mathcal{N}_i$ the composition has to be done $\mathcal{N}_i$-fold. This results in

$$\sum L(\varepsilon_i) = \mathcal{N}_i L(\varepsilon_i) = L(E_i). \tag{3.88}$$

Further composing these to the total system with overall number of states $\mathcal{N} = \sum_i \mathcal{N}_i$ we arrive at

$$\sum_i L(E_i) = \sum_i \mathcal{N}_i L(\varepsilon_i) = L(E). \tag{3.89}$$

Such a result is valid for *composable* constraints on the energy. They have the following form

$$C_E = \mathcal{N} \left(\sum_i p_i L(\varepsilon_i) \right) - L(E) = 0. \tag{3.90}$$

The Lagrange method leads us to the vanishing derivative

$$\frac{\partial}{\partial p_i} (S - \lambda C_E) = \mathcal{N} k_{\mathrm{B}} \left(1 - \ln \mathcal{N}\right) + k_{\mathrm{B}} \mathcal{N} \sigma'(p_i) - \lambda \mathcal{N} L(\varepsilon_i) = 0. \tag{3.91}$$

Remembering that we made use of the Stirling formula, we note that this relation is expected to be valid in the $\mathcal{N} \to \infty$ limit. The solution for the probability distribution, p_i is hence given by an equation of the form

$$k_{\mathrm{B}} \sigma'(p_i) = \lambda L(\varepsilon_i) + \alpha \tag{3.92}$$

with α being a state independent (but ensemble dependent) constant. For the Boltzmann–Gibbs entropy formula the elementary derivative, σ' is given as

$$\sigma'_{\mathrm{BG}}(p_i) = -1 - \ln p_i, \tag{3.93}$$

and the solution of the maximizing (3.92) turns out to be

$$p_i = \frac{1}{\mathcal{N}} \mathrm{e}^{-L(\varepsilon_i)/k_{\mathrm{B}} T}. \tag{3.94}$$

Checking it against the normalization condition,

$$\sum_i p_i = \frac{1}{\mathcal{N}} \sum_i \mathrm{e}^{-L(\varepsilon_i)/k_{\mathrm{B}} T} = 1, \tag{3.95}$$

it follows a remarkable expression for the number of all states:

$$\mathcal{N} = \sum_i \mathcal{N}_i = \sum_i \mathrm{e}^{-L(\varepsilon_i)/k_{\mathrm{B}} T}. \tag{3.96}$$

Since this quantity expresses at the same time the sum of degenerate quanta in a state with individual energy ε_i, it is called the *partition sum*.

Other constraints can be taken into account in a similar way. Using the *BG* entropy the grand canonical partition is given by

$$\ln \mathcal{N}_i = \ln(\mathcal{N} p_i) = -\frac{1}{k_{\mathrm{B}} T} L_{\mathrm{E}}(\varepsilon_i) + \frac{\mu}{k_{\mathrm{B}} T} L_N(n_i), \tag{3.97}$$

with the general particle number composition law

$$\sum_i \mathcal{N}_i L_N(n_i) = L_N(N). \tag{3.98}$$

Similarly, the pressure ensemble constrains the composed volume

$$\sum_i \mathcal{N}_i L_V(\mathrm{v}_i) = L_V(V), \tag{3.99}$$

and leads to

$$\ln \mathcal{N}_i = \ln(\mathcal{N} p_i) = -\frac{1}{k_{\mathrm{B}} T} L_{\mathrm{E}}(\varepsilon_i) - \frac{p}{k_{\mathrm{B}} T} L_V(\mathrm{v}_i). \tag{3.100}$$

In the box below we summarize the most important quantities and their relations to the Boltzmann–Gibbs partition process of all possible states, with X_a general displacement variables (they can be the energy, E, the volume V, the particle number N, etc.), their corresponding composition functions L_a and the Lagrange multiplier combinations $\lambda_a / k_{\mathrm{B}} = \mu_a / k_{\mathrm{B}} T$:

Number of specific states	$\mathcal{N}_i = \exp\left(-\sum_a \frac{\mu_a}{k_{\mathrm{B}} T} L_a(X_{ai}) \right)$
Partition sum	$\sum_i \mathcal{N}_i = \mathcal{N}$
Total composition	$\sum_i \mathcal{N}_i L_a(X_{ai}) = L_a(X_a)$
Probability distribution	$p_i = \frac{\mathcal{N}_i}{\mathcal{N}}$

3.3.3 Information and Knowledge

The extensive quantity associated to the absolute temperature, the entropy, also has different facets: (1) it describes a phenomenological thermodynamic potential to be maximized in equilibrium, (2) it is a logarithmic measure of the number of microstates realizing the same macrostate, (3) it is – in the Boltzmann–Gibbs scenario an additive – measure of the probability to find a given state in an ensemble. Satisfying the requirements of the most general theory of equilibrium, namely thermodynamics, the statistical entropy carries this bonus; it is connected to probability.

Let us write the BG entropy in a slightly different form, than previously:

$$\varsigma = \sum_i p_i \ln \frac{1}{p_i} = \left\langle \ln \frac{1}{p_i} \right\rangle, \tag{3.101}$$

with $S = k_{\mathrm{B}} \mathscr{N} \varsigma$ being the quantity discussed in the previous subsection. Perhaps one of the most important properties of the notion of probability is that rare events have a small probability. Our expectation for the number of finding a value (or state or event) with probability p_i is proportional to this probability. The quantity $1/p_i$ is therefore the greater the less probable a state (event) is in the studied ensemble. In a way its logarithm, $\ln(1/p_i)$, can be called with right *unexpectedness*.

Through this interpretation the idea of entropy can be connected to the measure of information. Observing a less probable event, one achieves a larger restriction with respect to making further predictions, than by observing a more common case. The above measure of unexpectedness describes the gain in information. More precisely the formula (3.101), containing the logarithm function, is predestined for being additive for probabilities, which are in form of a product. And exactly the *joint probability* of two events, say A and B, is then and only then a product, if the events are independent. Let the joint probability be p^{AB}, then the so called *marginal probabilities* are given as

$$p^A = \sum_B p^{AB}, \qquad p^B = \sum_A p^{AB}. \tag{3.102}$$

Here, the summation runs over all possibilities (states) of the respective event (physical system) A or B. This way p^{AB} is the joint probability for one subsystem being in a given state, A, *while* the other subsystem is in another given state, B. The marginal probability, p^A is the probability to find the first subsystem in state A *irrespective* to the state of the other subsystem. p^B is the same quantity by interchanging the roles. With the help of these quantities it is straightforward to define the *conditional probabilities*. The conditional probability for the subsystem to be in state A, while the other subsystem is in the state B is given by the normalized ratio

$$p^{A|B} = \frac{p^{AB}}{p^A}, \tag{3.103}$$

and correspondingly for the conditional probability $p^{B|A}$. This relation can be used to reconstruct the joint probability from marginal probabilities as

$$p^{AB} = p^A p^{A|B} = p^B p^{B|A}. \tag{3.104}$$

If the events (or states) are independent, then the condition is meaningless: $p^{A|B} = p^B$ and $p^{B|A} = p^A$ and one cannot gain any information on system B by observing (measuring the probability distribution of) system A, or vice verse. This is the case when the joint probability is the product of marginal probabilities:

$$p^{AB} = p^A p^B. \tag{3.105}$$

The BG-unexpectedness in this case is additive. The measure of information, gainable by the knowledge of the marginal probability p^A on the distribution p^B therefore relies in the entanglement or correlation of the respective states, in the deviation from the above multiplicative probability law. The *mutual information* is measured by the difference between the joint entropy and the sum of marginal entropies:

$$I(A:B) = \varsigma(A) + \varsigma(B) - \varsigma(AB). \tag{3.106}$$

This definition is symmetric and non-negative. It is only then zero, if the events (or systems) are independent. Let us describe one system with probabilities p_i for states i, and the other system with q_j for the states j. The joint states ij have a probability of r_{ij}. The sum of the normalized entropies is given by

$$\varsigma(A) + \varsigma(B) = \sum_i p_i \ln \frac{1}{p_i} + \sum_j q_j \ln \frac{1}{q_j}. \tag{3.107}$$

Using now the definition of marginal probabilities in the forefactors in front of the logarithms this can be written as

$$\varsigma(A) + \varsigma(B) = \sum_{i,j} r_{ij} \ln \frac{1}{p_i q_j}. \tag{3.108}$$

Based on this the mutual information (3.106) becomes

$$I(A:B) = \sum_{i,j} r_{ij} \ln \frac{r_{ij}}{p_i q_j}. \tag{3.109}$$

The state assumed with minimal knowledge has independent subsystems, $r_{ij} = p_i q_j$, and zero information, $I(A:B) = 0$. The independence criterion for canonical thermal states using $p_i \sim \exp(-\varepsilon_i/k_{\mathrm{B}}T)$, $q_j \sim \exp(-\varepsilon_j/k_{\mathrm{B}}T)$ and $r_{ij} \sim \exp(-\varepsilon_{ij}/k_{\mathrm{B}}T)$ is equivalent to

$$\varepsilon_{ij} = \varepsilon_i + \varepsilon_j. \tag{3.110}$$

Another form of energy distributions, e.g. a cut power-law,

$$p_i = \frac{1}{Z}\left(1 + a\varepsilon_i\right)^{-v}, \tag{3.111}$$

can describe a zero information state if

$$p_i q_j = \frac{1}{Z^2}\left(1 + a\varepsilon_i + a\varepsilon_j + a^2\varepsilon_i\varepsilon_j\right)^{-v} = r_{ij} = \frac{1}{Z_2}\left(1 + a\varepsilon_{ij}\right)^{-v}. \tag{3.112}$$

This requires a non-additive energy composition rule:

$$\varepsilon_{ij} = \varepsilon_i + \varepsilon_j + a\varepsilon_i\varepsilon_j. \tag{3.113}$$

3.4 The Temperature as a Property of the Noise

We have experienced different roles of the temperature in the theory of thermal, and in a general sense statistical, phenomena. As an intensive parameter describing equilibrium between energy distributed states of macroscopic systems, it has its most basic – and most phenomenological – thermodynamical description. Slow and mild changes, going through reversible or irreversible chains of macrostates, point out that $1/T$ can be used to define a variable of state, the entropy S, which value is independent of the way the state was achieved. Mathematically, then $1/T$ is an integrating factor, making it possible that a sum of non-differentials (mechanical and chemical work, heat, etc.) is related to the differential of entropy, $\mathrm{d}S$. Due to the kinetic and statistical foundation of the main anchor points of thermodynamics, the concept of entropy became based on the probability distribution of microstates. Thermal equilibrium maximizes the total entropy due to being most of the time in the most probable microstates. Constraints on the physical exchange of other quantities, however, enriches the maximum entropy principle by terms containing further functionals of the probability distribution: total energy, volume, particle number, etc. The inverse absolute temperature, $\beta = 1/k_{\mathrm{B}}T$, occurs in the correct handling of such situations as a Lagrange multiplier.

The mathematical role, the temperature plays in statistical models, and the physical properties of macrosystems in and near thermal equilibrium are therewhile intertwined. The quantity satisfying the zeroth law of thermodynamics and being a universal intensive variable of state is not guaranteed to be identical to a Lagrange multiplier of a constraint taken as an ansatz in a statistical model. In particular the constraint may have a meaning which is or is not realized by physical circumstances when bringing macroscopic bodies in contact with each other. Fortunately, many details do not count at the end: in the so called thermodynamical limit the behavior of big systems is more universal.

Considering possible generalizations of the classical thermodynamics – in order to describe phenomena not following the classical ideals – some basic assumptions can be loosened. Most prominently the additivity of the extensive variables of state, leading to working out a non-extensive thermodynamics, and the factorizing (independence) hypothesis about microstate probabilities, leading to a non-extensive statistical physics, using novel entropy formulas. One of the most intriguing questions by this research is that – by abandoning additivity and probabilistic independence – whether the classical equivalences between the role of intensive variables, in particular the temperature, remains intact. We have demonstrated by discussing the zeroth law that indeed the factor $1/T$ still can be used consequently and sensibly, but its relation to the entropy – energy relation may change.

We summarize these thoughts in the following statement: the concept of temperature can be used in a wider range of physical descriptions as it was envisioned by the classical, Gibbsean–Boltzmannian thermodynamics, but its correspondence with microscopic quantities may need a re-interpretation. In particular, calculating the temperature in relation with Lagrange multipliers to constraints, it will depend on the formulation of the constraint and the very entropy formula used, how it is related to properties of the probability distribution. And because in thermodynamics the most decisive distribution is that of the energy (irrespective to other details, like e.g. direction of the velocities of the constituents), the properties of the energy distribution have to be related to the temperature.

In the kinetic measurement of temperature, described in the previous chapter, we have seen that the average energy per particle is a simple function of the temperature. For ideal gases it is even proportional to that. In this section, we go after another connection: the relation between the width of the probability distribution and the temperature. Is only the average energy is determined by the temperature? The Lagrange multiplier role would suggest that. Or further properties, like the width, or perhaps the whole equilibrium distribution is determined by this single parameter? The ideal Maxwell–Boltzmann gas and the canonical Gibbs distribution support this view quite strongly. And what if further parameters influence the distribution, most prominently its width besides the expectation value? Can this further parameter comply with universality and independence requirements of the classical thermodynamics discussed so far? In such cases, is still a temperature there?

3.4.1 Brownian Motion and Einstein Temperature

The width of the energy distribution instead of the mean value plays the leading role in the studies of a wide class of physical phenomena. Most prominently diffusion is a phenomenon, where a material becomes dispersed in the medium of another, without any seeming preference to a direction or a place. The width of the distribution steadily grows, while no trend can be discovered for the mean value. Of course, the expectation value of the square of one quantity can be related to the expectation value of another one. Remarkably, this is the case between the kinetic energy and the momentum vector of non-relativistic, massive particles

$$E = \frac{1}{2m}\mathbf{p}^2. \tag{3.114}$$

Such particles move seemingly random, changing the direction of their motion nervously. This unpredictable motion can be described by modeling this randomness as an action of forces acting independently and uniformly in all directions in arbitrarily close time instants. The phenomenon of this motion has been experimentally observed by Robert Brown, studying the motion of pollen in water under the microscope in 1827. The theoretical description of the Brownian motion, in its simplest form as a random walk, is due to Albert Einstein in 1905.

Let us assume that the momentum is changing only by very short term, drastic interactions, the so called collisions. By a spherically symmetric elastic collision, the most common case for monoatomic gases, the magnitude of the momentum vector of the atoms is unchanged, only its direction changes. Assuming further a constant rate of collisions, the time between subsequent collisions, Δt, is also a constant. The change of a representative momentum vector under the action of the force **F** for a time $\delta t \ll \Delta t$ is described by the following equation

$$\mathbf{p}(t+\Delta t) = \mathbf{p}(t) + \delta t \mathbf{F}. \tag{3.115}$$

The force vector **F** is a *random variable*. All of its components are distributed symmetrically to the zero value, therefore its expectation (long time average) value vanishes

$$\langle \mathbf{F} \rangle = 0. \tag{3.116}$$

Due to elastic collisions the momentum vector, **p**, changes only its direction, but not its length. The expectation value of the energy per particle is given by[8]

$$\left\langle \frac{\mathbf{p}^2}{2m} \right\rangle = \frac{3}{2} k_\mathrm{B} T. \tag{3.117}$$

The position of a particle changes between two collisions by flying undisturbed with a velocity $\mathbf{p}/m$ for the mean inter-collision time, Δt. Therefore, the position vector, $\mathbf{r}(t)$, changes as

$$\mathbf{r}(t+\Delta t) = \mathbf{r}(t) + \Delta t \frac{\mathbf{p}}{m}. \tag{3.118}$$

Since the average momentum vector is zero, the position of the particle after several collisions is unpredictable. The squared distance from the starting point, however, can well be estimated:

$$\left\langle \mathbf{r}^2 \right\rangle (t+\Delta t) = \left\langle \mathbf{r}^2 \right\rangle (t) + 2\frac{\Delta t}{m} \langle \mathbf{r}\cdot\mathbf{p} \rangle + \frac{\Delta t^2}{m^2} \left\langle \mathbf{p}^2 \right\rangle. \tag{3.119}$$

The middle term in the above equation vanishes due to the random direction of the momentum vector: $\langle \mathbf{r}\cdot\mathbf{p} \rangle = 0$. The average value of $\mathbf{p}^2$ is obtained from the equipartition value of the kinetic energy (3.117). This way one concludes that the squared distance grows from collision to collision as

$$\left\langle \mathbf{r}^2 \right\rangle (t+\Delta t) = \left\langle \mathbf{r}^2 \right\rangle (t) + 3\frac{\Delta t^2}{m} k_\mathrm{B} T. \tag{3.120}$$

After a finite time t sufficient for $N = t/\Delta t$ collisions the distance squared from the original position of the particle grows linearly with this time. Starting at the origin, $\mathbf{r}(0) = \mathbf{0}$, and

---

[8] See the previous section about the kinetic temperature.

$$\left\langle \mathbf{r}^2 \right\rangle(t) = \frac{3\Delta t\, k_{\mathrm{B}} T}{m} t = 2Dt, \tag{3.121}$$

with $D = 3k_{\mathrm{B}}T\Delta t/2m$ being the diffusion constant. In fact the diffusion constant, measurable by observing the particles position vs. the time passed, is proportional to the temperature. The temperature obtained by using diffusion measurement is sometimes called the *Einstein temperature*.

3.4.2 Langevin and Fokker–Planck Equation

A description of the Brownian motion based on dynamics is given by the classical Langevin equation. A balance between damping and accelerating forces leads to a stationary state, with vivid microscopical dynamics, but macroscopically (on the average over many particle paths) it presents a thermodynamical equilibrium state. General statements about this balance are comprised in the fluctuation – dissipation theorem.

Let us consider a simple, one degree of freedom motion. The change of momentum p in time is given by a force depending on this momentum and on a noise variable z:

$$\dot{p} = F(p,z). \tag{3.122}$$

Such descriptions are called “mesoscopic,” since the dynamics of a selected particle is followed, but the effect of further particles is not calculated microscopically: it is comprised in using the notion of *noise*, and in assuming random distribution of the variable z. Following the method pioneered by Uhlenbeck and Ornstein [17], a distribution of many possible values of p at a time t can be considered. This $f(p,t)$ distribution governs average values of a smooth but otherwise arbitrary test function $R(p)$. The same integral over p can be expressed at the time $t+\Delta t$ assuming a statistical average over the noise z in the time interval passed since t:

$$\int \mathrm{d}p R(p) f(p,t+\Delta t) = \int \mathrm{d}p \left\langle R(p+\Delta t\, F(p,z)) \right\rangle f(p,t). \tag{3.123}$$

One assumes that the averaging of the force F over the noise z gives the result:

$$\begin{aligned} \langle F \rangle &= -G(p), \\ \langle F F \rangle - \langle F \rangle \langle F \rangle &= 2D(p)/\Delta t. \end{aligned} \tag{3.124}$$

The above scaling of the correlation with Δt follows from the Gaussian nature of the noise z. Expanding now (3.123) up to terms linear in Δt one arrives at:

$$\int \mathrm{d}p R(p) \frac{\partial f}{\partial t}(p,t) = \int \mathrm{d}p \left[-G(p)R'(p) + D(p)R''(p) \right] f(p,t). \tag{3.125}$$

After partial integration and considering arbitrary $R(p)$ one gets the Fokker–Planck equation:

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial p}(Gf) + \frac{\partial^2}{\partial p^2}(Df). \tag{3.126}$$

The original Langevin problem

The above Langevin and Fokker–Planck problem is still quite general. Damping and diffusion coefficients depend on the momentum p in a general way. Ergodization in phase space is achieved on the other hand when constant energy surfaces are covered. In such a situation, the distribution f, as well as the coefficients G and D (the latter related to the noise), depends on the energy $E(p)$ only. This case shall be discussed in Chap. 5.

The original Langevin equation [18] considers an energy independent diffusion and damping constant, D and G, respectively. This particular Langevin equation is given by

$$\dot{p} = z - G\frac{p}{m} \tag{3.127}$$

containing a damping proportional to the non-relativistic velocity, and a noise with zero mean $\langle z(t)\rangle = 0$, and with a correlation restricted to the same time instant only. The latter assumption is expressed in a correlation proportional to the Dirac-delta function,

$$\langle z(t)z(t')\rangle = 2D\delta(t-t'). \tag{3.128}$$

Equation (3.127) is linear, so it has a formal solution for $p(t)$:

$$p(t) = p(0)\mathrm{e}^{-Gt/m} + \int_0^t z(t')\mathrm{e}^{G(t'-t)/m}\mathrm{d}t'. \tag{3.129}$$

The expectation value of the momentum shows just a “forgetting” process of the initial value, since the noise term z has zero mean:

$$\langle p\rangle(t) = p(0)\mathrm{e}^{-Gt/m}. \tag{3.130}$$

After a long time, $t \to \infty$, this approaches zero. The kinetic energy, however, will have a contribution from the noise squared, and therefore does not vanish in the long term. By using the solution (3.129) one obtains

$$\langle E\rangle = \left\langle \frac{p^2}{2m} \right\rangle = E(0)\mathrm{e}^{-2Gt/m} + \frac{1}{2m}\int_0^t\int_0^t \langle z(t')z(t'')\rangle\,\mathrm{e}^{G(t'+t''-2t)/m}\,\mathrm{d}t'\,\mathrm{d}t''. \tag{3.131}$$

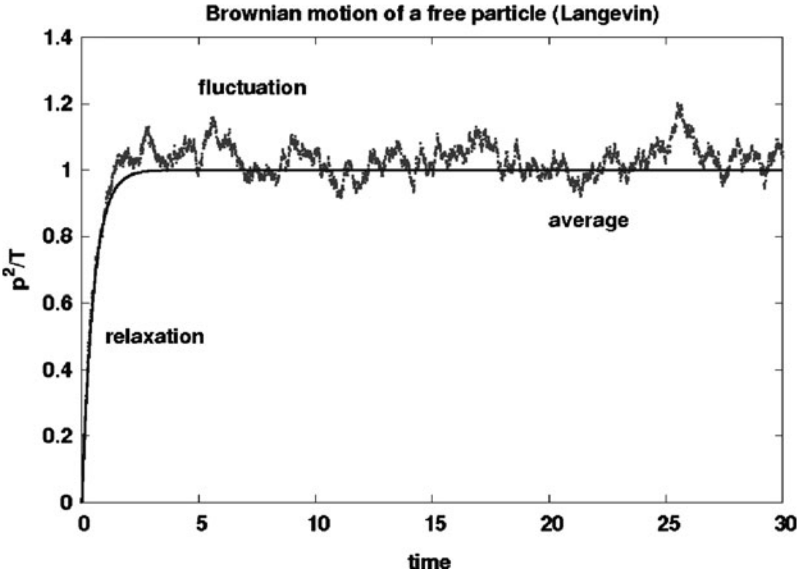

Fig. 3.3 The solution of the original Langevin equation, designed for a classical Brownian particle: the equilibration of the fluctuating kinetic energy averaged over 1,000 trajectories can be followed

Substituting now the noise correlator (3.128) one of the integrals can be carried out by using the Dirac-delta factor. We arrive at

$$\langle E \rangle = E(0)\mathrm{e}^{-2Gt/m} + \frac{D}{m}\int_0^t \mathrm{e}^{2G(t'-t)/m}\,\mathrm{d}t'. \tag{3.132}$$

The last integral can be carried out analytically, resulting in

$$\langle E \rangle = E(0)\mathrm{e}^{-2Gt/m} + \frac{D}{2G}\left(1-\mathrm{e}^{-2Gt/m}\right). \tag{3.133}$$

Finally, after a sufficiently long time, the energy of the particle in this one-dimensional model approaches

$$\lim_{t\to\infty}\langle E \rangle = \frac{D}{2G}. \tag{3.134}$$

Comparing this with the equipartition condition, $\langle E \rangle = k_{\mathrm{B}}T/2$, one obtains a relation between the damping and diffusion coefficients (Fig. 3.3):

$$D = k_{\mathrm{B}}T\,G. \tag{3.135}$$

This is a special case of the fluctuation – dissipation theorem.

The Fokker–Planck equation (3.126) contains in this case the factors D and Gp/m under the partial derivatives with respect to p, the factors D and G/m can be taken to the front. We obtain

$$\frac{\partial f}{\partial t} = \frac{G}{m}\frac{\partial}{\partial p}(pf) + D\frac{\partial^2}{\partial p^2} f. \tag{3.136}$$

The stationary distribution, f_{s}, is restricted by the detailed balance condition

$$\frac{Gp}{m} f_{\mathrm{s}} + D\frac{\partial}{\partial p} f_{\mathrm{s}} = 0. \tag{3.137}$$

This can easily be solved for the stationary momentum distribution:

$$f_{\mathrm{s}}(p) = C \exp\left(-\frac{Gp^2}{2mD}\right). \tag{3.138}$$

Considering this result as a distribution of the kinetic energy, $E = p^2/2m$, one arrives at

$$f_{\mathrm{s}}(p) = C \exp\left(-\frac{GE(p)}{D}\right). \tag{3.139}$$

This is a Boltzmann–Gibbs distribution with the Einstein-temperature, $k_{\mathrm{B}}T = D/G$.

3.4.3 Central Limit Theorem

There is a specific mathematical property supporting the applicability of statistical physics: The probability distribution of an appropriately scaled sum (average) of a large number of random variables fold to a Gaussian distribution. Moreover, the width of this "limiting distribution" scales down with increasing number of individual constituents. As a consequence, the most probable values and averages of quantities summed up from contributions of a great number of individual components (e.g. particles) do behave "almost" deterministically, as they had a sharp value. This property is expressed nicely in the central limit theorem [19, 20]. An enlightening example of this statistical phenomenon is presented by the distribution of the sum of random variables uniform on a finite interval.

Let x_i be a random variable, distributed according to the distribution $w(x_i)$. We are interested in the distribution of a scaled sum of $\mathscr{N}$ such, identically distributed variables. This is described by the following $\mathscr{N}$-fold integral:

$$P_{\mathscr{N}}(x) = \int \prod_{i=1}^{\mathscr{N}} w(x_i)\mathrm{d}x_i\, \delta\left(x - a_{\mathscr{N}} \sum_{k=1}^{\mathscr{N}} x_k\right). \tag{3.140}$$

Here, we assume that the joint probability is a product of the individual probabilities: This is the requirement of statistical independence. With this assumption the seeked probability distribution is an $\mathscr{N}$-fold convolution. Its Fourier transform,

$$\tilde{P}_{\mathscr{N}}(k) = \int \mathrm{d}x\, \mathrm{e}^{\mathrm{i}kx} P_{\mathscr{N}}(x), \tag{3.141}$$

then becomes a product of properly scaled Fourier transforms of the individual probabilities:

$$\tilde{P}_{\mathscr{N}}(k) = \prod_{i=1}^{\mathscr{N}} \tilde{w}(a_{\mathscr{N}} k). \tag{3.142}$$

From the Taylor expansion of $\ln \tilde{P}_{\mathscr{N}}(k)$ around $k = 0$ one obtains the *central moments* (correlations):

$$\sigma^{(\ell)} := \frac{1}{i^{\ell}} \frac{\partial^{\ell}}{\partial k^{\ell}} \ln \tilde{P}_{\mathscr{N}}(k) \bigg|_{k=0}. \tag{3.143}$$

The $\ell = 0$ central moment always vanishes since

$$\ln \tilde{P}(0) = \ln \int P(x) \mathrm{d}x = \ln 1 = 0 \tag{3.144}$$

due to the normalization of the integrated probability. The $\ell = 1$ central moment is the expectation value, $\langle x \rangle$, the $\ell = 2$ moment is the quadratic width, $\langle x^2 \rangle - \langle x \rangle^2$. Higher central moments prove to be the pure correlations, not expressed by lower order expectation values.

Now let us compare the central moments of the distributions $P_{\mathscr{N}}(x)$ and $w(x_i)$. The ℓ-th derivative of the logarithms of the respective Fourier transforms with respect to k differs in the scaling parameter, $a_{\mathscr{N}}$. This way one obtains

$$\sigma_{\mathscr{N}}^{(\ell)} = \sum_{i=1}^{\mathscr{N}} \sigma_i^{(\ell)} a_{\mathscr{N}}^{\ell} = \mathscr{N} \overline{\sigma}^{(\ell)} a_{\mathscr{N}}^{\ell}. \tag{3.145}$$

Here, we denoted the central moment of the $w(x_i)$ distribution by $\overline{\sigma}^{(\ell)}$. Now we would like to chose the scaling factor, $a_{\mathscr{N}}$, appropriately. Suppose that the first non-vanishing central moment of the distribution of the individual random variables is at ℓ_0. This can be $\ell_0 = 1$, but in this case one considers the distribution of $x - \langle x \rangle$ instead of that of x. In practice, therefore, $\ell_0 = 2$ (the width) is the first non-vanishing central moment.

We face the situation when $\sigma_i^{(\ell)} = 0$ for all $\ell < \ell_0$ values and $\sigma_i^{(\ell)}$ is finite for $\ell \geq \ell_0$. The essence of the central limit theorem is that all the higher moments for $\ell > \ell_0$ can be scaled down to zero in the folded distribution by choosing $a_{\mathscr{N}} \propto \mathscr{N}^{-1/\ell_0}$. The resulted scaling, $\sigma_{\mathscr{N}}^{(\ell)} = \mathscr{N}^{1-\ell/\ell_0} \overline{\sigma}^{(\ell)}$, in the $\mathscr{N} \to \infty$ limit leaves us with only one nonzero central moment, the ℓ_0-th one.

The $\ell = 0$ central moment is zero due to the normalization of the probability: $\ln \tilde{P}(0) = \ln 1 = 0$. The first moment ($\ell = 1$) can be made zero by a simple shift in the variables x_i. The second central moment is then the first nontrivial nonzero value. The resulted distribution of the scaled sum has a second moment with all higher moments vanishing, therefore $\ln \tilde{P}(k)$ is quadratic in k,

$$\ln \tilde{P}(k) = -\frac{1}{2}\overline{\sigma}^{(2)} k^2. \tag{3.146}$$

This way $\tilde{P}(k)$ – and with that $P(x)$ – can only be a Gaussian:

$$P(x) = \frac{1}{\sqrt{2\pi\overline{\sigma}^{(2)}}} \, \mathrm{e}^{-\frac{x^2}{2\overline{\sigma}^{(2)}}}. \tag{3.147}$$

We note that the necessary scaling factor by considering the sum is $a_{\mathscr{N}} \propto 1/\sqrt{\mathscr{N}}$.

A nice, simple example is given for x_i-s distributed evenly in the interval $(-1,+1)$. In this case – according to the central limit theorem – the distribution of

$$x = \frac{\sqrt{3}}{\sqrt{\mathscr{N}}} \sum_{i=1}^{\mathscr{N}} x_i \tag{3.148}$$

approaches the normalized Gaussian. Due to the convolution the Fourier transform is a product:

$$\lim_{\mathscr{N}\to\infty} \tilde{P}_{\mathscr{N}}(k) = \lim_{\mathscr{N}\to\infty} \left(\frac{\sin(k\sqrt{3/\mathscr{N}})}{k\sqrt{3/\mathscr{N}}} \right)^{\mathscr{N}}. \tag{3.149}$$

Here, we made use of the fact that the Fourier transform of the uniform distribution on a finite interval is the function $\sin(k)/k$. Using the Taylor-expansion of the $\sin(k)/k$ function one has

$$\frac{\sin(k\sqrt{3/\mathscr{N}})}{k\sqrt{3/\mathscr{N}}} = 1 - \frac{1}{3!}\frac{3}{\mathscr{N}}k^2 + \cdots \tag{3.150}$$

This leaves us with

$$\lim_{\mathscr{N}\to\infty} \tilde{P}_{\mathscr{N}}(k) = \lim_{\mathscr{N}\to\infty} \left(1 - \frac{1}{2\mathscr{N}}k^2\right)^{\mathscr{N}} = \exp(-k^2/2) \tag{3.151}$$

upon using Euler's famous formula for the exponential function. In the Fig. 3.4, the numerical distribution histograms are shown for several values of $\mathscr{N}$. Already the $\mathscr{N} = 3$ case, glued together from three parabola segments, is irritatingly close to the Gaussian at the first sight. This fact should warn us: In order to justify that a distribution is Gaussian, a very large number of elements have to be drawn and analyzed on a logarithmic plot.

A counterexample to "the distribution of a sum were a Gaussian" is given by the Cauchy–Lorentz distribution. It has the Fourier transform $\tilde{w}_i(k) = \exp(-|k|)$. Now there is a limiting distribution with an altered scaling for

$$x = \frac{1}{\mathscr{N}} \sum_{i=1}^{\mathscr{N}} x_i. \tag{3.152}$$

The limiting distribution itself is, however, Lorentzian, it is not the Gauss distribution:

$$\lim_{\mathscr{N}\to\infty} \tilde{P}_{\mathscr{N}}(k) = \lim_{\mathscr{N}\to\infty} \left(\mathrm{e}^{-|k|/\mathscr{N}}\right)^{\mathscr{N}} = \exp(-|k|). \tag{3.153}$$

The Cauchy–Lorentz distribution is a special example for the general class of self-similar Lévy distributions [21].

Challenging the four laws

Finally we summarize again the four laws of classical thermodynamics, discussed in this chapter. The zeroth law derives from the transitivity property of thermal equilibrium the empirical temperature scale and its relation to the equation of state, to the

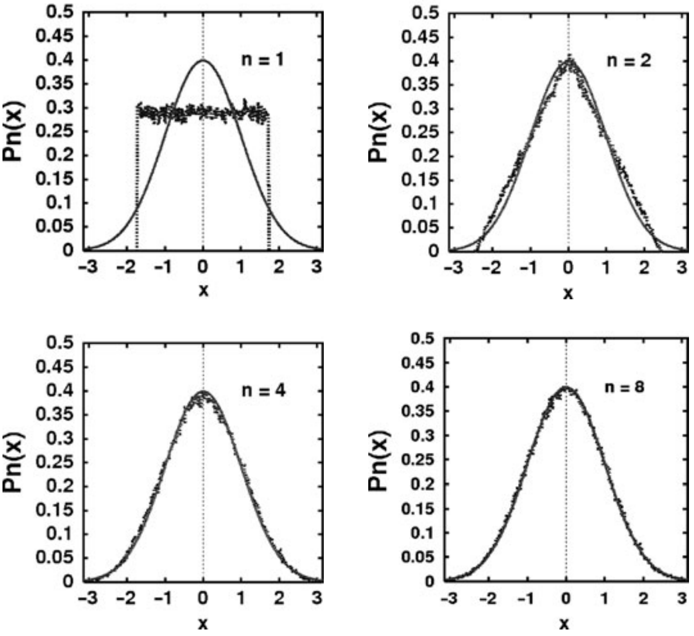

Fig. 3.4 Histograms over the distribution of scaled sums of random variables uniformly distributed in the interval $(-1,+1)$. Inspected on a linear scale already a few terms suffice to simulate a Gaussian distribution, which is the limiting distribution for infinitely many addenda

entropy–energy relation. It is challenged by situations where the energy content cannot be treated additively, but still an equilibrium (or at least a long living stationary state) occurs. In particular, when the "area/volume argument" supporting the neglection of non-additive effects does not hold: in case of experiencing a fractal surface or phase space filling pattern, for unscreened long range interaction and quantum entanglement. We indicate this in the first row in the greybox below.

The first law recovers energy conservation. Historically, it does it in a special context discovering the energy contribution from internal motion as heat (this is the kinetic theory of heat). By taking into account changes of entropy and the work of all thermodynamical forces a differential balance equation has to be satisfied. This is written in the second row.

The second law has several formulations. On the one hand it says that entropy is a variable of state obtained by using an integrating factor $1/T$ to the heat. Therefore, its value is independent of the path along which the state has been reached. In a closed system, it cannot be decreased macroscopically and as a consequence heat always flows from higher temperature bodies to lower temperature ones. The third row in the table below indicates this.

Finally, the third law sets the entropy at zero absolute temperature to be zero. This is a postulate which had to be added to thermodynamics. In quantum systems, this property emerges naturally by the ground state of minimal energy being a pure state: such states have zero Boltzmann entropy.

This time we summarize the laws of thermodynamics in terms of comprehensive formulas:

0. $T_1 = T_2 = \cdots = T_N$ in equilibrium
1. $T\mathrm{d}S = \mathrm{d}E + p\mathrm{d}V - \mu\mathrm{d}N + \cdots$
2. $\mathrm{d}S \geq 0$ for closed systems
3. $S = 0$ at $T = 0$

Problems

3.1. Prove the two leading orders in the Stirling formula for $\ln N!$.

3.2. Determine the occupation probabilities for three states having zero, one and two quanta of the energy ε by excluding all other states. The average energy is fixed to be $\bar{\varepsilon}$.

3.3. Determine the grand-canonical equilibrium distribution for a fractionally fermionic-bosonic system: maximum the fraction qN can be in an indistinguishable state of K states.

3.4. Prove the generalized Markov inequality (3.52).

3.5. What is the distribution of energy differences in an ideal Maxwell–Boltzmann gas?

3.6. The Jensen inequality,

$$\prod_{i=1}^{\mathscr{N}} a_i^{p_i} \leq \sum_{i=1}^{\mathscr{N}} p_i a_i$$

for all $a_i > 0$, $p_i \in [0,1]$ and $\sum_i p_i = 1$ is the generalization of the traditional inequality between the geometric and arithmetic means. Prove this inequality. What does it say for the information entropy?

3.7. Second Law and Life

By thermal equilibration between two subsystems the colder heats up and the warmer body cools down until a common temperature is achieved. How is it possible then, that on the Earth, while steadily gaining energy from the hotter Sun, entropy is virtually reduced by the spontaneous evolution of highly improbable – as highly correlated – structures, shortly named Life.

Chapter 4
Fluctuating Temperature

Differences between ensembles in finite systems, near-equilibrium fluctuations of thermodynamical quantities, correlated particle production and multiplicity distributions.

Challenges of a special kind emerge for the use of classical thermodynamical concepts, in particular the temperature, in "small" systems. In terms of physics, this "smallness" can be expressed in several ways: The geometrical size vs. the correlation range, the system size vs. the spatial extension of typical density fluctuations may as well characterize this feature as the uncertainty of thermodynamical intensives – most prominently the temperature. These challenges to the concept of temperature arise in physical situations when the *thermodynamical limit* is not realized to a satisfactory degree.

Typically, such a case is given in the study of systems with a limited number of degrees of freedom. In nuclear physics, measuring the number and energy of fragments stemming from energetic collisions of atomic nuclei, the distribution of the secondaries reveals information not only about the strong forces acting in the reaction zone but also about the statistical fluctuations varying event by event. These variations, even more pronounced in high energy particle producing experiments, carry information about the "statistical size" of the typical event. This being restricted, the theoretical thermodynamical limit can be very far from reality in such experiments. By considering extended volumina of fireballs emitting hadrons, it is not easy to distinguish between this finite size microcanonical statistical effect on the temperature fitted to spectra and between the local fluctuation of temperature inside a single fireball [22–24].

It is furthermore customary to analyze a huge number of independent collision events, in order to collect enough examples for making a good statistics. In such "averaged" spectra some properties, like the average energy per particle or the mean of the momentum squared, remind us to the most basic thermodynamical concepts. An associated "temperature" can be calculated on this basis; some examples we have presented in the previous chapter. Another measure of the temperature can be accessed by analyzing the typical size of fluctuations, e.g. by studying the distribution

T.S. Biró, *Is There a Temperature? Conceptual Challenges at High Energy, Acceleration and Complexity*, Fundamental Theories of Physics 171,
DOI 10.1007/978-1-4419-8041-0_4,

of the number of produced particles in elementary collision events. The event by event distribution around a mean multiplicity is characteristic to the statistics of independently generated microstates of a few (sometimes several) particles. In such analyses, depending on what is counted for, sometimes independent, another time correlated properties are investigated. The difference between the number distribution of independently produced charges and those which can only be made in pairs is significant. The more significant the less particle is produced in a single collision event. Effects related to this distinction are referred to as a distinction between the canonical and the grand canonical approach to thermodynamics. In a special context, considering light hadron production in heavy ion collisions, it was named to *canonical enhancement*.

4.1 Microcanonical Temperature Distribution

The temperature derived from thermodynamical principles, as we have discussed it in the previous chapter, and the Lagrange multiplier associated to fixing the total energy are related in the canonical distribution as $\beta = 1/k_{\mathrm{B}}T$. In the microcanonical ensemble there is no β parameter, the partition function depends on the total energy. Assuming possible states indexed by n with energy E_n the respective partition functions are defined as

$$\begin{aligned} Z_{\mathrm{C}}(\beta) &= \sum_n \mathrm{e}^{-\beta E_n}, \\ Z_{\mathrm{M}}(E) &= \sum_n \delta(E - E_n). \end{aligned} \tag{4.1}$$

Here, we used the Dirac delta notation for counting $1/\Delta E$ each time the energy of the state equals to the value E within a fixed precision, ΔE. For calculating expectation values and correlations such a constant factor in the partition function does not count at the end.

There is a relation between the canonical and microcanonical approach, derived from the Fourier representation

$$\delta(E - E_n) = \int_{-\pi}^{+\pi} \frac{\mathrm{d}\varphi}{2\pi}\, \mathrm{e}^{\mathrm{i}\varphi(E-E_n)}. \tag{4.2}$$

The microcanonical partition function namely can be expressed as

$$Z_{\mathrm{M}}(E) = \sum_n \int_{-\pi}^{+\pi} \frac{\mathrm{d}\varphi}{2\pi}\, \mathrm{e}^{\mathrm{i}\varphi(E-E_n)}, \tag{4.3}$$

and in the exponential factor one recognizes the formal continuation of the canonical exponential to imaginary arguments, $Z_C(i\varphi)$. Denoting $i\varphi$ by β we arrive at

$$Z_M(E) = \frac{1}{2\pi i} \int_{-i\pi}^{+i\pi} d\beta \, e^{\beta E} Z_C(\beta). \tag{4.4}$$

This is nothing else than the formula for the inverse Laplace transform. The opposite transformation can be derived directly from (4.1):

$$Z_C(\beta) = \int_0^\infty dE \, e^{-\beta E} Z_M(E). \tag{4.5}$$

The canonical probability of being in state n is given by

$$P_{nC} = \frac{1}{Z_C(\beta)} e^{-\beta E_n}, \tag{4.6}$$

while the microcanonical probability is

$$P_{nM} = \frac{1}{Z_M(E)} \delta(E - E_n). \tag{4.7}$$

These two expressions are quite different functions of E_n; moreover, one is parametrized by β and the other by E. In the thermodynamical limit, however, expectation values are important only, since the typical width of these distributions is decreasing with the size of the system. At least for weakly correlated systems we expect this behavior.

Let us start with investigating the expectation value of the energy in the canonical and microcanonical ensemble. In the canonical ensemble one gets

$$\langle E \rangle_C = \sum_n P_{nC} E_n = \frac{1}{Z_C(\beta)} \sum_n E_n e^{-\beta E_n} = -\frac{\partial}{\partial \beta} \ln Z_C(\beta) \tag{4.8}$$

for the expectation value of the energy and – using similar formal transformations –

$$\delta E_C^2 = \left\langle E^2 \right\rangle_C - \langle E \rangle_C^2 = \frac{\partial^2}{\partial \beta^2} \ln Z_C(\beta) \tag{4.9}$$

for its second central moment, for the quadratic width. Whenever $\ln Z_C$ is an extensive quantity, being proportional either to the particle number, N, or to the volume, V, the relative measure of energy fluctuation,

$$\frac{\delta E_C}{\langle E \rangle_C} = \frac{\sqrt{\frac{\partial^2}{\partial \beta^2} \ln Z_C(\beta)}}{-\frac{\partial}{\partial \beta} \ln Z_C(\beta)}, \tag{4.10}$$

scales like $1/\sqrt{N}$ or $1/\sqrt{V}$, respectively. In the $N \longrightarrow \infty$ ($V \longrightarrow \infty$) limit the width tends to zero and the energy distribution $P_{n\mathrm{C}}(E_n)$ is a Gaussian, determined by the first two moments, $\langle E \rangle_\mathrm{C}$ and δE_C, only.

In the microcanonical ensemble, on the other hand, the energy distribution is sharp at any size; the expectation value is fixed,

$$\langle E \rangle_\mathrm{M} = \sum_n E_n P_{n\mathrm{M}} = E, \tag{4.11}$$

and the width is zero, $\delta E_\mathrm{M} = 0$. The temperature is not directly defined. It can, however, be introduced based on the inverse Laplace transformation formula (4.4), formally. Based on the microcanonical probability factor, $1/Z_\mathrm{M}(E)$, $S = k_\mathrm{B} \ln Z_\mathrm{M}(E)$ is the entropic equation of state. From this the reciprocal of the thermodynamic temperature is derived as being

$$\frac{1}{T} = \frac{\partial S}{\partial E} = k_\mathrm{B} \frac{\partial}{\partial E} \ln Z_\mathrm{M}(E). \tag{4.12}$$

The quantity, defined as $\bar{\beta} = 1/k_\mathrm{B}T$, is therefore given by

$$\bar{\beta} = \frac{\partial}{\partial E} \ln Z_\mathrm{M}(E) = \frac{\int w(\beta)\beta \, \mathrm{d}\beta}{\int w(\beta) \mathrm{d}\beta} \tag{4.13}$$

with the formal "distribution" of complex β values[1]

$$w(\beta) = K \mathrm{e}^{\beta E} Z_\mathrm{C}(\beta). \tag{4.14}$$

Here, K is a normalization constant fitted to achieve

$$\int w(\beta) \mathrm{d}\beta = 1 = \int_{-\mathrm{i}\pi}^{+\mathrm{i}\pi} \frac{\mathrm{d}\beta}{2\pi i} \mathrm{e}^{\beta E} \frac{Z_\mathrm{C}(\beta)}{Z_\mathrm{M}(E)}. \tag{4.15}$$

Now $w(\beta)$ for a fixed energy E can be viewed as a "distribution" of possible β-values. In this view the thermodynamical inverse temperature is the "expectation value" of the integration variable β with the weight $w(\beta)$:

$$\bar{\beta} = \langle \beta \rangle_\mathrm{M} = \frac{\partial}{\partial E} \ln Z_\mathrm{M}(E). \tag{4.16}$$

Continuing this chain of thoughts, the squared width is given by

$$\delta\beta_\mathrm{M}^2 = \frac{\partial^2}{\partial E^2} \ln Z_\mathrm{M}(E). \tag{4.17}$$

---

[1] One rather should talk about a complex weight factor under the integral. Just like the Wigner function, it cannot be interpreted strictly as a probability.

Again, for an extensive microcanonical system $\ln Z_{\mathrm{M}}(E)$ scales with the size and therefore the relative magnitude of the dispersion of the relevant β values around the expectation value, $\bar{\beta}$, scales down like $1/\sqrt{N}$.

Let us demonstrate this behavior on the example of the ideal Maxwell–Boltzmann gas. The canonical partition function is given as

$$Z_{\mathrm{C}}(\beta) = V^N \prod_{j=1}^{N} \mathrm{d}^3 p_j \, \mathrm{e}^{-\beta \sum\limits_{i=1}^{N} \mathbf{p}_i^2/2m}. \tag{4.18}$$

Due to the factorizing property of the exponential of a sum, the above integral can be carried out easily. It turns out to be the N-th power of the single Gauss integral:

$$Z_{\mathrm{C}}(\beta) = \left[V \mathrm{d}^3 p \mathrm{e}^{-\beta \mathbf{p}^2/2m} \right]^N = V^N \left(\frac{m}{2\pi\beta} \right)^{3N/2} \tag{4.19}$$

This way $\ln Z_{\mathrm{C}} \propto N$, the ideal gas is – as expected – extensive. The expectation value of the energy is given by $\langle E \rangle_{\mathrm{C}} = 3N/2\beta = 3Nk_{\mathrm{B}}T/2$. The relative width of the energy distribution – a good measure of characteristic energy fluctuations at a fixed temperature – fulfills the inverse square root law:

$$\frac{\delta E_{\mathrm{C}}}{\langle E \rangle_{\mathrm{C}}} = \sqrt{\frac{2}{3N}}. \tag{4.20}$$

In the microcanonical ensemble, the energy is fixed and the partition function is a constrained integral in the N-particle phase space:

$$Z_{\mathrm{M}}(E) = V^N \prod_{j=1}^{N} \mathrm{d}^3 p_i \, \delta \left(\sum_{i=1}^{N} \mathbf{p}_i^2/2m - E \right). \tag{4.21}$$

The $3N$-dimensional integral with a single constraint is effectively a $3N-1$-dimensional integral. In order to evaluate this we introduce the $3N$-vector

$$\mathbf{P} = \left(\frac{\mathbf{p}_1}{\sqrt{2m}}, \frac{\mathbf{p}_2}{\sqrt{2m}}, \ldots, \frac{\mathbf{p}_N}{\sqrt{2m}} \right). \tag{4.22}$$

Its squared length is given by

$$P^2 = \mathbf{P}^2 = \sum_{i=1}^{N} \mathbf{p}_i^2/2m. \tag{4.23}$$

The microcanonical partition function hence becomes

$$Z_{\mathrm{M}}(E) = V^N \left(\frac{\sqrt{2m}}{2\pi} \right)^{3N} \Omega_{3N-1} \int_0^{\infty} \delta(P^2 - E) P^{3N-1} \mathrm{d}P, \tag{4.24}$$

with Ω_{3N-1} being the $3N-1$ dimensional surface of the $3N$-dimensional sphere with unit radius (cf. problem 7.6). The last integral over P can be easily evaluated considering the correct Jacobian,

$$\delta(P^2 - E) = \frac{1}{2\sqrt{E}}\delta(P - \sqrt{E}). \tag{4.25}$$

The final result is

$$Z_{\mathrm{M}}(E) = V^N \left(\frac{\sqrt{2m}}{2\pi}\right)^{3N} \Omega_{3N-1}\,\frac{1}{2}\,E^{3N/2-1}. \tag{4.26}$$

Its logarithm is also proportional to N, so the microcanonical description of the ideal gas converges to the canonical one in the thermodynamical limit. The expectation value of the β variable is the thermodynamical temperature,

$$\frac{1}{k_{\mathrm{B}}T} = \langle \beta \rangle_{\mathrm{M}} = \left(\frac{3N}{2} - 1\right)\frac{1}{E}. \tag{4.27}$$

The relative width is given by

$$\frac{\delta\beta_M}{\langle \beta \rangle_{\mathrm{M}}} = \frac{1}{\sqrt{\frac{3N}{2} - 1}}. \tag{4.28}$$

It can be seen that for $N \to \infty$ the canonical and microcanonical descriptions lead to equivalent results. However, for a finite number of particles this is not the case. Assuming the same energy the canonical temperature is slightly smaller than the microcanonical one (the inverse of the average β):

$$T_{\mathrm{C}} = \left(1 - \frac{2}{3N}\right)T_{\mathrm{M}}. \tag{4.29}$$

In the extreme case of $N = 1$ the difference is two third of the total value. The mean value of the microcanonical temperature distribution for this case is plotted against the particle number in Fig. 4.1. The error bars represent the width of the microcanonical distribution.

4.2 Fluctuations in Finite Phase Space

Another way to conceive the effect of finite size on thermodynamical properties is to ask the question that how a subsystem of a large body behaves statistically. What is the optimal subsystem to total system ratio for the possibly fastest maintenance of thermal equilibrium?

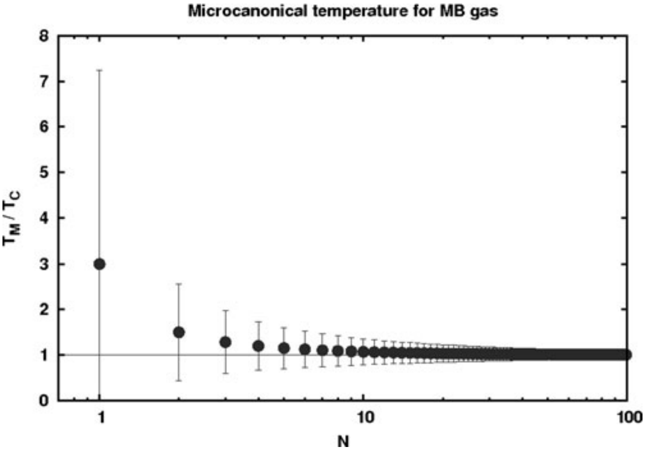

Fig. 4.1 The ratio of microcanonical and canonical mean temperatures as a function of the particle number in MB-gas is plotted. The error bars are proportional to the width of the microcanonical temperature distribution

4.2.1 Maximal Probability State

For this purpose, we consider a system of altogether N quanta distributed in K possible slots. We ask for the average values and eventually the probability distribution of having n quanta in k slots under this condition. First, we put limits on the characteristic deviation form the average level occupancy, $f = N/K$. In the grand canonical approach for fermions – as we have discussed it previously – the entropy maximum principle requires that

$$\Omega(N) = \ln \binom{K}{N} - \beta\omega(N+1/2) + \beta\mu N = \max. \tag{4.30}$$

for N quanta of each having an energy ω, at the temperature $T = 1/\beta$ and chemical potential μ (we use $\hbar = 1$ and $k_B = 1$ units). Regarding this maximization problem with discrete values for N, the maximum at a given N is defined by the inequalities

$$\Omega(N+1) \leq \Omega(N), \qquad \text{and} \qquad \Omega(N-1) \leq \Omega(N). \tag{4.31}$$

This condition gives limits for the maximally probable value of N as follows. Using the abbreviation $\ln x = \beta(\omega - \mu)$ we consider

$$\begin{aligned} \Omega(N+1) - \Omega(N) &= \ln \frac{K-N}{N+1} - \ln x \leq 0, \\ \Omega(N) - \Omega(N-1) &= \ln \frac{K-N+1}{N} - \ln x \geq 0, \end{aligned} \tag{4.32}$$

It is equivalent with the following restriction

$$\frac{K-N}{N+1} \leq x \leq \frac{K-N+1}{N}. \tag{4.33}$$

Denoting the total occupancy ratio by $\bar{f} = N/K$, this restriction can be re-arranged to

$$w - \frac{1}{K}(1-w) \leq \bar{f} \leq w + \frac{1}{K}w \tag{4.34}$$

with

$$w = \frac{1}{x+1} = \frac{1}{e^{\beta(\omega-\mu)}+1}. \tag{4.35}$$

Possible deviations from the Fermi distribution, valid in the $K \to \infty$ limit, must be in the order of or less than the occupancy divided by the number of all possible quanta.

4.2.2 Fermions in Finite Subvolume

We would like to estimate the probability of having n quanta in k slots while in the total configuration there are N quanta in K slots. Considering independent filling, this probability is proportional to the number of ways of this choice in the subsystem and in the rest of the total body:

$$P_n = \frac{\begin{pmatrix} k \\ n \end{pmatrix} \begin{pmatrix} K-k \\ N-n \end{pmatrix}}{\begin{pmatrix} K \\ N \end{pmatrix}}. \tag{4.36}$$

This expression is normalized to one by summing over all possible values of n between zero and k. Its generating function is proportional to the ${}_2F_1$ hypergeometric function.

We consider now this expression in the small subsystem limit, $k \ll K$ and correspondingly $n \ll N$. The second binomial factor is expanded using the approximation

$$(N-n)! \approx N! N^{-n}, \tag{4.37}$$

with the result

$$P_n \approx \frac{\begin{pmatrix} k \\ n \end{pmatrix}}{\begin{pmatrix} K \\ N \end{pmatrix}} \frac{K! K^{-k}}{N! N^{-n} (K-N)! \, (K-N)^{n-k}}. \tag{4.38}$$

Here, the binomial in the denominator cancels and we are left with

$$P_n = \begin{pmatrix} k \\ n \end{pmatrix} \left(\frac{K-N}{K} \right)^k \left(\frac{N}{K-N} \right)^n. \tag{4.39}$$

Using from now on the notation $\bar{f} = N/K$ for the average occupancy in the total system we arrive at the (properly normalized) Bernoulli distribution

$$P_n = \binom{k}{n} \bar{f}^n (1-\bar{f})^{k-n}. \tag{4.40}$$

For inspecting expectation values and the characteristic width of this distribution it is purposeful to compute the generating function

$$Z(\gamma) = \sum_{n=0}^{k} P_n \mathrm{e}^{n\gamma} = \left(\bar{f} e^{\gamma} + 1 - \bar{f}\right)^k. \tag{4.41}$$

The normalization can be checked by $Z(0) = 1$. The expectation value is given by

$$\langle n \rangle = \left. \frac{\partial}{\partial \gamma} \ln Z(\gamma) \right|_{\gamma=0} = k\bar{f}, \tag{4.42}$$

and the squared width

$$\delta n^2 = \left. \frac{\partial^2}{\partial \gamma^2} \ln Z(\gamma) \right|_{\gamma=0} = k\bar{f}(1-\bar{f}). \tag{4.43}$$

The relative magnitude of occupancy fluctuation is therefore

$$\frac{\delta n}{\langle n \rangle} = \frac{1}{\sqrt{k}} \sqrt{\frac{1-\bar{f}}{\bar{f}}} = \frac{1}{\sqrt{k}} \mathrm{e}^{x/2}. \tag{4.44}$$

Finally, we note that the low average occupation limit of the Bernoulli distribution is the Poisson distribution. Utilizing the approximation formula for $(k-n)!$ in the case of $n \ll k$ one obtains

$$\binom{k}{n} \approx \frac{k^n}{n!}. \tag{4.45}$$

Based on this the Bernoulli distribution (4.40) is approximated by

$$P_n \approx (1-\bar{f})^k \frac{1}{n!} \left(\frac{k\bar{f}}{1-\bar{f}} \right)^n. \tag{4.46}$$

Recognizing that $\bar{f}/(1-\bar{f}) = \mathrm{e}^{-x}$ the low-density small-subsystem probability distribution of n quanta is given by

$$P_n = C_k(x) \frac{1}{n!} \left(k\mathrm{e}^{-x}\right)^n. \tag{4.47}$$

Here, $C_k(x) = \exp(-k\mathrm{e}^{-x})$ is the proper normalization factor.

4.2.3 Bosons in Finite Subvolume

The analysis for the ideal gas of bosons is analogous to the above. Now the probability of distributing quanta in slots after a division to two independent subsystems with n and $N-n$ quanta and k and $K-k$ slots, respectively, is given by the formula

$$P_n = \frac{\binom{k+n}{n}\binom{K-k+N-n}{N-n}}{\binom{K+N+1}{N}}. \tag{4.48}$$

The small subsystem limit, $n \ll N$ and $k \ll K$ leads to the Bernoulli type distribution

$$P_n = \binom{k+n}{n} \bar{f}^n (1+\bar{f})^{-n-k-1} \tag{4.49}$$

with $\bar{f} = N/K$. The logarithmic generating function is given by

$$Z(\gamma) = \sum_{n=0}^{\infty} \binom{k+n}{n} (\bar{f}\mathrm{e}^{\gamma})^n (1+\bar{f})^{-k-n-1} = \left(1+\bar{f}-\bar{f}\mathrm{e}^{\gamma}\right)^{-k-1}. \tag{4.50}$$

The expectation value of quanta in k slots of the subsystem becomes

$$\langle n \rangle = (k+1)\bar{f}, \tag{4.51}$$

and the squared width from the second derivative of $\ln Z(\gamma)$ is given by

$$\delta n^2 = (k+1)\bar{f}(1+\bar{f}). \tag{4.52}$$

The relative importance of occupation number fluctuations is suppressed by the subsystem size as

$$\frac{\delta n}{\langle n \rangle} = \frac{1}{\sqrt{k+1}} \mathrm{e}^{x/2} \tag{4.53}$$

with $x = \ln(\bar{f}/(1+\bar{f}))$ being the logarithm of the average particle to hole ratio.

It is interesting to note at this point that the independent distribution of bosonic quanta among slots realizes a *negative binomial* distribution. The name stems from the generalization of the Euler Gamma function (factorial), $\Gamma(n) = (n+1)!$, to negative integers. Relying on the basic property

$$\Gamma(z+1) = z\Gamma(z), \tag{4.54}$$

accepted to be valid even for complex arguments, at negative integer arguments, for $z = -r$ one obtains infinite values. The recursion

$$\begin{aligned}\Gamma(-r+1) &= (-r)\Gamma(-r) = (-r)(-r-1)\Gamma(-r-1) \\ &= (-r)(-r-1)\ldots(-r-j)\Gamma(-r-j)\end{aligned} \tag{4.55}$$

namely never stops, contrary to the case of positive integer arguments. However, after a finite number of recursive steps, say j, the following ratio is well defined:

$$\frac{\Gamma(-r+1)}{\Gamma(-r-j)} = (-1)^{j+1} r(r+1)\ldots(r+j) = (-1)^{j+1}\frac{(r+j)!}{(r-1)!} \tag{4.56}$$

In the binomial coefficient one considers ratios of factorials, so it may have a finite value when some of its arguments are negative integers. Let us use the notation $(-r)! = \Gamma(-r+1)$. We rewrite the above equation as

$$\frac{(-r)!}{(-r-j-1)!} = (-1)^{j+1}\frac{(r+j)!}{(r-1)!}. \tag{4.57}$$

Dividing now both sides by $(j+1)!$ one recognizes the formal definitions of the binomial coefficients, on the left hand side with some negative integers:

$$\binom{-r}{j+1} = (-1)^{j+1}\binom{r+j}{r-1}. \tag{4.58}$$

Utilizing this result for $j = n-1$ and $r = k+1$ we arrive at

$$\binom{-k-1}{n} = (-1)^n\binom{n+k}{k} = (-1)^n\binom{n+k}{n}. \tag{4.59}$$

This relation generalizes the binomial formula for negative powers:

$$\sum_{n=0}^{\infty}\binom{-k-1}{n} a^n b^{-k-1-n} = (a+b)^{-k-1}. \tag{4.60}$$

The bosonic probability (4.49) can formally be written as a negative binomial distribution:

$$P_n = \binom{-k-1}{n}(-\bar{f})^n(1+\bar{f})^{-k-1-n} \tag{4.61}$$

Owing to the generalized binomial formula above (4.60), its normalization to 1 became transparent.

It is interesting to note that the negative binomial distribution can be viewed as a product of two Poisson distributions, integrated over the mean-value parameter of these distributions. In this case, $\bar{f}$ denotes the ratio of the parameters of the two respective Poisson distributions; one in n, the other in k. To prove this, one utilizes the identity

$$\int_0^{\infty} x^N \mathrm{e}^{-ax}\mathrm{d}x = \frac{N!}{a^{N+1}}. \tag{4.62}$$

This way we can write that

$$P_n = \binom{k+n}{n} \bar{f}^n (1+\bar{f})^{-n-k-1} = \frac{\bar{f}^n}{k!n!} \int_0^\infty \mathrm{e}^{-(1+\bar{f})x} x^{k+n} \,\mathrm{d}x, \tag{4.63}$$

where we have applied the above identity to $N = k+n$ and $a = 1+\bar{f}$. The integrand in the above expression can be then factorized as follows:

$$P_n = \int_0^\infty \frac{(x\bar{f})^n}{n!} \mathrm{e}^{-\bar{f}x} \frac{x^k}{k!} \mathrm{e}^{-x} \,\mathrm{d}x. \tag{4.64}$$

With the help of this integral representation it is especially straightforward to obtain the inversion property of the negative binomial distribution,[2]

$$P_n(k;\bar{f}) = \bar{f}^{-1} P_k\left(n;\bar{f}^{-1}\right). \tag{4.65}$$

We note that while

$$\Pi(k;x) = \frac{x^k}{k!} \mathrm{e}^{-x} \tag{4.66}$$

is a *Poisson distribution* in the variable k (with mean value $\langle k \rangle = x$ and with $\delta k^2 = x$), it is also an *Euler Gamma distribution* in the variable x (with mean value $\langle x \rangle = k+1$ and the same squared width $\delta x^2 = k+1$).

4.2.4 Fluctuations in a Subvolume

The $\delta n^2 \sim 1/k$ dependence is quite general, it is not only for the low density limit discussed so far. For a large number of states (particles with a given energy, or quanta with given properties) the factorials can be approximated by Stirling's formula. The distribution (4.36) for fermionic quanta and (4.48) for bosonic ones incorporate finite phase space effects already for independent systems. Now we investigate the dependence of the equilibrium density and its mean squared fluctuations in the thermodynamical limit: $K \longrightarrow \infty$ while the ratios $\bar{f} = N/K$ and $v = k/K$ are kept fixed. The distributed variable is the occupation density in the subvolume, $f = n/k$ and the corresponding ratio in the rest of the system ("reservoir") is given as

$$\hat{f} = \frac{N-n}{K-k} = \frac{\bar{f} - vf}{1-v}. \tag{4.67}$$

---

[2] One has to replace the integration variable x by $y/\bar{f}$.

Under such circumstances the binomial terms occurring in the expression (4.36) will have the following limits:

$$\begin{aligned} \binom{k}{n} &\longrightarrow k\,\sigma(f), \\ \binom{K-k}{N-n} &\longrightarrow (K-k)\,\sigma(\hat{f}), \\ \binom{K}{N} &\longrightarrow K\,\sigma(\bar{f}). \end{aligned} \tag{4.68}$$

The entropy per state (using $k_\mathrm{B} = 1$ units) is hence given as

$$S = \lim_{K\to\infty} \frac{1}{K} \ln P_n(k;N,K) \;=\; \left\{ v\,\sigma(f) + (1-v)\,\sigma(\hat{f}) - \sigma(\bar{f}) \right\}, \tag{4.69}$$

with the Boltzmann–Fermi expression [cf. (3.27)]:

$$\sigma(f) = -f\ln f - (1-f)\ln(1-f). \tag{4.70}$$

The equilibrium value for f is determined by the stationarity of (4.69). One obtains

$$\frac{\partial S}{\partial f} = v\,\sigma'(f) + (1-v)\frac{\mathrm{d}\hat{f}}{\mathrm{d}f}\sigma'(\hat{f}) = 0, \tag{4.71}$$

with

$$\frac{\mathrm{d}\hat{f}}{\mathrm{d}f} = -\frac{v}{1-v}. \tag{4.72}$$

upon using (4.67). The stationarity condition (4.71) this way becomes equivalent to

$$\sigma'(f) = \sigma'(\hat{f}), \tag{4.73}$$

which leads to $f = \hat{f}$. Utilizing again the definition (4.67) one concludes that in equilibrium also $f = \bar{f}$; all mean densities are equal. We note that this is just the microcanonical result. Considering other ensembles this result would change if the energy or charge associated to the subsystem and to the reservoir part differed.

The typical fluctuations near the equilibrium on the other hand are inversely proportional to the second derivative of the entropy. While this feature, as a general property of the thermodynamical equilibrium, will be discussed in the next section, in the special case considered here one can rely on the independent occupancy picture. For large K, and k with a fixed finite ratio $v = k/K$, the variance of the subvolume occupation is related to the variance of the ratio f: $\delta n^2 = K^2 v^2 \delta f^2$. In this limit $\ln P_n(k;N,K)$ is expanded around the equilibrium value, $n = \langle n \rangle = kN/K$, up to second order terms, since for the variance all higher order terms vanish at equilibrium. One obtains

$$\frac{\partial^2 S}{\partial f^2} = v\frac{\delta}{\delta f}\left\{\sigma'(f) - \sigma'(\hat{f})\right\} = v\left\{\sigma''(f) + \frac{v}{1-v}\sigma''(\hat{f})\right\}. \tag{4.74}$$

Here

$$\sigma''(f) = -\frac{1}{f(1-f)}. \tag{4.75}$$

This quantity is negative, the entropy functional being concave once near to its maximum. It is the leading estimate for the squared fluctuations:

$$\frac{1}{\delta f^2} = -\frac{\partial^2 S}{\partial f^2}. \tag{4.76}$$

This relation together with the equilibrium condition $f = \hat{f} = \bar{f}$ gives rise to

$$\delta f^2\big|_{\text{eq}} = \frac{1-v}{v}\bar{f}(1-\bar{f}). \tag{4.77}$$

For bosons all these steps can be repeated, but $\sigma(f) = -f\ln f + (1+f)\ln(1+f)$ [cf. (3.34)] has to be used. The final result is

$$\delta f^2\big|_{\text{eq}} = \frac{1-v}{v}\bar{f}(1+\bar{f}). \tag{4.78}$$

At the same time the squared fluctuations in the rest of the system, $\delta\hat{f}^2$, can be obtained by interchanging v and $1-v$. This way the optimal relative size of the subsystem is $v = 1/2$, at this value is the total equilibrium fluctuation minimal: The expression

$$\delta f^2 + \delta\hat{f}^2\big|_{\text{eq}} = \bar{f}(1\pm\bar{f})\left(\frac{1-v}{v} + \frac{v}{1-v}\right) \tag{4.79}$$

has its minimum in v at this value. Here the $+$ $(-)$ sign is valid for bosons (fermions).

4.3 Near-equilibrium Fluctuations

If the deviations from the average values of thermodynamical quantities are relatively small, then their distribution is well approximated by a Gaussian. Assuming that $S(X_i)$ is the entropic equation of state in terms of the variables $X_i = E, V, N, \ldots$, the maximum of

$$-\beta\Phi = S(X_i) - \sum_i Y^i X_i \tag{4.80}$$

determines the equilibrium. Here, the Lagrange multipliers are given by

$$Y^i = \frac{\partial S}{\partial X_i}. \tag{4.81}$$

Considering now near-equilibrium states the thermodynamical variables reach values $X_i + \Delta X_i$. The distribution of these off-equilibrium values is proportional to the exponential of the altered entropic thermodynamical potential due to the Boltzmannian definition of entropy:

$$\mathscr{P}(\Delta X) \propto \mathrm{e}^{S(X+\Delta X) - \sum_i Y^i (X_i + \Delta X_i)}. \tag{4.82}$$

We consider this at fixed intensives, Y^i. The notation X stands for the multitude of components, X_i. Expanding the exponential to second order terms in the fluctuations, ΔX_i, one utilizes the Gaussian approximation for their distribution. Since the entropy is maximal at equilibrium, its second derivative matrix must be negative definite. Therefore, one defines the positive definite metric tensor

$$g^{ij} = -\frac{\partial^2 S}{\partial X_i \partial X_j}. \tag{4.83}$$

Using this notation and the relation (4.81) we obtain

$$\mathscr{P} \propto \mathrm{e}^{S(X) - \sum_i Y^i X_i} \, \mathrm{e}^{-\frac{1}{2} \sum_{ij} \Delta X_i g^{ij} \Delta X_j}. \tag{4.84}$$

Here the prefactor is independent of the fluctuations, so it can be absorbed into the normalization of the probability. The normalized Gaussian distribution is given by

$$\mathscr{P} = \frac{1}{\sqrt{(2\pi)^r g}} \, \mathrm{e}^{-\frac{1}{2} \sum_{ij} \Delta X_i g^{ij} \Delta X_j}, \tag{4.85}$$

with r variables and $g = \det g^{ij}$ being the determinant of the matrix defined in (4.83). The inverse of the matrix (existent for $g \neq 0$) we denote by g_{ij}. Due to elementary properties of the multi-Gaussian distribution (4.85), the correlated expectation values of the near-equilibrium fluctuations of the thermodynamical extensive quantities are given by this inverse metric matrix

$$\left\langle \Delta X_i \Delta X_j \right\rangle = g_{ij}. \tag{4.86}$$

In the above derivation, we assumed that the intensive quantities, Y^j, do not fluctuate. Keeping their value fixed we dealt with a maximally grand-grand-canonical approach. In the other extreme one considers the fluctuations of the intensives, ΔY^j, keeping the extensive variables, X_i fixed. In this microcanonical situation the variables X and Y change place and one arrives at

$$\left\langle \Delta Y^i \Delta Y^j \right\rangle = g^{ij}. \tag{4.87}$$

The fluctuations of the intensive thermodynamical variables, like $1/T, p/T, -\mu/T, \ldots$ can therefore be estimated by considering the minus of the second derivative matrix of the microcanonical equation of state $S(E,V,N,\ldots)$. In this case the X_i-s are fixed and the corresponding Y^j-s fluctuate with a nearly Gaussian distribution in the statistical ensemble.

Let us consider some simple examples. Disregarding cross-correlations with other variables, the fluctuation of the temperature in the microcanonical ensemble (at fixed energy) is given by

$$\left\langle \Delta T^2 \right\rangle = -T^4 \frac{\partial^2 S}{\partial E^2}, \tag{4.88}$$

while the relation

$$\frac{1}{T} = \frac{\partial S}{\partial E} \tag{4.89}$$

holds. Regarding the following volume-homogeneous class of possible microcanonical equation of states,

$$S(E,V) = Vs(E/V), \tag{4.90}$$

one obtains

$$\frac{1}{T} = s'(E/V) \tag{4.91}$$

and

$$\frac{\partial^2 S}{\partial E^2} = \frac{1}{V} s''(E/V). \tag{4.92}$$

This gives rise to the following Gaussian estimate for the temperature fluctuation

$$\left\langle \Delta T^2 \right\rangle = -\frac{T^4}{V} s''(E/V). \tag{4.93}$$

For the well-known black body radiation, $s(\varepsilon) = a\varepsilon^{3/4}$. The first derivative becomes

$$s' = \frac{3}{4} a\varepsilon^{-1/4} = \frac{3s}{4\varepsilon} = \frac{1}{T}, \tag{4.94}$$

while the second derivative is given by

$$s'' = -\frac{3}{16} a\varepsilon^{-5/4} = -\frac{3s}{16\varepsilon^2} = -\frac{1}{4T\varepsilon}. \tag{4.95}$$

The characteristic magnitude of Gaussian temperature fluctuations near to the thermal equilibrium state is estimated as being

$$\left\langle \Delta T^2 \right\rangle = \frac{T^4}{V} \frac{1}{4T\varepsilon} = \frac{T^3}{4E}. \tag{4.96}$$

The inverse square root scaling of $\sqrt{\left\langle \Delta T^2 \right\rangle}$ with the total energy involved in the radiation can be observed clearly.

4.4 Superstatistics

Based on the above experience the idea of considering a general distribution of the temperature or its inverse, $\beta = 1/k_\mathrm{B}T$, occurs. In situations when the microcanonical equilibrium description is insufficient, either due to dealing with non-equilibrium systems or systems of too small size, or – as it will be discussed in Chap. 5 – with long range correlations destroying the simple picture of Gaussian distributed deviations from the thermal equilibrium value, this more general view may come to help.

In particular, in several statistical phenomena instead of the Gaussian or exponential form a power-law tailed distribution emerges. An energy distribution of this special form,

$$f(E) = (1 + aE)^{-v}, \tag{4.97}$$

with parameters a and v, can be formally regarded as an integral over canonical Gibbs–Boltzmann distributions. In fact, an Euler Gamma distribution of the inverse temperature,

$$w(\beta) = \frac{c^n}{\Gamma(n)} \beta^{n-1} \mathrm{e}^{-c\beta}, \tag{4.98}$$

leads to

$$\int_0^\infty w(\beta) \mathrm{e}^{-\beta E} \mathrm{d}\beta = \left(1 + \frac{E}{c}\right)^{-n}. \tag{4.99}$$

Here, the identification $a = 1/c$ and $v = n$ delivers the seeked power-law form. The parameters a and v or c and n respectively, can be associated to the properties of the distribution of β. Based on (4.98) the mean value is given by

$$\langle \beta \rangle = \frac{n}{c} = av. \tag{4.100}$$

One also may inspect the mean value of the temperature,

$$T = \left\langle \beta^{-1} \right\rangle = \frac{c}{n-1} = \frac{1}{a(v-1)}, \tag{4.101}$$

in $k_\mathrm{B} = 1$ units.

Now the question arises what is behind the Euler Gamma distribution of the (inverse) temperature, why is it special. The answer is that it is "simple" in the same sense than the Gaussian distribution: it can be obtained as a limiting distribution under some basic assumptions. Most remarkably it is the distribution of the sum of the squares of identically distributed Gaussian variables. The particular use of this mathematical fact in statistical physics of power-law tailed distributions was pointed out by Christian Beck and Ezekiel Cohen originally [25].

The name *superstatistics* was coined to reflect that the statistics of the β parameter is superimposed on the ordinary canonical statistical distribution of energy.

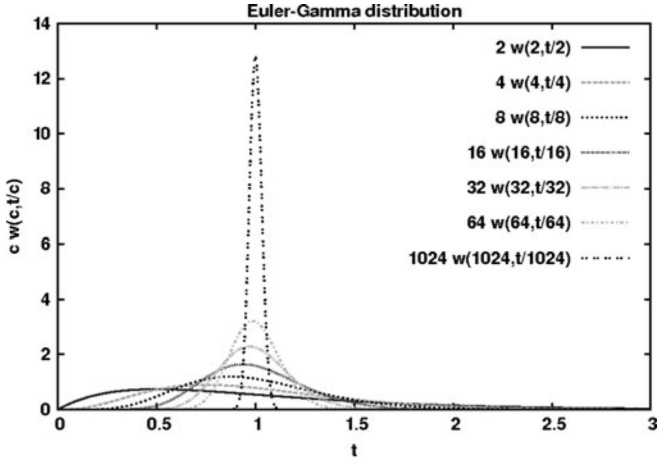

Fig. 4.2 Euler Gamma distributions for different width parameter. All curves are scaled as $f(t) = cw(t/c)$ at $n = 1/c$ in order to have the maximum at $t = 1$

Superstatistics describes complex systems, characteristically far from equilibrium in dynamical changes of the thermodynamical intensive variables on a large spatio-temporal scale. This "second" averaging over possible Lagrange multipliers gives rise to effective canonical factors and due to this to altered formulas of thermodynamics. This way it is equivalent to considering non-additive composition laws for the corresponding thermodynamical extensives. In the case of energy and temperature one defines the correspondence by requiring

$$\int_0^\infty \mathrm{e}^{-\beta E} w(\beta) \mathrm{d}\beta = \mathrm{e}^{-\langle\beta\rangle L_a(E)}. \tag{4.102}$$

The emergence of the Euler Gamma distribution can be conjectured in several ways. In the framework of superstatistics the following argumentation has been used: By its very construction only non-negative values of β carry a physical meaning, so one looks for a procedure to obtain a distribution which reflects this property. Considering mesoscopic random variables, β can be interpreted as a sum related to random quantities in a way always being positive or zero. The simplest construction with these properties is the sum of the squares of $2n$ identically distributed Gaussian random variables. The distribution of this quantity is given by

$$P(\beta) = \int \left(\prod_{j=1}^{2n} \mathrm{d}x_j w(x_j) \right) \delta \left(\beta - \frac{1}{2} \sum_{i=1}^{2n} x_i^2 \right), \tag{4.103}$$

with

$$w(x) = \sqrt{\frac{c}{2\pi}} \mathrm{e}^{-cx^2/2} \tag{4.104}$$

This $2n$-fold integral can easily be evaluated after introducing the Fourier representation of the Dirac-delta condition, this way all integrals over the individual x_j variables factorize:

$$P(\beta) = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi} \mathrm{e}^{\mathrm{i}k\beta} \left(\int_{-\infty}^{\infty} \mathrm{d}x \sqrt{\frac{c}{2\pi}} \, \mathrm{e}^{-cx^2/2} \mathrm{e}^{-\mathrm{i}\frac{kx^2}{2}} \right)^{2n} \tag{4.105}$$

The Gauss integrals are straightforward to evaluate, resulting

$$P(\beta) = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi} \mathrm{e}^{\mathrm{i}k\beta} \, (1 + ik/c)^{-n} . \tag{4.106}$$

This final integration features an n-fold pole on the positive imaginary axis at $k = ic$. The integration along the real k axis leads to the Euler Gamma distribution,

$$P(\beta) = \frac{c^n}{\Gamma(n)} \beta^{n-1} \, \mathrm{e}^{-c\beta} \tag{4.107}$$

for $\beta \geq 0$ and zero otherwise.

This distribution can be generalized to any real parameter n, not only the integer ones. In the original argumentation, $2n$ is an integer, so n itself can be a half-integer value. In fact, many power-law tailed distributions, found in Nature, show a power close to a half-integer. We note that the $n \to \infty$ limit of the Euler Gamma distribution is extremely narrow – and its integral is still normalized to one. This way the "conventional" canonical statistics is re-established in this limit.

The idea of superstatistics and its use is subject to contemporary development [26]. There is a superstatistical generalization of the fluctuation – dissipation relation, a generalization of the proper thermodynamical potential used as a variational principle and a generalization of the definition of the entropy. Besides the power-law tails, also stretched exponentials are applied quite often for the description of various phenomena. Microcanonical treatment with a non-Gaussian temperature fluctuation, fractional reaction equations occurring in physical chemistry, the superstatistical version of random matrix theory – just to mention a few. Superstatistical network analysis, path integrals and time series analysis are contemporary topics of research.

But also practical applications do not come short: turbulent flow in fluids and in the atmosphere, elementary particle statistics in cosmic ray and accelerator experiments all can be described by such distributions more accurately than with the "old fashioned" Gaussian. One of the most vivid area of applications is in financial models, and in statistics over everyday life phenomena, like traffic delays or heart signals. In fact some cases of chaotic dynamics, the so called weak chaos, also shows non-Gaussian tailed distributions of energy.

Finally, it has to be noted that also T may be Euler Gamma distributed if it is derived as a sum of squares of a finite number of Gaussian random variables. Or the logarithm as well may be Gauss-distributed resulting in a "log-normal" distribution of the (inverse) temperature. In fact, this is a major concern that the superstatistical distribution, $P(\beta)$, can be a priori anything. Following principles, like the least bias with some constraints given, one may select out some particular classes of such distributions. We expect that once the proper maximum entropy principle [27] is formulated with generalized entropy formula and generalized constraints, the superstatistical distribution follows.

4.5 Canonical Enhancement

It is often so, in particular in relativistic heavy ion collisions observing thousands of newly produced particles in an event, that only statistical information is available for tracing back characteristica of an earlier stage of interacting matter. Aiming at a possible discovery it is especially important to be aware of an unavoidable loss of information due to the very nature of statistics. Selecting out relevant control parameters, on the other hand, even statistical information can be used to make qualitative distinctions with respect to the kind of matter existed for a while in such experiments, in particular drawing conclusions about a possible equation of state.

A truly interesting control parameter is the size of the reacting system, which is often regarded as infinite in theory (as the so called thermodynamical limit). In reality it is, however, finite and only to a certain degree controllable in experiments, e.g. by varying the target nucleus and triggering measurements by centrality (produced multiplicity, transverse energy) of a collision. But even surmising an infinite volume a further distinction can be done according to the mean particle number in an event.

Two opposite limits are worthwhile to be considered: (1) the case of frequent events producing many particles on the mean, approximately described by the Gaussian distribution, and (2) rare events with very few (on the mean less than one) particles, covered by the Poisson distribution. A characteristic finite size effect in relativistic heavy ion collisions, named *canonical enhancement*, can also be understood as originating in the difference between rare and frequent events, between sparse and copious particle production. Mathematically, this reveals itself in the difference between a large and a small mean particle number. The large number case gives results equivalent to those stemming from a Gaussian distribution.

The Gaussian approximation is the basis of the equivalence of the canonical and grand canonical approaches in the thermodynamical limit. On the other hand the Poisson statistics with a small mean number markedly characterizes the "small world" effects. The ratio of the canonical and grand canonical result in small systems is less than one, the same result can be obtained simply relying on the Poisson distribution alone.

The importance of this finite size effect for relativistic heavy ion collisions, in particular its explanation power for finding more produced strange mesons per colliding participant particles in ion–ion than in proton–proton collisions (the so called *strangeness enhancement*), was first realized by Redlich [28] and Oeschler et al. [29]. Originally presented as a constraint stemming from the proper statistical treatment of a U(1) symmetry in the canonical approach (whence the name canonical enhancement) [30], and referring to volume and temperature during the derivation of the result, soon was it re-derived on the basis of rate equations [31], and has been shown that there can be an underlying master equation with the Poisson distribution as stationary solution. Rafelski and Letessier emphasized that this phenomenon is strongly related to pair statistics (to associated production of conserved charge and anticharge) and it holds also out of chemical equilibrium with general fugacity factors [32]. Also a debate has been conducted about the relevance of this effect on the strangeness enhancement in heavy ion collisions, especially at CERN SPS using 40, 60 and 160 GeV/nucleon beam energies.

Here, we derive the canonical enhancement factor relying on the Poisson distribution. We do not directly refer either to temperature nor to volume in this derivation, – even if also thermal systems in a given volume may show Poisson statistics, this is not their only possible origin. Then we apply this finite number suppression factor to an analysis of particle production in the framework of the sudden quark coalescence picture of hadron formation [33]. We recover qualitatively the linear coalescence formula for the low particle number case, by the virtue of which the number of composite objects (mesons and baryons) are proportional to the product of the numbers of its constituents (the quarks and antiquarks).

From the probability $P(n)$ of getting n particles of a certain kind the expectation value $\langle n\rangle$ and higher moments like quadratic spread can easily be obtained by the use of the generating function:

$$Z(\gamma) = \sum_n P(n)\, \mathrm{e}^{\gamma n}. \tag{4.108}$$

The mean number becomes

$$\langle n \rangle = \frac{\partial}{\partial \gamma} \ln Z \bigg|_{\gamma=0}. \tag{4.109}$$

Under certain circumstances we are particularly interested in pairs of particles carrying a sum or a difference of a given physical quantity (like electric or baryonic charge, or strangeness number). On the basis of independent one-particle distributions the pair statistics and the distribution of the sum can be calculated. Without any constraint on the difference, the distribution of the sum is described by the convolution of the corresponding distributions:

$$P_U(s) = \sum_{n,m} P_1(n)P_2(m)\delta_{m+n,s} = \sum_n P_1(n)P_2(s-n). \tag{4.110}$$

Here, $P_U(s)$ denotes the *unconstrained* distribution of the sum s. This is the relevant quantity, whenever there is no information on the difference. On the other hand the production of given charged particles and antiparticles happens always in pairs due to charge conservation. This process is called associated production. As a consequence, even if the production process is statistical, the difference in their number is bound to be zero. In this case we obtain the following *constrained* distribution of the sum:

$$P_C(s|0) = \frac{1}{P_0}\sum_{m,n} P_1(n)P_2(m)\delta_{m+n,s}\delta_{m-n,0} = \frac{P_1(s/2)P_2(s/2)}{\sum_n P_1(n)P_2(n)}. \tag{4.111}$$

This is a conditional probability with the factor P_0 being the probability of getting zero difference in the number statistically, which ensures the normalization of the result to one. Figure 4.1 shows a geometrical interpretation of the distinction between these two pair statistics: the unconstrained distribution can be obtained by adding all points in (n,m) space over a given bin of the diagonal representing a given sum $s = n+m$, while in case of the fixed zero difference only hits in the diagonal stripe count. The ratio of the stripe to the total area reflects the $1/P_0$ normalization factor (Fig. 4.3).

Applying this idea to restless coalescence of quarks into hadrons, we still constrain the difference to zero, but this time due to a confinement principle. The number of coalesced hadrons is the half sum in this case. Caring for pions only in a simplified world of light quarks and antiquarks, we arrive at having n from both, with zero difference and a sum of $2n$ forming exactly n pions. The generating function of the constrained distribution $P_C(s|0)$ in this case reads as

$$Z_C(\gamma) = \frac{1}{P_0}\sum_n P_q(n)\,P_{\overline{q}}(n)\,e^{\gamma n}. \tag{4.112}$$

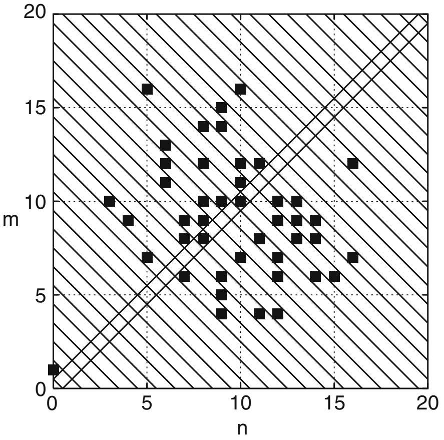

Fig. 4.3 The constrained (*main diagonal stripe*) and unconstrained (*the whole square*) distribution of the sum of two Poisson deviates with the mean value ten

Assuming Poisson distribution both for the quarks and antiquarks this generating function becomes

$$Z_C(\gamma) = \frac{1}{P_0} \sum_n \frac{\langle q \rangle^n}{n!} e^{-\langle q \rangle} \frac{\langle \bar{q} \rangle^n}{n!} e^{-\langle \bar{q} \rangle} e^{\gamma n} = \frac{1}{P_0} e^{-\langle q \rangle - \langle \bar{q} \rangle} I_0(2e^{\gamma} \sqrt{\langle q \rangle \langle \bar{q} \rangle}). \quad (4.113)$$

with $I_0(x)$ being the Bessel function of the first kind with imaginary argument. The normalization factor $1/P_0$ can be obtained from $Z(0) = 1$, giving

$$Z_C(\gamma) = \frac{I_0(2e^{\gamma} \sqrt{\langle q \rangle \langle \bar{q} \rangle})}{I_0(2\sqrt{\langle q \rangle \langle \bar{q} \rangle})}. \quad (4.114)$$

The expectation value of the pions can be derived by computing the logarithmic derivative. We obtain

$$\langle \pi \rangle_P = \frac{1}{2} \langle s \rangle = \sqrt{\langle q \rangle \langle \bar{q} \rangle} \; \frac{I_1(2\sqrt{\langle q \rangle \langle \bar{q} \rangle})}{I_0(2\sqrt{\langle q \rangle \langle \bar{q} \rangle})}, \quad (4.115)$$

with the label P reminding us to the Poisson distribution. For small mean number of quarks this leads to the product assumption of the simple linear coalescence model:

$$\langle \pi \rangle_P \approx \langle q \rangle \langle \bar{q} \rangle, \quad (4.116)$$

due to $I_1(x)/I_0(x) \approx x/2$ for small argument. For large mean numbers on the other hand the ratio of the Bessel functions, I_1/I_0 approaches one. For finite mean quark numbers this ratio remains less than one; this is the *canonical suppression* factor (cf. Fig. 4.4).

As opposed to the above analysis of the Poisson distribution, for the Gaussian distribution both the unconstrained and the zero difference constrained pair statistics

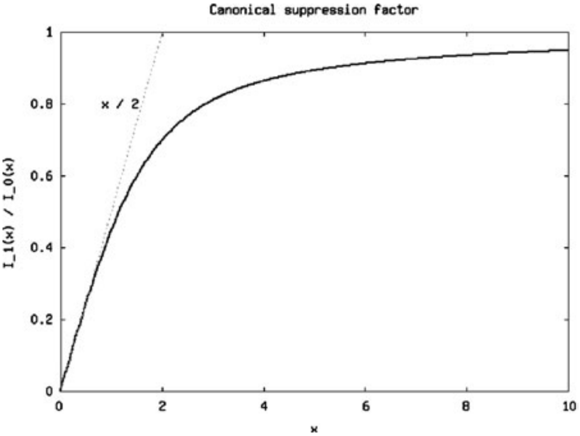

Fig. 4.4 The canonical suppression factor as a ratio of Bessel functions

leads again to a Gaussian distribution (but with a larger width). Assuming so distributed quark and antiquark numbers with respective square widths equal to the mean values, as it is typical for near-equilibrium ideal gases, the expectation value of the half sum, the pion number becomes the harmonic mean of the expectations (because by convolution of Gaussian distributions the inverse square widths are additive):

$$\langle \pi \rangle_{\mathrm{G}} = \frac{2\langle q \rangle \langle \bar{q} \rangle}{\langle q \rangle + \langle \bar{q} \rangle}. \tag{4.117}$$

In case of zero baryon charge $\langle q \rangle = \langle \bar{q} \rangle$ and these formulas reduce to a very simple result:

$$\langle \pi \rangle_{\mathrm{G}} = \langle q \rangle; \qquad \langle \pi \rangle_{\mathrm{P}} = \langle q \rangle \ \frac{I_1(2\langle q \rangle)}{I_0(2\langle q \rangle)}. \tag{4.118}$$

As a consequence one can express the canonical enhancement factor in this case as the ratio of Poissonian and Gaussian expectation values:

$$\frac{\langle \pi \rangle_{\mathrm{P}}}{\langle \pi \rangle_{\mathrm{G}}} = \frac{I_1(2\langle q \rangle)}{I_0(2\langle q \rangle)}. \tag{4.119}$$

It is particularly interesting when we compare rare particles, for example K^+ mesons coalesced from Poisson distributed u and $\bar{s}$ quarks with copiously produced π^+ pions glued from u and $\bar{d}$ quarks. The expected meson numbers,

$$\left\langle K^+ \right\rangle_{\mathrm{P}} = \sqrt{u\bar{s}} \ \frac{I_1(2\sqrt{u\bar{s}})}{I_0(2\sqrt{u\bar{s}})}, \tag{4.120}$$

for kaons and

$$\left\langle \pi^+ \right\rangle_{\mathrm{G}} = \frac{2u\bar{d}}{u+\bar{d}} \tag{4.121}$$

for pions (with u, $\bar{s}$ and $\bar{d}$ denoting here the expectation values of the respective quark numbers) for a baryon free and strangeness free, and isotropically symmetric fireball due to $\bar{d} = d = \bar{u} = u$ and $\bar{s} = s = f\bar{d}$ with a fixed strangeness ratio $f = \bar{d}/\bar{s}$ reduce to

$$\left\langle K^+ \right\rangle_{\mathrm{P}} = u\sqrt{f} \ \frac{I_1(2u\sqrt{f})}{I_0(2u\sqrt{f})} \tag{4.122}$$

and

$$\left\langle \pi^+ \right\rangle_{\mathrm{G}} = u. \tag{4.123}$$

In this simplified scenario, the kaon to pion ratio can be expressed as a function of the pion number and so can be compared with experimental results. Of course the result can only be qualitative on this level, since by using the above assumptions for the quark and antiquark numbers, one is bound to predict the same ratio for K^+/π^+ and for K^-/π^-. It is not quite fulfilled in experiments: comparing the heavy ion results with those of proton–proton collisions, these ratios increase by a factor of roughly 2 and 1.6, respectively.

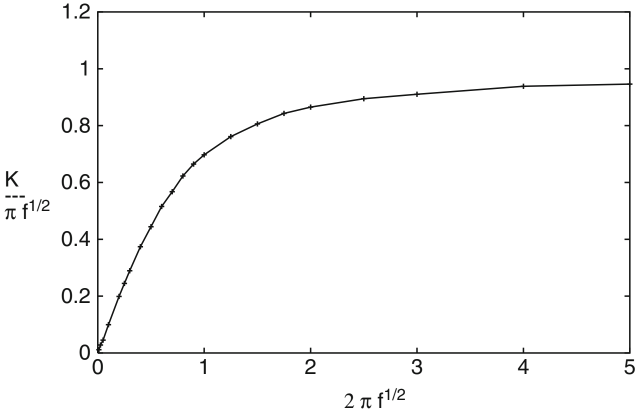

Fig. 4.5 Canonical suppression factor obtained from the expectation value of the sum of two (numerically simulated) Poisson distributions. It coincides with the analytically derived ratio of two Bessel functions I_1/I_0

The result of this simple idea can be inspected in Fig. 4.2, where the normalized ratio $\langle K^+\rangle_{\mathrm{P}}/(\langle\pi^+\rangle_{\mathrm{G}}\sqrt{f}$ is plotted vs. the scaled pion number, $2\langle\pi^+\rangle_{\mathrm{G}}\sqrt{f}$. This is exactly the canonical suppression factor. Using the value $f \approx 0.5$ for estimating the Wroblinski factor, f, one concludes that the kaon/pion ratio falls to its half at an expected pion number of about 0.5 as compared to large pion numbers. This value corresponds to a situation before resonance decays, so it is not directly observable in experiments, but correcting for resonance decays is always possible in the framework of a theoretical model (Fig. 4.5).

Assuming that both pions and kaons are constructed from Poisson distributed quarks, their ratio changes between two limiting values corresponding to few and many quarks respectively:

$$\frac{\langle K\rangle_{\mathrm{P}}}{\langle\pi\rangle_{\mathrm{P}}} = \sqrt{f}\quad\frac{I_1(2u\sqrt{f})}{I_0(2u\sqrt{f})}\quad\frac{I_0(2u)}{I_1(2u)}, \tag{4.124}$$

gives f for $u \ll 1$ and $\sqrt{f}$ for $u \gg 1$. Considering the light quark (pion) number before resonance decay the former case is realized in "pp" collisions (according to ALCOR [33] $\langle\pi\rangle \sim 0.1$) and the latter case in "PbPb" collisions ($\langle\pi\rangle \sim 10$, before resonance decay). The double ratio,

$$\frac{(K/\pi)_{\mathrm{PbPb}}}{(K/\pi)_{\mathrm{pp}}} \approx \frac{1}{\sqrt{f}} \tag{4.125}$$

would be about 1.4, which is to be compared with the experimental values 1.6 for negative and 2 for positive kaon to pion ratios. The transition is around $\langle\pi\rangle \approx 0.7\ldots1.4$, probably occurring in a collision of relatively light ions.

Problems

4.1. Prove the rule for the Pascal triangle,

$$\binom{k}{n} = \binom{k-1}{n} + \binom{k-1}{n-1}.$$

4.2. What is the Pascal triangle-like recursion rule for the probabilities in the Bernoulli distribution?

4.3. What is the Pascal triangle-like recursion rule for the probabilities in the hypergeometric distribution?

4.4. What is the triangle recursion rule for the probabilities in the bosonic Bernoulli distribution?

4.5. Derive the generating function $Z(\gamma)$ for the bosonic occupation probability, given in (4.50).

4.6. Determine the double generating function,

$$Z_P(\gamma,\alpha,f) = \sum_{n=0}^{\infty}\sum_{k=0}^{\infty} P_n(k;f)\mathrm{e}^{\gamma n}\,\mathrm{e}^{\alpha k}$$

for the negative binomial distribution $P_n(k;f)$. It plays the role of the partition function in the pressure ensemble.

4.7. Find a transformation formula between the fermionic and bosonic type Bernoulli distributions.

4.8. Estimate the magnitude of energy fluctuations near to thermal equilibrium for the non-extensively modified black body radiation, described by the equation of state

$$S(E,V) = \frac{4}{3}\sigma^{1/4}V\left(\frac{L(E)}{V}\right)^{3/4}.$$

Assuming $L(E) = \frac{1}{a}\ln(1+aE)$ with a small parameter $a > 0$, how do these fluctuations behave with a?

Chapter 5
Complications with the Temperature

The spectral temperature in case of multiplicative noise, generalized fluctuation–dissipation relation. Stochastic volatility models. The thermodynamics of abstract composition rules and alternative entropy formulas.

In this chapter we deal with some challenges of a special art: the challenges emerging from the complexity of the physical system under study. This includes a variety of phenomena. First, we review mesoscopic approaches to thermal phenomena, where the temperature may be interpreted characterizing the property of noise. Here we go beyond the additive white noise, already considered in the classical Langevin equation: Some other possibilities will be presented. Most prominently the multiplicative noise and in general the effect of stochastic factors in the dynamical evolution equation on the stationary distribution of possible momentum values are investigated. This case is equivalent to considering a "colored" noise, when the correlation width of the random terms depend on the state of the mesoscopic variable, say on the momentum of a "pointer" particle. Based on the lessons of this study we formulate a generalization of the fluctuation–dissipation theorem for particular colored noises, we call ergodic noise, where the momentum dependence is restricted to a dependence via the total energy.

Following these presentations we make a trip to the field of financial models, in order to demonstrate how coupled stochastic equations in a given approximation describe the presence of ergodic colored noise. In such cases the effective stationary distribution is again non-Gaussian, simulating an energy-dependent ("sliding") spectral temperature. Such phenomena are a common cause for the so called "fat tail" distributions.

Then anomalous behaviour in the diffusion problem will be addressed in order to learn about the leading order deformation of results known from classical studies. As an example we show the correspondence between non-Gaussian (non-Gibbsean) momentum (energy) distributions and the negative binomial multiplicity distribution seen in high energy particle physics experiments.

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DOI 10.1007/978-1-4419-8041-0_5,

Finally, we present a formal approach to generalize thermodynamics: the treatment of abstract composition rules and the thermal equilibrium properties following from them.

5.1 Colored and Multiplicative Noise

A description of the Brownian motion based on dynamics is given by the classical Langevin equation (cf. Chap. 3). A balance between damping and accelerating forces leads to a stationary state, with vivid microscopical dynamics, but macroscopically (on the average over many particle paths) it presents a thermodynamical equilibrium state. General statements about this balance are comprised in the fluctuation–dissipation theorem.

Let us consider first a simple, one degree of freedom motion. The change of momentum p in time is given by a force depending on this momentum and on a noise variable z:

$$\dot{p} = F(p,z). \tag{5.1}$$

Such descriptions are called "mesoscopic," since the dynamics of a selected "pointer" particle is followed, but the effect of further particles is not calculated microscopically: rather it is pressed into using the notion of *noise*, into an *assumed* random distribution of the variable z. The dependence of the evolution of the pointer variable, p, on itself and on the noise not always can be disentangled. If the noise, z, can be singled out as a lonely source term, i.e. when the above equation can be casted into a form

$$H(\dot{p},p) = z, \tag{5.2}$$

then we call this an *additive noise*. If the noise occurs as a factor to p-dependent terms, one uses the term *multiplicative noise*. Finally, if the noise (or its combination with a deterministic effect) has a correlation depending on p we talk about a *colored noise*

$$\dot{p} + \Gamma(p) = z(p). \tag{5.3}$$

The method of Ornstein and Uhlenbeck, presented in Chap. 3, can be used also in the general case to predict the distribution of p values from parallel evolutions, upon knowing the probabilistic properties of the noise variable, z. This $f(p,t)$ distribution is governed by the general Fokker–Planck equation (3.126).

5.1.1 Stochastic Damping Coefficient

In what follows we demonstrate that the well-known linear Langevin equation, modeling the Brownian motion and leading to a Gaussian stationary distribution of the corresponding Fokker–Planck equation, is altered by the multiplicative noise. This effect leads to a power-law tail in the stationary distribution of particle momenta. At a finite ratio of the correlation strength for the multiplicative and additive noise the stationary energy distribution becomes a cut power-law distribution [34].

Power-law tails are present in numerous distributions studied in physics or elsewhere when dealing with complex systems. These are often contrasted to the traditional statistical system, showing the Gibbs distribution ($\exp(-E/T)$) in energy, which is Gaussian in the momenta of free, non-relativistic particles ($\exp(-p^2/2mT)$). The latter is considered as the generic case for thermal equilibrium of non-correlated or short-range correlated systems. This concept has been carried far beyond of its original field describing monoatomic ideal gas (the Maxwell–Boltzmann statistics), by applying the Gibbs distribution in thermal equilibrium to areas such as particle physics and field theory.

A very simple and elegant, microdynamical explanation for the Maxwell–Boltzmann statistics is offered by the Langevin equation, describing a free particle moving under the influence of a deterministic damping force and a stochastic drive. It seems that in many statistical considerations of complex physical models from that on it is tacitly assumed that the presence of this additive noise is a dominant effect: the equilibrium distribution follows Gibbs' formula (the Gaussian distribution in momentum for a free, massive particle). Since the harmonic oscillator is just the extension of this free motion Langevin equation into the phase space, also for free quantum systems the above picture is generally accepted.

Now we treat the damping constant in the Langevin equation also stochastically (considering this way both multiplicative and additive noise). Our goal is to derive a generic stationary distribution for the Langevin-type equation with both additive and multiplicative noise. Conform to the original assumptions both noise terms are white (Dirac delta correlated in time), but in general they may show cross-correlations. Our starting point is the linear equation:

$$\dot{p} + \gamma p = \xi, \tag{5.4}$$

where now both ξ and γ are stochastic variables. They both may have a non-zero mean value,

$$\langle \xi(t) \rangle = F, \qquad \langle \gamma(t) \rangle = G, \tag{5.5}$$

and are subject to extremely short-term correlations:

$$\begin{aligned} \langle \xi(t)\xi(t') \rangle - \langle \xi(t) \rangle \langle \xi(t') \rangle &= 2D\,\delta(t-t'), \\ \langle \gamma(t)\gamma(t') \rangle - \langle \gamma(t) \rangle \langle \gamma(t') \rangle &= 2C\,\delta(t-t'), \\ \langle \gamma(t)\xi(t') \rangle - \langle \gamma(t) \rangle \langle \xi(t') \rangle &= 2B\,\delta(t-t'), \\ \langle \xi(t)\gamma(t') \rangle - \langle \xi(t) \rangle \langle \gamma(t') \rangle &= 2B\,\delta(t-t'), \end{aligned} \tag{5.6}$$

This problem, contained in (5.4–5.6), can be solved analytically. We determine the time dependence of the distribution of p values, denoted by $f(p,t)$ using the Fokker–Planck equation. In this notation, $f(p_0,t)\mathrm{d}p$ is the probability that after time t the variable p has the value in the range $[p_0, p_0 + \mathrm{d}p]$. We rewrite (5.4) as a finite difference equation

$$p(t+\mathrm{d}t) = p(t) + \int_t^{t+\mathrm{d}t} \mathrm{d}t' \left(\xi(t') - \gamma(t')\, p(t')\right), \tag{5.7}$$

Assuming that $p(t)$ is a smooth enough function, we replace $p(t')$ either by $p(t)$ or by $p(t+\mathrm{d}t)$, or any value in between. We fix ourselves to the Ito prescription, which uses $p(t)$ under the integral in the $\mathrm{d}t \to 0$ limit. In order to simplify notation we write the integral term as $\mathrm{d}t\,\langle x \rangle$, with x denoting the general integrand.

Now we are ready to follow the steps of the general derivation of the Fokker–Planck equation by Wang and Uhlenbeck. We start with

$$f(p,t+\mathrm{d}t) = \int \mathrm{d}\xi\, \mathrm{d}\gamma P(\xi,\gamma)\, f(p - \mathrm{d}t\,\langle \xi \rangle + p\mathrm{d}t\,\langle \gamma \rangle). \tag{5.8}$$

According to the method of Wang and Uhlenbeck we take a trial function $R(p)$ that is smooth enough and compute its average over the noise, as a function of time,

$$\langle R(t) \rangle = \int \mathrm{d}p R(p)\, f(p,t). \tag{5.9}$$

Applying this form to (5.8) we obtain

$$\begin{aligned} &\int \mathrm{d}p R(p)\, f(p,t+\mathrm{d}t) \\ &= \int \mathrm{d}\xi\, \mathrm{d}\gamma P(\xi,\gamma) \int \mathrm{d}p R(p + \mathrm{d}t\,\langle \xi \rangle - p\,\mathrm{d}t\,\langle \gamma \rangle)\, f(p,t). \end{aligned} \tag{5.10}$$

By Taylor expanding $R(p)$ and integrating over the noise distribution we get

$$\begin{aligned} &\langle R(p + \mathrm{d}t\,\langle \xi \rangle - p\,\mathrm{d}t\,\langle \gamma \rangle) \rangle \\ &= \left\langle R(p) + \mathrm{d}t R'(p)\, K_1(p) + \mathrm{d}t R''(p)\, K_2(p) + \mathcal{O}(\mathrm{d}t^2) \right\rangle \end{aligned} \tag{5.11}$$

with

$$K_1 = F - Gp, \qquad K_2 = D - 2Bp + Cp^2 \tag{5.12}$$

in the present case. This is equivalent to the following Fokker–Planck equation

$$\frac{\partial f}{\partial t} = -\frac{\partial (K_1 f)}{\partial p} + \frac{\partial^2 (K_2 f)}{\partial p^2}. \tag{5.13}$$

The stationary, detailed balance solution satisfies

$$\frac{\mathrm{d}}{\mathrm{d}p}\left(K_2 f_0\right) = K_1\, f_0, \tag{5.14}$$

which is analytically solvable for the stationary distribution.

We arrive at

$$f_0(p) = f(0)\,\frac{K_2(0)}{K_2(p)}\,\exp(L(p)) \tag{5.15}$$

with $f(0)$ being an integration constant and

$$L(p) = \int_0^p \mathrm{d}q\,\frac{K_1(q)}{K_2(q)}. \tag{5.16}$$

In the case of two noises correlated the way given in (5.6) we obtain the following logarithm of the stationary distribution (see problem 5.1):

$$\ln\frac{f_0(p)}{f(0)} = -\left(1+\frac{G}{2C}\right)\ln\frac{K_2(p)}{D} - \frac{\alpha}{\vartheta}\,\mathrm{atn}\left(\frac{\vartheta\, p}{D-Bp}\right), \tag{5.17}$$

with

$$\vartheta = \sqrt{CD-B^2} \qquad \text{and} \qquad \alpha = G\frac{B}{C} - F. \tag{5.18}$$

Here "atn" denotes the inverse of the tangent function, not always taking the first principle value, but rather continuing at $p > D/B$ smoothly.

Considering physical applications the noise correlation amplitudes, D, C and B build a positive semidefinite matrix. This ensures that C and D are non-negative values, and the determinant ϑ is real and also non-negative. The same applies for the function $K_2(p)$ occurring under the logarithm. In this context zero values for any of the correlation amplitudes are limiting cases, and in fact the stability of the stationary solution (5.17) against choosing a small positive value in principle has to be investigated.

Let us analyze some different limiting cases. First we consider the case of the original Langevin equation: $C = B = 0$. By doing so we do not allow for any noise (stochastic behavior) in the damping constant γ. This choice leads us back to the familiar Gauss distribution as the stationary solution of the corresponding Fokker–Planck equation:

$$f(p) = f(0)\mathrm{e}^{-\frac{G}{2D}p^2}\mathrm{e}^{\frac{F}{D}p}. \tag{5.19}$$

Here also a shift in the mean momentum occurs in case of a mean driving force $\langle\, \xi\, \rangle = F$.

Another interesting limiting case is that of the purely multiplicative noise with $D = 0, B = 0$. It has been applied among others for the heat conduction equation in fireballs produced in high-energy particle collisions [35]. In that model a Gamma distribution for the inverse temperature, $1/T$, has been obtained. The stationary solution in this case becomes

$$f(p) = f(p_1)\, p^{-2-G/C}\, \mathrm{e}^{-\frac{F}{C|p|}} \tag{5.20}$$

which is an Euler Gamma distribution in $1/p$. For large p this function approaches a pure power-law.

It is particularly amazing to investigate the degenerate case of $\vartheta = 0$. Now $K_2(p)$ reaches zero at a finite maximal momentum, $p_m = \sqrt{D/C}$, meaning zero probability in the stationary distribution $f(\sqrt{D/C}) = 0$. This “limiting momentum” – and with that a limiting energy – occurs only by this fine tuning of noise correlations in the physical system.

All limiting cases rely on an expansion of the generic solution for the small value of one or another parameter. Their validity is limited to certain ranges of momenta and energy: the classical Gaussian solution is always fine for small values of the argument of the inverse tangent function,

$$x = \frac{\vartheta p}{D - Bp}. \tag{5.21}$$

The Euler Gamma distribution on the other hand emerges for large vales of this quantity. Correspondingly, the widely applied Gaussian distribution can be a good approximation to the stationary solution only for momenta $p \ll \sqrt{D/C}$. (For $C = 0$ strictly, of course this is “the” solution for any finite momentum.) Generally the small argument of the inverse tangent is fulfilled for

$$p \ll \frac{D}{\vartheta + B}. \tag{5.22}$$

This result also means that *for the smallest fluctuation in the multiplicative factor the stationary Gauss distribution develops a power-law tail.* The power in this tail, p^{-2v}, is given by

$$v = 1 + \frac{G}{2C}. \tag{5.23}$$

In order to offer a visual insight into the nature of the generic stationary solution we show stationary spectra for different parameters (cf. Fig. 5.1).

In the case $B = 0$ (no cross correlation between the noises), and $F = 0$ (no drift term due to the additive noise), the *exact* stationary distribution is the Tsallis distribution

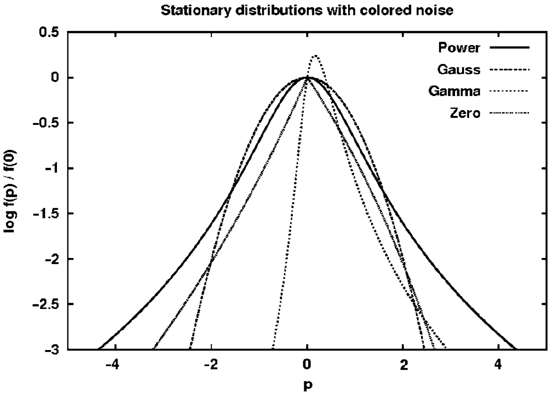

Fig. 5.1 Comparison of the generic stationary distributions of the Langevin-type equation with both additive and multiplicative noise. Limiting cases, as the Gauss-, the Gamma- and the Power-Law distribution are labeled correspondingly. The label "Zero" refers to the case with $\vartheta = 0$. The following parameters have been used: For the curve "Power" $B = 0, C = 1, D = 1, G = 1, F = 0$. For "Gauss" $B = 0, C = 0, D = 1, G = 1$ and $F = 0$. For "Gamma" $B = 0, C = 1, D = 0.1, G = 1, F = 1$. Finally, for the curve "Zero" $B = 1, C = 0.1, D = 10, G = 1$ and $F = 0$

$$f(p) = f(0)\left(1 + \frac{C}{D}p^2\right)^{-\nu}. \tag{5.24}$$

By using the energy of the free particle, $E = p^2/2m$ as the distribution variable and (5.17) we get

$$f(E) = f_0\left(1 + (q-1)\frac{E}{T}\right)^{\frac{q}{1-q}}, \tag{5.25}$$

where the parameters of the Tsallis distribution are given by

$$T = \frac{D}{mG}, \qquad q = 1 + \frac{2C}{G}. \tag{5.26}$$

Again for $C = 0$ (only additive noise) $q = 1$ and the Tsallis distribution goes over into the Gibbs distribution,

$$f(E) = f_0 \exp(-E/T). \tag{5.27}$$

Tsallis and others have worked out a thermodynamical framework [36] offering the distribution (5.25) as the canonical distribution.

We note that the presence of the two uncorrelated noise and the corresponding Fokker–Planck equation also can be obtained from a single momentum-dependent diffusion coefficient. Instead of (5.4) one may consider

$$\dot{p} + Gp = \eta\,\sqrt{D + Cp^2}, \tag{5.28}$$

with a single noise η, normalized to unity:

$$\langle\, \eta(t)\,\rangle = 0, \qquad \langle\, \eta(t)\eta(t')\,\rangle = 2\delta(t-t'). \tag{5.29}$$

This is a particular case of a more general field-dependent noise considered by Arnold, Son and Yaffe in the context of non-abelian plasmas. For a non-relativistic particle, its energy being $E = p^2/2m$ this is also a purely energy-dependent, i.e. ergodic noise. In the following sections we have a closer look on such systems.

5.1.2 Energy-dependent Noise

The Langevin and Fokker–Planck problems are quite general. Damping and diffusion coefficients may depend on the momentum p in a general way. Ergodization in phase space on the other hand achieved only when constant energy surfaces are covered uniformly. In such a situation the distribution f, as well as the coefficients G and D (the latter related to the noise), depends on the energy $E(p)$ only. Note, however, that they are not constant.

A corresponding particular Langevin equation is given by [37]

$$\dot{p} = z - G(E)\frac{\partial E}{\partial p} \tag{5.30}$$

containing an energy dependent damping term proportional to the general velocity $v = \partial E/\partial p$, and a zero-average noise, $\langle z(t)\rangle = 0$, with a correlation

$$\langle z(t)z(t')\rangle = 2D(E)\delta(t-t'). \tag{5.31}$$

The Fokker–Planck equation contains in this case the factors $D(p) = D(E)$ and $G(p) = -G(E)\partial E/\partial p$. Its stationary solution is given by

$$f(p) = \frac{A}{D(E)}\exp\left(-\int\frac{G(E)}{D(E)}\mathrm{d}E\right) = A\exp\left(-\int\frac{\mathrm{d}E}{\mathscr{T}(E)}\right). \tag{5.32}$$

This result is not readily the Boltzmann–Gibbs distribution, $\exp(-E/T)$, only in the case of energy-independent damping and noise coefficients. A general equilibrium is able to feature almost any other distribution of the energy of a single degree of freedom picked out of its environment. Instead of a constant temperature, T, in the general case a sliding inverse logarithmic slope is characteristic to such states. From $1/\mathscr{T}(E) = -\mathrm{d}\ln f(E)/\mathrm{d}E$ its relation to the damping and diffusion coefficients follows:

$$\mathscr{T}(E) = \frac{D(E)}{G(E) + D'(E)}. \tag{5.33}$$

The low-energy limit of this expression, pretending as $G(E)$ and $D(E)$ were constant, leads to an experimentally feasible definition of the Gibbs temperature, $T_{\text{Gibbs}} = D(0)/G(0)$. From the viewpoint of the Brownian motion another temperature may be used, the Einstein temperature $T_{\text{Einstein}} = \lim_{E\to\infty} D(E)/G(E)$. None of these two approximations are, however, coincident with the sliding slope of particle spectra given by (5.33) (Fig. 5.2).

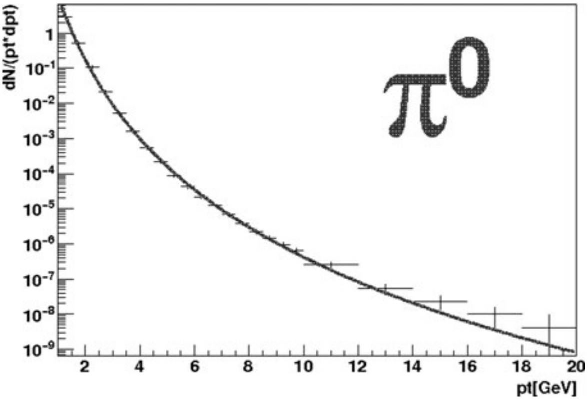

Fig. 5.2 Experimental spectrum of pions as measured in RHIC experiment and the fitted cut power-law distribution with $q = 1.22$. Reprinted from Fig. 5.1. in "Pions and Kaons from Stringy Quark Matter" (J. Phys. G 30: 064044, 2009) written by T.S. Biró and K. Urmossy

An important and historically considered particular case is given by the constant slope distribution, the Boltzmann–Gibbs distribution: $\mathscr{T}(E) = T$. The Tsallis distribution (5.25), obtained in the previous subsection, seems to be the next simplest, having a linear inverse slope–energy relation:

$$\mathscr{T}(E) = \frac{1}{q}T + \left(1 - \frac{1}{q}\right)E. \tag{5.34}$$

The corresponding equilibrium distribution in this case turns out to be an exponential of a logarithm, which is a power-law:

$$f(p) = \frac{1}{Z}\left(1 + (q-1)\frac{E}{T}\right)^{\frac{q}{1-q}} \tag{5.35}$$

It has the interesting property, that the parameter T is the fixed point of the sliding (linear) slope: $\mathscr{T}(T) = T$. This parameter may be referred to as the *Tsallis temperature.*

The classical mesoscopic models of temperature from the random walk picture of the Brownian motion til the corresponding Langevin and Fokker–Planck equations often assume constant properties of the diffusion and the damping term.

Relating them via the fluctuation–dissipation theorem makes it possible to conjecture a temperature. This we refer to as the "Einstein temperature." Interesting, and still analytically treatable complications arise, when the medium producing the noise is no more "democratic": the noise' strength itself depends on the state of the observed slow degree of freedom (e.g. a Brownian particle). Such in general $(\mathbf{p},\mathbf{q})$ - dependent noises are called *colored*. Such systems are difficult to solve. However, if the "colorization" of the noise, comprised in the dependence of the noise correlation on the state of the observed, slow degree of freedom, is only indirect, only via the energy of the observed subsystem, then the classical formulas can be generalized analytically. As a consequence the renown fluctuation–dissipation theorem, relating dissipative and noisy terms in the mesoscopic equations of motion, holds in a more general form. This, at the end, effects the formula and interpretation of the Einstein temperature, too.

In a realistic system there are many microscopic degrees of freedom to be considered. Denoting a point in the $6N$-dimensional phase space by π_i, the first $3N$ part being generalized coordinates, $\mathbf{q}$, the second $3N$ part generalized momenta, $\mathbf{p}$, the Langevin equation can be implemented in the form

$$\dot{\pi}_i = (S_{ij} - G_{ij})\nabla_j E + z_i. \tag{5.36}$$

The symplectic coefficient, S_{ij}, has a block structure in the phase space: a block of unity between momenta and coordinates produces the $\dot{\mathbf{q}} = \frac{\partial E}{\partial \mathbf{p}}$ like equations of motion and the corresponding block of minus unity produces the $\dot{\mathbf{p}} = -\frac{\partial E}{\partial \mathbf{q}}$ ones. All other entries in the matrix S_{ij} are zero. These contributions to the evolution in phase space do not change the total energy of the system, $E(p_i)$, they just cause conservative motion inside a given energy shell only. For considering the thermal evolution of the energy distribution it is therefore not interesting and shall be omitted in the followings. Also the noise terms are active only as forces, giving a source term to the equation of motion for momenta only. This way we reduce the dissipative phase space dynamics to a Langevin-type equation for the momentum components only.

The damping and dissipation terms with the respective symmetric coefficients G_{ij} and D_{ij} keep balance on the long term. An ergodized equilibrium distribution of the momenta can be a single function of the energy variable E only, therefore these coefficient matrices have to be connected by a single function of energy, too. In this spirit we consider the following type of Langevin equation:

$$\dot{p}_i = -G_{ij}(E)\nabla_j E + z_i. \tag{5.37}$$

with the noise correlation

$$\left\langle z_i(t) z_j(t') \right\rangle = 2D_{ij}(E)\,\delta(t-t'). \tag{5.38}$$

We are interested in the evolution of the distribution over ensembles of $p_i(t)$ values, $f(\mathbf{p},t)$.

One uses the general Fokker–Planck equation (3.126):

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial p_i}\left(G_{ij}(E)\frac{\partial E}{\partial p_j} f \right) + \frac{\partial^2}{\partial p_i \partial p_j}\left(D_{ij}(E) f \right). \tag{5.39}$$

The stationary solution, $f_0(E)$, satisfies not only the $\frac{\partial f}{\partial t} = 0$ requirement, but also the detailed balance condition:

$$G_{ij}(E)\frac{\partial E}{\partial p_j} f_0(E) + \frac{\partial}{\partial p_j}\left(D_{ij}(E) f_0(E) \right) = 0. \tag{5.40}$$

Now due to the assumption of E-dependence only we get

$$G_{ij}(E)\frac{\partial E}{\partial p_j} f_0(E) + D'_{ij}(E)\frac{\partial E}{\partial p_j} f_0(E) + D_{ij}(E) f'_0(E)\frac{\partial E}{\partial p_j} = 0. \tag{5.41}$$

This result should hold for any value of the generalized $3N$-velocity vector, $\frac{\partial E}{\partial p_j}$. This is achieved only if the coefficient vanishes:

$$G_{ij}(E) f_0(E) + D'_{ij}(E) f_0(E) + D_{ij}(E) f'_0(E) = 0. \tag{5.42}$$

Dividing this equation by $f_0(E)$ one obtains

$$G_{ij}(E) + D'_{ij}(E) + D_{ij}(E)\frac{\mathrm{d}}{\mathrm{d}E}\ln f_0(E) = 0. \tag{5.43}$$

Now let us abbreviate the logarithmic slope of the $f_0(E)$ energy distribution by

$$\frac{1}{\mathcal{T}} := -\frac{\mathrm{d}}{\mathrm{d}E}\ln f_0(E). \tag{5.44}$$

Doing all these steps gives rise to a general fluctuation dissipation theorem:

$$D_{ij}(E) = \mathcal{T}(E)\left(G_{ij}(E) + D'_{ij}(E) \right). \tag{5.45}$$

It is highly nontrivial that two high-dimensional matrix functions of the phase space coordinates p_i would be related by a single scalar function of energy only! Recalling that $\mathcal{T}(E)$ is the inverse logarithmic slope of the equilibrium distribution, the fluctuation–dissipation relation can be expressed using an integral with $f_0(E)$:

$$D_{ij}(E) = \frac{1}{f_0(E)}\int_E^{\infty} G_{ij}(x) f_0(x)\,\mathrm{d}x. \tag{5.46}$$

Still, quite general diffusion and damping coefficient matrices are allowed, but D_{ij} is connected to G_{ij} via an energy dependent scalar, the equilibrium energy distribution, $f_0(E)$. This distribution can be anything, provided that it is derived as a canonical distribution from thermodynamically consistent composition rules discussed in Chap. 3. We note that for a constant (energy-independent) damping coefficient, the energy-dependent diffusion coefficient matrix, $D_{ij}(E)$, is proportional to the *probability of having energy larger than E* in the stationary distribution. This way the fluctuation–dissipation balance theorem is related to a continuous version of the extreme value probability.

A simple realization of the correspondence (5.46) is given by such matrices D_{ij} and G_{ij} which are proportional to the same constant matrix: $D_{ij}(E) = D(E)\gamma_{ij}$, and $G_{ij}(E) = G(E)\gamma_{ij}$. For this class of solutions the integral equation (5.46) simplifies to a scalar requirement,

$$D(E) = \frac{1}{f_0(E)} \int_E^{\infty} G(x)\, f_0(x)\, \mathrm{d}x. \tag{5.47}$$

Expressing the reciprocal of logarithmic slope from (5.44, 5.45) in this case we obtain

$$\frac{1}{\mathscr{T}} = \frac{G(E)}{D(E)} + \frac{D'(E)}{D(E)}. \tag{5.48}$$

The equilibrium energy distribution can be reconstructed by using (5.44). The result is

$$f_0(E) = C \exp\left(- \int \frac{\mathrm{d}E'}{\mathscr{T}(E')} \right) = \frac{C}{D(E)} \exp\left(- \int \frac{G(E')}{D(E')} \mathrm{d}E' \right). \tag{5.49}$$

It is enlightening to discuss some particular cases of the stationary energy distribution. The use of the Boltzmann–Gibbs distribution, $f(E) \propto \exp(-E/T)$, leads to $D_{ij} = TG_{ij}$ with energy-independent matrices (this is the usual textbook case). The use of a cut power-law energy distribution,

$$f(E) = C\,(1 + aE)^{-\nu} \tag{5.50}$$

with an energy-independent damping coefficient, G, gives rise to

$$D(E) = \frac{G}{\nu - 1} \left(\frac{1}{a} + E \right) \tag{5.51}$$

i.e. to a diffusion coefficient which is a linear function of the energy. It is interesting to note that such an energy distribution is the canonical energy distribution to a non-additive energy composition law, $E_1 \oplus E_2 = E_1 + E_2 + aE_1E_2$, discussed previously. In this case $\nu = 1/aT$.

A further interesting case is presented by assuming that both the damping and the diffusion coefficient matrix follow the same function of the energy, but their ratio (the Einstein temperature) is constant.[1] Due to (5.45) the sliding slope is, however, not constant; it rather interpolates between a low- and high-energy and behavior. From $D_{ij}(E) = TG_{ij}(E) = \gamma_{ij} T g(E)$ it follows

$$\gamma_{ij} T g(E) \,=\, \mathscr{T}(E)\,\left(\gamma_{ij} g(E) + \gamma_{ij} T g'(E)\right). \tag{5.52}$$

We can express the sliding slope parameter from this equation as being

$$\frac{1}{\mathscr{T}} \,=\, \frac{1}{T} + \frac{g'(E)}{g(E)}. \tag{5.53}$$

Integrating this over the energy variable leads to the logarithm of the detailed balance distribution

$$\ln f_0(E) = \int\limits_E^{\infty} \frac{\mathrm{d}x}{\mathscr{T}(x)} = -E/T - \ln g(E) + \text{const.} \tag{5.54}$$

One inspects that the detailed balance contribution is not solely the Boltzmann–Gibbs exponential; it is modified by the same energy-dependent factor in this case:

$$f_0(E) \,=\, C\,\frac{1}{g(E)}\,\mathrm{e}^{-E/T}. \tag{5.55}$$

5.1.3 Coupled Stochastic Dynamics

Stationary energy distributions differing from the Gibbs–Boltzmann exponential may emerge not only as energy-dependent (sliding) slopes, $\mathscr{T}(E)$, due to non-trivial correlations in the noise, but also due to nontrivial dynamics of the correlation amplitude itself. Instead of being a function of the energy of the pointer particle in the mesoscopic approach, one considers phenomena where the noise property itself is a function of time, sampled from another distribution. This *superstatistical* approach has been circumvented in Chap. 4.

Here we consider a case where the noise is also governed by background stochastic processes, underlying some dynamical equations. In particular the noise correlation, $D(t)$, itself becomes a stochastic variable. This way two simple, but coupled Langevin type equations have to be solved.

This approach is most relevant when time series of data have to be studied, like by signal processing or by considering statistical models for the financial market. This new branch of physics, econophysics, deals with wildly fluctuating variables, i.e. stock prices. However, also the statistical properties of the noise on the top of mean trends is seemingly subject to random effects: this property is called "volatility."

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[1] This assumption is typical to field theory calculations.

In the following sections we present such a model, originally published in [38]. We inspect the price of a share, $s(t)$, as a stochastic variable on the top of a deterministic exponential growth (with inflation rate $\mu > 0$). It is customary to regard the modified log-return, the profit in original sense, i.e.

$$x = \ln \frac{s_t}{s_0} - \mu t, \tag{5.56}$$

as the indicator variable. For its evolution a Langevin equation of type

$$\mathrm{d}x = -a(v)\mathrm{d}t + \sqrt{v}\,W_1 \tag{5.57}$$

can be written down, with W_1 being a so called Wiener process, a Gaussian white noise, with zero mean and unit width. The function $a(v)$ reflects the prescription when deriving the x-process with additive noise from the s-process with multiplicative noise. In the Ito-scheme it is given by $a(v) = v/2$. There exist, however, one particular Strotanovich scheme where it vanishes $a(v) = 0$.

The volatility, $v = \sigma^2$ itself is governed by stochastic effects according to phenomenological observations on financial markets. Contemporary models, of which we shall present one in more details, usually have a first order deterministic part, causing an exponential approach to the mean volatility, θ, and a noise term possibly influenced by the volatility itself. We consider another stochastic equation for the time evolution of the volatility:

$$\mathrm{d}v = -\gamma(v-\theta)\mathrm{d}t + b(v)W_2. \tag{5.58}$$

The second Wiener process, W_2, may be or may not be correlated with the first one. It is customary to use $b(v) = \kappa v$ (Hull–White model) or $b(v) = \kappa\sqrt{v}$ (Heston model), in particular.

Born–Oppenheimer approximation

We put an emphasis here on approximations which enable a simplified treatment predicting the distribution of x (or s) as a function of time. Namely we assume that the stochastic volatility variable, v, reaches more or less its stationary distribution – due to being influenced by a number of factors – and then acts for the dynamics of the log-return, x, as an instantaneous, time-independent parameter. This assumption is analog to the Born–Oppenheimer approximation applied successfully in solid state and atomic physics. The v-process can be then solved in itself. The corresponding Fokker–Planck equation is given as

$$\frac{\partial \Pi}{\partial t} + \frac{\partial}{\partial v}\gamma(v-\theta)\Pi + \frac{1}{2}\frac{\partial^2}{\partial v^2}b^2(v)\Pi = 0. \tag{5.59}$$

The stationary detailed balance solution satisfies

$$\frac{\partial}{\partial v} b^2(v)\Pi = -2\gamma(v-\theta)\Pi. \tag{5.60}$$

The balanced distribution of the volatility, v, is given by

$$\Pi(v) = \frac{N}{b^2(v)} \exp\left(-2\gamma \int \frac{v-\theta}{b^2(v)} \mathrm{d}v\right). \tag{5.61}$$

According to the Born–Oppenheimer approximation we average over this stationary balance probability of v the solution of the primary diffusion process described by (5.57),

$$P(x;v,t) = \frac{1}{\sqrt{2\pi vt}} \exp\left(-\frac{(x+a(v)t)^2}{2vt}\right). \tag{5.62}$$

We obtain the following approximation for the time evolution of the log-return probability:

$$P_t(x) = \int_0^\infty \mathrm{d}v\, \Pi(v)\, P(x;v,t). \tag{5.63}$$

Collecting all terms together we arrive at

$$P_t(x) = \frac{N}{\sqrt{2\pi t}} \int_0^\infty \mathrm{d}v \frac{1}{b^2(v)\sqrt{v}} \exp\left(-\frac{(x+a(v)t)^2}{2vt} - 2\gamma \int \frac{v-\theta}{b^2(v)} \mathrm{d}v\right). \tag{5.64}$$

Heston model

For the Heston model, $b(v) = \kappa\sqrt{v}$ the stationary distribution is an Euler Gamma distribution:

$$\Pi(v) = \frac{\alpha^\alpha}{\theta^\alpha \Gamma(\alpha)} v^{\alpha-1} \mathrm{e}^{-v\alpha/\theta} \tag{5.65}$$

with $\alpha = 2\gamma\theta/\kappa^2$. In the Ito-scheme $a(v) = v/2$, and the above integral (5.64) can be determined analytically. We obtain

$$P_t(x) = \frac{1}{\Gamma(\alpha)} \left(\frac{2\alpha|x|}{ft}\right)^\alpha \sqrt{\frac{f}{\pi|x|}} \mathrm{e}^{-x/2} K_{\alpha-1/2}\left(\frac{f|x|}{2}\right) \tag{5.66}$$

with

$$f = \sqrt{1 + \frac{16\kappa^2}{\gamma t}} \tag{5.67}$$

and $K_\nu(z)$ Bessel K-function. For large times the factor $f \to 1$ approaches unity.

For large positive x arguments, i.e. for extreme large wins on s, the Bessel function is dominated by an exponential, so

$$P_t^{(\mathrm{win})}(x) \sim x^n \mathrm{e}^{-\frac{f+1}{2}x} \tag{5.68}$$

and for large negative x, i.e. for extreme losses, it is dominated by another exponential

$$P_t^{(\mathrm{loss})}(x) \sim x^n \mathrm{e}^{\frac{f-1}{2}x}. \tag{5.69}$$

Since $f > 1$ at all times, it means that in this model losses tend to show a fatter tail (a slower decrease) in x than wins. For very large times this difference, however, reduces. Note that $\mathrm{e}^{-xf_\pm} = s^{-f_\pm}$ is in fact a power-law behavior in s, using the notation $f_\pm = (f \pm 1)/2$.

In the case of $a(v) = 0$ this model is also subject to the scaling $P_t(x) = \rho(x/\sqrt{t})/\sqrt{t}$ just like the normal diffusion. Now the $\mathrm{e}^{-x/2}$ factor is not present and $f = 4\kappa/\sqrt{\gamma t}$ in (5.66). The distribution $P_t(x)$ in this case becomes symmetric for wins and losses (relative to the mean trend).

Hull–White model

In order to compare the power of different approximations let us consider another model, the Hull–White model, which leads to simpler result with interesting thermodynamical analogies. Using $b = \kappa v$ the balanced volatility follows again an Euler Gamma distribution, now in in the reciprocal variable $y = 1/v$:

$$\Pi(y) = \frac{(\beta\theta)^{\beta+1}}{\Gamma(\beta+1)}\, y^\beta\, \mathrm{e}^{-\beta\theta y} \tag{5.70}$$

with $\beta = 2\gamma/\kappa^2$. The approximated x distribution in the special scheme with $a(v) = 0$ becomes:

$$P_t(x) = \frac{1}{\sqrt{2\pi t}} \int\limits_0^\infty \mathrm{d}y\, \Pi(y) \sqrt{y} \mathrm{e}^{-\frac{x^2}{2t}y}. \tag{5.71}$$

Regarding the quantity $E = x^2/2t$ as an abstract "energy" the above formula represents a Boltzmann–Gibbs energy distribution under the influence of a "fluctuating temperature" $k_\mathrm{B}T = 1/y$. In particular a Gamma-distributed inverse temperature is known to lead to a cut power-law (Tsallis) distribution in the energy variable:

$$P_t(x) = N(\beta, \beta\theta t)\left(1 + \frac{x^2}{2\beta\theta t}\right)^{-(\beta+3/2)} \tag{5.72}$$

with

$$N(\beta, z) = \frac{1}{\sqrt{2z}} \frac{\Gamma(\beta+3/2)}{\Gamma(\beta+1)\Gamma(1/2)}. \tag{5.73}$$

The above ratio of Γ functions actually constitutes Bernoulli's Beta-function $B(\beta+1, 1/2)$.

This result is symmetric in win and loss percentages, i.e. for all positive and negative x values, due to the $a(v) = 0$ choice. This is a nice symmetry property of this model. On the other hand here the large x behavior is a power-law in x, not in s. Nevertheless, for large powers β the cut power-law (Tsallis) distribution comes quite close to the exponential for small and intermediate arguments, so the difference may influence the extreme large x (s) values only (Fig. 5.3).

The scaling is universal as long as $a(v) = 0$ can be taken, in this case

$$P_t(x) = \frac{1}{\sqrt{t}} f\left(\frac{x}{\sqrt{t}}\right) \tag{5.74}$$

for any time-lag t. This is testable on the (detrended and normalized) data (cf. Fig. 5.4). Since these data are detrended and normalized, the Gaussian curve to be followed by a simple – traditional – stochastic white noise is unique. The background-stationary distribution in the Hull–White model on the other hand includes the parameters $a(v)$ and β. They can be fitted to the shape of the scaling function in (5.74). One gets $f(x) \approx -2.36\ln(1 + x^2/1.78) - 0.62$.

5.2 Fisher Entropy

Sir Ronald Aylmer Fisher (1890–1962) was a statistician, evolutionary biologist and geneticist. He was described as "a genius who almost single-handedly created the foundations for modern statistical science."

Fisher invented the technique of maximum likelihood and originated the concepts of sufficiency, ancillarity, Fisher's linear discriminator and Fisher information. His 1924 article "On a distribution yielding the error functions of several well known statistics" presented Pearson's χ^2 and Student's t distributions in the same framework as the Gaussian distribution, and his own "analysis of variance" distribution z (more commonly used today in the form of the F distribution). These contributions made him renown in the field of statistics.

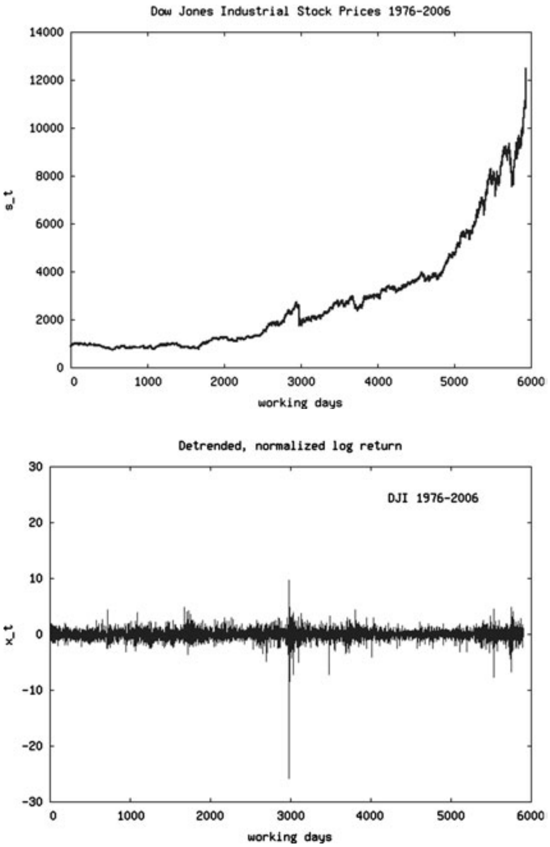

Fig. 5.3 The distribution of normalized and detrended log-returns $P_t(x)$ for Dow Jones data 1996–2006, compared with the Gaussian curve of the normal distribution and with predictions of the Hull–White model in the Born–Oppenheimer approximation

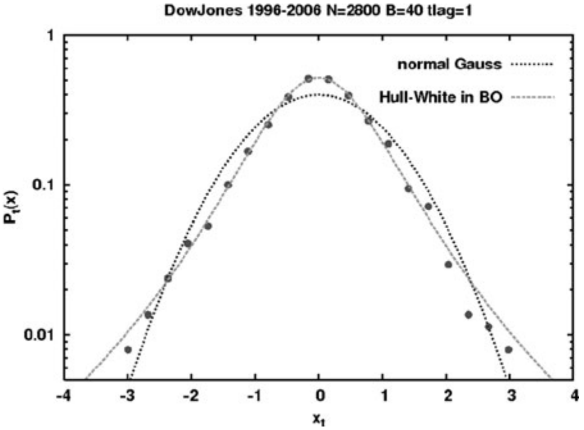

Fig. 5.4 Time data of Dow Jones daily closing average s_t and the detrended and normalized log return x_t

Originally, Fisher's entropy or information formula [39–41],

$$I(\Theta) = -S_{\mathrm{F}}(\Theta) = \left\langle \left(\frac{\partial}{\partial \Theta} \ln f(x,\Theta) \right)^2 \right\rangle, \tag{5.75}$$

stems from searching for the best fit of a distribution formula, $f(x,\Theta)$, to statistical data. The distribution over x defines the expectation value in the above formula, while Θ is a fit parameter. This information measure is additive for independent sets of data x and y, i.e. $I_{xy}(\Theta) = I_x(\Theta) + I_y(\Theta)$. In the followings we consider its thermodynamical analogue, where both the distributed variable $x = \Delta p_i$ and the parameter $\Theta = p_i$ describe a deviation and a starting point for it in the phase space. In the sense of Fisher's statistics the optimal description of an uncertainty of knowing a point in the phase space is measured.

5.2.1 Taylor Expansion of the Entropy in Phase Space

Starting with the Boltzmann–Gibbs–Shannon (BGS) entropy formula an expression reminding to Fisher's entropy can be constructed, as it stemmed from the second order term in a Taylor expansion. Considering the entropy as the phase space integral with the high-dimensional integration measure $\mathrm{d}\Gamma$,

$$S = \langle \sigma \rangle = \int \sigma(p_i) f(p_i) \mathrm{d}\Gamma, \tag{5.76}$$

the BGS entropy is defined by $\sigma = -\ln f$ (in $k_{\mathrm{B}} = 1$ units). Let us regard now fluctuations (or a given degree of uncertainty) in the classical phase space position by taking the entropy formula at $p_i + \Delta p_i$. The Taylor expansion of σ includes the following derivatives:

$$\frac{\partial}{\partial p_i} \sigma = -\frac{1}{f} \frac{\partial}{\partial p_i} f \tag{5.77}$$

for the first order term and

$$\frac{\partial}{\partial p_i} \frac{\partial}{\partial p_j} \sigma = \frac{1}{f^2} \frac{\partial f}{\partial p_i} \frac{\partial f}{\partial p_j} - \frac{1}{f} \frac{\partial}{\partial p_i} \frac{\partial}{\partial p_j} f \tag{5.78}$$

for the second order term. Using the abbreviating notation $\nabla^i f = \partial f / \partial p_i$, the expansion of σ is given by

$$\sigma(p_i + \Delta p_i) = -\ln f - \frac{1}{f} \Delta p_i \nabla^i f + \frac{1}{2} \Delta p_i \left(\frac{1}{f^2} \nabla^i f \nabla^j f - \frac{1}{f} \nabla^i \nabla^j f \right) \Delta p_j. \tag{5.79}$$

By the virtue of (5.76) the entropy functional becomes

$$S = -\int f \ln f \mathrm{d}\Gamma - \int \Delta p_i \nabla^i f \mathrm{d}\Gamma + \frac{1}{2}\int \Delta p_i \Delta p_j \left(\frac{1}{f}\nabla^i f \nabla^j f - \nabla^i \nabla^j f\right) \mathrm{d}\Gamma. \tag{5.80}$$

Now we assume that the deviations (uncertainties) around the classical phase space point are symmetric. Up to second order (in the Gaussian approximation) one has

$$\langle \Delta p_i \rangle = 0, \qquad \langle \Delta p_i \Delta p_j \rangle = \kappa^2 \delta_{ij}. \tag{5.81}$$

Averaging now the entropy functional in (5.80) by using these properties one obtains

$$S = -\int f \ln f \mathrm{d}\Gamma + \frac{\kappa^2}{2}\int \left(\frac{1}{f}(\nabla f)^2 - \nabla^2 f\right) \mathrm{d}\Gamma. \tag{5.82}$$

Here the first order term has vanished due to the assumed isotropy of the phase space delocalization. In the second order term still there is a contribution, the one with $\nabla^2 f$, which is a total derivative, so its integral contributes only by a surface term in the phase space. This contribution will be neglected. After all this considerations we arrive at two main contributions to the entropy functional:

$$S = S_{\mathrm{B}} + S_{\mathrm{F}} \tag{5.83}$$

with the original Boltzmann entropy formula,

$$S_{\mathrm{B}} = -\int f \ln f \,\mathrm{d}\Gamma, \tag{5.84}$$

and with Fisher's entropy[2]

$$S_{\mathrm{F}} = \frac{\kappa^2}{2}\int \frac{1}{f}(\nabla f)^2 \,\mathrm{d}\Gamma. \tag{5.85}$$

As it is shown by the solution of problem (5.2) the total entropy assuming an isotropic Gaussian distribution of the uncertainty Δp_i can also be written as

$$S = \int f \mathrm{e}^{\kappa^2 \nabla^2/2} (-\ln f) \,\mathrm{d}\Gamma. \tag{5.86}$$

By seeking for an equilibrium distribution the entropy has to be maximized. Depending on different constraints, the functional derivative of $S[f]$ is needed for the determining equation. The formula (5.86) leads to the following variation

$$\frac{\delta S}{\delta f} = -\left[\mathrm{e}^{\kappa^2 \nabla^2/2}(\ln f) + \frac{1}{f}\mathrm{e}^{\kappa^2 \nabla^2/2} f\right]. \tag{5.87}$$

---

[2] This formula coincides with (5.75) by regarding the phase space point itself as the Θ parameter.

Expansion up to terms in the order of $\mathscr{O}(\nabla^2)$ one gets

$$\frac{\delta S}{\delta f} = -(1+\ln f) + \kappa^2 \left(\frac{(\nabla f)^2}{2f^2} - \frac{\nabla^2 f}{f} \right). \tag{5.88}$$

In the general canonical equilibrium the distribution is determined by a differential equation

$$\frac{\delta S}{\delta f} = \alpha + \beta E(p_i). \tag{5.89}$$

5.2.2 Fisher Entropy of the Maxwell–Boltzmann Gas

The differential equation determining the optimal distribution to maximize the Fisher-expanded shifted Boltzmann-entropy, S, to second order is in general hard to solve. For a non-relativistic ideal gas, the Maxwell–Boltzmann (MB) gas, however, an analytic solution can be obtained. It is worth to inspect it.

The non-relativistic kinetic energy of N particles is additive, it defines the radius squared of the $D = 3N$-dimensional sphere in phase space:

$$E(p_i) = \frac{1}{2m} \sum_{i=1}^{D} p_i^2 = \frac{p^2}{2m}. \tag{5.90}$$

We assume that the distribution is a function of this radius only, $f(p_i) = f(p)$. In this case $\nabla_i f = f'(p) p_i / p$ and the D-dimensional Laplacean is given by

$$\nabla^2 f = f'' + \frac{D-1}{p} f'. \tag{5.91}$$

The canonical entropy supplemented by the Fisher-type second order term achieves its maximum if the following ordinary differential equation is fulfilled:

$$-(1+\ln f) + \kappa^2 \left(\frac{f'f'}{2f^2} - \frac{f''}{f} - \frac{D-1}{p} \frac{f'}{f} \right) = \alpha + \beta \frac{p^2}{2m}. \tag{5.92}$$

This has a special analytical solution with the Gaussian ansatz:

$$\ln f = A - Bp^2/2. \tag{5.93}$$

Replacing this ansatz into (5.92) we obtain two constraints for the variables A and B:

$$\begin{aligned} -(1+A) + \kappa^2 DB &= \alpha, \\ B - \kappa^2 B^2 &= \frac{\beta}{m}. \end{aligned} \tag{5.94}$$

For the microcanonical distribution $\beta = 0$ and the $B = 0$ solution holds with constant probability f. There is, however, another solution with $B = 1/\kappa^2$ in this case: *a Gaussian equilibrium distribution with microcanonical constraint*! This seems to be an oddity, and one is tempted to throw away this solution as non-physical one. For the canonical case $\beta > 0$, and the solution contiguous with $B = 0$ may be chosen:

$$B = \frac{1}{2\kappa^2} - \frac{1}{\kappa}\sqrt{\frac{1}{4\kappa^2} - \frac{\beta}{m}}. \tag{5.95}$$

In this case the canonical equilibrium distribution is Gaussian, but the relation between the Lagrange multiplier β and the width of the Maxwell–Boltzmann distribution has been changed. Another odd property of this approach is that there is a maximal β for the real solution; so there is a minimal temperature below which no canonical equilibrium can be established with the entropy formula (5.83). It is given by

$$T \geq T_{\text{min}} = \frac{4\kappa^2}{m}. \tag{5.96}$$

5.3 Thermodynamics of Abstract Composition Rules

Non-extensive thermodynamics is required whenever the "normal" addition rule for extensive variables, in particular the central quantity, entropy, is violated [36]. In such cases the additive Boltzmann–Gibbs–Shannon (BGS) formula cannot be applied, because it would become a non-extensive quantity, whose value – related to the number of microstates realizing a given macrostate, $\mathcal{N}$, – grows with the number of degrees of freedom, N, faster than linear. On the other hand, in a given "universality class" of entanglements, another entropy formula may be obtained. It follows then a more complicated composition rule than the simple addition, which in turn – for a special value of a scale parameter – can be extensive, i.e. linearly growing with N.

There is a physical consequence of this treatment.

Since due to the classical logarithmic formula the BGS entropy is then and only then additive, when the probabilities of microstates are independent and therefore the *joint probability* is a product of the respective probabilities, we may also say that for non-extensive systems the statistical independence assumption is violated. This alone were a common property of any finite system treated microcanonically, but non-extensive thermodynamics applies to those systems, which persist this violation even in the $N \to \infty$ (so called "thermodynamical") limit.

Let us investigate this correspondence more closely. Let p_{ij}^{A+B} the joint probability of the event when the subsystem A is in the state i and the subsystem B is in its state j. The respective number of possible states be N_A and N_B. Then two *marginal probabilities* can be defined: one for the system A being in its state i irrespective to the state of the system B,

$$q_i^A = \sum_{j=1}^{N_B} p_{ij}^{A+B}, \tag{5.97}$$

and another one for the system B being in state j irrespective to the status of A,

$$q_j^B = \sum_{i=1}^{N_A} p_{ij}^{A+B}. \tag{5.98}$$

The *conditional probabilities* express the odds for a system to be in a given state while the other system is in another definite state:

$$\begin{aligned} w_{i(j)}^A &= \frac{p_{ij}^{A+B}}{q_j^B}, \\ w_{j(i)}^B &= \frac{p_{ij}^{A+B}}{q_i^A}. \end{aligned} \tag{5.99}$$

Even if there are correlations between the subsystems A and B, from the above definitions it is obvious that the common microstate probability is always a product of a marginal and a conditional probability:

$$p_{ij}^{A+B} = q_j^B w_{i(j)}^A = q_i^A w_{j(i)}^B. \tag{5.100}$$

In the particular case of *statistically independent* systems the micro-probability is a product of the marginal probabilities

$$p_{ij}^{A+B} = q_i^A q_j^B. \tag{5.101}$$

All these probabilities are normalized to one.

The generalization of the BGS entropy is not additive at the product of probabilities, the addition "$+$" is replaced by another composition rule, "$\oplus$." The entropy as a functional of the joint probability distribution is in general a non-additive composition of entropy terms belonging to the corresponding marginal and conditional probabilities,

$$S\left(p_{ij}^{A+B}\right) = S\left(q_i^A\right) \oplus S\left(w_{j(i)}^B\right) = S\left(w_{i(j)}^A\right) \oplus S\left(q_j^B\right), \tag{5.102}$$

or with a more compact notation for the marginal and conditional probabilities,

$$S(A+B) = S(A) \oplus S(B|A) = S(A|B) \oplus S(B). \tag{5.103}$$

This relation is really general, valid even for correlated, in particular for quantum-entangled systems.

A necessary condition for the above equation to be true is its fulfillment in the equipartition case. Now all microstate probabilities are given by $p_{ij}^{A+B} = c$, with c being a constant value. In this case the marginal probabilities are also constant, $q_i^A = N_B c$ and $q_j^B = N_A c$. The conditional probabilities become $P(A|B) = w_{i(j)}^A = 1/N_A$ and $P(B|A) = w_{j(i)}^B = 1/N_B$. The general entropy rule (5.102) reads as

$$S(c) = S(N_B c) \oplus S(1/N_B) = S(1/N_A) \oplus S(N_A c). \tag{5.104}$$

It means that the entropy function at equipartition satisfies a general, not necessarily additive composition rule for the product of arguments:

$$S(xy) = S(x) \oplus S(y). \tag{5.105}$$

In the traditional statistical physics the composition of entropies is by addition, and therefore the equipartition entropy function must be proportional to the logarithm. In fact $S = k \ln W$ with W being the number of states (and $1/W$ the probability to be in one given state) is Boltzmann's famous formula. For W states the equal probabilities are given as $c = 1/W$ and $S(c) = Wc\sigma(c) = \sigma(1/W)$ if using the entropy density function $\sigma(c)$.

In thermodynamics not a single pairing of two subsystems counts at the end, but a huge number of repetition of such compositions. The basic question is whether after many – in the mathematical model infinitely many – steps the effective composition of two large, "pre-composed" subsystems may be well described by a simple addition rule or not. This question is not easy to answer in general, although conventional thermodynamic textbooks frequently argue that for a large number of degrees of freedom the general rule for extensive quantities becomes close to the addition, because all interaction and correlation contributions grow less than the volume. This is true for most interactions, definitely for the short ranged ones. For long range interactions, however, causing entanglement between microstates or non-vanishing energy contributions due to fractal surfaces in their phase space filling pattern, more general composition rules may apply.

Typical physical systems showing non-extensive thermodynamical behavior are strongly coupled, show long-range correlations and correspondingly long-range forces. Many of them are not in a real equilibrium but in long-lived metastable states. Most studied examples for long-range correlated matter is given by glasses, in particular spin glasses (and an uncountable number of mathematical models for neural networks were triggered by an analogy to glassy systems). Another examples are Bose condensed ("cold") atomic systems and materials capable of high-T_c superconductivity. Further instances of non-extensive physical systems are rather known from long-range forces acting in their inside: gravitating clusters, charged plasmas and quark matter (the primordial cosmic soup) at hadronization. Yet another examples – treated in the framework of models using the concept of a non-extensive entropy formula – are given by "unpredictable" phenomena, like earthquakes, turbulence and in general chaotic Hamiltonian dynamics. Since – as we shall see – a non-extensive entropy formula leads to fat tailed distributions in a formally canonical equilibrium state, it also has been applied to describe such (mostly power-law tailed) distributions in all areas of statistical physics: in the description of fluctuation distributions in financial markets as well as for anomalous diffusion in systems studied for the development of nanotechnology.

5.3.1 Asymptotic, General Composition Rules

In this subsection we seek answer to the question "what is the result of infinitely many repetition of a composition?" for a given class of composition rules[3] for real quantities [42], like the thermodynamical entropy, internal energy or particle number. Let a composition rule for two values of such a real quantity be given by

$$x \oplus y = h(x,y). \tag{5.106}$$

We require that this composition function is differentiable and satisfies the following triviality rule

$$h(x,0) = x. \tag{5.107}$$

This way it is quite general. Among all possible rules the simple addition plays a very special role: its repetitions always remain an addition. Adding N_1 pieces on the one hand and N_2 ones on the other hand makes two big systems. A final addition of these two leads to a system of size $N_1 + N_2$, and our quantity $x_{N_1+N_2} = x_{N_1} + x_{N_2}$ is combined evenly by the same addition. This survives the $N_i \to \infty$ limit, particularly considered in thermodynamics.

What is, however, the situation for a general rule? Its repetition by a huge number of times may lead to another effective rule, to an *asymptotic rule* of composition in the thermodynamical limit. It turns out that several different rules may lead to the same asymptotic rule, which has a number of nice properties: it is associative and commutative and hence can be described by a simple mapping to the addition, $L(x)$. We shall construct this strict monotonic function which maps a general asymptotic (infinitely many times repeated) composition rule to the simple addition. Reminding to the role of the logarithm function, which maps the product to the addition, we call this function *formal logarithm*.

Let us add up a quantity y in small, Δy steps. Then in a general recursive step we have already x_{n-1} in the sum and construct

$$x_n = h(x_{n-1}, \Delta y). \tag{5.108}$$

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[3] Not just for the composition of entropy, but any, originally extensive quantity, like energy, particle number, volume, etc.

Subtracting $x_{n-1} = h(x_{n-1}, 0)$ form both sides of this equation we get

$$x_n - x_{n-1} = h(x_{n-1}, \Delta y) - h(x_{n-1}, 0). \tag{5.109}$$

Now composing a finite quantity y in infinitely many steps N makes the one step quantity Δy infinitesimally small. In this case the differentiable function $h(x,y)$ can be Taylor-expanded in its second argument around zero. So one arrives at the following differential equation:

$$\frac{\mathrm{d}x}{\mathrm{d}y} = \frac{\partial}{\partial y} h(x,y)\bigg|_{y=0} = h_2'(x, 0^+), \tag{5.110}$$

where we have introduced a particular short hand notation for the partial derivative with respect to the second argument at its zero value. The solution of this scaling equation gives a relation between the additive index variable, $t = n\Delta y$ ($t = y$ for $n = N$ only) and the composed – not necessarily additive – quantity x:

$$t = L(x) = \int_0^x \frac{\mathrm{d}z}{h_2'(z, 0^+)}. \tag{5.111}$$

Considering now large N_1 and N_2 composites, their asymptotic composition rule for the $N_1 + N_2$-repeated rule satisfies

$$L\left(x_{N_1+N_2}\right) = L\left(x_{N_1}\right) + L\left(x_{N_2}\right). \tag{5.112}$$

From this the asymptotic rule to a general composition rule is given via its formal logarithm defined in (5.111):

$$\varphi(x_1, x_2) = L^{-1}\left(L(x_1) + L(x_2)\right). \tag{5.113}$$

A general condition for this formula for the asymptotic rule is that the inverse function to the formal logarithm, L^{-1}, exists; among real functions this is the case for strict monotonic functions $L(x)$ (otherwise the inverse cannot be unique).

5.3.1.1 Properties of Asymptotic Rules

Asymptotic rules have interesting special properties. As it easily can be inspected from (5.113) $\varphi(x,y)$ is symmetric in its arguments. We have not required such a property for the rule, $h(x,y)$ we started with. The asymptotic rule is associative, too. It is easy to prove in a few lines.

Associativity means that

$$(x \oplus y) \oplus z = x \oplus (y \oplus z). \tag{5.114}$$

This property is satisfied by the rules given by (5.113):

$$\begin{aligned}\varphi\left(x,\varphi(y,z)\right) &= L^{-1}\left(L(x)+L\left(\varphi(y,z)\right)\right)\\ &= L^{-1}\left(L(x)+L(y)+L(z)\right)\\ &= L^{-1}\left(L\left(\varphi(x,y)\right)+L(z)\right)\\ &= \varphi\left(\varphi(x,y),z\right).\end{aligned} \tag{5.115}$$

On the other hand associative rules have themselves as asymptotic counterparts. It is an important property enforcing that associative rules build an attractor among all pairwise rules in the thermodynamical limit.

Whenever $h(x,y)$ is associative, there exists a formal logarithm function associated to it. We denote this function by $\Lambda(x)$, so

$$\Lambda\left(h(x,y)\right) = \Lambda(x)+\Lambda(y) \tag{5.116}$$

is satisfied. Inspecting the partial derivative of this equation with respect to y one gets

$$\Lambda'(h)\frac{\partial h}{\partial y} = \Lambda'(y), \tag{5.117}$$

which at $y=0$ in turn delivers

$$\Lambda'(x)h_2'(x,0^+) = \Lambda'(0), \tag{5.118}$$

when using the triviality property $h(x,0)=x$. The formal logarithm for the corresponding asymptotic rule is then determined by using (5.111). We obtain

$$L(x) = \int_0^x \frac{\Lambda'(z)}{\Lambda'(0)}\mathrm{d}z = \frac{1}{\Lambda'(0)}\Lambda(x). \tag{5.119}$$

Since the asymptotic formal logarithm is a constant times the original one and such a factor automatically cancels by applying L^{-1}, we conclude that the asymptotic rule to an associative rule is itself: $\varphi(x,y)=h(x,y)$ in this case.

This result strongly motivates to select out that formal logarithm for each pairwise asymptotic rule, which have the property $L'(0)=1$.

5.3.1.2 Scaling the Formal Logarithm

Before studying examples of useful composition rules applied for physical systems and its correspondence to entropy formulas and to the generalization of canonical equilibrium, we deal with a very important property: due to applying both L and its inverse function L^{-1} in the construction of the asymptotic composition rule, a multiplicative factor in the argument cancels. This scaling property is fulfilled by an arbitrary factor but zero. Let be $K(x)=cL(x)$ a scaled formal logarithm, then the equation $K(\varphi(x,y))=K(x)+K(y)$ is just c times the equation $L(\varphi(x,y)) = L(x)+L(y)$, so they are equivalent.

This particular freedom in the choice of the formal logarithm allows us to use a standard one satisfying the property $L'(0)=1$. This requirement fixes the multiplicative constant.

On the other hand by scaling the argument of the formal logarithm function (which we have to because of the physical units of different quantities), we handle a whole, continuously deformable class of non-additive composition rules in the thermodynamical limit. We define the *scaled formal logarithm* by

$$L_a(x) := \frac{1}{a} L(ax). \tag{5.120}$$

It is easy to see by setting $t = L_a(x)$ that its inverse function reflects the same scaling:

$$L_a^{-1}(t) := \frac{1}{a} L^{-1}(at). \tag{5.121}$$

Choosing the special value $a=1$, one gets back the fiducial formal logarithm: $L_1(x) = L(x)$ Finally in the $a \to 0$ limit, due to the $L'(0)=1$ property the Taylor expansion of (5.120) starts with the identity:

$$L_0(x) = x. \tag{5.122}$$

This way we consider a continuous set of formal logarithms with the deformation parameter a, giving at $a=0$ the identity. This parameter may in principle have any real, even negative, values. Its deviation from zero is a quantitative measure of the non-additivity of the composition rule.

We list some examples of interesting composition rules and the corresponding scaled formal logarithms.

1. The classical rule is trivially the addition, $h(x,y) = \varphi(x,y) = x+y$. In this case the formal logarithm is the identity: $L_a(x) = x$ for any value of a.

2. Somewhat more complicated is the rule $h(x,y) = x+y+axy$. Its derivative is given by $h_2'(x,0) = 1+ax$ and therefore the formal logarithm of the asymptotic rule is
$$L(x) = \int_0^x \frac{\mathrm{d}z}{1+az} = \frac{1}{a}\ln(1+ax).$$
Since $L'(0)=1$ this is already the fiducial formal logarithm and its scaling by b replaces only the parameter a by ab. Therefore, the above form is also the general scaled formal logarithm.

3. Einsteins' relativistic velocity addition formula gives rise to another interesting composition rule:
$$h(u,v) = \frac{u+v}{1+uv/c^2}.$$

The derivative with respect to the second argument at zero gives $h_2'(u,0) = 1 - u^2/c^2$, by using this the formal logarithm becomes

$$L(u) = \int_0^u \frac{\mathrm{d}w}{1 - w^2/c^2} = c\,\mathrm{Arth}\frac{u}{c}.$$

The additive quantity is a multiple of the rapidity, defined by $z = \mathrm{Arth}(u/c)$; the velocity u follows another, more complicated composition rule. Here again the speed of light, c, functions as a general scaling parameter.

4. All composition rules of the type $h(x,y) = x + y + G(xy)$ lead to $h_2'(x,0) = 1 + xG'(0)$. For any finite value of $G'(0)$ these belong to the case 2 in this list with $a = G'(0)$, so the asymptotic rule is $\varphi(x,y) = x + y + xyG'(0)$. In addition $G(0) = 0$ has to be satisfied in order to cope with the triviality rule $h(x,0) = x$.

5. Another general functional type of composition, $h(x,y) = (x+y)f(xy)$, leads to $h_2'(x,0) = f(0) + x^2 f'(0)$. Due to $h(x,0) = x$ it has to be $f(0) = 1$. This type of composition rule asymptotically belongs to case 3 with $c^2 = -f'(0)$.

6. Many rules can be imagined, a few of them – the simple ones – occur in physical models. In order to interpolate between addition and multiplication, as an alternative to the rule 2, the following rule was suggested:

$$h(x,y) = x\sqrt{1 + \kappa^2 y^2} + y\sqrt{1 + \kappa^2 x^2}.$$

In this case $h_2'(x,0) = \sqrt{1 + \kappa^2 x^2}$. The formal logarithm becomes

$$L(x) = \int_0^x \frac{\mathrm{d}z}{\sqrt{1 + \kappa^2 z^2}} = \frac{1}{\kappa}\mathrm{Arsh}(\kappa x).$$

The asymptotic rule coincides with the original one (proving that it was associative), $\varphi(x,y) = h(x,y)$.

5.3.2 Deformed Exponential and Logarithm Functions

As the classical BGS formula for entropy is based on the natural logarithm, mapping the product formula to an addition, generalizations of this formula are supplemented by another mapping between addition and the more general asymptotic composition rule. This second mapping is performed by the formal logarithm. The composition of the natural and the formal logarithm should be then at the heart of a non-extensive entropy formula: this functional composition is called the *deformed* *logarithm*. This composition, $\ln_a = L_a^{-1} \circ \ln$, has its inverse function, the *deformed exponential*, $e_a = \exp \circ L_a$:

$$\begin{aligned} \ln_a(x) &= L_a^{-1}(\ln x), \\ e_a(x) &= \mathrm{e}^{L_a(x)}. \end{aligned} \tag{5.123}$$

It is straightforward to see that the following properties are satisfied:

$$\begin{aligned} \ln_a(1/x) &= -\ln_{-a}(x), \\ 1/e_a(x) &= e_{-a}(-x). \end{aligned} \tag{5.124}$$

The $a \leftrightarrow -a$ duality, inherent in these formulas, complements the known properties of reciprocals and negatives of the natural logarithm and exponential functions. Certainly, for $a = 0$ all the known classical results are recovered.

The deformed logarithm and exponential functions for the examples listed in the previous subsection are given as follows.

1. For the simple addition $L(x) = x$ and $\ln_a(x) = \ln(x)$, $e_a(x) = \mathrm{e}^x$; everything is familiar.

2. For $h(x,y) = x + y + axy$ we obtain

$$\begin{aligned} e_a(x) &= \mathrm{e}^{L_a(x)} = (1+ax)^{1/a}, \\ \ln_a(t) &= L_a^{-1}(\ln t) = \frac{1}{a}\left(t^a - 1\right). \end{aligned} \tag{5.125}$$

   The original a parameter can be used as a general scaling parameter.

3. Einstein's velocity addition formula leads to the following deformed functions:

$$\begin{aligned} e_c(u) &= \mathrm{e}^{L_c(u)} = \left(\frac{c+u}{c-u}\right)^{c/2}, \\ \ln_c(z) &= L_c^{-1}(\ln z) = c\,\mathrm{th}\frac{\ln z}{c} = c\frac{z^{1/c} - z^{-1/c}}{z^{1/c} + z^{-1/c}}. \end{aligned} \tag{5.126}$$

   Physically $e_c(u)^{1/c}$ is the relativistic Doppler-factor belonging to the velocity u.

4. Rule 6 with the fiducial formal logarithm of the inverse sine hyperbolic function leads also to a deformed exponential resembling power-law tails for large arguments:

$$\begin{aligned} e_\kappa(x) &= \left(\kappa x + \sqrt{1+\kappa^2 x^2}\right)^{1/\kappa}, \\ \ln_\kappa(t) &= \frac{1}{2\kappa}\left(t^\kappa - t^{-\kappa}\right). \end{aligned} \tag{5.127}$$

Considering $\kappa x = p/mc$, related to the relativistic momentum p of a particle with mass m, one obtains $e_\kappa(p/mc) = \mathrm{e}^{\zeta/\kappa}$ with the particle rapidity ζ. Such functions has been fitted to cosmic ray spectra showing a power-law tail at high energy over several orders of magnitude [43].

5.3.3 Generalized Entropy Formulas

From the viewpoint of thermodynamics both the entropy and another extensive quantity, most prominently the energy, may violate the additivity rule due to correlations between the elementary degrees of freedom. If someone tries to interpret such total systems on a "per particle" basis, then the extensivity – the proportionality of the total energy, entropy, etc., with the particle number also turns out to be violated. A generalized entropy formula therefore is additive for non-factorizing sub-state probabilities and is non-additive for factorizing probabilities.

In order to satisfy an equation like (5.105), the formal logarithm may be used. The entropy composition rule for a joint system with factorizing probability is formulated as

$$\sum_{i,j} w_{ij}\sigma(w_{ij}) = h\left(\sum_i p_i\sigma(p_i), \sum_j q_j\sigma(q_j)\right), \tag{5.128}$$

with $w_{ij} = p_i q_j$. Let us consider the microcanonical, the equipartition case. Now only the number of microstates are different between the subsystems, but each single one has the same occupation probability. This way we have $p_i = a = 1/N_1$ and $q_j = b = 1/N_2$. Furthermore, due to the factorization assumption, $w_{ij} = ab$. The elementary entropy function satisfies the following equation:

$$\sigma(ab) = h(\sigma(a), \sigma(b)). \tag{5.129}$$

Applying this to the general formula (5.128), the rule of *h-extensivity* emerges:

$$\sum_{i,j} p_i p_j h(\sigma(p_i), \sigma(q_j)) = h\left(\sum_i p_i\sigma(p_i), \sum_j q_j\sigma(q_j)\right). \tag{5.130}$$

An arbitrary rule does not satisfy this requirement for uneven p_i and q_j distributions, although it is trivial for the equipartition case. However for the Tsallis' rule, containing the product term, the normalization of the probabilities and the factorization of the double sum ensures that this is satisfied. Since

$$\sum_{i,j} p_i q_j(\sigma_i + \sigma_j + a\sigma_i\sigma_j) = \sum_i p_i\sigma_i \cdot \sum_j q_j + \sum_i p_i \cdot \sum_j q_j\sigma_j + a\sum_i p_i\sigma_i \cdot \sum_j q_j\sigma_j, \tag{5.131}$$

the total entropy satisfies the same rule, namely $S_{12} = S_1 + S_2 + aS_1S_2$, than the micro-rule.

A general entropy formula containing $\sigma(p)$, a contribution depending on the microstate probability, has to satisfy further constraints. For a pure state, say $q_0 = 1$ and all other $q_j = 0$, the σ function should ensure sensible answers. Substituting first 1 and then 0 into (5.129) one obtains

$$\begin{aligned} \sigma(p_i) &= h(\sigma(p_i), \sigma(1)) = \sigma(p_i) \oplus \sigma(1), \\ \sigma(0) &= h(\sigma(p_i), \sigma(0)) = \sigma(p_i) \oplus \sigma(0). \end{aligned} \tag{5.132}$$

With respect to the composition $\oplus$ $\sigma(1)$ behaves like zero and $\sigma(0)$ like infinity. The sure event must have zero entropy even in the generalized formula, while the impossible event gives an infinite contribution – and therefore it never occurs.

In the limit of infinitely many repetitions the effective composition rule is associative and possesses a formal logarithm, $L(x)$. The entropy composition rule in this limit satisfies

$$L(\sigma(ab)) = L(\sigma(a)) + L(\sigma(b)). \tag{5.133}$$

The general solution of this function equation is the logarithm for the composed function “L of sigma”:

$$L(\sigma(p)) = \beta \ln p. \tag{5.134}$$

Inverting this relation and fitting to the Boltzmann case one arrives at the (scaled) deformed logarithm of $1/p$ as a general entropy formula:

$$\sigma(p) = L^{-1}(-\ln p) = \ln_a \frac{1}{p}. \tag{5.135}$$

Another question arises when one would like to construct an entropy formula which is additive for non-factorizing, correlated sub-state probabilities following a prescribed law. Instead of the product, which is the exponential of the sum of the logarithms, let w_{ij} be constructed as the exponential of the generalized sum of logarithms. This generalizes the product formula to

$$w_{ij} = \mathrm{e}^{\ln p_i \oplus \ln q_j} = \mathrm{e}^{h(\ln p_i, \ln q_j)}. \tag{5.136}$$

Now we would like to construct an entropy formula using a σ function which satisfies

$$\sum_{ij} w_{ij} \sigma(w_{ij}) = \sum_i p_i \sigma(p_i) + \sum_j q_j \sigma(q_j). \tag{5.137}$$

Let us consider the microcanonical equilibrium again, where all a priori probabilities are equal. Then we have $p_i = a$, $q_j = b$ and $w_{ij} = c$. These quantities satisfy (5.136) meaning

$$\ln c = h(\ln a, \ln b). \tag{5.138}$$

The additivity of entropy can be satisfied by normalized probabilities if

$$w_{ij} \sigma(w_{ij}) = p_i q_j (\sigma(p_i) + \sigma(q_j)), \tag{5.139}$$

although $w_{ij} \neq p_i q_j$, but given by (5.138). Using the simplifying notation a, b, c for p_i, q_j and w_{ij} respectively, we seek for an entropy density function, σ which fulfills the relation

$$c\sigma(c) = ab\,(\sigma(a) + \sigma(b))\,. \tag{5.140}$$

This functional equation is to be solved for σ. Let us regard first the derivative of c with respect to b taken at $b = 1$. We get

$$\frac{\partial c}{\partial b} = \mathrm{e}^{h(\ln a, \ln b)}\, h_2'(\ln a, \ln b)\, \frac{1}{b}, \tag{5.141}$$

which at $b = 1$ turns out to be

$$\left.\frac{\partial c}{\partial b}\right|_{b=1} = a\, h_2'(\ln a, 0). \tag{5.142}$$

Remember that $h_2'(x, 0)$ is related to the formal logarithm function, $L(x)$ via an integral, therefore the above equation is equivalent to

$$\left.\frac{\partial c}{\partial b}\right|_{b=1} = \frac{1}{\frac{\mathrm{d}L}{\mathrm{d}a}} \tag{5.143}$$

using $L(\ln a)$. We execute now the derivation with respect to b on the right hand side of (5.140) resulting in

$$\left.\frac{\partial}{\partial b}\,(ab\sigma(a) + ab\sigma(b))\right|_{b=1} = a\left(\sigma(a) + \sigma(1) + \sigma'(1)\right). \tag{5.144}$$

Using now the property that $\sigma(1) = 0$ we simplify this expression. The left hand side also will be derived and then taken at $b = 1$:

$$\left.\frac{\partial}{\partial b}\,(c\sigma(c))\right|_{b=1} = \left(\sigma(a) + a\sigma'(a)\right)\left.\frac{\partial c}{\partial b}\right|_{b=1}. \tag{5.145}$$

Substituting the result (5.143) we arrive at

$$\left(\sigma(a) + a\sigma'(a)\right)\frac{1}{\frac{\mathrm{d}L(\ln a)}{\mathrm{d}a}} = a\left(\sigma(a) + \sigma'(1)\right). \tag{5.146}$$

Introducing the notation $x = \ln a$ the following differential equation follows from the above:

$$\mathrm{e}^{-x}\frac{\mathrm{d}}{\mathrm{d}x}\left[\mathrm{e}^{x}\sigma(\mathrm{e}^{x})\right] = L'(x)\left[\sigma(\mathrm{e}^{x}) + \sigma'(1)\right]. \tag{5.147}$$

The solution of this differential equation can be expressed by analytic quadrature formulas. In order to achieve this we introduce the function $g(x)$ satisfying

$$\mathrm{e}^{x}\sigma(\mathrm{e}^{x}) = g(x)\mathrm{e}^{L(x)}. \tag{5.148}$$

Now the derivations in (5.147) are carried out with the result

$$e^{L(x)-x}g'(x)+g(x)e^{L(x)-x}L'(x)=L'(x)\left(g(x)e^{L(x)-x}+\sigma'(1)\right). \tag{5.149}$$

Here the terms containing $g(x)$ cancel and we are left with a simple, integrable equation:

$$g'(x)=\sigma'(1)L'(x)e^{x-L(x)}. \tag{5.150}$$

This general result includes the classical formula as a particular case for $L(x)=x$: then $L'(x)=1$, $g'(x)=\sigma'(1)$ and therefore $g(x)=\sigma(e^x)=\sigma'(1)x$. This is the famous logarithm formula since $x=\ln a$: $\sigma(a)=\sigma'(1)\ln a$. According to the classical Boltzmann formula $\sigma'(1)=-k_B$, the negative of the Boltzmann constant.

Let us integrate the general equation (5.150) by setting $\sigma'(1)=-k_B$. We obtain

$$g(x)=-k_B\int_0^x L'(u)\,e^{u-L(u)}\,du. \tag{5.151}$$

Expressing out σ from the definition (5.148) we have

$$\sigma(e^x)=g(x)\,e^{L(x)-x}\;=\;-k_B e^{L(x)-x}\int_0^x L'(u)\,e^{u-L(u)}\,du. \tag{5.152}$$

Replacing finally x by $\ln a$ we obtain the entropy density function we were seeking for as

$$\sigma(a)=-k_B e^{L(\ln a)-\ln a}\int_0^{\ln a} L'(u)\,e^{u-L(u)}\,du. \tag{5.153}$$

Summarizing, by using this formula the entropy $S=\sum_i p_i\sigma(p_i)$ is additive at the non-factorizing probabilities which satisfy

$$L(\ln w_{ij})=L(\ln p_i)+L(\ln q_j). \tag{5.154}$$

Finally, it is interesting to note that while (5.138) corresponds to a given way of generalizing the product formula, i.e.

$$\ln c=\ln a\oplus\ln b=L^{-1}\left(L(\ln a)+L(\ln b)\right), \tag{5.155}$$

there is another "natural" way to generalize by using the deformed logarithm function. Requiring

$$\ln_d c=\ln_d a+\ln_d b, \tag{5.156}$$

leads to

$$\ln c=L_d\left(L_d^{-1}(\ln a)+L_d^{-1}(\ln b)\right) \tag{5.157}$$

upon using the definition of the deformed logarithm. Comparison with the form (5.155) reveals that the formal logarithm functions used in the respective definitions of a formal product formula are inverse functions to each other.

5.3.3.1 Generalized Stosszahlansatz: Entropic Non-additivity

A particularly interesting and useful instance of generalizing the product formula emerges in attempts to generalize the Boltzmann equation [43–48]. The original Boltzmann equation, describing the time evolution of the one-particle phase space distribution, uses the so called "Stosszahlansatz," a definite assumption about the probability rate of pairwise particle collisions. The essential physical assumption is that by a micro-collision the partners have already forgotten their previous momentum- (and in inelastic collisions energy-) exchange. From this follows that the collision rate is simply proportional to the phase space density of both partners. The Boltzmann equation then accounts for both scattering in and scattering out with respect to a given momentum state (a point in phase space).

For our argumentation here only the very abstract structure of the Boltzmann equation is important and its connection to entropy production. Our questions are: (1) how to generalize the Stosszahlansatz and (2) what is the "proper" entropy formula satisfying the second law of thermodynamics. We use therefore a compact notation, simply indices $1, 2, 3$ and 4 denote quantities and the corresponding phase space integrals associated to the colliding partners 1 and 2 before, 3 and 4 after the pairwise collision, respectively. The differential cross section governing the rate of events as well as energy and momentum conserving constraints will be comprised in a single factor, w_{1234}. This way both the original Boltzmann equation and its possible generalized pendants have the following form

$$\dot{f}_1 = \int\limits_{234} w_{1234} \left(G_{34} - G_{12} \right). \tag{5.158}$$

Here the gain and loss factors are composed in the knowledge of the individual phase space densities. In the original Stosszahlansatz Boltzmann assumed

$$G_{ij} = f_i \cdot f_j. \tag{5.159}$$

We note that also the Uehling–Uhlenbeck extension, using blocking factors of the type $1 - f_k$, can be casted into the above form. Assuming namely

$$\dot{f}_1 = \int\limits_{234} w_{1234} \left[f_3 f_4 (1 - f_1)(1 - f_2) - f_1 f_2 (1 - f_3)(1 - f_4) \right], \tag{5.160}$$

the positive and – more important – in all of the four indices entirely symmetric factor $(1 - f_1)(1 - f_2)(1 - f_3)(1 - f_4)$ can be attached to the rate-and-constraint factor, w_{1234}, having the same index permutation symmetry properties. This way one achieves the equation

$$\dot{f}_1 = \int\limits_{234} \tilde{w}_{1234} \left[\frac{f_3 f_4}{(1-f_3)(1-f_4)} - \frac{f_1 f_2}{(1-f_1)(1-f_2)} \right], \tag{5.161}$$

with

$$\tilde{w}_{1234} = w_{1234}(1-f_1)(1-f_2)(1-f_3)(1-f_4). \tag{5.162}$$

It reveals the following generalized product formula underlying the modified Stosszahlansatz:

$$G_{ij} = \frac{f_i}{1-f_i} \cdot \frac{f_j}{1-f_j}. \tag{5.163}$$

In both the Boltzmann and Boltzmann–Uehling–Uhlenbeck cases the factor formula is really a product of simple functions of the respective one-particle phase space distributions.

We shall show below that the generalization of the Stosszahlansatz via the deformed logarithm function, i.e. the ansatz

$$\ln_a G_{ij} = \ln_a f_i + \ln_a f_j, \tag{5.164}$$

leads to a physically meaningful generalization of the Boltzmann equation. Two important features have to be analyzed: the detailed balance solution and the entropy production during the evolution according to the general Boltzmann equation.

The detailed balance solution is set whenever the value inside the bracket in (5.158) is zero. In the original equation this means

$$f_1 f_2 = f_3 f_4. \tag{5.165}$$

Since the one-particle energies are assumed to be additive in such collisions, i.e. $E_1 + E_2 = E_3 + E_4$ is required, the detailed balance equation (5.165) actually maps the addition of energy onto the product of phase space densities. This way the energy dependence of the individual particle distributions in the detailed balance state can only be[4] the exponential function:

$$f_{\mathrm{eq}}(E) = \mathrm{e}^{\beta(\mu - E)}. \tag{5.166}$$

In the Uehling–Uhlenbeck case from the factorized form (5.163)

$$\frac{f_1}{1-f_1} \cdot \frac{f_2}{1-f_2} = \frac{f_3}{1-f_3} \cdot \frac{f_4}{1-f_4} \tag{5.167}$$

it follows that the exponential function of the energy has to be the following expression:

$$\frac{f_{\mathrm{eq}}(E)}{1-f_{\mathrm{eq}}(E)} = \mathrm{e}^{\beta(\mu - E)}. \tag{5.168}$$

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[4] More than that, the chemical potential terms, μ, may also differ as long as their sum satisfies $\mu_1 + \mu_2 = \mu_3 + \mu_4$.

Expressing from this the equilibrium distribution one naturally arrives at the Fermi–Dirac formula

$$f_{\text{eq}}(E) = \frac{1}{\mathrm{e}^{\beta(E-\mu)}+1}. \tag{5.169}$$

We note that using the enhancement factors, $(1+f_k)$ instead of the blocking factors, one arrives at the Bose–Einstein formula with a similar effort:

$$f_{\text{eq}}(E) = \frac{1}{\mathrm{e}^{\beta(E-\mu)}-1}. \tag{5.170}$$

Now the question arises, what is the detailed balance one-particle energy distribution relying on a more general Stosszahlansatz of the type formulated in (5.164). In this case the energy addition $E_1+E_2=E_3+E_4$ is mapped to the general detailed balance condition,

$$G_{12} = G_{34} \tag{5.171}$$

meaning the equality of deformed exponentials of respective sums of deformed logarithms. Since, however, the deformed exponential – at a fixed deformation scale parameter a – is a strict monotonic function, it means the equality of the respective sums of deformed logarithms:

$$\ln_a f_1 + \ln_a f_2 = \ln_a f_3 + \ln_a f_4. \tag{5.172}$$

Following the above argumentation we arrive at the conclusion that the one-particle energy distributions in the detailed balance state in this case should be the deformed exponentials

$$f_{\text{eq}}(E) = e_a^{-\beta E}. \tag{5.173}$$

5.3.3.2 Generalized Pair Condition: Energetic Non-additivity

In principle not only the entropy may be a non-additive function of the number of the physical degrees of freedom, but any other, in the classical treatment extensive quantity. Most prominently, the energy may follow a nontrivial composition rule when unifying two subsystems. Universality class in thermodynamical sense may emerge only if this energy composition law is expressible as a function of the individual subsystem energies: $E_1 \oplus E_2 = h(E_1, E_2)$. In the view of the Boltzmannian approach, this time not the form of the Stosszahlansatz, but the energy constraint is modified.

It is important to emphasize that the energy conservation is not violated: in $1+2 \to 3+4$ type two-body collision the total composite energy of the pair is the same before and after the collision:

$$E_1 \oplus E_2 = E_3 \oplus E_4. \tag{5.174}$$

However, the composition prescription is not necessarily additive, nor it becomes close to additive after infinitely many repetitions when simulating a genuinely entangled internal energetics. The usual argumentation for neglecting such effects relies on the conjecture, that the additive part of the subsystem energies – in the extreme case that of single particles – grows with the volume, while the interaction part among them, which may deform the addition rule, grows less. In the thermodynamical limit therefore the additivity is established.

These classical arguments do not hold for physical systems not conforming with this negligibility rule. Measured in terms of the number of degrees of freedom, N, instead of the less easily described volume variables, large systems sometimes have an energy component which is more than linear (superlinear) in N. Such systems are *non-extensive* systems. What physical factors may compromise the neglection of energetic entanglement terms besides the additive ("N-extensive") ones? First of all a fractal phase space filling pattern, meaning an effective dimensionality less than required for the proportionality to N, leads to a situation, where the additive and non-additive contributions may re-define the chances in the race towards the thermodynamical limit. This pattern may be only metastable, long but not ever lasting in the real physical world, but mathematical models handling them as quasi-equilibrium states unavoidably lead to a version of non-extensive thermodynamics. Another broad class of possibility is long range interaction. Speaking in geometrical terms the non-additive to additive ratio in the composition of thermodynamical energy is formulated as

$$\frac{\text{non}-\text{additive terms}}{\text{additive terms}} \sim \frac{\text{interface area} \times \text{interaction range}}{\text{volume}} \sim \frac{A\ell}{V} \sim N^{\alpha-1/3}. \tag{5.175}$$

Traditional thermodynamics applies whenever $\alpha < 1/3$. However, already in the marginal case, when $\alpha = 1/3$, (as in the case of a linear potential signaling confinement of pairs of particles), non-additive terms may survive the thermodynamical limit of $N \to \infty$ [36].

The Boltzmann equation can be generalized also alongside the line of applying non-additive energy composition rules. A chance for success in this description is rooted in the separability of the interaction events into pairwise interactions. But this alone does not forces the energy additivity formula upon us. Let us inspect the general situation of three consecutive pairwise microcollision events (cf. the Fig. 5.5). We denote these microscopic interaction events by A, B and C. The involved particles shall have indices 1, 2 and 3. In the event A particles 1 and 2 interact, then in the event B particles 2 and 3, finally in the event C particles 1 and 2 again. Admittedly, such a situation is not typical if the events are rare – an assumption Boltzmann originally applied. The energy compositions for all three particles now has to be regarded. At the beginning $E_A = (E_1 \oplus E_2) \oplus E_3$. After the collision event A $E'_A = (E'_1 \oplus E'_2) \oplus E_3$, the energy is conserved as $E'_A = E_A$. Now in event B particles 2 and 3 collide. The question is whether particle 2 had forgotten its previous collision (interaction with partner 1) by this time. Similarly we have

$$E_B = E'_1 \oplus (E'_2 \oplus E_3) = E'_1 \oplus (E''_2 \oplus E'_3) = E'_B$$

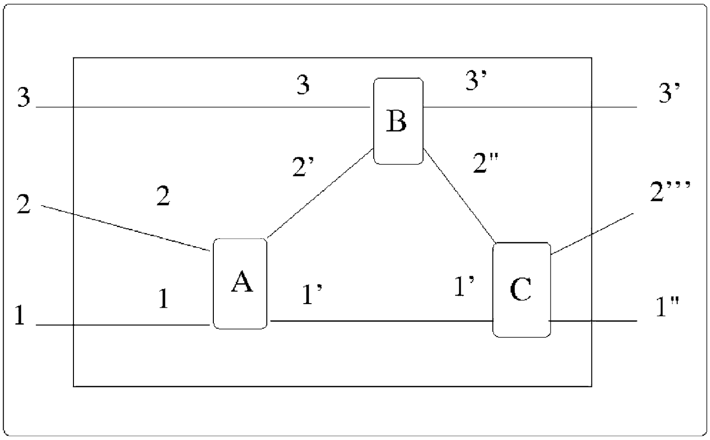

Fig. 5.5 Schematic graph of consecutive pairwise two-body collisions requiring associativity of the energy composition law

before and after event B. If forgetting is statistically relevant and dynamically allowed, then E_B has nothing to do with E'_A. On the other hand, if the *same* particle 2 takes part in both the A and B interaction events and nothing else happens, then obviously $E_B = E'_A$. This equality requires

$$(E'_1 \oplus E'_2) \oplus E_3 = E'_1 \oplus (E'_2 \oplus E_3)$$

i.e. exactly the associativity of the composition rule. Although the simple addition is definitely a particular solution to this requirement, this is not the only solution. The energy composition rule being, however, associative, there is an additive quantity, $L(E)$ as we have shown in previous subsections.[5]

A non-extensive Boltzmann equation can be then used [49] to model such a chain of events, containing a general formula for the pair-energy expression before and after collisions. In its general structure,

$$\dot{f}_1 = \int\limits_{234} w_{1234}\delta_{1234}\left(f_3 \otimes f_4 - f_1 \otimes f_2\right), \tag{5.176}$$

the constraint δ-factor is generalized to

$$\delta_{1234} = \delta\left(h(E_1,E_2) - h(E_3,E_4)\right)\delta^3\left((\mathbf{p}_1 + \mathbf{p}_2) - (\mathbf{p}_3 + \mathbf{p}_4)\right). \tag{5.177}$$

In principle the momentum composition formula also may be more general than the addition, but for the sake of simplicity we do not pursue that possibility here.

An interesting and immediate consequence of this assumption is that now the (generalized) product formula maps a generalized addition by fulfilling the detailed balance condition

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[5] The corrections need to depend on the energies only, otherwise it is not so simple.

$$\begin{aligned} f(E_1) \otimes f(E_2) &= f(E_3) \otimes f(E_4), \\ L(E_1) + L(E_2) &= L(E_3) + L(E_4). \end{aligned} \tag{5.178}$$

The general stationary solution in a detailed balance state then is composed from a deformed exponential due to the generalization of the product formula in the Stosszahlansatz and from the formal logarithm of the generalized energy composition rule:

$$f_{\mathrm{eq}} = \mathrm{e}_a^{\beta(\mu - L(E))} \tag{5.179}$$

with $\beta = 1/T$ playing the role of the absolute temperature and μ that of a chemical potential associated to the mean additive-energy, $L(E)/N$ and to the particle number N, respectively.

In computer simulations all traditional Monte Carlo methods can be used with the caveat that $L(E)$ and the function e_a^x are to be utilized in place of E and the exponential function e^x. For theoretical studies up to now only the one or the other generalization has usually been studied [50], but physically the statistical (entropic) and dynamical (energetic) entanglement of individual degrees of freedom (particles) may emerge due to the same cause. More complete treatments, also in terms of thermodynamical studies, are waited for.

5.3.3.3 Generalized Evolution: The H-theorem

The very essence of Boltzmann's equation was not the detailed balance solution leading to the Maxwell–Boltzmann distribution of velocities of atoms in an ideal gas upon using the non-relativistic energy formula $E = \mathbf{p}^2/2m$. The greater part of excitement was caused by the proof of irreversibility; by showing that the entropy defined by Boltzmann's logarithmic formula cannot be decreased during the evolution described by the Boltzmann equation. This was much of a wonder, since all quantities related to micro-collisions, comprised in the factor w_{1234}, were symmetric to the direction of time: exchange of quantities between indices 1 and 2 with 3 and 4, respectively. A time-reversible microdynamics seemingly led to an irreversible growth of the macroscopic entropy,[6]

$$S = -\int f \ln f. \tag{5.180}$$

The time-reversal symmetry is broken in the difference between a typical initial state, described by a one-particle phase space distribution, f at time zero, and the statistically most probable final state after a long time. This result contradicts to the "recurrence lemma" of Poincare, who mathematically had proved that by an ergodic dynamics any mechanical system returns to an arbitrary close vicinity of its starting point in the phase space. The resolution of this contradiction lies in the hierarchy

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[6] Boltzmann originally presented his proof for the negative of the entropy, called a quantity H, hence the name "H-theorem." H cannot be increased in this case.

of typical times characteristic to these two statements: In order to come close to a detailed balance solution of the Boltzmann equation on the average $2-3$ collisions per particle are needed, so altogether $\sim N$ collisions in a gas of N particles. For a recurrence near to a single arrangement of N particles in the phase space, even if each may have only a few different states, like half spin particles with fixed position would have only 2, the necessary time is in the order of $\mathcal{N} \sim 2^N$. In case of an infinite time observation, one observes a configuration near to the detailed balance solution much more frequently than near to a recurrent configuration. For $N \to \infty$ the latter is statistically irrelevant, since $N/\mathcal{N} \to 0$.

We do not repeat Boltzmann's original proof here, it can be found in several textbooks on statistical mechanics. Instead, we deal with the same problem for the generalized Boltzmann equation right away [51]. In this respect we include generalizations of the Stosszahlansatz as well as that of the energy composition rule. Furthermore, the evolution operator, so far denoted by an overdot in the equations of the previous subsections, also will be generalized. The more classical generalization is that of Vlasov, describing the evolution in collisionless plasmas, the so called "free streaming." In that case the phase space density at a given point, x in configuration space also changes due to streams of incoming and outgoing particles. The corresponding currents are convective, they are equal to the product of density and velocity. For relativistic momenta, $\mathbf{p}$, particles have the velocity $\mathbf{v} = \mathbf{p}/E$. Comprising energy and momentum in a four-momentum, $p^\mu = (E, \mathbf{p})$ (in units where $c = 1$), the energy itself is the first component of the four-momentum, denoted by index 0. Similarly, partial derivatives with respect to time and space are comprised into a four-gradient operator, $\partial_\mu = (\frac{\partial}{\partial t}, \nabla)$. Collecting all terms together, convective currents generalize the evolution operator to

$$\dot{f} = \frac{p^\mu}{p^0}\,\partial_\mu f = \frac{\partial f}{\partial t} + (\mathbf{v}\cdot\nabla) f. \tag{5.181}$$

In this setting the energy of individual particles $E = p^0$ may depend on the three-vector momentum, but not on the position in ordinary space. This way the phase space density is local in space and is evolving in time, $f = f(t, \mathbf{x}, \mathbf{p})$.

The most general Boltzmann equation, we are going to present an H-theorem for, includes one more possible extension: It is possible that not f, but a certain function of it, say $F(f)$, describes the quantity whose phase space integral is normalized. To give an example, several authors describe non-extensive plasmas by using a power of the original quantity, $F(f) = f^q$ with the parameter q being near to one. This means that while still the f densities enter into the probabilistic formula of the Stosszahlansatz, the normalized quantity over one-particle phase distribution is $F(f)$. Therefore the Boltzmann-type evolution equation has the following form:

$$\frac{p^\mu}{p^0}\partial_\mu F(f_1) = \int\limits_{234} w_{1234}\left(G_{34} - G_{12}\right). \tag{5.182}$$

Here the fully index-symmetric rate factor, w_{1234} includes energy and momentum conserving constraints, too. We shall see, that Boltzmann's result on entropy growth by approaching the detailed balance solution, depends only on the use of index-symmetry and antisymmetry properties. All other details are irrelevant.

Now the question is, how to compute the entropy. Since we are considering now the general situation which counts also for streaming in configuration space, we have to use an entropy four-current. It is considered to be convective, similar to the normalizable (conserved) current expression. The only part which is unclear at this moment is the correspondence between local entropy density in the comoving frame and the normalized particle density $F(f)$. To start with, we assume a general functional form, $\sigma(F)$ for the entropy density in the frame comoving with the local streaming. Our formula becomes

$$S^{\mu} = \int \frac{p^{\mu}}{p^{0}} \sigma(F(f)). \tag{5.183}$$

The local and Lorentz-covariant balance equation for this entropy current is then given by

$$\partial_{\mu} S^{\mu} = \int_{1} \sigma'(F(f_1)) \frac{p^{\mu}}{p^{0}} \partial_{\mu} F(f_1). \tag{5.184}$$

Replacing now the very evolution equation (5.182) into this result one obtains

$$\partial_{\mu} S^{\mu} = \int_{1234} w_{1234}\, \sigma_1' (G_{34} - G_{12}). \tag{5.185}$$

Here we used the shorthand notation $\sigma_i' = \sigma'(F(f_i)) = \mathrm{d}\sigma/\mathrm{d}F$ for $i = 1$. Now the index symmetries are utilized. Since this integral is over all phase space coordinates of 1, 2, 3 and 4, these are just dummy indices. We can exchange 1 and 2, or 3 and 4 and still have the same quantity. Furthermore, an exchange between the index block 1,2 and 3,4 – physically reversing the microcollision – also can be done, with the caveat, however, that in this case the G-terms also change place and an overall minus sign emerges. Summing up the same integral in four different notations, with two of them with a relative minus sign, one arrives at

$$\partial_{\mu} S^{\mu} = \frac{1}{4} \int_{1234} w_{1234} \left(\sigma_1' + \sigma_2' - \sigma_3' - \sigma_4'\right) (G_{34} - G_{12}). \tag{5.186}$$

There is a general way to keep this quantity non-negative, even to do this irrespective to the rate-and-constraint factor w_{1234}. The product of the two bracketed quantities in the above equation show the same index permutation structure. The respective sums of σ' terms has to be then correlated to the gain and loss terms, G, in a way that the product of the two brackets remains non-negative. We demand that

$$(\Phi(G_{12}) - \Phi(G_{34})) (G_{34} - G_{12}) \geq 0. \tag{5.187}$$

This is ensured for any monotonic falling function $\Phi(z)$. Only if $\Phi(G_{34}) < \Phi(G_{12})$ at $G_{34} > G_{12}$ and $\Phi(G_{34}) > \Phi(G_{12})$ at $G_{34} < G_{12}$ is fulfilled, is the above product (5.187) positive. The third possibility is that both factors are zero. It happens due to $\Phi(G_{12}) = \Phi(G_{34})$ at $G_{12} = G_{34}$. This equality is nothing else than the detailed balance condition. This way the evolution governed by the generalized Boltzmann equation always increases the accordingly constructed entropy, unless the detailed balance distribution is achieved. Then the entropy is maximal.

In conclusion the entropy density has to be constructed as an expression satisfying

$$\sigma'(F(f_1)) + \sigma'(F(f_2)) = \Phi(G_{12}), \tag{5.188}$$

with Φ being a strict monotonic falling function. Remembering that the gain and loss terms are expressed via the deformed exponential and logarithm functions as $G_{ij} = e_a(\ln_a(f_i) + \ln_a(f_j))$, the only such entropy definition is given if we satisfy

$$\sigma'(F(f)) = -\alpha \ln_a(f) + K, \tag{5.189}$$

with a positive α and an yet undetermined constant, K. The monotonic falling function in this case is given by

$$\Phi(G) = -\alpha \ln_a(G) + 2K. \tag{5.190}$$

The differential equation (5.189) is solvable by quadrature with the formal result

$$\sigma(f) = \int (-\alpha \ln_a f + K) F'(f) \mathrm{d}f. \tag{5.191}$$

The constant K is set by requiring $\sigma(1) = 0$, a further constant stemming from the integration by $\sigma(0) = 0$, in the result. Finally α can be fitted to the traditional Boltzmann formula in the limit $F(f) \to f$ and $a \to 0$. By doing so we arrive at the Boltzmann constant, $\alpha = k_{\mathrm{B}}$.

The general conclusion is, that a convective entropy four-current constructed in accordance with the deformed logarithm of the one-particle phase space density will never decrease during the evolution governed by a generalized Boltzmann equation. Statistical irreversibility is robust against changing quite a few ingredients in Boltzmann's original equation.

5.3.4 Generalized Canonical Formula and Thermal Equilibrium

Armored with these experiences with a possible generalization of the Boltzmann equation a generalized canonical formula at equilibrium can be formulated. The volume integral of the entropy density – neglecting currents – is given by

$$S = \int \mathrm{d}^3x \int \frac{\mathrm{d}^3p}{(2\pi\hbar)^3}\,\sigma(f). \tag{5.192}$$

This quantity has to be maximized while seeking for an equilibrium state. For the sake of brevity we shall denote the phase space integrals by a simple integration sign. There are still further constraints. In the generalized setting $F(f)$ is the normalized quantity, so one constraint is

$$\int F(f) = N. \tag{5.193}$$

Not using further constraints one arrives at a microcanonical equilibrium. Using a Lagrange multiplier $\bar{\alpha}$, one requires

$$\frac{\delta}{\delta f}\int (\sigma(f) - \bar{\alpha}F(f)) = 0. \tag{5.194}$$

Using the general entropy form (5.191) its derivative with respect to f can be obtained by using the chain rule:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}f} = \sigma' F' = (-\alpha \ln_a f + K)\,F'(f). \tag{5.195}$$

Utilizing this result at the evaluation of the variational equation (5.194) we arrive at

$$(-\alpha \ln_a f + K)\,F'(f) = \bar{\alpha}F'(f). \tag{5.196}$$

Its resolution for f is independent of the actual form of $F(f)$ and is expressed by the parameters α, a and $\bar{\alpha}$. Anyway the result is independent of the phase space position, in particular of the particle energy. Microcanonical equilibrium is always realized by equipartition.

The canonical equilibrium on the other hand also utilizes a further constraint: that of the total, in general non-additive, energy,

$$\int L(E)\,F(f) = L(E_{\mathrm{tot}}). \tag{5.197}$$

In this case the variational problem is supported by a new Lagrange multiplier ($\bar{\beta}$) times this constraint and one arrives at the following condition for the canonical equilibrium

$$(-\alpha \ln_a f + K)\,F'(f) = \bar{\alpha}F'(f) + \bar{\beta}L(E)F'(f). \tag{5.198}$$

Again the equilibrium solution is independent of the very functional form of $F(f)$, but now it includes besides the deformed logarithm $\ln_a f$ due to probability entanglement also the formal logarithm of one-particle energy $L(E)$. The canonical distribution coincides with the result of the generalized Boltzmann equation,

$$f = e_a^{\bar{\beta}(\mu - L(E))}. \tag{5.199}$$

The canonical distribution is hence not always exponential in the individual energies, like the Gibbs–Boltzmann distribution. It can be deformed essentially in two ways: (1) by the formal logarithm of the energy composition rule and (2) by a deformed logarithm counting for correlations in the entropy formula or equivalently in the underlying generalization of the product formula for entangled individual probabilities. Already one of these effects suffices to have a non-exponential, in particular a power-law tailed distribution in a formally canonical equilibrium state. On the other hand the question of normalization to particle number, i.e. the very choice of the function $F(f)$ does not disturb at all the familiar derivation of the equilibrium distribution. The only condition is that all constraints, e.g. both the number normalization and summing up of the additive formal logarithm of the energy uses the *same* function $F(f)$.

Finally, we summarize the four laws of general thermodynamic composition rules:

1. Repetition of general composition rules – by coupling small amounts to an accumulating result – leads asymptotically to *associative* rules.
2. All associative rules are mapped to addition by their *formal logarithm*.
3. In terms of these additive formal logarithms all classical *thermodynamic* formulas apply.
4. The equilibrium distribution of measured quantities are the usual functions of formal logarithms: they are *deformed*.

Problems

5.1. Derive the general result (5.17) by executing the integration (5.16) and substituting into the formula (5.15). What can one tell about the limits $D \to 0$ and $C \to 0$?

5.2. Consider the expectation value of the Taylor expansion with a Gauss-distributed deviation. What could be the next term continuing the construction recipe for Fisher entropy?

5.3. What is the asymptotic rule to Einstein's velocity addition rule:

$$u \oplus v = \frac{u+v}{1+uv/c^2}?$$

5.4. Is the following rule associative?

$$x \oplus y = x + y + \frac{a}{\frac{1}{x}+\frac{1}{y}}$$

5.5. Obtain the formal particle–hole correspondence for the deformed Fermi and Bose distributions:

$$f_a(x) = \frac{1}{e_a(x)+1}, \qquad \text{and} \qquad g_a(x) = \frac{1}{e_a(x)-1}.$$

What replaces the known results, $f_0(-x) = 1 - f_0(x)$ and $-g_0(-x) = 1 + g_0(x)$ for general values of the parameter a?

5.6. What is the canonical energy distribution with an additive energy and the following entropy composition rule?

$$S_{12} = S_1\sqrt{1+a^2S_2^2} + S_2\sqrt{1+a^2S_1^2}.$$

5.7. Obtain the canonical energy distribution for the following class of pairwise energy composition rule:

$$E_1 \oplus E_2 = E_1 + E_2 + \frac{a}{2}(E_1+E_2)^2.$$

5.8. Verify that the Rényi entropy is additive for factorizing probabilities.

5.9. Construct a composition rule which does not have a thermodynamical limit.

5.10. Compare the Rényi and Tsallis entropy formulas for binary (1.bit) events, $p_1 = p, p_2 = 1-p$. Discuss the location and value of maximum and the convexity.

5.11. Calculate the pressure for a massless ideal Boltzmann gas with canonical Tsallis-Pareto energy distribution with no chemical potential.

Chapter 6
The Temperature of Moving Bodies

We present the debate about the correct relativistic transformation formula for the temperature and its modern resolution based on relativistic hydrodynamics. Thermal-like particle spectra from high-energy heavy-ion collisions are shown and interpreted.

In this chapter, we deal with those challenges for basic thermal concepts which are related to the relativistic motion. When massive bodies move with a speed close to that of the light, or when considering the thermodynamics of radiation itself (when the particles of the statistical system all move exactly with the speed of light), we cannot avoid a relativistic statistical mechanics. It is, however, not so that only some formulas would have to be changed, like the Maxwell–Boltzmann distribution to its relativistic version. Some of the basic concepts of classical thermodynamics, most prominently the "timelessness" of the equilibrium state, are challenged by special relativity. The concept of "equal time" can be established without problem only locally when dealing with relativistic systems. Synchronization of time over an extended volume becomes a nontrivial issue in the relativistic thermodynamics. While the particle picture may choose to consider eigentimes along individual particle paths, the continuum approach to substances, like hydrodynamics, has to carefully establish local quantities as building blocks of the theory.

We review in this chapter some amazing problems related to the concept of thermodynamical temperature in relativistic systems. We start with issues of relativistic thermodynamics, joining to a classical debate about the proper relativistic transformation formula for the absolute temperature. This leads us over to the relativistic hydrodynamical approach with an emphasis on the treatment of the energy dissipation and heat transfer processes. By doing so we deliver a possible modern resolution of the classical controversy about the relativistic temperature [52]. Following this the handling of a possibly non-local entropy in a local theory of continuums is demonstrated.

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6.1 Relativistic Thermodynamics

Relativistic thermodynamics, may it sound surprising, is not yet an established theory. The origin of seeming paradoxes and unsettled notions lies in the controversy between the classical thermodynamical limit of *extended* systems and the ideal of a *local* description of relativistic dynamics satisfying principles of causality and stability. Although the most known laws of thermodynamics refer to an ideal, long-term equilibrium state, in fact most of its statements foot on real or just imagined processes, changing among such states. The theory of special relativity poses a constraint on the speed of the propagation of any physical signal, and with that on the speed of change of the thermal state.

An important example is the propagation of heat. Fourier's heat-diffusion equation, describing an average distance of an energy packet from its origin growing like $r \sim \sqrt{t}$, in fact assumes a velocity for this special kind of energy transfer as $v \sim 1/\sqrt{t}$. This formula, however, collides with the relativistic limitation on the velocity, $v \leq c$. The worse that this conflict occurs at short time. Of course, one may claim that the diffusion equation is invalid for short times, but the quantitative value of this t_0 will then depend on material properties, like the diffusion constant (or in case of the Fourier equation on the heat conductivity coefficient). Such a solution is not satisfying. One would better like to have a relativistic equation for heat conduction, which in the limit of low energy transport speed comes close to the classical diffusion-like equation. Such a relativistic equation in fact must contain a description of heat waves, never propagating faster than the speed of light.

In the next section, we select out the concept of temperature to face with requirements of the theory of special relativity. We present contradicting views about the correct transformation formula of the absolute temperature by relativistic motion and a possible generalization starting from a local description in the framework of relativistic hydrodynamics.

6.2 Disputes About the Temperature at Relativistic Velocities

Albert Einstein's famous paper about the electrodynamics of moving bodies, "Zur Elektrodynamik bewegter Körper" [53], opened the road for the theory of special relativity by pointing out that the Lorentz transformation inherent in the Maxwell equations can be derived starting from simple mechanical postulates about the motion in general. Combining the relativity principle – known since Galilei – with the invariance of the speed of light all rules of the Lorentz transformation can be easily derived. This was a major step towards generalizing our concepts about motion, space and time and correspondingly about momentum and energy. Following this step, in fact all classical physical quantities have to face the "relativity test."

It might be less known that in particular the concept of temperature was also in the focus of interest of Einstein, Planck, and several colleagues. Contemporary debates inflamed about the proper Lorentz transformation formula for the temperature when moving a heated body. There were, however, several, mutually excluding answers. Einstein himself has varied his point of view. This problem has some intricacies not settled until today.

How large is the temperature of a body moving with relativistic speed? This question – however naive it seems – is not easy to answer. Planck and Einstein concluded that it appears cooler by a Lorentz factor. But Einstein, in private correspondence to Laue, also argued for the opposite case, i.e. that it appeared hotter by a Lorentz factor. Heinrich Ott, a student of Sommerfeld attacked the "official" opinion and argued for the hotter apparent temperature. His article, published in 1963, caused some uncertainty among experts. Preceding this debate, in 1947 a study has been published in French in a local Croatian journal by Danilo Blanusa, a mathematics professor in Zagreb "About the paradox notion of energy." His result was Ott's formula: moving bodies appear hotter by a Lorentz factor. But this publication remained widely unknown. Not much later than Ott, in 1965, Peter Landsberg wrote a couple of articles in Nature. He stated that using the correct logic the temperature of the moving body is unchanged (so the temperature is a Lorentz scalar quantity). Both the Planck–Einstein and the Blanusa–Ott opinion can be true, only if there is no apparent change in the temperature due to a moving observer. This debate and its "resolution" reminds to the famous *twin paradox*.

In the afterlife of this debate, several facets of the problem have been discussed. Several authors pointed out the fact that the apparent temperature must depend on the way it is measured or defined. In particular, considering the radiation of a thermal black body there is a relativistic version of the Doppler effect. Bodies moving towards the detector look hotter, their spectra undergoes a blue shift, while departing bodies appear cooler, showing a red shift. In this case, not only a Lorentz factor, but also the classical Doppler factor occurs in the proper temperature transformation formula.

Moreover, this problem has been investigated from the viewpoint of the zeroth law of thermodynamics, too. Here, the focus question is how shall thermal equilibrium be established between bodies moving with relativistic speed, or between parts of a gas cloud with relativistically moving particles. For ideal gases, without internal energy dissipating currents, it turned out that the relative velocity has to vanish in thermal equilibrium. Naturally, in this case, the temperatures are equal [54].

In order to analyze this problem closer we have to deal with a local version of thermodynamics, since only this can be handled relativistically at the end. This local thermodynamics, based on the densities of extensive variables and their currents, is hydrodynamics. Relativistic hydrodynamics is based on energy and momentum conservation and on the assumption that the equation of state can be formulated locally, as a relation solely between densities of the thermodynamical extensives.

6.3 Thermodynamics of Energy and Momentum Exchange

The key point is that relativistically energy and momentum are just projections of a more complex quantity, the four-momentum. The density and current of the four-momentum is then described by a four-tensor in spacetime, by the *energy-momentum tensor*, T_{ij}. Considering moving bodies, moving sources and detectors of energy as well as moving observers, this tensor occurs by different projections in the different systems. Here is in fact room for apparent differences in the results of local measurements, while there are some invariant combinations. The very question is, how they relate to the thermodynamical temperature.

A minimalistic description of special relativistic continua considers the local energy and momentum conservation law,

$$\partial_i T^{ij} = 0. \tag{6.1}$$

Here, the indices i and j run over all four spacetime directions. By building a bridge to the language of classical thermodynamics one has to deal with extended bodies. The local four-momentum conservation law (6.1) has to be integrated over larger volumina occupied by the considered bodies. By doing so the question of time synchronization emerges. While there is no general, global solution to this synchronization problem, thermal equilibrium itself – being an infinite time stationary state in *all* respective reference frames – can be defined independently of the movement of possible observers. Based on this view one can determine corresponding volume-integrals of the internal and of the dissipated energy and momentum. The consideration of the momentum balance, besides that of the energy, is the essential novelty in relativistic thermodynamics with respect to the classical thermodynamics of standing bodies.

The local conservation of energy and momentum is in fact related to the Gibbs relation, to the equation describing the transformation of internal energy to heat and mechanical work.[1] Considering relativistic energies, the transfer and change of momentum is inherently connected to this law. This fact is expressed by new "work type" (i.e. nontotal differential) terms. Due to the occurrence of these terms the concept of temperature also picks up new additives.

Also the condition for thermal equilibrium, i.e. the zeroth law of thermodynamics and with that the definition of absolute temperature can be treated in a way conform to relativistic hydrodynamics. In the equilibrium state (living long – infinite – time subject to all reference frames) the entropy is maximal, isolated systems tend to realize this macrostate most of their eigentime. The conditions for this equilibrium, however, can be various: constraining on the total energy is only one of the possibilities. Such conditions are taken into account with associated Lagrange multipliers by the thermodynamical variational principle discussed in Chap. 3 at length. We are

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[1] Also frequently cited as being the first law of thermodynamics.

going to identify the proper Lagrange multiplicator to the energy constraint in the relativistic case; this will be the reciprocal of the absolute temperature, $\beta = 1/k_{\mathrm{B}}T$. But since the energy cannot be treated independently of the momentum in relativistic approaches, our result will include a relation to the speed of the equilibrating bodies, too.

Rigid bodies, strictly speaking, cannot exist. Assuming such bodies lead to a number of paradoxes in the theory of special relativity. Considering extended pieces of matter together with relativistic motion, it comes the closest to this concept a body, inside which the time can be synchronized; i.e. a "system-time" can be extracted from measurements. This is doable in a fluent environment only then, if the local four-velocity, $u^i(x)$, is not accelerating: $\dot{u}^i = 0$. Namely in this case all hypersurfaces (in particular three-volumes) labeled by a given synchron-time remain synchronized during the evolution. Such a special situation can only be achieved if the locally spacelike derivatives of the pressure vanish, otherwise they would cause an acceleration of the flow according to the Euler equation. We consider $\nabla^i p = 0$ while $u^i \nabla_i = 0$, i.e. in the four-dimensional spacetime the local vector field u^i signals the system of comoving observers having the system-time as their proper time coordinate. This way the spatial derivative four-vector is a projection orthogonal to the "time-direction":

$$\nabla^i = \partial^i - u^i(u_k \partial^k). \tag{6.2}$$

6.3.1 Perfect Relativistic Fluid

Let us consider now the basic equation of relativistic hydrodynamics. The dynamical equation describing the evolution of flow patterns, $u^i(x) = u^i(t, \mathbf{r})$, is the Euler equation. In the non-relativistic version, it describes the accelerating flow of particles due to the pressure differences in the medium. Relativistically, it describes the spacetime evolution of the density and current of energy and momentum. The familiar continuity equation for the "number density of atoms," n, is in the relativistic context just the leading term in the energy conservation: it describes the density of the rest mass energy nmc^2. The description of phenomena related to heat conductivity and viscosity, the leading order dissipative effects, emerge then in next to leading order in the $1/c^2$ expansion. Such terms lead to the Navier–Stokes and Fourier equations.

First, we consider the idealistic case, the perfect fluid. In this case the dissipative effects are neglected and the energy–momentum tensor, T_{ij}, shows a simple structure. Being in general a 4×4, symmetric tensor it has four real eigenvalues: the energy density, e, and the pressure eigenvalues p_1, p_2, and p_3. In isotropic systems there is a common hydrostatic pressure (it is called Pascal's law) $p_1 = p_2 = p_3 = p$. There belong four eigenvectors to the four eigenvalues. These span out a reference frame in the spacetime, a so called tetrad. Due to the Minkowski metric exactly one of the eigenvectors is timelike. Choosing this for the description of the flow, one describes the relativistic flow in a frame locally comoving with the energy. The eigenvector is normalized: $u_i u^i = 1$.

A comoving observer's own four velocity is the same as that of the flow, consequently she/he measures $u^i = (1,0,0,0)$, i.e. a standing fluid. At the same time T_{ij} is observed to be diagonal in this frame. The energy–momentum tensor for a perfect fluid hence can be reconstructed in a general frame as being

$$T^{ij} = eu^i u^j - p\left(g^{ij} - u^i u^j\right). \tag{6.3}$$

The energy density, e, and pressure, p, locally characterizes the flowing medium. The conservation equation (6.1) suffices to determine four independent quantities, say e and u^i (since u^i is normalized, it contains only three unknowns). The fifth variable, in this case p, has to be specified as a function of the energy density. The relation $p(e)$, being the same everywhere in the same fluid, is characterizing the quality of the flowing matter. This is the hydrodynamical version of the equation of state. In practice, a parametric representation, $p(T), e(T)$, is used, relying on the temperature dependence of the local pressure and energy density.

We note by passing that further conserved currents (Noether currents) may also occur; their flow is described by extra conditions

$$\partial_i J^i = 0. \tag{6.4}$$

In relativistic theories dealing with particle physics, such a current can be the current of electric charge, or that of the baryonic charge or any other current related to a conserved charge carried by the particles. By analyzing accelerator experiments or cosmic rays often several conserved currents occur at the same time.

It is noteworthy that any such $J^i = nv^i$ four vector defines now a unit length four vector, v^i, which also may be regarded as a flow field. This flow field is then associated to that particular charge. There is, however, no guarantee that the flow of energy and another flow, say that of the baryon number, a difference between the charges of baryons and antibaryons, would point out the same flow field. In fact one has a choice in the relativistic hydrodynamical description. We use the convention of Landau which relates the flow field to the energy, since it is generally accepted.[2] In a non-perfect fluid, showing internal dissipation, there remains however no reason for any specific choice.

It is enlightening to consider some specific projections of the energy–momentum conservation equation. The energy conservation – one basic column of thermodynamics – in the comoving frame is given by

$$u_i \partial_j T^{ij} = u_i \partial_j \left(wu^i u^j - pg^{ij}\right) = 0, \tag{6.5}$$

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[2] The fixing to the particle number is called the Eckart convention.

with $w = e + p$ being the enthalpy density. Carrying out the derivations term by term and using $u_j u^j = 1$ we get

$$u_i \partial_j T^{ij} = \partial_j (w u^j) + w u_i u^j \partial_j u^i - u^j \partial_j p = 0. \tag{6.6}$$

Here, the several terms contain a derivation with respect to the comover's proper time, $u^j \partial_j = \mathrm{d}/\mathrm{d}\tau$, this operation we shall denote by an overdot. The quantity $u_i \dot{u}^i$ in the second term vanishes, since the length of the four vector is constant: $(u_i u^i)^{\cdot} = 2u_i \dot{u}^i = 0$. Using again the $w = e + p$ relation the rest leads to

$$u_i \partial_j T^{ij} = \partial_i (e u^i) + p\, \partial_i u^i = 0. \tag{6.7}$$

This form already reminds to the first law of thermodynamics. In fact the contributions of the internal energy change and mechanical work can be recognized after an integration of the above equation over a four dimensional region of spacetime.

As a matter of fact all expressions in the form $\partial_i (f u^i)$ can be integrated over a time-dependent local three-volume, V giving[3]

$$\partial_i (f u^i)\, V\, \mathrm{d}\tau = \mathrm{d}(fV). \tag{6.8}$$

This correspondence is Reynold's transport law. In particular, for $f = 1$ the change of the volume-like quantity V is related to the four-divergence of the four-velocity field:

$$\partial_i u^i = \frac{1}{V} \frac{\mathrm{d}V}{\mathrm{d}\tau} = (\ln V)^{\cdot}. \tag{6.9}$$

It actually describes a local expansion factor, well known in general relativity and cosmological models as the Hubble constant. On the other hand the product of the volume V and the energy density e can be regarded as the internal energy inside V, $E = eV$ with right. Using these interpretations equation (6.7) transforms to

$$\left(u_i \partial_j T^{ij}\right) V\, \mathrm{d}\tau = \mathrm{d}E + p\,\mathrm{d}V = 0. \tag{6.10}$$

The right hand side is zero only for perfect fluids. Dissipative processes producing heat or changing particle numbers due to chemistry eventually complete this relation to the familiar Gibbs relation:

$$\mathrm{d}E + p\mathrm{d}V = T\mathrm{d}S + \mu\mathrm{d}N. \tag{6.11}$$

The particular condition $\mathrm{d}E + p\mathrm{d}V = 0$ in the absence of processes changing particle numbers, $\mathrm{d}N = 0$, is equivalent to constant entropy: $\mathrm{d}S = 0$. The motion of the perfect relativistic fluid this way is always *adiabatic*.

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[3] Strictly speaking this is valid in the limit $V \to 0$. In this sense V is only an auxiliary variable.

6.3.2 Dissipative Hydrodynamics

Let us now try to quantify the dissipation and entropy change in the framework of relativistic hydrodynamics. The perfect fluid is only an idealization; in physical matter, there is always dispersion of energy and momentum at finite temperature.

Classical thermodynamics dealt with the exchange of heat and mechanical work between extended bodies. Relativistic hydrodynamics is on the other hand a local theory, otherwise it could not conform with requirement of causality, restricting the propagation speed of physical effects. In the thermodynamical analysis, the world is divided into an inner and an outer region, inside and outside the extended body. In the relativistic thermodynamics the energy and momentum conservation is satisfied locally, but its integrals over spacetime regions can be separated to volume and surface contributions. As a consequence the external work and the heat exchange can be identified and separated from the change of internal energy.

The energy momentum tensor contains in this case new contributions. The formula (6.3) is modified. Now the tensor T^{ij} has some further non-vanishing projections:

$$T^{ij} = eu^i u^j + q^i u^j + u^i q^j + P^{ij}, \tag{6.12}$$

where $u_i q^i = 0$ and $u_i P^{ij} = 0$, $P^{ij} u_j = 0$. With this the above expression is the general expansion. Since u^i is timelike ($u_i u^i = 1 \geq 0$), a four vector orthogonal to it is spacelike, $q_i q^i \leq 0$. The spacelike tensor P^{ij} contains terms related to the pressure; it is no more isotropic nor diagonal. The deviations from the perfect fluid are emphasized if one separates its isotropic, hydrostatic part:

$$P^{ij} = p(u^i u^j - g^{ij}) + \Pi^{ij}. \tag{6.13}$$

In a perfect fluid Π^{ij} vanishes therefore, $T_i^{\ i} = e - 3p$. In a dissipative fluid the bulk viscosity causes a deviation from this formula. The additional terms in a dissipative fluid emerge as

$$T^{ij} = \left(wu^i u^j - pg^{ij}\right) + \left(u^i q^j + q^i u^j + \Pi^{ij}\right). \tag{6.14}$$

It pays off to introduce some more compact notations. The vectors and tensors parallel and orthogonal to the velocity field u^i lead to separate equations. The local four-current of energy density can be composed from a parallel and from an orthogonal component:

$$\varepsilon^j = eu^j + q^j. \tag{6.15}$$

The hydrostatic pressure contains a projector orthogonal to u,

$$\Delta^{ij} = g^{ij} - u^i u^j, \tag{6.16}$$

and finally the rest can be summarized in a tensor which is orthogonal to u_i, but has an u^j-projection equal to q_i:

$$\Sigma^{ij} = q^i u^j + \Pi^{ij}. \tag{6.17}$$

According to this classification the total energy–momentum tensor consists of three terms:

$$T^{ij} = u^i \varepsilon^j - \Delta^{ij} p + \Sigma^{ij}. \tag{6.18}$$

The derivation with respect to the spacetime coordinates also splits into components parallel and orthogonal to u_i: $\partial_i = u_i \mathrm{d}/\mathrm{d}\tau + \nabla_i$, as already mentioned above. The local energy- and momentum conservation in a dissipative fluid then includes the following contributions:

$$\partial_i T^{ij} = u_i \dot{T}^{ij} + \nabla_i T^{ij} = \left(u_i T^{ij}\right)^{\cdot} - \dot{u}_i T^{ij} + \nabla_i T^{ij}. \tag{6.19}$$

The first term in this expression is simply the proper-time derivative of $u_i T^{ij} = \varepsilon^j$. In the second term those parts of T^{ij} which contain u^i give no contribution since $\dot{u}_i u^i = 0$. The rest is given by $\dot{u}_i T^{ij} = -\dot{u}^j p - \dot{u}_i \Sigma^{ij}$. Finally the spacelike derivative ("nabla"-) term requires a little longer analysis. Considering the identity $u^i \nabla_i = 0$ we first obtain

$$\nabla_i T^{ij} = \varepsilon^j (\nabla_i u^i) - \nabla^j p - p \nabla_i \Delta^{ij} + \nabla_i \Sigma^{ij}. \tag{6.20}$$

In the spacelike derivative of the projector Δ^{ij}, however, this operation acts only on the flow velocity field, therefore $\nabla_i \Delta^{ij} = -\nabla_i (u^i u^j) = -u^j (\nabla_i u^i)$. Putting all this together we gain the following expression:

$$\nabla_i T^{ij} = \left(\varepsilon^j + p u^j\right) \nabla_i u^i - \nabla^j p + \nabla_i \Sigma^{ij}. \tag{6.21}$$

The three contributions together establish the following conservation equation:

$$\partial_i T^{ij} = \dot{\varepsilon}^j + p \dot{u}^j - \dot{u}_i \Sigma^{ij} + (\varepsilon^j + p u^j) \nabla_i u^i - \nabla^j p + \nabla_i \Sigma^{ij} = 0. \tag{6.22}$$

It is furthermore useful to combine the effects of factors due to the acceleration of velocity field and the effect of the spacelike nabla operator in a single operation, orthogonal to u: $D^j = \nabla^j - \dot{u}^j$. This way $u_j D^j = 0$, and the conservation law appears in the following, thermodynamically suggestive form:

$$\partial_i T^{ij} = \dot{\varepsilon}^j + (\varepsilon^j + p u^j) \nabla_i u^i - D^j p + D_i \Sigma^{ij} = 0. \tag{6.23}$$

We note that due to $u_i \dot{u}^i = 0$ it is $\nabla_i u^i = \partial_i u^i = D_i u^i$. Now it is easy to obtain the u_j-projection of the above equation. Let us consider the terms individually. The projection of the first term is given by

$$u_j \dot{\varepsilon}^j = \dot{e} + u_j \dot{q}^j. \tag{6.24}$$

The second term's projection is simply the enthalpy density:

$$u_j(\varepsilon^j + pu^j) = e + p = w. \tag{6.25}$$

The u_j-projection of the third term vanishes, the corresponding projection of the fourth term can be listed as follows:

$$u_j D_i \Sigma^{ij} = u_j \left(\nabla_i - \dot{u}_i\right)\left(q^i u^j + \Pi^{ij}\right) = \nabla_i q^i - \dot{u}_i q^i + u_j \nabla_i \Pi^{ij}. \tag{6.26}$$

Collecting these four terms one obtains the energy conservation equation in the frame comoving with the flow:

$$u_j \partial_i T^{ij} = \dot{e} + u_j \dot{q}^j + w \nabla_i u^i + \nabla_i q^i - \dot{u}_i q^i + u_j \nabla_i \Pi^{ij} = 0. \tag{6.27}$$

Using finally the orthogonality of q and Π to the velocity field u one arrives at the following energy balance equation:

$$\dot{e} + w \nabla_i u^i = 2 q_i \dot{u}^i - \nabla_i q^i + \Pi^{ij} \nabla_i u_j. \tag{6.28}$$

It is evident that, due to the q^i heat four current, in relativistic dissipative systems the energy balance equation is not independent from the momentum balance equation (Euler equation) which determines the acceleration of the velocity field, $\dot{u}^j$. Even restricting to non-accelerating flows, there remains a source term in form of $-\nabla_i q^i$, indicating that the Gibbs relation does contain an energy-leak term. Therefore, $T\mathrm{d}S$ is not zero, but equals to the heat dissipated through the boundary surface of the integration volume.

6.3.3 Dissipation in Extended Regions

In order to return to the relativistic thermodynamics of moving bodies we consider non-accelerating flow, $\dot{u}^i = 0$. This can only be achieved if the spatial gradient of the pressure also vanishes, $\nabla^i p = 0$. Using these conditions, (6.23) can be simplified to

$$\partial_i T^{ij} = \dot{\varepsilon}^j + (\varepsilon^j + pu^j) \nabla_i u^i + \nabla_i \Sigma^{ij} = 0. \tag{6.29}$$

This form can be easily integrated over a hypersurface, $H(\tau)$, which includes a volume $V(\tau)$ slowly changing as a function of the comover's proper time, τ. We note that the flow field, $u^i(x)$, is not necessarily homogeneous, it is just non-accelerating.

Such an integration leads to a relation between the change of total energy and momentum and the change of the volume and heat. Utilizing that $\nabla_i u^i = \dot{V}/V$ [cf. (6.9)], one arrives at

$$\dot{E}^j + p\bar{u}^j \dot{V} = -\int\limits_{H(\tau)} \nabla_i \Sigma^{ij} \, \mathrm{d}V, \tag{6.30}$$

with

$$E^j = E\bar{u}^j + G^j, \tag{6.31}$$

$E = \int e\,\mathrm{d}V = eV$ total energy, $G^j = \int q^j\,\mathrm{d}V$ total conductive energy current and $\bar{u}^j = \int u^j \mathrm{d}V/V$ average flow velocity of the body. The latter, assuming homogeneous energy density, coincides with the velocity of the energy center. The volume integral on the right hand side of (6.30) is that of a total divergence, therefore, it can be written as a surface contribution. The total dissipated energy and momentum in a short proper time, $\mathrm{d}\tau$, is the correct relativistic four-vector generalization of the heat transfer. Since $\mathrm{d}E^j = \bar{u}^j \mathrm{d}E + \mathrm{d}G^j$ contributes to (6.30) by the total τ-derivative of the internal energy and momentum, $\mathrm{d}G^j$ itself is also a total differential and not a work-like term. We obtain the following relation:

$$(\mathrm{d}E + p\mathrm{d}V)\bar{u}^j + \mathrm{d}G^j = \delta Q^j. \tag{6.32}$$

Here, the term $\mathrm{d}G^j$ is novel compared to the classical Gibbs relation. The rest is just the familiar $\mathrm{d}E + p\mathrm{d}V$ term carried on a flow. One also should note that although u_i and q^i are locally orthogonal, their volume integrals are not necessarily so. One may feel necessary to rearrange the integrals again to terms parallel and orthogonal to $\bar{u}^i$. We may include the part of G^j, which is parallel to $\bar{u}^j$, into the internal energy E. The rest of G^j will then be orthogonal to $\bar{u}^j$. In the following discussion we tacitly assume that E and G^j stand for such corrected quantities.

Now we seek for an integrating factor to the relativistic four vector of heat. In this process also a four vector, A^j, appears in place of $1/T$.

$$(\mathrm{d}E + p\mathrm{d}V)\bar{u}^j + \mathrm{d}G^j = A^j \mathrm{d}S + \sigma^j \mathrm{d}\tau. \tag{6.33}$$

where σ^j comprises terms orthogonal to A^j. Projecting this equation with A^j we obtain a total differential of the comover entropy

$$\mathrm{d}S = \frac{A_j \bar{u}^j}{A_k A^k}(\mathrm{d}E + p\mathrm{d}V) + \frac{A_j}{A_k A^k}\mathrm{d}G^j. \tag{6.34}$$

It is obvious that the traditional $1/T$ factor of thermodynamics has to be the coefficient of the first two terms. By fixing this correspondence, however, the coefficient of the novel term is still not determined entirely. It is a four vector, indicating that besides the temperature, T, another quantity must be balanced between two bodies in relativistic thermal equilibrium. The corresponding intensive variable of state, following the tradition, can be defined by factorizing out $1/T$:

$$\frac{g^j}{T} = \frac{A^j}{A_k A^k}. \tag{6.35}$$

Now $g_i \bar{u}^i = 1$ is required for obtaining $1/T$ as a factor of the classical term $\mathrm{d}E + p\mathrm{d}V$. However, it does not follow that in general $g^i = \bar{u}^i$. This is only a particular solution, even if a particularly simple one. Of course, this *assumption* has been made by several authors. Considering namely $g^i = \bar{u}^i$ leads to the canonical equilibrium distribution $\exp(-\bar{u}_i E^i/T)$, occurring to be a natural generalization of the Boltzmann–Gibbs factor $\exp(-E/T)$. In fact this has been proposed by Jüttner already in 1911 [55–58]. Also by Israel and Stewart, when pioneering a relativistic dissipative hydrodynamical description, this simplification has been utilized [59–61].

Since according to our synchronization assumption the flow is stationary and therefore the total differential of the global flow field of the body vanishes, $\mathrm{d}\bar{u}^j = 0$. The carried (convective) energy current and the four vector orthogonal to $\bar{u}^i$ describing spacelike energy conduction can be summarized in a single vector, $E^j = E\bar{u}^j + G^j$. Using this notation the relativistic Gibbs relation can be written as

$$\mathrm{d}S = \frac{g_j}{T}\mathrm{d}E^j + \frac{p}{T}\mathrm{d}V. \tag{6.36}$$

We consider now a general intensive parameter, $g^j = \bar{u}^j + w^j$. Here, the second vector is spacelike. Due to the requirement $g^j \bar{u}_j = 1$ it is perpendicular to the four velocity of the moving body: $w_j \bar{u}^j = 0$. At the same time the total vector, g^j, has to be timelike, because the growth of entropy physically happens in timelike regions of the spacetime. This way the vector A^j in (6.33) itself is timelike leading to the above property of g^j. Therefore we have

$$g_j g^j = (\bar{u}_j + w_j)(\bar{u}^j + w^j) = 1 + w_j w^j \geq 0. \tag{6.37}$$

It follows then $w_j w^j \geq -1$. Being a spacelike vector this expression is also smaller than zero. In conclusion, the velocity defined by the ratio of the current component of w^j to its density component can only be *subluminal*. Here, is the final test of relativistic thermodynamics: velocities associated to energy and momentum transfer are always less than the speed of light. In Fig. 6.1, the possible endpoints of the vector w^i for a given timelike $\bar{u}^i$ lie on a line, Minkowski-orthogonal to the direction of $\bar{u}^i$ and restricted between the spacelike hyperboles of unit apex.

In order to gain a visual picture we shall restrict the discussion to one time and one space dimension in the followings. The motion of the thermodynamical body is then described by the Lorentz vector $\bar{u}^j = (\gamma, \gamma v)$, while the energy conduction by the spacelike vector $w^j = (\gamma v w, \gamma w)$ orthogonal to $\bar{u}^j$. Here, v is the Newtonian velocity of the body and $\gamma = 1/\sqrt{1-v^2}$ is the Lorentz factor in $c = 1$ units. The velocity parameter w describes the velocity of conductive energy currents. Neither v nor w may exceed the speed of light.

6.4 Relativistic Thermal Equilibrium

Let us consider now the thermal equilibrium between two bodies in relative motion to each other and to the observer's frame. In the equilibrium state, the entropy is maximal, under the condition that certain relations hold. By now, the energy and momentum conservation has to be regarded in a unified view. The changes in the energy–momentum four-vectors of the respective interacting bodies balance each other: $\mathrm{d}E_1^j + \mathrm{d}E_2^j = 0$. The situation is analog with the total volume considering non-penetrating bodies, $\mathrm{d}V_1 + \mathrm{d}V_2 = 0$. Since the total additive entropy is at its maximum, its total differential is also zero: $\mathrm{d}S_1 + \mathrm{d}S_2 = 0$.

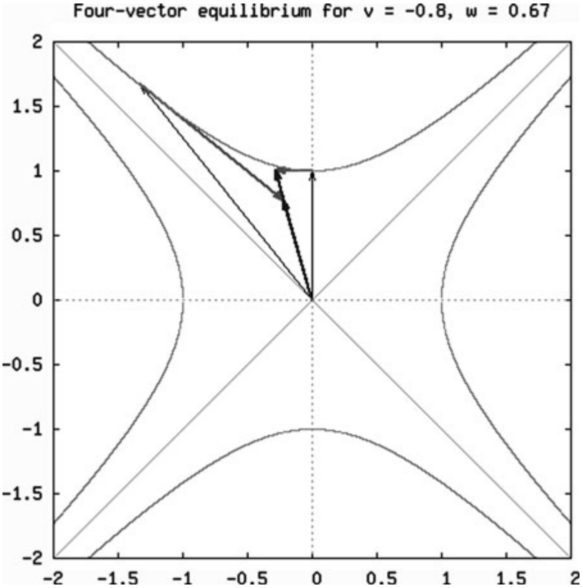

Fig. 6.1 Thermal equilibrium of important four vectors: a general case. The magnitude of the relative velocity is $v = -0.8$, the heat current velocity in the observed body is $w_2 = 0.67$. The g-vectors have to be parallel, but not necessarily of equal length in equilibrium

The general, relativistic entropy depends on the internal energy, E, on the volume, V, but also on the energy current G^j! Therefore, the proper relativistic equation of state is of the following form: $S = S(E^j, V)$. In thermal equilibrium, taking the partial derivatives of the entropy from (6.36) we obtain

$$\mathrm{d}S_1 + \mathrm{d}S_2 = \left(\frac{g_1^j}{T_1} - \frac{g_2^j}{T_2} \right) \mathrm{d}E_1^j + \left(\frac{p_1}{T_1} - \frac{p_2}{T_2} \right) \mathrm{d}V_1 = 0. \tag{6.38}$$

Here, each term has to vanish independently, i.e. for any combination of the infinitesimal changes $\mathrm{d}E_1^j$ and $\mathrm{d}V_1$. Annulling the second bracket the familiar condition $p_1/T_1 = p_2/T_2$ emerges, representing the equity of intensive parameters associated to the volume change.

Equating the first bracket to zero, however, gives more than the usual equity of temperatures! The condition

$$\frac{g_1^j}{T_1} = \frac{g_2^j}{T_2} \tag{6.39}$$

requires the equity of two Lorentz vectors.

This requirement can be viewed as the equity of lengths and unit vectors (directions in the spacetime). The squared Minkowski length of the intensive Lorentz vector, $g_j g^j = 1 + w_j w^j = 1 - w^2 \geq 0$, contains the velocity of heat conduction. This way we arrive at the following equation containing both the temperature and this velocity:[4]

$$\frac{\sqrt{1-w_1^2}}{T_1} = \frac{\sqrt{1-w_2^2}}{T_2}. \tag{6.40}$$

This wonderful formula demonstrates strongly the origin of the "thermal twin paradox": for $w_1 = 0$ the one, for $w_2 = 0$ the other view about the modifying Lorentz factor to the temperature is obtained. Viewing from a system where the total energy conduction is zero, $w_1 + w_2 = 0$, obviously leads to $T_1 = T_2$, to the opinion expressed by Landsberg. It should be clear, that by a Lorentz transformation from the general case to any particular observer's system, at one time only one of these conditions can be fulfilled.

Without restricting the generality of the discussion we regard the body with the index 1 as the thermometer. It means that w_1 and T_1 quickly obtain their value prescribed by the equilibrium condition, it will be read out by the observer moving with velocity v_1, without disturbing the values w_2 and T_2 established by physical processes in the body 2 (Figs. 6.2–6.6).

6.4.1 *Relativistic Doppler Effect and Beyond*

What have the Lorentz factors, associated to the internal heat conduction speed, and the (average) velocities of the moving bodies, to do with each other? These

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[4] The velocity of the body is v, the heat conduction velocity with respect to the body is w. For a general observer the latter appears as combined velocity, $v \oplus w = (v+w)/(1+vw)$.

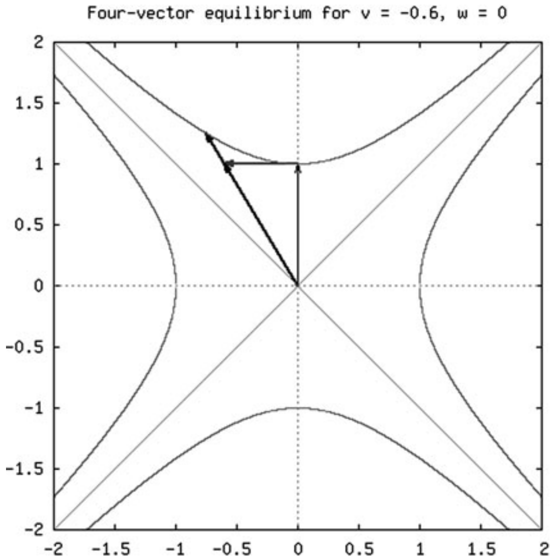

Fig. 6.2 Important four-vectors in relativistic thermal equilibrium. The relative velocity is $v = -0.6$, the observed body shows no heat conduction, $w_2 = 0$. The velocity of the induced heat current in the thermometer is $w_1 = v$, and it indicates a temperature cooler by a Lorentz factor: $T_1/T_2 = \|g_1\|/\|g_2\| = 0.8$

factors, independent in their origin, became related in thermal equilibrium, due to the parallelization of the g^j intensive four vectors. This fact hides the relativistic Doppler formula as well as the correct answer to the thermal twin paradox. This component of the equilibrium condition also explains why in thermal equilibrium also the velocities of the bodies must become into relation.

We divide (6.39) by its Minkowski-length expressed by (6.40). We obtain

$$\frac{\bar{u}_1^j + w_1^j}{\sqrt{1-w_1^2}} = \frac{\bar{u}_2^j + w_2^j}{\sqrt{1-w_2^2}}. \tag{6.41}$$

This formula equates unit length Lorentz vectors. Extracting the equation of the spacetime directional tangents, the respective ratios of the spacelike and timelike components, we arrive at

$$\frac{w_1 + v_1}{1 + v_1 w_1} = \frac{w_2 + v_2}{1 + v_2 w_2}. \tag{6.42}$$

This is nothing else than Einstein's relativistic velocity addition formula. In this sense, the velocities of the respective heat currents seen by respective body

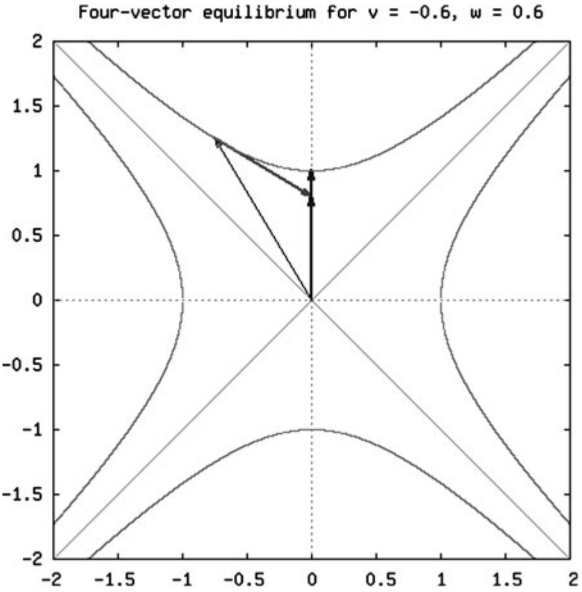

Fig. 6.3 Important four vectors in relativistic thermal equilibrium. The relative velocity is $v = -0.6$, the observed body shows a heat conduction velocity of $w_2 = -v$. The velocity of the induced heat current in the thermometer is none in this case $w_1 = 0$, and the thermometer indicates a temperature hotter by a Lorentz factor: $T_1/T_2 = \|g_1\|/\|g_2\| = 1.25$

comovers becomes equal. Expressing relative velocities from this equation, one also inspects that the relative velocity of the moving bodies in thermal equilibrium will be compensated by the relative velocity of heat currents inside the bodies:

$$\frac{w_1 - w_2}{1 - w_1 w_2} = \frac{v_2 - v_1}{1 - v_1 v_2} = v. \tag{6.43}$$

Here, v is the (observer independent) relative velocity of the two bodies. Expressing say w_1 by v and w_2 from the above equilibrium condition one gets

$$w_1 = \frac{w_2 + v}{1 + v w_2}. \tag{6.44}$$

Finally, utilizing the Lorentz factor $\gamma = 1/\sqrt{1 - v^2}$, associated to the relative velocity, the ratio of temperatures in (6.40) becomes

$$\frac{T_2}{T_1} = \gamma(1 + v w_2). \tag{6.45}$$

This generalized Doppler formula contains two parameters: the relative velocity v and the velocity of heat current in the observed body, w_2. This quantities are physical, they cannot be changed by varying the frame of reference (Figs. 6.7 and 6.8).

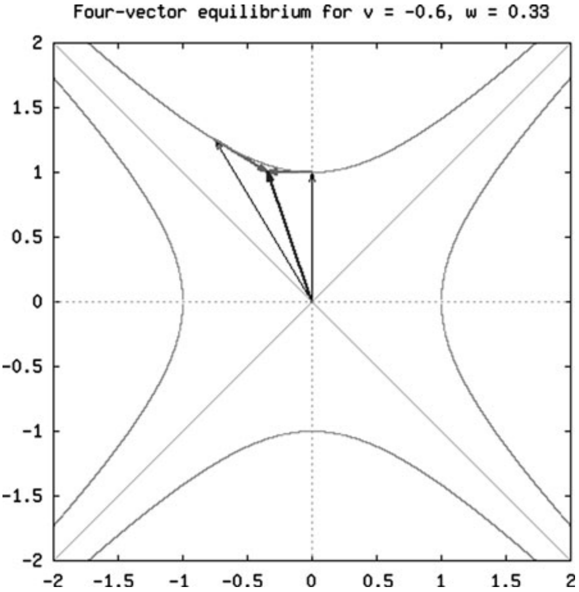

Fig. 6.4 Important four vectors in relativistic thermal equilibrium. The relative velocity is $v = -0.6$, the observed body shows a heat conduction velocity of $w_2 = 0.33$ which induces an opposite velocity in the thermometer, $w_1 = -0.33$. The thermometer shows the same temperature as the body has: $T_1/T_2 = \|g_1\|/\|g_2\| = 1$

Let us list again those particular cases which coincide with one or the other formulas proposed during historical debates.

1. In case of $w_2 = 0$ there is no heat current relative to the observed, moving body. In the observing body (in the thermometer) there is an induced heat current with the equilibrium velocity $w_1 = v$, being equal to the relative velocity of the two bodies. The temperature in body 1 (the thermometer) is given by $T_1 = T_2/\gamma$, so it appears cooler by a Lorentz factor than the comoving temperature. This conclusion was put forward by Max Planck and Albert Einstein.
2. In the opposite case one considers a thermometer not showing any heat current. Then $w_1 = 0$, conjecturing $w_2 = -v$, a very special heat current in the observed body. It means that while the observed body moves, the energy current seems to stand relative to the thermometer: the conductive part compensates the convective part. This way the ratio of temperatures satisfies $T_1 = T_2\gamma$, so the measured temperature is hotter by a Lorentz factor. This was the opinion of Heinrich Ott and Danilo Blanusa.
3. In the case when the total system has standing energy, (i.e. we are in the Landau frame of the total system $1+2$), one sets $w_1 + w_2 = 0$. By this condition in the equilibrium state $w_2 = (-1+\sqrt{1-v^2})/v = -w_1$ and of course $T_1 = T_2$. One measures the "correct" temperature by a particular coincidence of different effects, although there is a non-vanishing relative velocity, v, between the

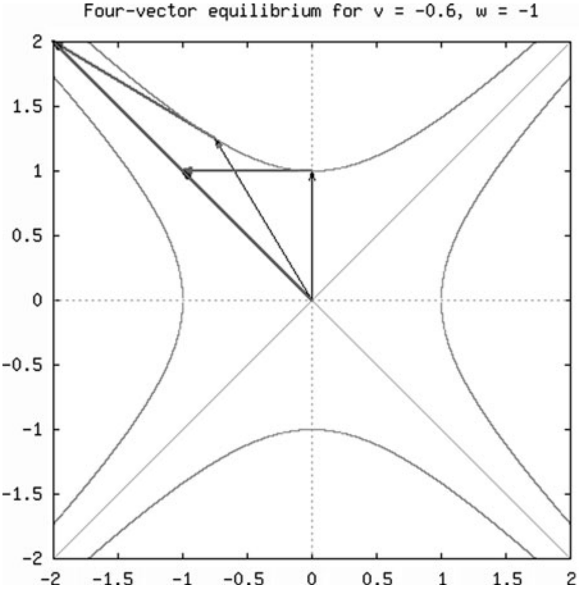

Fig. 6.5 Important four vectors in relativistic thermal equilibrium. The relative velocity is $v = 0.6$, the observed body departs filled with radiation. The induced energy current in the thermometer has also a velocity of light, $w_1 = 1$. The temperature indicated by the thermometer shows a relativistic Doppler red shift: $T_1/T_2 = \|g_1\|/\|g_2\| = 0.5$

thermometer and the measured body. This position was argued for by Peter Landsberg, as the “symmetric solution” to the thermal twin paradox.

4. Finally, if the body is filled with radiation, the energy current cannot be stopped inside. It always goes with the velocity of light. For a body radiating photons towards the thermometer one has $w_2 = -1$ and obtains the relativistic Doppler formula

$$\frac{T_2}{T_1} = \sqrt{\frac{1-v}{1+v}}. \tag{6.46}$$

For a parting body $v > 0$ ($v_2 > v_1$), and one measures a red-shifted temperature, $T_2 < T_1$, while for a closing body due to $v < 0$ ($v_2 < v_1$) a blue-shifted value, $T_2 > T_1$, is obtained. The former phenomenon is met frequently in astronomical observations, especially by studying far objects, since the space inside our Universe is expanding. The latter is rather typical for observations of particle spectra in high energy accelerator experiments, stemming from a fireball expanding outwards, approaching the detectors with speeds close to that of the light.

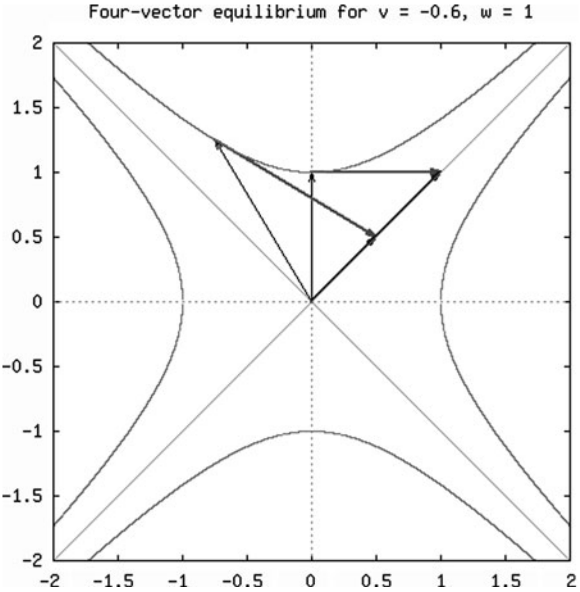

Fig. 6.6 Important four vectors in relativistic thermal equilibrium. The relative velocity is $v = -0.6$, the observed body closes filled with radiation, $w_2 = 1$. The induced energy current in the thermometer has also a velocity of light, $w_1 = 1$. The temperature indicated by the thermometer shows a relativistic Doppler blue shift: $T_1/T_2 = \|g_1\|/\|g_2\| = 2.0$

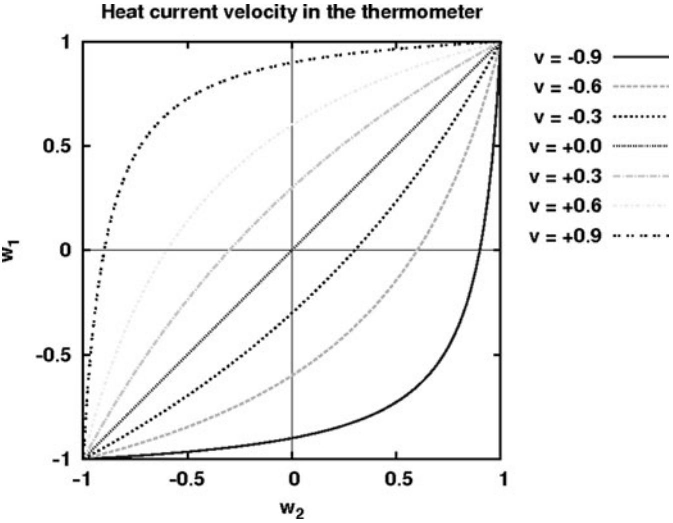

Fig. 6.7 The equilibrium heat current shown by the thermometer, w_1, as a function of the heat current in the observed body, w_2, moving by a relative velocity of v (see legend)

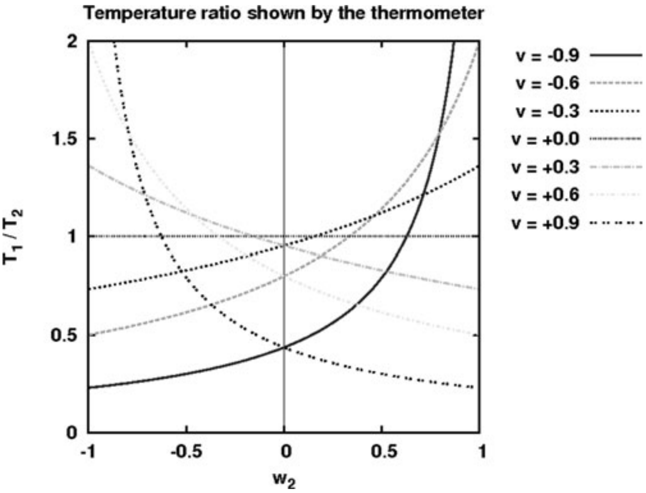

Fig. 6.8 The ratio of the temperature shown by a thermometer to that of the one in comoving frame, T_1/T_2, as a function of the heat current in the observed body, w_2. The different curves belong to different relative velocities from $v = -0.9$ to $v = +0.9$ (see legend)

Problems

6.1. Express temperature transformation in rapidity variables.

6.2. Can it be that $T_1/T_2 \leq |w_1/w_2|$? What does it mean for the measured value T_1?

6.3. At what special values of the relative velocity can it be $T_1 = 2T_2$?

Chapter 7
The Temperature of no Return

The Unruh temperature for constant acceleration, black hole thermodynamics, and Hawking radiation. String theory, higher dimensional gravity, dual field theory. Applications to viscosity and Yang–Mills equation of state. Gravity emerging from information.

To begin this chapter we face the shocking fact that a uniform accelerating observer experiences a Planck distribution for a monochromatic light-wave. The equivalent temperature due to this Unruh effect is proportional to the acceleration. As it is expressed by Einstein's equivalence principle – formulating the very physical content of general relativity – a constant acceleration is physically equivalent to an also constant gravitational field. Such a constant field occurs at the event horizon of a black hole (its constancy actually defines the event horizon).

At this point we briefly recall what is a black hole and elaborate on analogies between classical black hole properties and thermodynamics. The Hawking radiation, as a suggested physical mechanism for measuring black hole temperature and evaporating small black holes from the universe (and according to some speculations in high energy accelerator experiments), will be discussed separately. Finally, contemporary models of high energy particle collisions, based on the AdS/CFT[1] correspondence, are reviewed in this chapter. Since one of the most characteristic outcome of this analogy is the prediction of a lower bound for shear viscosity, we deal with the question, how the energy and momentum flow, in particular dissipation, are treated in this framework. The energy conservation is complicated by the equivalence principle: any accelerating observer feels gravitational fields, which are among others also energy stores. The consequent handling of general relativistic hydrodynamics including local thermodynamics is, however, not yet clarified to a satisfactory depth.

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[1] AdS: Anti de Sitter spacetime, CFT: conformal field theory.

T.S. Biró, *Is There a Temperature? Conceptual Challenges at High Energy, Acceleration and Complexity*, Fundamental Theories of Physics 171,
DOI 10.1007/978-1-4419-8041-0_7,

7.1 Temperature due to Acceleration: The Unruh Effect

A correspondence between temperature and acceleration can in fact already be established in the framework of special relativity. An observer with constant acceleration measures a thermal spectrum for a field which is a monochromatic plane wave for a static observer. This is called the *Unruh effect* after its first investigator (Unruh) [62,63].

It is a surprising result, since no heat bath, no noisy environment, no Brownian motion is involved – simply a Fourier analysis in terms of the static time coordinates, t and in terms of the comoving (co-accelerating) proper time, τ, gives different results. But why this result looks like the Planck spectrum, is a mystery. The derivation namely nowhere but at the last step has a reference to Planck's constant (and hence to quantum physics), when reinterpreting the result in terms of the black body radiation.

The equivalent temperature, T, is proportional to the acceleration, g:

$$k_{\mathrm{B}}T = \frac{\hbar g}{2\pi c}. \tag{7.1}$$

For a sizable effect, however, one needs enormous acceleration: at Earth gravitational acceleration, $g \approx 10\ \mathrm{m\,s^{-2}}$, the thermal energy is in the order of magnitude of $k_{\mathrm{B}}T \approx 10^{-29}$ eV; to be compared to the room temperature which is about $k_{\mathrm{B}}T \approx 2.5 \times 10^{-3}$ eV. In particle accelerators, on the other hand, one estimates a deceleration stopping from nearly light speed to zero on a distance of 0.3 fm inside an atomic nucleus; to this value it corresponds $k_{\mathrm{B}}T \approx 100$ MeV, a temperature which can in fact be observed in the spectra of produced particles in the same order of magnitude [64,65].

In this section, we present a – relatively simple – derivation of the Unruh effect. First, we describe relativistic motion with constant acceleration, and then analyze a plane wave seen from a co-accelerating frame.

It is sufficient to consider one spatial dimension, the direction of motion. The four velocity, tangent to the world line of the motion, is normalized to one: $u^{\mu} = (\sqrt{1+v^2}, v, 0, 0)$. The four-acceleration vector, $a^{\mu} = \mathrm{d}u^{\mu}/\mathrm{d}\tau$, is orthogonal to this vector. Fixing its constant length according to $a_{\mu}a^{\mu} = -g^2$, i.e. fixing the acceleration experienced by the comoving observer to g, we consider the four-acceleration vector $a^{\mu} = (gv, g\sqrt{1+v^2}, 0, 0)$. This leads us to the following ordinary differential equation for $v(\tau)$ to be solved:

$$\frac{\mathrm{d}v}{\mathrm{d}\tau} = g\sqrt{1+v^2}. \tag{7.2}$$

This is an integrable problem with the general result $v = \sinh(g\tau + c_1)$. Having zero velocity at proper time $\tau = 0$, the integration constant vanishes. The path of the motion is readily obtained from $\mathrm{d}t/\mathrm{d}\tau = \sqrt{1+v^2}$ and $\mathrm{d}x/\mathrm{d}\tau = v$ in a parametric form:

$$\begin{aligned} x &= \frac{1}{g}\left(\cosh(g\tau)-1\right)+x(0), \\ t &= \frac{1}{g}\sinh(g\tau). \end{aligned} \tag{7.3}$$

Considering $x(0) = 1/g$ as a starting coordinate we obtain the simplest path to a constant acceleration (Fig. 7.1).

Now let us consider a plane wave described by the scalar field

$$\phi(t,x) = \frac{1}{\sqrt{2\omega}}\mathrm{e}^{-\mathrm{i}(\omega t - kx)}. \tag{7.4}$$

For a photon moving into the positive x-direction the dispersion relation $\omega = k$ holds, and the phase of the complex amplitude becomes $\varphi = \omega t - kx = \omega(t-x)$. For an observer moving with a constant velocity v the path would be parametrically given as $t = \gamma\tau$, $x = \gamma v\tau$, with the Lorentz factor $\gamma = 1/\sqrt{1-v^2}$. Such an observer experiences another plane wave,

$$\phi_v(t,x) = \frac{1}{\sqrt{2\omega}}\mathrm{e}^{-\mathrm{i}\omega_v\tau}, \tag{7.5}$$

with a lowered frequency

$$\omega_v = \omega\gamma(1-v) = \omega\sqrt{\frac{1-v}{1+v}}. \tag{7.6}$$

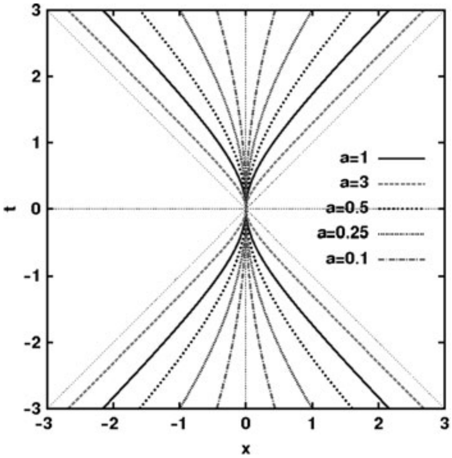

Fig. 7.1 Trajectories in spacetime crossing $x_0 = 0$ at $t = 0$, for different constant accelerations, $g = \pm a$, follow hyperbolas according to (7.3)

This "red shift" of the frequency is the (special) relativistic Doppler effect, and it is widely known.

For a constant acceleration path, however, the functional form of the phase of the wave differs for a comoving observer: as a function of the proper time τ we have $\omega t - kx = -(\omega/g)\mathrm{e}^{-g\tau}$ and therefore the wave field,

$$\phi_a(t,x) = \frac{1}{\sqrt{2\omega}} \mathrm{e}^{-\mathrm{i}\left(\frac{\omega}{g}\mathrm{e}^{-g\tau}\right)}, \tag{7.7}$$

for him does not look monochromatic at all. In fact we have to Fourier analyze this waveform now for the comover: we Fourier transform it as a function of τ. We get

$$f(\nu) = \frac{1}{\sqrt{2\omega}} \int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}\frac{\omega}{g}\mathrm{e}^{-g\tau}} \mathrm{e}^{\mathrm{i}\nu\tau} \mathrm{d}\tau. \tag{7.8}$$

This integral can be analytically expressed by Euler's Gamma function. To achieve this we introduce the variable $z = \mathrm{e}^{-g\tau}$ for integration. Note that in this case $z(-\infty) = +\infty$ and $z(+\infty) = 0$ while $\mathrm{d}\tau = -\mathrm{d}z/zg$. We arrive at

$$f(\nu) = \frac{1}{g\sqrt{2\omega}} \int_{0}^{\infty} z^{-1-\mathrm{i}\nu/g} \mathrm{e}^{-\mathrm{i}\omega z/g} \, \mathrm{d}z. \tag{7.9}$$

This form contains the standard type for Euler's Gamma function,

$$\int_{0}^{\infty} z^{c-1} \mathrm{e}^{-bz} \mathrm{d}z = b^{-c} \Gamma(c), \tag{7.10}$$

with $c = -\mathrm{i}\nu/g$ and $b = \mathrm{i}\omega/g$. The result of the Fourier transformation associated to the proper time of the co-accelerating observer hence is given by

$$f(\nu) = \frac{1}{g\sqrt{2\omega}} \left(\frac{\mathrm{i}\omega}{g}\right)^{\mathrm{i}\nu/g} \Gamma\left(-\frac{\mathrm{i}\nu}{g}\right). \tag{7.11}$$

The imaginary power of an imaginary quantity is the exponential of the logarithm of the base multiplied by the power, which contains an $\ln \mathrm{i} = \mathrm{i}\pi/2$:

$$\left(\frac{\mathrm{i}\omega}{g}\right)^{\mathrm{i}\nu/g} = \mathrm{e}^{\frac{\mathrm{i}\nu}{g}\ln\left(\frac{\mathrm{i}\omega}{g}\right)} = \mathrm{e}^{\frac{\mathrm{i}\nu}{g}\left(\frac{\mathrm{i}\pi}{2}+\ln\frac{\omega}{g}\right)}. \tag{7.12}$$

Finally, we obtain

$$f(\nu) = \frac{1}{g\sqrt{2\omega}} \mathrm{e}^{\mathrm{i}\frac{\nu}{g}\ln\frac{\omega}{g}} \mathrm{e}^{-\pi\nu/2g} \Gamma\left(-\frac{\mathrm{i}\nu}{g}\right). \tag{7.13}$$

However, what we actually need in order to describe the physically observed spectrum is the absolute value squared of this quantity: The energy density in the co-accelerating frame is expressed as

$$\varepsilon_a = \int \frac{d^3\nu}{(2\pi)^3} \frac{\nu^2}{2} |f(\nu)|^2 . \tag{7.14}$$

Interpreting this as stemming from a spectrum of photons, we express the energy density with the help of a spectral density, $w(\nu)$:

$$\varepsilon_a = \int \frac{d^3\nu}{(2\pi)^3} \frac{\nu}{2} w(\nu). \tag{7.15}$$

So, in order to determine the spectral density $w(\nu) = \nu|f(\nu)|^2/2$, we calculate the absolute value squared of the expression given in (7.13). It is given as

$$|f(\nu)|^2 = f(\nu)f^*(\nu) = \frac{1}{2g^2\omega} e^{-\pi\nu/g} \Gamma\left(-i\frac{\nu}{g}\right) \Gamma\left(i\frac{\nu}{g}\right). \tag{7.16}$$

We simplify this result. For this purpose two well-known properties of the Euler Gamma function shall be used: (1) due to $\Gamma(z+1) = z\Gamma(z)$ we have $\Gamma(1 - i\nu/g) = (-i\nu/g)\Gamma(-i\nu/g)$ and (2) due to $\Gamma(z)\Gamma(1-z) = \pi/\sin(\pi z)$ we obtain

$$|f(\nu)|^2 = \frac{1}{2g\nu\omega} e^{-\pi\nu/g} \frac{\pi}{\sinh(\pi\nu/g)}. \tag{7.17}$$

Now it is relatively easy to obtain the spectral density $w(\nu)$ by the normalized formula $w(\nu) = \nu|f(\nu)|^2/2$. It contains the Planck spectrum (including the Bose–Einstein distribution function factor for photons):

$$w(\nu) = \frac{1}{2\omega} \frac{\pi}{g} \frac{1}{e^{2\pi\nu/g} - 1}. \tag{7.18}$$

This is like a thermal black body radiation with the temperature

$$T = \frac{g}{2\pi}, \tag{7.19}$$

in units where $k_B = \hbar = c = 1$, or – restoring the physical units of natural constants – we have

$$\frac{2\pi c\nu}{g} = \frac{\hbar\nu}{k_B T} \tag{7.20}$$

in the exponential of the Bose distribution function, and therefore

$$T = \frac{\hbar}{k_{\mathrm{B}}c}\frac{g}{2\pi}. \tag{7.21}$$

It is noteworthy that the formal continuation of the motion with constant acceleration to imaginary time, $\tau = \mathrm{i}\beta$, leads to periodic paths in spacetime with the period $\beta = 2\pi/g$, and therefore – in precise agreement with the KMS relations discussed in thermal field theory (see Chap. 8) – the Unruh temperature $T = 1/\beta = g/2\pi$ emerges as the physical temperature of the quantum gas of photons. Seemingly, this very same periodicity is explored by the Fourier-transformation and the complex properties of Euler's Gamma function.

7.2 Formal Entropy and Temperature for Black Holes

Analogs to the basic laws of thermodynamics can be found formally, by studying the Schwarzschild black hole solution of classical general relativity: (1) the zeroth law is represented by the fact that gravitational acceleration, $g = c^2/2R$, is constant on the event horizon at radius $R = 2GM/c^2$ surrounding the black hole – so it can be viewed as an equilibrium state with a universal (therefore absolute) Unruh temperature $T = \hbar g/(2\pi c k_{\mathrm{B}})$ with k_{B} being the Boltzmann constant and $\hbar = h/2\pi$ the reduced Planck's constant; (2) the first law is represented by the analogy between entropy and the event horizon surface, $A = 4\pi R^2$ at the Schwarzschild radius $R = 2GM/c^2$, so the change of the total mass-energy content of a black hole is obtained as[2]

$$c^2\mathrm{d}M = \frac{c^4}{2G}\mathrm{d}R = \frac{c^4}{2G}\frac{\mathrm{d}A}{8\pi R} = \frac{c^4}{4G}\frac{k_{\mathrm{B}}T}{\hbar c}\,\mathrm{d}A,$$

offering the analogy to

$$\mathrm{d}E = T\mathrm{d}S,$$

and from this constructing an entropy proportional to the surface of the event horizon,

$$S = \frac{c^3 k_{\mathrm{B}}}{4\hbar G}A;$$

---

[2] As in the classical thermodynamics, black hole thermodynamics can be supported by further work-terms as $\Omega \mathrm{d}J$ due to the change in total angular momentum, J, of a rotating black hole, or as $\Phi \mathrm{d}Q$ due to the change of its total electric charge, Q. Such terms are analogs to the mechanical work, $p\mathrm{d}V$ and to the chemical work $-\mu\mathrm{d}N$, respectively.

and finally (3) the second law, describing irreversibility, is mirrored in the playful fact, that any matter with positive energy density crossing the horizon increases the mass and hence the radius and the surface of the black hole: $\mathrm{d}A \geq 0$ is analogous to $\mathrm{d}S \geq 0$. However, the third law of thermodynamics is not satisfied by this analogy, since at $g \to 0(T \to 0)$ we do not have $A \to 0(S \to 0)$. To the contrary, a Schwarzschild black hole with diminishing radius has an unbounded gravitational acceleration at its horizon ($g(0) \to \infty$) while its area (entropy) tends to zero.

In this section, we review the emergence of these analogies and the main cornerstones in the struggle for the comprehension of their physical background. Is the formal entropy of a black hole really has to do with the logarithm of the number of microstate permutations? Does the gravitational acceleration at the black hole horizon surface really act as an intensive and absolute parameter for the thermal equilibrium? Is there a temperature at all?

7.2.1 *What is a Black Hole?*

An old – classical – idea considers the escape velocity from a very heavy star: if it reaches the velocity of light, then even light cannot escape from its surface to infinity. The region beyond that altitude, the classical black hole radius, cannot ever be observed by a far outside observer: it appears to be absolutely black.

Considering Newton's gravitational potential, the escape velocity from a given distance r from the center of gravity is given by the condition that at radial infinity there still remains some kinetic energy:

$$\frac{mv^2}{2} - \frac{GMm}{r} \geq 0. \tag{7.22}$$

Here, M is the mass of the star, G the constant of Newtonian gravity, v the velocity of a probe with mass m at the radius r.

The radius, where darkness starts is easy to obtain by formally substituting the velocity of light ($v = c$):

$$r_{\mathrm{d}} = \frac{2GM}{c^2}. \tag{7.23}$$

From $r < r_{\mathrm{d}}$ light cannot escape to infinity.

The idea of a "dark star" was first raised by John Michell in 1784. A derivation, similar to the above, is due to Pierre Simon de Laplace [66], with the conclusion that some – and especially the heavy – objects in universe would not be seen by astronomers.

However, the Michell–Laplace dark body is not a black hole in today's sense [67]. Particles – and in the present consideration also particles of light, the Newtonian corpuscles – with a velocity smaller than that of the escape velocity would leave the surface at radius r, emerge and fall back in due of time. They just cannot become free. Therefore such stars look dark for (cannot be seen by) an infinitely distant observer, but they still gleam for near astronomers. They do it even twice; once in emerging light and a second time in a back-falling light.

A black hole in the theory of general relativity is surrounded by an even horizon, in the simplest, spherical case at the radius R. Below this horizon nothing can escape, all particles, even photons fall inwards. From the horizon nothing, not even a photon, may emerge and take off: classically it is dark even for a very near orbiting observer. Close above the horizon gravity is still important, bodies are falling towards the center while orbiting, but they can escape to spatial infinity with a high enough outward radial velocity component.

Precisely, this critical radius, $R = 2GM/c^2$, occurs in an ansatz of Schwarzschild solving Einstein's equations for general relativity.[3] As a matter of history, Schwarzschild's solution was not a black hole, either. He considered a static solution to the Einstein equation, with vacuum everywhere, except a mass point. He communicated this to Einstein on a military postcard in 13 January 1916. Einstein was so surprised, that he immediately published this communication to him. Then on February 24, 1916 Karl Schwarzschild communicated a solution outside of a homogeneous sphere filled with an incompressible liquid. Actually, he himself never considered gravitational collapse, he was looking for *static* solutions.

Johannes Droste was the first who anticipated the imploding black hole solution, by finding the solution of Schwarzschild independently of him in December 1916 and communicating this to Hendrik Lorentz. He stated that this would be a "non-static solution to a static problem," and as such, it has to be omitted. The Schwarzschild solution, as referred to under this name since, was actually presented first by David Hilbert, regarding R just as a real valued parameter in the solution. In 1922, the possibility of gravitational collapse, as an admissible solution to the Einstein equations has been discussed, but no mathematical proof of the existence of such a solution arose. Marcel Brillouin has obtained a new exact solution in 1923 by a valid transformation of coordinates in Schwarzschild's solution. It still describes a static vacuum solution with the "boundary condition" of a point particle with mass M at $r = 0$, not a black hole. The collapsing black hole solution with an event horizon is derivable from Hilbert's solution; it just cannot be described by admissible coordinate transformations. Sometime later, in 1960, Mihail D. Kruskal and Gabor Szekeres independently have published an "extension" of Schwarzschild's solution to the region beyond the even horizon. In the same year, John Wheeler baptized such an object to a "black hole."

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[3] He sent his solution from the Russian front in 1916, soon after Einstein's publication of his equation in 1915. Schwarzschild has, unfortunately, died in the First World War, shortly after this (May 1916).

Criticizers of the black hole idea often mention, that so far only a single spherical solution is known wrapped in an event horizon from which nothing (even light) cannot take off. Talking about binary black holes and collisions or fusion of black holes is just a conjecture. Also, the observation of black holes – e.g. by gravitational lensing – does not mean the observation of an event horizon, the latter should be left in darkness forever. In spite of these critique, raising physical considerations, creative mathematical games have been continued and led us to the semiclassical and quantum treatment of strong gravity objects. In the following sections, we review the classical equations describing the object which we call black hole today.

The Hilbert–Einstein action can be taken as a starting point of classical general relativity. It formulates the principle that the covariant four-volume integral of the scalar curvature of empty spacetime is extremal. Adding the action of further "matter" terms represented by their respective Lagrange densities the action becomes

$$S = \int \mathrm{d}^4x \, \sqrt{-\det g} \left(\frac{c^4}{16\pi G} \mathscr{R} + \mathscr{L} \right). \tag{7.24}$$

Variation with respect to the metric tensor components, g_{ik} leads to the Einstein equations

$$\mathscr{R}^{ik} - \frac{1}{2} g^{ik} \mathscr{R} = \frac{8\pi G}{c^4} T^{ik}. \tag{7.25}$$

Here, $\mathscr{R} = \mathscr{R}^{ik} g_{ik}$ is the scalar curvature obtained from the Ricci tensor $\mathscr{R}^{ik}$, whose components are on the other hand contractions of the four-index Riemann tensor

$$\mathscr{R}^{ik} = R^{iakb} g_{ab}. \tag{7.26}$$

The energy–momentum tensor of matter, T^{ik}, is obtained from the corresponding action part also by varying the metric tensor:

$$T^{ik} = \frac{1}{K} \frac{\partial \mathscr{L} K}{\partial g_{ik}} - \frac{1}{K} \frac{\partial}{\partial x^\ell} \frac{\partial \mathscr{L} K}{\partial \frac{\partial g_{ik}}{\partial x^\ell}} \tag{7.27}$$

with $K = \sqrt{-\det g}$. For studying black holes in most of the space (and time) the vacuum solution is taken with $T^{ik} = 0$ or, considering the idea of a cosmological constant, with $T^{ik} = \lambda g^{ik}$. The latter corresponds to a constant, positive or negative energy density, which fills the "empty" space.

Solutions to the Einstein equation (7.25) are not known in full generality; obeying some symmetry constraints, however, several exact analytic forms have been studied already. Static and radial symmetric solutions, like the Schwarzschild solution, are so simple, that they can be obtained by the substitution method: designing a g_{ik}

metric tensor with unknown one-variable functions, and substituting this ansatz into the Einstein equations leaves us with a system of ordinary differential equations which – sometimes – even have analytic solutions [68].

In order to derive the Schwarzschild radial black hole solution, and its counterparts with nonzero cosmological constant, the de Sitter and "anti" de Sitter solutions, we utilize the computational method described in the classical gravity book by Misner, Thorne, and Wheeler [69]. This method is based on the use of differential forms in a locally Lorentzian basis. Curvature two-forms are then obtained via the Cartan derivative, a generalization of the vector product, lifting differential arc objects to small parallelograms and so forth in higher dimensions. The procedure can be summarized in the following list:

1. Obtain the Lorentzian one-forms based on the invariant arc length squared,

$$\mathrm{d}s^2 = g_{ik}\mathrm{d}x^i \otimes \mathrm{d}x^k = \eta_{ik}\omega^i \otimes \omega^k$$

   where $\eta_{ik} = (-,+,+,+)$ is the flat Minkowski metric tensor. The differential one-forms ω^i will span the basis of the calculation.
2. Index pull-down and lift-up is understood by $v^i = \eta^{ij} v_j$ and $v_i = \eta_{ij} v^j$ (we use the convention of summing over indices occurring once in the upper and once in the lower position).
3. The Cartan derivatives of the basis differentials can be arranged as sums of elementary (parallelogram) two-forms:

$$\mathrm{d}\omega^a = -c_{\mu\nu}{}^a\, \omega^\mu \wedge \omega^\nu .$$

   The lowered index coefficients $c_{\mu\nu b} = \eta_{ba} c_{\mu\nu}{}^a$ are obviously antisymmetric in their first two indices.
4. From the coefficients of these expansions an antisymmetric two-index differential one-form (related to the Christoffel symbols) can be constructed:

$$\Omega_{\mu\nu} = \frac{1}{2}\left(c_{\mu\nu a} + c_{\mu a\nu} - c_{\nu a\mu}\right)\omega^a .$$

   By doing so the Ω-covariant Cartan derivatives of the basis one-forms vanish, $D\omega^a = \mathrm{d}\omega^a + \Omega^a{}_b \wedge \omega^b = 0$.
5. The curvature two-form can be constructed now in a straightforward manner:

$$R^\mu{}_\nu = D\Omega^\mu{}_\nu = \mathrm{d}\Omega^\mu{}_\nu + \Omega^\mu{}_a \wedge \Omega^a{}_\nu .$$

   This two-form contains the entries of the Riemann tensor in the Lorentzian basis:

$$R^\mu{}_\nu = R^\mu{}_{\nu ab}\,\omega^a \wedge \omega^b .$$

6. The Ricci tensor is obtained from the Riemann tensor by contracting a curvature direction and a basis index:
$$\mathscr{R}_{\nu b} = R^{a}{}_{\nu ab}.$$
7. The scalar curvature is the trace of the Ricci tensor, $\mathscr{R} = \mathscr{R}^{b}{}_{b}$, and the components of the Einstein tensor can be built:
$$\mathscr{G}_{\nu b} = \mathscr{R}_{\nu b} - \frac{1}{2}\eta_{\nu b}\mathscr{R}.$$
8. Finally, using the frame independence of tensors, the components in the original coordinate differential basis can be obtained by comparison:
$$\mathscr{G}_{\nu b}\,\omega^{\nu} \otimes \omega^{b} = G_{ij}\,\mathrm{d}x^{i} \otimes \mathrm{d}x^{j}.$$
   The energy–momentum tensor due to the Einstein equation equals to
$$G_{ij} = \frac{8\pi G}{c^4} T_{ij}.$$
   It remains to resolve these equalities for the unknown functions in the original ansatz for the metric.

In what follows, we obtain the most general static and radial solution to the Einstein equations with and without a cosmological constant. The ansatz for the metric contains two unknown functions of the radius, $a(r)$ and $b(r)$:

$$\mathrm{d}s^2 = -\mathrm{e}^{2a}\mathrm{d}t^2 + \mathrm{e}^{2b}\mathrm{d}r^2 + r^2\mathrm{d}\theta^2 + r^2\sin^2\theta\,\mathrm{d}\phi^2. \tag{7.28}$$

The one-forms spanning a Lorentzian basis of differentials can be read off as being $\omega^0 = e^a\mathrm{d}t$, $\omega^1 = e^b\mathrm{d}r$, $\omega^2 = r\mathrm{d}\theta$ and $\omega^3 = r\sin\theta\,\mathrm{d}\phi$. Their Cartan derivatives are as follows

$$\begin{aligned}
\mathrm{d}\omega^0 &= a'e^a\mathrm{d}r\wedge\mathrm{d}t = -a'\mathrm{e}^{-b}\omega^0\wedge\omega^1,\\
\mathrm{d}\omega^1 &= 0,\\
\mathrm{d}\omega^2 &= \mathrm{d}r\wedge\mathrm{d}\theta = \frac{1}{r}\mathrm{e}^{-b}\omega^1\wedge\omega^2,\\
\mathrm{d}\omega^3 &= \sin\theta\,\mathrm{d}r\wedge\mathrm{d}\phi + r\cos\theta\,\mathrm{d}\theta\wedge\mathrm{d}\phi =\\
&= \frac{1}{r}\mathrm{e}^{-b}\,\omega^1\wedge\omega^3 + \frac{\mathrm{ctg}\theta}{r}\,\omega^2\wedge\omega^3.
\end{aligned} \tag{7.29}$$

Here, the prime denotes the ordinary derivative with respect to the radial coordinate, $a' = \mathrm{d}a/\mathrm{d}r$. Owing to the general formula

$$\mathrm{d}\omega^a = -c_{\mu\nu}{}^{a}\omega^{\mu}\wedge\omega^{\nu} \tag{7.30}$$

the non-vanishing coefficients are

$$\begin{aligned} c_{01}{}^{0} &= a' \mathrm{e}^{-b}, \\ c_{12}{}^{2} &= -\frac{1}{r}\mathrm{e}^{-b}, \\ c_{13}{}^{3} &= -\frac{1}{r}\mathrm{e}^{-b}, \\ c_{23}{}^{3} &= -\frac{\mathrm{ctg}\theta}{r}. \end{aligned} \tag{7.31}$$

Index pull-down is done by using the Minkowski metric $\eta_{ij} = (-,+,+,+)$ to obtain $c_{100} = -c_{010} = a'\mathrm{e}^{-b}$, $c_{212} = -c_{122} = c_{313} = -c_{133} = \mathrm{e}^{-b}/r$, and $c_{323} = -c_{233} = \mathrm{ctg}\theta/r$. Now the connection forms according to the formula

$$\Omega_{\mu\nu} = \frac{1}{2}\left(c_{\mu\nu\alpha} + c_{\mu\alpha\nu} - c_{\nu\alpha\mu}\right)\omega^{\alpha} \tag{7.32}$$

are given as

$$\begin{aligned} \Omega_{01} &= c_{010}\omega^{0} = -a'\mathrm{e}^{-b}e^{a}\,\mathrm{d}t, \\ \Omega_{02} &= 0, \\ \Omega_{03} &= 0, \\ \Omega_{13} &= c_{133}\omega^{3} = -\mathrm{e}^{-b}\sin\theta\,\mathrm{d}\phi, \\ \Omega_{23} &= c_{233}\omega^{3} = -\cos\theta\,\mathrm{d}\phi, \\ \Omega_{12} &= c_{122}\omega^{2} = -\mathrm{e}^{-b}\,\mathrm{d}\theta. \end{aligned} \tag{7.33}$$

The same entries, but with the first index uplifted, differ from these only in $\Omega^{0}{}_{1}$ in a sign. We are ready now to obtain the curvature two-form according to the general formula

$$R^{\mu}{}_{\nu} = \mathrm{d}\Omega^{\mu}{}_{\nu} + \Omega^{\mu}{}_{\alpha}\wedge\Omega^{\alpha}{}_{\nu}. \tag{7.34}$$

We start with $R^{0}{}_{1}$. Since $\Omega^{0}{}_{2} = \Omega^{0}{}_{3} = 0$ only the Cartan derivative term contributes:

$$R^{0}{}_{1} = \mathrm{d}\Omega^{0}{}_{1} = \left(a'\mathrm{e}^{a-b}\right)'\,\mathrm{d}r\wedge\mathrm{d}t. \tag{7.35}$$

Re-expressed in terms of the Lorentzian one-form basis we have $R^{0}{}_{1} = A\omega^{0}\wedge\omega^{1}$ with

$$A = -\mathrm{e}^{-a-b}\left(a'\mathrm{e}^{a-b}\right)' = (a'b' - a'a' - a'')\mathrm{e}^{-2b}. \tag{7.36}$$

Similarly, we obtain (but now having only wedge contribution)

$$R^{0}{}_{2} = \Omega^{0}{}_{1}\wedge\Omega^{1}{}_{2} = -a'\mathrm{e}^{a-2b}\,\mathrm{d}t\wedge\mathrm{d}\theta \tag{7.37}$$

or re-expressed $R^0{}_2 = -B\omega^0 \wedge \omega^2$ with

$$B = \frac{a'}{r} \mathrm{e}^{-2b}. \tag{7.38}$$

Following the general formulas one also obtains $R^0{}_3 = -B\omega^0 \wedge \omega^3$. The remaining curvature forms all have contributions both from Cartan derivatives and wedge products. We obtain

$$R^1{}_2 = \mathrm{d}\Omega^1{}_2 + \Omega^1{}_3 \wedge \Omega^3{}_2 = \mathrm{d}(-\mathrm{e}^{-b}\mathrm{d}\theta) + (-\mathrm{e}^{-b}\sin\theta\mathrm{d}\phi) \wedge (\cos\theta\mathrm{d}\phi). \tag{7.39}$$

Carrying out the derivations we have a cancellation in the wedge product and obtain $R^1{}_2 = C\omega^1 \wedge \omega^2$ with

$$C = \frac{b'}{r} \mathrm{e}^{-2b}. \tag{7.40}$$

The next component of the curvature two-forms is

$$R^1{}_3 = \mathrm{d}\Omega^1{}_3 + \Omega^1{}_2 \wedge \Omega^2{}_3 = \mathrm{d}(-\mathrm{e}^{-b}\sin\theta\mathrm{d}\phi) + (-\mathrm{e}^{-b}\mathrm{d}\theta) \wedge (-\cos\theta\mathrm{d}\phi). \tag{7.41}$$

Here, two contributions, namely the one from the derivative of $\sin\theta$ in the first term and the wedge product, cancel. The remaining result is simply $R^1{}_3 = C\omega^1 \wedge \omega^3$. Finally, we have to obtain $R^2{}_3$. According to the general formula (7.34) we have

$$R^2{}_3 = \mathrm{d}\Omega^2{}_3 + \Omega^2{}_1 \wedge \Omega^1{}_3 = \mathrm{d}(-\cos\theta\mathrm{d}\phi) + (\mathrm{e}^{-b}\mathrm{d}\theta) \wedge (-\mathrm{e}^{-b}\sin\theta\mathrm{d}\phi). \tag{7.42}$$

This provides a new combination of the parametrizing functions: $R^2{}_3 = E\omega^2 \wedge \omega^3$ with

$$E = \frac{1}{r^2}\left(1 - \mathrm{e}^{-2b}\right). \tag{7.43}$$

Collecting our results we have the following table of curvature two-forms, reflecting the nonzero entries of the Riemann tensor:

$$\begin{aligned} &R^0{}_1 = A\,\omega^0 \wedge \omega^1, \qquad R^0{}_2 = -B\,\omega^0 \wedge \omega^2, \qquad R^0{}_3 = -B\,\omega^0 \wedge \omega^3, \\ &R^1{}_2 = C\,\omega^1 \wedge \omega^2, \qquad R^1{}_3 = C\,\omega^1 \wedge \omega^3, \qquad R^2{}_3 = E\,\omega^2 \wedge \omega^3. \end{aligned} \tag{7.44}$$

The Riemann tensor, $R^\mu{}_{\nu\alpha\beta}$ is nonzero only for those index combinations when $(\mu = \alpha, \nu = \beta)$ or $(\mu = \beta, \nu = \alpha)$. As a consequence the Ricci tensor is again diagonal (but not proportional to the unity matrix!). According to the general definition

$$\mathscr{R}_{\nu\beta} = R^\alpha{}_{\nu\alpha\beta}, \tag{7.45}$$

we obtain

$$\begin{aligned} \mathscr{R}_{00} &= R^1{}_{010} + R^2{}_{020} + R^3{}_{030} = -A + B + B, \\ \mathscr{R}_{11} &= R^0{}_{101} + R^2{}_{121} + R^3{}_{131} = +A + C + C, \\ \mathscr{R}_{22} &= R^0{}_{202} + R^1{}_{212} + R^3{}_{232} = -B + C + E, \\ \mathscr{R}_{33} &= R^0{}_{303} + R^1{}_{313} + R^2{}_{323} = -B + C + E. \end{aligned} \tag{7.46}$$

The scalar curvature of static radial ansatz is hence determined as

$$\mathscr{R} = -\mathscr{R}_{00} + \mathscr{R}_{11} + \mathscr{R}_{22} + \mathscr{R}_{33} = 2A - 4B + 4C + 2E. \tag{7.47}$$

Finally, this gives rise to the following nonzero components of the Einstein tensor

$$\begin{aligned} \mathscr{G}_{00} &= \mathscr{R}_{00} + \frac{1}{2}\mathscr{R} = 2C + E, \\ \mathscr{G}_{11} &= \mathscr{R}_{00} - \frac{1}{2}\mathscr{R} = 2B - E, \\ \mathscr{G}_{22} &= \mathscr{R}_{00} - \frac{1}{2}\mathscr{R} = B - C - A, \\ \mathscr{G}_{33} &= \mathscr{R}_{00} - \frac{1}{2}\mathscr{R} = B - C - A. \end{aligned} \tag{7.48}$$

We consider now the Einstein equation in the Lorentzian basis with a possible cosmological constant

$$\mathscr{G}_{\nu\beta} = \frac{8\pi G}{c^4} T_{\nu\beta} + \lambda\, \eta_{\nu\beta}. \tag{7.49}$$

A vacuum solution has $T_{\nu\beta} = 0$ and hence

$$\begin{aligned} \mathscr{G}_{00} &= 2C + E = -\lambda, \\ \mathscr{G}_{11} &= 2B - E = \lambda, \\ \mathscr{G}_{22} &= B - C - A = \lambda, \\ \mathscr{G}_{33} &= B - C - A = \lambda. \end{aligned} \tag{7.50}$$

Adding the 00 and 11 components we realize that for such solutions $B + C = 0$ has to be required. This means $a' + b' = 0$. Putting the integration constant to zero (since a constant factor can be absorbed in the radial coordinate r without problem), we obtain $a = -b$. This way only one function, say $b(r)$ is left to be obtained.

Substituting this result into the 22 (and equivalently 33) component equation and comparing to the 11 component one arrives at $\lambda = 2B - A = 2B - E$. This means that $A = E$ and $a = -b$ have to be replaced in order to distillate the final equation

$$A = \left(-2b'b' + b''\right) \mathrm{e}^{-2b} = \frac{1 - \mathrm{e}^{-2b}}{r^2} = E. \tag{7.51}$$

This equation is analytically solvable. In order to obtain its solution we introduce the following function of the radial variable:

$$Y(r) = 1 - \mathrm{e}^{-2b(r)}. \tag{7.52}$$

This way we have $Y' = 2b'\mathrm{e}^{-2b}$ and $Y'' = (2b'' - 4b'b')\mathrm{e}^{-2b}$. We realize that $A = Y''/2 = E = Y/r^2$. So we have to solve the following differential equation

$$Y'' = \frac{2}{r^2}Y. \tag{7.53}$$

Its general solution is a power law in the radius. The ansatz $Y \sim r^\alpha$ leads to the algebraic equation $\alpha(\alpha-1) = 2$, which has two solutions: $\alpha = -1$ and $\alpha = 2$. Therefore, the general solution is given by

$$Y(r) = \frac{c_1}{r} + c_2 r^2. \tag{7.54}$$

One of the integration constants can be related to the cosmological constant, λ. In fact, expressing $b = -\frac{1}{2}\ln(1-Y)$ we obtain

$$b' = -\frac{1}{2}\frac{-Y'}{1-Y} = \mathrm{e}^{2b}\left(-\frac{c_1}{2r^2} + c_2 r\right) \tag{7.55}$$

whence

$$C = \frac{b'}{r}\mathrm{e}^{-2b} = -\frac{c_1}{2r^3} + c_2 \tag{7.56}$$

and

$$B = -C = \frac{c_1}{2r^3} - c_2. \tag{7.57}$$

On the other hand

$$A = \frac{1}{2}Y'' = \frac{1}{r^2}Y = \frac{c_1}{r^3} + c_2. \tag{7.58}$$

Using these results we obtain the following connection to λ:

$$2B - A = 2\left(\frac{c_1}{2r^3} - c_2\right) - \left(\frac{c_1}{r^3} + c_2\right) = -3c_2 = \lambda. \tag{7.59}$$

Therefore, the general static radial vacuum solution with a cosmological constant of the theory of general relativity is given by

$$\mathrm{e}^{2a} = \mathrm{e}^{-2b} = 1 - Y(r) = 1 - \frac{c_1}{r} + \frac{\lambda}{3}r^2. \tag{7.60}$$

The metric tensor has the form

$$\mathrm{d}s^2 = -\left(1 - \frac{c_1}{r} + \frac{\lambda}{3}r^2\right)\mathrm{d}t^2 + \frac{\mathrm{d}r^2}{1 - \frac{c_1}{r} + \frac{\lambda}{3}r^2} + r^2\left(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\phi^2\right). \tag{7.61}$$

Without the (in)famous cosmological term, i.e. for $\lambda = 0$, one obtains the Schwarzschild solution with the horizon radius $r_\mathrm{H} = c_1$. The $\lambda < 0$ assumption, being equivalent with a positive energy density of the vacuum, is a solution found by de Sitter. Finally, the $\lambda > 0$ value belongs to a negative energy density in the vacuum: a strange, but consequent picture of strongly interacting field theory. Such solutions are called an "Anti de Sitter" spacetime, briefly *AdS*-spacetime. They can be generalized to higher dimensions, too.

Finally, the integration constant c_1 can be obtained from a comparison of the metric tensor at $\lambda = 0$ and $r \to \infty$ to the one resulting from Newtonian gravity. Let us regard a slow motion ($|\mathbf{v}| \ll c$) and a weak gravitational potential. Then the Lagrangian describing the movement of a testing mass point with mass m in the weak gravitational field $-GM/r$ of a far center with mass M is given by

$$L = -mc^2\sqrt{1-\mathbf{v}^2/c^2} + m\frac{GM}{r}. \tag{7.62}$$

The corresponding action is

$$S = -mc^2 \int \left(\sqrt{1-\mathbf{v}^2/c^2} - \frac{GM}{rc^2}\right) \mathrm{d}t = -mc^2 \int \mathrm{d}\tau. \tag{7.63}$$

The second equality implies that this action can be regarded as the action of a freely moving mass point in the language of appropriate coordinates (comoving proper time); this is the equivalence principle. This leaves us with the following approximation to the arc length in spacetime:

$$\mathrm{d}\tau = \left(\sqrt{1-\mathbf{v}^2/c^2} - \frac{GM}{rc^2}\right) \mathrm{d}t. \tag{7.64}$$

Utilizing the definition of velocity we have $\mathbf{v}\mathrm{d}t = \mathrm{d}\mathbf{r}$, and squaring the above expression to leading order in $1/c^2$ we obtain

$$\mathrm{d}s^2 = -c^2\mathrm{d}\tau^2 = -\left(c^2 - 2\frac{GM}{r}\right)\mathrm{d}t^2 + \mathrm{d}r^2 + r^2\mathrm{d}\theta^2 + r^2\sin^2\theta\mathrm{d}\phi^2. \tag{7.65}$$

Comparing this expression with (7.61) for $\lambda = 0$, i.e. with the Schwarzschild solution, we conclude that

$$1 - \frac{2GM}{rc^2} = 1 - \frac{c_1}{r}. \tag{7.66}$$

This leads to the famous Schwarzschild radius, $r_{\mathrm{H}} = c_1 = 2GM/c^2$.

The classical solution for a *charged black hole* can be obtained with just a little extra effort. A point charge has a static, radial symmetric electric field, so the spacetime metric for an observer outside the charge distribution is also static and spherical symmetric. The ansatz (7.28) is still proper for this problem.

The electromagnetic field strength can be described by an antisymmetric tensor or equivalently by a differential two-form. It can be given both in the coordinate system of the far, static observer and in local Lorentzian basis:

$$F = E_r \mathrm{d}t \wedge \mathrm{d}r = \mathrm{e}^{-(a+b)} E_r \omega^0 \wedge \omega^1. \tag{7.67}$$

The radial electric field component, E_r, is a function of the radius, r, only. The Gauss law is given by the divergence of this field, which vanishes outside the region where the charge is located – it is imagined to be restricted to the singular point at $r = 0$. Since the divergence is given via the dual differential form as $\mathrm{Div}F =^{*} d^{*}F$, we consider the dual of the electromagnetic field strength form,

$${}^{*}F = \mathrm{e}^{-(a+b)} E_r \omega^2 \wedge \omega^3. \tag{7.68}$$

It can be expressed with the help of the far observer's coordinate differentials, too:

$${}^{*}F = \mathrm{e}^{-(a+b)} E_r r^2 \sin\theta \, \mathrm{d}\theta \wedge \mathrm{d}\phi. \tag{7.69}$$

The Cartan derivative of this expression contains the derivative with respect to the radius:

$$\mathrm{d}^{*}F = \frac{\partial}{\partial r}\left(\mathrm{e}^{-(a+b)} E_r r^2\right) \sin\theta \, \mathrm{d}r \wedge \mathrm{d}\theta \wedge \mathrm{d}\phi. \tag{7.70}$$

This expression is the dual of the divergence, so it vanishes everywhere in space-time, where charges and currents are absent. Hence, according to our assumption, the expression inside the parentheses of the radial partial derivative is constant. According to the local Gauss' law,[4] we denote this constant by $Q/4\pi\varepsilon_0$ and arrive at

$$E_r(r) = \frac{Q}{4\pi\varepsilon_0 r^2} \mathrm{e}^{a+b}. \tag{7.71}$$

The energy density, carried by a static electric field, in the Lorentzian frame is given by

$$e = \frac{\varepsilon_0}{2} E_r^2. \tag{7.72}$$

The energy–momentum tensor contains this energy density, a radial pressure with the same magnitude (in $c = 1$ units) but with opposite sign, and the tangential pressure components with positive sign:

$$T = T_{ij} \omega^i \otimes \omega^j = e\left(\omega^0 \otimes \omega^0 - \omega^1 \otimes \omega^1 + \omega^2 \otimes \omega^2 + \omega^3 \otimes \omega^3\right). \tag{7.73}$$

This tensor is traceless, $\eta^{ij} T_{ij} = 0$, a typical feature of energy–momentum tensor of massless quanta.

---

[4] Referring to the vacuum dielectric constant as ε_0.

With this energy–momentum tensor entries the Einstein equations (7.50) are now supplemented:

$$\begin{aligned}
\mathscr{G}_{00} &= 2C+E=-\lambda+w,\\
\mathscr{G}_{11} &= 2B-E=\lambda-w,\\
\mathscr{G}_{22} &= B-C-A=\lambda+w,\\
\mathscr{G}_{33} &= B-C-A=\lambda+w.
\end{aligned} \tag{7.74}$$

Here, $w=8\pi Ge$ (in $c=1$ units) is expressed with the radius and the constant by using (7.72) as

$$w=\frac{GQ^2}{4\pi\varepsilon_0}\frac{1}{r^4}=\frac{\tilde{Q}^2}{r^4}. \tag{7.75}$$

Solving the Einstein equations (7.74) in this case one realizes that $B+C=0$ still holds. Therefore, $a+b=0$ for any solution (up to a re-scaling of the radial coordinate). Repeating the $Y=1-\mathrm{e}^{-2b}$ notation one has $A=Y''/2$, $C=-B=Y'/2r$ and $E=Y/r^2$. This way we arrive at the following two differential equations for the unknown function $Y(r)$:

$$\begin{aligned}
\frac{1}{2}Y''+\frac{1}{r}Y' &= -\lambda+\frac{\tilde{Q}^2}{r^4},\\
\frac{1}{r}Y'+\frac{1}{r^2}Y &= -\lambda-\frac{\tilde{Q}^2}{r^4}.
\end{aligned} \tag{7.76}$$

It is easy to check that the general solution is given by

$$Y(r)=c_1r^2+\frac{c_2}{r}+\frac{c_3}{r^2}. \tag{7.77}$$

Noting namely that the first and second derivatives are

$$\begin{aligned}
Y'(r) &= 2c_1r-\frac{c_2}{r^2}-2\frac{c_3}{r^3},\\
Y''(r) &= 2c_1+2\frac{c_2}{r^3}+6\frac{c_3}{r^4},
\end{aligned} \tag{7.78}$$

one satisfies both equations in (7.76) provided that $c_1=-\lambda/3$ and $c_3=\tilde{Q}^2$. The constant $c_2=2GM$, was already obtained in the Schwarzschild solution by fitting the asymptotic spacetime to that of Newtonian gravity; it is not determined by the energy–momentum tensor, it is related to the vacuum solution.

This solution provides the metric factor $f(r)=\mathrm{e}^{2a}=\mathrm{e}^{-2b}=1-Y(r)$ as being

$$f(r)=1+\frac{\lambda}{3}r^2-2GM\frac{1}{r}+\tilde{Q}^2\frac{1}{r^2}. \tag{7.79}$$

The metric,

$$ds^2 = -f(r)dt^2 + \frac{dr^2}{f(r)} + r^2 d\Omega_2^2, \tag{7.80}$$

with $d\Omega_2^2 = d\theta^2 + \sin^2\theta\, d\phi^2$ being the two-dimensional angle differential on a unit radius sphere, is the Reissner–Nordstrøm (abbreviated: RN-) metric.

This metric has some interesting properties. Using the notation, $\tilde{M} = GM/c^2$ the Schwarzschild horizon is at the radius $r_H = 2\tilde{M}$. The Reissner–Nordstrøm metric also has coordinate singularity; an event horizon for the far observer, at $f(r) = 0$. This condition is fulfilled by the equation

$$r^2 f(r) = r^2 - 2\tilde{M}r + \tilde{Q}^2 + \frac{\lambda}{3}r^4 = 0. \tag{7.81}$$

Without the cosmological constant term (i.e. for $\lambda = 0$) it has two solutions describing an inner and an outer spherical horizon at

$$r_\pm = \tilde{M} \pm \sqrt{\tilde{M}^2 - \tilde{Q}^2}. \tag{7.82}$$

This solution makes sense for $\tilde{M} \geq \tilde{Q}$ only. The case $\tilde{M} = \tilde{Q}$ is called an *extremal black hole*; then the inner and outer horizons coincide: $r_+ = r_-$ (Fig. 7.2).

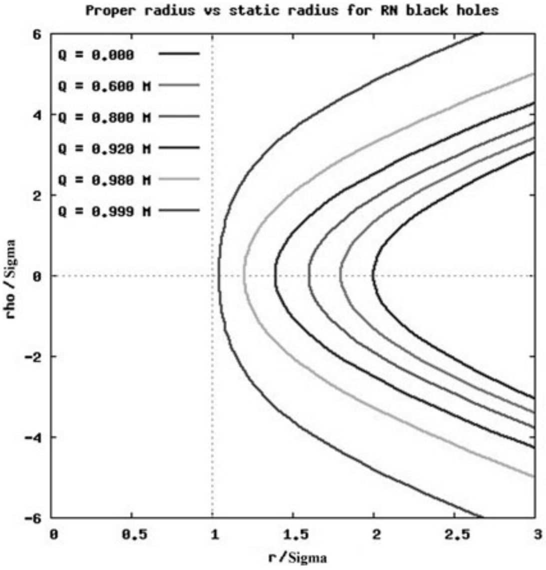

Fig. 7.2 The proper radial distance coordinate for differently charged Reissner–Nordstrøm *black hole* are plotted as functions of the radial coordinate measured by a static, far observer [cf. (7.84)]. Both axes are scaled with arithmetic mean of the radii of the inner and outer horizons, $\Sigma = (r_+ + r_-)/2$, and the legend shows the relation between the scaled charge and mass units, $\tilde{Q}$ and $\tilde{M}$, respectively

It is instructive to study the RN-metric near to the outer horizon, but outside. The proper radial distance, ρ, which can be used as a "better" coordinate than r, is given by

$$\rho = \int \frac{\mathrm{d}r}{\sqrt{f(r)}}. \tag{7.83}$$

This definition gives $\mathrm{d}\rho^2 = \mathrm{d}r^2/f(r)$, and – it is important – it shows no singularity at the horizon. Without cosmological constant ($\lambda = 0$) the above integral can be calculated analytically. In the region $r \geq r_+$ the following parametric solution can be given

$$\begin{aligned} r &= \Sigma + \Delta \cosh \alpha, \\ \rho &= \Sigma \alpha + \Delta \sinh \alpha. \end{aligned} \tag{7.84}$$

Here, $\Sigma = (r_+ + r_-)/2$ and $\Delta = (r_+ - r_-)/2$.

It is easy to check that

$$r^2 f(r) = (r - r_+)(r - r_-) = \Delta^2 \sinh^2 \alpha \tag{7.85}$$

is valid and the metric becomes

$$\mathrm{d}s^2 = -\left(\frac{\Delta \sinh \alpha}{\Sigma + \Delta \cosh \alpha} \mathrm{d}t \right)^2 + (\Sigma + \Delta \cosh \alpha)^2 \left(\mathrm{d}\alpha^2 + \mathrm{d}\Omega^2 \right) \tag{7.86}$$

Near to the outer horizon $r \to r_+$ and $\alpha \to 0$. The effective metric here becomes

$$\mathrm{d}s^2 \approx -\frac{\Delta^2 \alpha^2}{r_+^2} \mathrm{d}t^2 + r_+^2 \left(\mathrm{d}\alpha^2 + \mathrm{d}\Omega^2 \right). \tag{7.87}$$

This form can be written locally as a Minkowski metric after corresponding coordinate transformations; this is a Rindler spacetime. The physical message from this is that near to the horizon the spacetime looks exactly as it would be observed from a uniformly accelerating frame.

Near to the horizon $r_+^2 \mathrm{d}\Omega^2 = \mathrm{d}\hat{x}^2 + \mathrm{d}\hat{y}^2$ is a flat transverse plane. Since $\rho \approx r_+ \alpha$ is the proper radial coordinate, the near-horizon metric becomes

$$\mathrm{d}s^2 = -\frac{\Delta^2}{r_+^4} \rho^2 \mathrm{d}t^2 + \mathrm{d}\rho^2 + \mathrm{d}\hat{x}^2 + \mathrm{d}\hat{y}^2. \tag{7.88}$$

Now new time and space coordinates, the Rindler coordinates, can be introduced in analogy to the description of the Unruh trajectory in (7.3):

$$
\begin{aligned}
\hat{t} &= \rho \sinh \frac{\Delta}{r_+^2} t, \\
\hat{z} &= \rho \cosh \frac{\Delta}{r_+^2} t.
\end{aligned}
\tag{7.89}
$$

In terms of these new coordinates, the spacetime metric near to the outer Reissner–Nordstrøm horizon becomes a plain Minkowski form,

$$
\mathrm{d}s^2 = -\mathrm{d}\hat{t}^2 + \mathrm{d}\hat{z}^2 + \mathrm{d}\hat{x}^2 + \mathrm{d}\hat{y}^2. \tag{7.90}
$$

It is important to note that using the flat time coordinate, $\hat{t}$, the equations (7.89) describe a relativistic path with uniform acceleration (Fig. 7.3).

The corresponding Unruh temperature,

$$
T = \frac{g}{2\pi} = \frac{1}{2\pi} \frac{\Delta}{r_+^2} = \frac{1}{4\pi} \frac{r_+ - r_-}{r_+^2}, \tag{7.91}
$$

is regarded as the temperature of the black hole horizon.

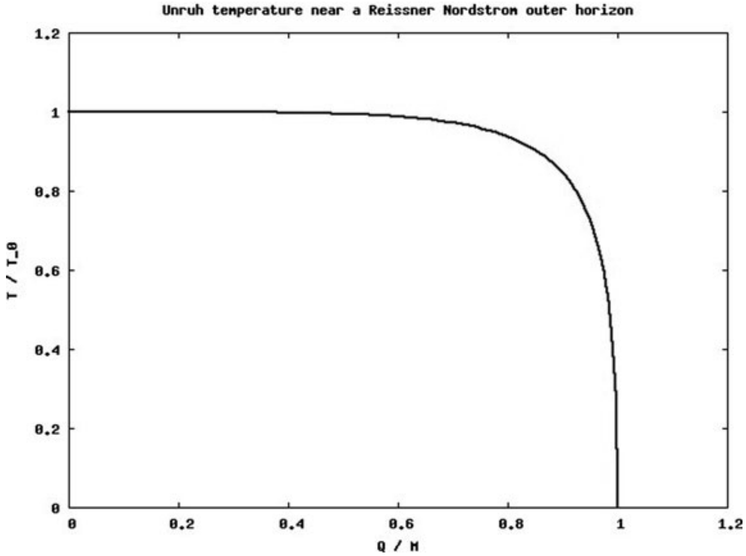

Fig. 7.3 The Unruh temperature near to the outer horizon of classical charged (Reissner–Nordstrøm) *black hole* relative to that of a neutral (Schwarzschild) *black hole* [cf. (7.91)]

Not only in this special case, but quite generally, near to such a horizon the acceleration is constant and the Rindler coordinates give a good approximate description. This coordinate system, on the other hand, always looks like a frame attached to a uniformly accelerating point, its monochromatic light emission will be measured as a Planck distribution with the corresponding Unruh temperature by a far, static observer.[5]

In the case $\tilde{Q} = 0$ we have $r_- = 0$, $r_+ = 2\tilde{M}$ – a neutral Schwarzschild black hole. The corresponding Unruh temperature becomes

$$T = \frac{1}{4\pi r_+} = \frac{1}{8\pi\tilde{M}}. \tag{7.92}$$

On the other hand for an extremal Reissner–Nordstrøm black hole $\tilde{Q} = \tilde{M}$ and $r_+ = r_-$, so the Unruh temperature of such a horizon is the absolute zero, $T = 0$. The corresponding entropy is finite, however! We meet again the weakest point of the black hole thermodynamics.

7.2.2 A Formal Analogy to the Entropy

As we have seen in the previous subsection, Schwarzschild black hole event horizons have a radius proportional to the mass of the black hole: $R = 2GM/c^2$. From this result a surprising property follows (noted by Bekenstein in 1973 [70]): the energy content, $E = Mc^2$ of such a black hole, additive by a fusion of two black holes, is accompanied by an irreversible growth of the surface of the even horizon. Since $M = M_1 + M_2$ by a conjectured adiabatic fusion of two black holes, the radii of the static horizons are additive either: $R = R_1 + R_2$. But this leads to an ever growing surface, since $A = 4\pi R^2 = 4\pi(R_1^2 + R_2^2 + 2R_1R_2) \geq A_1 + A_2$. So the area of the event horizon never decreases, behaving exactly so, as the total entropy.[6]

This gives rise to the conjecture that the entropy content of a black hole (i.e. the information lost under the event horizon) would be proportional to the horizon area – and not the inside volume, as naively expected. Assuming hence

$$S = \alpha A = 4\pi\alpha\left(\frac{2GM}{c^2}\right)^2 \tag{7.93}$$

as the entropy, and the mass-energy, $E = Mc^2$ as thermodynamical internal energy of a black hole, the inverse temperature as a Lagrange multiplier maximizing the entropy with a fixed energy constraint becomes

---

[5] This is the mirror image of the effect discussed in the Sect. 7.1; we shall derive it later.

[6] It means that a fusion of black holes would be a spontaneous process, while their fission into smaller ones cannot happen without an outsider – and quite dramatic – action.

$$\beta = \frac{1}{k_{\mathrm{B}}T} = \frac{\partial S}{\partial E} = \frac{32\pi\alpha}{c^6} G^2 M = \frac{16\pi\alpha}{c^4} GR. \tag{7.94}$$

There are two surprising facts about this result. One is classical, connecting the general relativity analog of surface acceleration (gravitational "constant") on the Schwarzschild event horizon to the radius, R. The other is connecting a constant acceleration to a thermal looking environment in the field theoretical vacuum (this is the Unruh effect) and hence the formal black hole horizon temperature to a temperature obtainable from irradiated field quanta near the horizon: the Hawking temperature [71].

7.2.3 Hawking Radiation

In some sense the Hawking radiation is alike the Unruh effect: here, the far observer in a flat Minkowskian spacetime receives radiation from a source freely falling near the black hole horizon. Essentially, the principle of relativity teaches us that only the relative motion is relevant physically; from this viewpoint it should not be much of a surprise, that the Hawking temperature equals to the Unruh temperature belonging to the acceleration of a free falling particle near the horizon.

In order to obtain this temperature, we calculate the proper time acceleration of a free falling mass point near the black hole horizon, as it is seen by a far, static observer. In general, the motion of a free particle of mass m is described by the relativistic Maupertuis action:

$$S = -\int E\mathrm{d}t + \int p\mathrm{d}x = \int p_i \mathrm{d}x^i = mc \int \mathrm{d}s. \tag{7.95}$$

Variation of the trajectories, $\delta x^i(s)$, lead to the description of the free fall. Assuming a general metric, $\mathrm{d}s^2 = g_{ij}\mathrm{d}x^i\mathrm{d}x^j$, this variational principle leads to the description of geodesic motion. It is straightforward to show by noting that the variation of the proper distance differential can be written as

$$\delta(\mathrm{d}s) = \frac{1}{2\mathrm{d}s}\delta(\mathrm{d}s^2) = \frac{1}{2\mathrm{d}s}\delta\left(g_{ij}\mathrm{d}x^i\mathrm{d}x^j\right). \tag{7.96}$$

Considering the variation $\delta x^i(s)$ three terms occur:

$$\delta \mathrm{d}s = \frac{\mathrm{d}s}{2}\left\{\frac{\partial g_{ij}}{\partial x^k}u^i u^j \delta x^k + g_{ij}u^i \frac{\mathrm{d}\delta x^j}{\mathrm{d}s} + g_{ij}\frac{\mathrm{d}\delta x^i}{\mathrm{d}s}u^j\right\}, \tag{7.97}$$

with $u^i = \mathrm{d}x^i/\mathrm{d}s$ being the components of the four-velocity. The Maupertuis action (7.95) therefore has the variation

$$\delta S = mc\int \delta(\mathrm{d}s) = \int \left\{\frac{1}{2}\frac{\partial g_{ij}}{\partial x^k}u^i u^j - \frac{\mathrm{d}}{\mathrm{d}s}(g_{ik}u^i)\right\}\delta x^k \mathrm{d}s, \tag{7.98}$$

after performing partial integration in the second and third term, change of indices to factorize out δx^k, and utilizing the symmetry of the metric tensor. The variational equation $\delta S = 0$ for arbitrary path variation $\delta x^i(s)$ leads to the following general equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}s}\left(g_{ik}u^i\right) = \frac{1}{2}\frac{\partial g_{ij}}{\partial x^k}u^i u^j. \tag{7.99}$$

Using now the chain rule for the s-derivation on the left hand side, rearranging and symmetrizing the coefficient of the term $u^i u^j$ we arrive at

$$g_{ik}\frac{\mathrm{d}u^i}{\mathrm{d}s} = \frac{1}{2}\left(\frac{\partial g_{ij}}{\partial x^k} - \frac{\partial g_{ik}}{\partial x^j} - \frac{\partial g_{jk}}{\partial x^i}\right)u^i u^j. \tag{7.100}$$

Finally, multiplying by the inverse metric tensor, g^{nk} and arranging to zero one recognizes the Christoffel symbol in the expression in the large brackets and concludes to the equation of the geodesic motion:

$$\frac{\mathrm{d}u^n}{\mathrm{d}s} + \Gamma^n_{ij}u^i u^j = 0. \tag{7.101}$$

Knowing of this equivalence one can obtain the trajectory of geodesic motion, the solution of (7.101), also by varying the Maupertuis action (7.95) directly. This method is especially fruitful if the metric shows high symmetry.

The general spacetime metric of a static, radially symmetric black hole is given by

$$\mathrm{d}s^2 = -f(r)\mathrm{d}t^2 + \frac{\mathrm{d}r^2}{f(r)} + r^2\mathrm{d}\Omega^2. \tag{7.102}$$

Denoting the total s-derivatives by an overdot, the Maupertuis action is expressed in terms of the coordinate derivatives:

$$S = mc\int\sqrt{-f\dot{t}^2 + \frac{1}{f}\dot{r}^2 + r\dot{\theta}^2 + r^2\sin^2\theta\dot{\phi}^2}\quad \mathrm{d}s. \tag{7.103}$$

This integral has the shape of $S = mc\int L(\dot{t},\dot{r},\dot{\theta},\dot{\phi},r,\theta)\mathrm{d}s$. The integrand, L, is proportional to the Lagrangian. Not depending explicitly on t and ϕ there are two constants of the free motion. The Euler–Lagrange type equations belonging to this action describe the trajectory of the free fall of the particle with the mass m:

$$\frac{\partial L}{\partial t} - \frac{\mathrm{d}}{\mathrm{d}s}\frac{\partial L}{\partial \dot{t}} = -\frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{-2f\dot{t}}{2L}\right) = 0,$$

$$\begin{aligned}
\frac{\partial L}{\partial r}-\frac{\mathrm{d}}{\mathrm{d}s}\frac{\partial L}{\partial \dot r} &= \frac{1}{2L}\left(-f'\dot t^2-\frac{f'}{f^2}\dot r^2+2r(\dot\theta^2+\sin^2\theta\dot\phi^2)\right)-\frac{\mathrm{d}}{\mathrm{d}s}\frac{2\dot r}{2Lf}=0,\\
\frac{\partial L}{\partial \theta}-\frac{\mathrm{d}}{\mathrm{d}s}\frac{\partial L}{\partial \dot\theta} &= \frac{1}{2L}\left(2r^2\sin\theta\cos\theta\,\dot\phi^2\right)-\frac{\mathrm{d}}{\mathrm{d}s}\frac{2r^2\dot\theta}{2L}=0,\\
\frac{\partial L}{\partial \phi}-\frac{\mathrm{d}}{\mathrm{d}s}\frac{\partial L}{\partial \dot\phi} &= -\frac{\mathrm{d}}{\mathrm{d}s}\frac{2r^2\sin^2\theta\,\dot\phi}{2L}=0.
\end{aligned} \tag{7.104}$$

Due to the very definition of the metric (7.102), however,

$$L^2=-f\dot t^2+\dot r^2/f+r^2\dot\theta^2+r^2\sin^2\theta\,\dot\phi^2=-1 \tag{7.105}$$

for a particle moving on a timelike path. Using this simplification we utilize three of the four equations of motion (7.104)

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}s}\left(f(r)\frac{\mathrm{d}t}{\mathrm{d}s}\right) &= 0,\\
\frac{\mathrm{d}}{\mathrm{d}s}\left(r^2\sin^2\theta\frac{\mathrm{d}\phi}{\mathrm{d}s}\right) &= 0,\\
\frac{\mathrm{d}}{\mathrm{d}s}\left(r^2\frac{\mathrm{d}\theta}{\mathrm{d}s}\right) &= r^2\sin\theta\,\cos\theta\,\dot\phi^2,
\end{aligned} \tag{7.106}$$

and instead of the fourth one we use the $L^2=-1$ condition (7.105):

$$\dot r^2=f\left(-1+f\dot t^2-r^2\dot\theta^2+r^2\sin^2\theta\,\dot\phi^2\right). \tag{7.107}$$

Two of the equations can readily be integrated

$$\begin{aligned}
f\dot t &= K,\\
r^2\sin^2\theta\,\dot\phi &= J.
\end{aligned} \tag{7.108}$$

Starting in the equatorial plane, $\theta=\pi/2$, $\dot\theta=0$, the third equation in (7.106) ensures that the trajectory remains in this plane. Studying in particular radial motion, $\dot\phi=0$ at the beginning, and so it remains. In this case, one of the integration constants in (7.108) vanishes, $J=0$. The radial motion is then described by (7.107),

$$\dot r^2=f(-1+f\dot t^2)=-f+K^2. \tag{7.109}$$

The second equality is a consequence of the first line in (7.108).

It is particularly interesting to study the free falling trajectory near to the black hole horizon; here we expect universal behavior. Taking the s-derivative of the square root of the left hand side in (7.109) we obtain the proper acceleration of a free falling particle:

$$\frac{\mathrm{d}^2r}{\mathrm{d}s^2}=-\frac{f'}{2\sqrt{-f+K^2}}\frac{\mathrm{d}r}{\mathrm{d}s}=-\frac{1}{2}f'(r). \tag{7.110}$$

Near to the black hole horizon this quantity behaves regularly featuring a constant acceleration

$$\left.\frac{\mathrm{d}^2r}{\mathrm{d}s^2}\right|_{r=R} = -\frac{1}{2}f'(R). \tag{7.111}$$

Although $f(R) = 0$ causing the coordinate singularity for the far observer, $f'(R) \neq 0$ is a finite value. In particular for a Schwarzschild black hole $f(r) = 1 - R/r$ with $R = 2GM/c^2$ being the Schwarzschild radius. In this case $g = \ddot{r}(R) = f'(R)/2 = c^2/2R$ is the acceleration on the trajectory of a free falling particle at the horizon.[7] The corresponding Unruh temperature, T satisfies

$$\frac{k_\mathrm{B}T}{\hbar c} = \frac{1}{2\pi}\frac{g}{c^2} = \frac{1}{4\pi R} = \frac{c^2}{8\pi GM}. \tag{7.112}$$

From this result we can determine the coefficient α in the $S = \alpha A$ formula. For this purpose, we use the $\mathrm{d}(Mc^2) = T\mathrm{d}S$ correspondence. On the one hand

$$T\mathrm{d}S = \frac{k_\mathrm{B}T}{\hbar c}\mathrm{d}\left(\hbar c\frac{S}{k_\mathrm{B}}\right), \tag{7.113}$$

which – replacing $S = \alpha A = \alpha 4\pi R^2$ becomes

$$T\mathrm{d}S = 2\alpha\frac{\hbar c}{k_\mathrm{B}}\mathrm{d}R. \tag{7.114}$$

On the other hand expressing the black hole mass with the Schwarzschild radius $M = Rc^2/2G$ and

$$\mathrm{d}(Mc^2) = \mathrm{d}\left(\frac{R}{2G}c^4\right), \tag{7.115}$$

which must be equal to $T\mathrm{d}S$ obtained in (7.114). This leads to

$$\frac{c^4}{2G} = \frac{\hbar c}{k_\mathrm{B}}2\alpha. \tag{7.116}$$

Expressing α we conclude that

$$\alpha = \frac{1}{4}\frac{k_\mathrm{B}}{\hbar c}\frac{c^4}{G} = \frac{k_\mathrm{B}}{4}\frac{c^3}{\hbar G}. \tag{7.117}$$

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[7] The negative sign reflects the property that all radially moving particles (outbound or inbound) feel an acceleration towards the center of the black hole.

Here, the factor $1/4$ is the famous result, the other factors are combinations of different natural constants. In particular it is customary to introduce at this point the Planck length, $L_{\mathrm{P}} = \sqrt{\hbar G/c^3}$, in which units the black hole horizon area contributes to the formal entropy:

$$\frac{1}{k_{\mathrm{B}}} S = \frac{1}{4} \frac{A}{L_{\mathrm{P}}^2}. \tag{7.118}$$

Of course, not only for the Schwarzschild black hole, but near to any horizon a free falling particle is locally isometric to a Rindler space describing constant acceleration. It is easy to recognize again in the radial case.

Let us consider the metric (7.102) around $r = R$ with $f(R) = 0$ defining the horizon. Expanding in $\varepsilon = r - R$ near to the horizon one considers $f = \varepsilon f'(R)$. With this the metric to leading order becomes

$$\mathrm{d}s^2 = -\varepsilon f'(R)\mathrm{d}t^2 + \frac{\mathrm{d}\varepsilon^2}{\varepsilon f'(R)} + R^2 \mathrm{d}\Omega^2. \tag{7.119}$$

We follow now the same steps as by the study of the Reissner–Nordstrøm metric. Introducing the coordinate ρ by requiring

$$\mathrm{d}\rho^2 = \frac{\mathrm{d}\varepsilon^2}{\varepsilon f'(R)} \tag{7.120}$$

we obtain

$$\int \sqrt{f'} \mathrm{d}\rho = \int \frac{\mathrm{d}\varepsilon}{\sqrt{\varepsilon}} = 2\sqrt{\varepsilon}. \tag{7.121}$$

From here, $\rho = 2\sqrt{\varepsilon/f'}$ follows. Substituting this result back into the spacetime metric expression and noting that $R^2\mathrm{d}\Omega^2 = \mathrm{d}\hat{x}^2 + \mathrm{d}\hat{y}^2$ is a flat subspace, we arrive at

$$\mathrm{d}s^2 = -\frac{1}{4} f'^2 \rho^2 \mathrm{d}t^2 + \mathrm{d}\rho^2 + \mathrm{d}\hat{x}^2 + \mathrm{d}\hat{y}^2. \tag{7.122}$$

Noting now that $g = f'(R)/2$ is the magnitude of the proper acceleration of a free falling particle at the horizon, this metric can be made locally Minkowskian by the correspondence

$$\begin{aligned} \hat{t} &= \rho \sinh(gt), \\ \hat{z} &= \rho \cosh(gt) \end{aligned} \tag{7.123}$$

with the obvious result $\mathrm{d}s^2 = -\mathrm{d}\hat{t}^2 + \mathrm{d}\hat{z}^2 + \mathrm{d}\hat{x}^2 + \mathrm{d}\hat{y}^2$.

Since the near-horizon metric in the coordinates $(\hat{t}, \hat{z}, \hat{x}, \hat{y})$ is Minkowskian, a plane wave described in this metric shall be analyzed by the far observer in terms of his/her time coordinate t. Similarly, as in the case of the special relativistic Unruh effect, this Fourier re-analysis gives a thermal black body radiation for a single photon of frequency ω. For the sake of definiteness we spell here explicitly out this consideration.

The coordinate ρ is treated approximately as a constant in the near-horizon analysis, its value will not enter into the formula of the equivalent Unruh temperature. The frequency dependent complex amplitude of a wave in terms of the far static observer's time, t, is given by

$$F(\nu) = \int\limits_{-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}k\hat{z} - \mathrm{i}\omega\hat{t}}\, \mathrm{e}^{\mathrm{i}\nu t} \mathrm{d}t. \tag{7.124}$$

Considering radiated photons in the positive radial direction, $k = \omega$, while $\hat{t}$ and $\hat{z}$ are given in (7.123). Using this we have

$$F(\nu) = \int\limits_{-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}\omega\rho \mathrm{e}^{-gt}}\, \mathrm{e}^{\mathrm{i}\nu t} \mathrm{d}t. \tag{7.125}$$

We introduce again the integration variable $z = \omega\rho\mathrm{e}^{-gt}$ which has the value $+\infty$ at the infinite past, $t = -\infty$, and the value zero at the infinite future, $t = +\infty$ for the far observer. Its differential, $\mathrm{d}z = -gz\mathrm{d}t$, relates the t-integration to the z-integration:

$$F(\nu) = \int\limits_{0}^{\infty} \frac{\mathrm{d}z}{gz}\, \mathrm{e}^{\mathrm{i}z}\, \mathrm{e}^{-\frac{\mathrm{i}\nu}{g} \ln \frac{z}{\omega\rho}} \tag{7.126}$$

From this result a phase factor can be separated and the rest is an Euler Gamma type integral

$$F(\nu) = \frac{1}{g} \mathrm{e}^{\frac{\mathrm{i}\nu}{g} \ln(\omega\rho)} \int\limits_{0}^{\infty} \mathrm{d}z\, z^{i\nu/g - 1}\, \mathrm{e}^{\mathrm{i}z} \tag{7.127}$$

The result of integration is described by the Euler Gamma function

$$F(\nu) = \frac{1}{g} \mathrm{e}^{\frac{\mathrm{i}\nu}{g} \ln(\omega\rho)}\, i^{i\nu/g}\, \Gamma(i\nu/g). \tag{7.128}$$

The $i\nu/g$-th power of $i = \mathrm{e}^{\mathrm{i}\pi/2}$ gives the unique real factor, $\mathrm{e}^{-\pi\nu/2g}$. The absolute value squared of this wave amplitude for the far observer is given by

$$|F(\nu)|^2 = \frac{1}{g^2} \mathrm{e}^{-\frac{\pi\nu}{g}}\, \Gamma\left(\frac{i\nu}{g}\right) \Gamma\left(-\frac{i\nu}{g}\right). \tag{7.129}$$

Finally, utilizing a certain mathematical property of the Euler Gamma function, namely that $\Gamma(iA)\Gamma(-iA) = \pi/A \sinh(\pi A)$, we obtain a result proportional to the Planck distribution:

$$|F(\nu)|^2 = \frac{2\pi}{g\nu} \frac{1}{e^{2\pi\nu/g} - 1}. \tag{7.130}$$

In conclusion, a photon, radiated mono-chromatically near the horizon, looks like a Planck distributed, thermal black body radiation when detected by a far, static observer. The equivalent temperature satisfies the relation

$$\frac{k_B T}{\hbar c} = \frac{1}{2\pi} \frac{g}{c^2}. \tag{7.131}$$

We note, that the essence of this effect is entirely classical, describing the influence of curved spacetime on the propagation of massless plane waves. Planck's constant enters solely in the interpretation of the frequency distribution of the classical wave as an energy distribution of a particle, called photon, in the detection process.

Also, the entropy formula (7.93), connected to the area of the event horizon surrounding a black hole, is more general. Here we sketch some ideas, how it can be applied to more general – but still radial symmetric – spacetimes, than the Schwarzschild one.

Noting that the near horizon acceleration, $g = \frac{c^2}{2} f'(R)$, is related to the seeming temperature from spatial infinity [cf. (7.131)], the seeming entropy represented by such a horizon can be calculated in a way, which follows the classical approach of Clausius. Using namely, $1/T$ as an integrating factor – assuming that other extensive quantities are kept constant – the entropy is integrated as

$$S = \int \frac{d(Mc^2)}{T} = k_B \frac{4\pi c}{\hbar} \int \frac{dM}{f'(R)}. \tag{7.132}$$

The value of the derivative of the metric factor, $f(r)$ is to be taken at the horizon, which is defined by the constraint $f(R) = 0$. We use this implicit definition in the above equation by inserting a formal integration over r with a Dirac-delta distribution:

$$S = k_B \frac{4\pi c}{\hbar} \iint \frac{\delta(r - R)}{f'(r)} \, dr \, dM. \tag{7.133}$$

The important step is to realize that $f'(r)$ actually is the Jacobian of the variable change from r to $f(r)$, therefore we can equivalently write

$$S = k_B \frac{4\pi c}{\hbar} \iint \delta(f(r)) \, dr \, dM. \tag{7.134}$$

Interchanging now the order of integration, $f(r)$ will be treated as a function containing the total mass M. The integration over M can now be done by using the Dirac-delta, and we arrive at a formula with a new Jacobian in the denominator

$$S = k_{\mathrm{B}} \frac{4\pi c}{\hbar} \int \frac{\mathrm{d}r}{\left| \frac{\partial f}{\partial M} \right|_{f(r,M)=0}} . \tag{7.135}$$

This formula already includes the Reissner–Nordstrøm case as well as a possible cosmological constant term. We can do the integral for all type of solutions of the Einstein equations containing a factor of the following type:

$$f(r) = 1 - \frac{2GM}{c^2 r} - \hat{f}(r). \tag{7.136}$$

The only assumption we need is that $\hat{f}(r)$ is independent of M. This is a physically well-supported assumption, since far from the horizon Newtonian gravity has to be re-established. This is reflected in the first two terms of the general expression. For such spacetimes one obtains

$$\frac{\partial f}{\partial M} = -\frac{2G}{c^2 r}. \tag{7.137}$$

The integration in the formula (7.135) now can be done analytically. and in the result the radius at the horizon has to be taken. This leads to

$$S = \frac{1}{4} k_{\mathrm{B}} \frac{A}{L_{\mathrm{P}}^2} \tag{7.138}$$

with the horizon area, $A = 4\pi R^2$, and $L_{\mathrm{P}}^2 = \hbar G / c^3$ being the square of the Planck length.

It is interesting to note that the Planck scale, represented by either the length L_{P} or the mass M_{P}, can also be related to a smallest amount of information [70]. Information and entropy are intimately related by noting that knowledge itself can be quantified along a process of restricting probabilities. Probabilities prior knowledge are more uniform than after any restriction; this way maximal entropy states represent the least knowledge about a physical system. The negative entropy as a measure of information has been proposed by Claude Shannon [72], practically coincident with the Boltzmann formula:

$$S = k_{\mathrm{B}} \sum_{i=1}^{N} -w_i \ln w_i$$

– without further constraints – is maximal at equiprobability, $w_i = 1/N$, with N possible alternatives. The minimal information on the other hand is defined by the gain in information, or equivalently by the loss in entropy, due to an answer to a single "yes/no" question.[8] The smallest possible unit of information is the negative of a change in the entropy of a system with two, mutually excluding alternative states by changing from equiprobability state to a pure state. Before the measurement process we have the probabilities $w_1 = 1/2, w_2 = 1/2$, and after obtaining the full information (a definitive yes or no) $w_1 = 1, w_2 = 0$. Due to the Shannon–Boltzmann formula the change is

$$\frac{1}{k_\mathrm{B}} \Delta S = (-1\ln 1 - 0\ln 0) - \left(-\frac{1}{2}\ln\frac{1}{2} - \frac{1}{2}\ln\frac{1}{2} \right) = -\ln 2. \tag{7.139}$$

Applying this to the black hole entropy, one concludes that the 1-bit information black hole should have a horizon area satisfying

$$\frac{1}{4}\frac{A}{L_\mathrm{P}^2} = \ln 2. \tag{7.140}$$

The corresponding radius of a Schwarzschild black hole would be

$$R_{1-\mathrm{bit}} = L_\mathrm{P}\sqrt{\frac{\ln 2}{\pi}} \approx 0.47 L_\mathrm{P}, \tag{7.141}$$

about the half of the Planck length. Certainly, this is an interesting numerical coincidence, but the very black hole entropy formula, (7.138), might be invalidated at this distance scale. Here quantum gravity should describe the core physics.

When black holes radiate, it has serious physical consequences. These consequences can be analyzed without referring to quantum gravity; they are comprehensible already in a semiclassical context.

The Hawking radiation has been described as a spontaneous particle production from the vacuum at the horizon. A pair of positive and negative energy fluctuations, quantum mechanically always present, can be separated due to the strong gravitational field. While the positive energy excitation propagates to radial infinity and eventually will be detected, the negative energy partner falls below the event horizon and eventually will be absorbed by the massive singularity which generates the black hole. This process reduces the energy of the black hole with the same amount, that is carried away by the black body radiation.

This way the Hawking radiation means an outwards directed thermal radiation from the event horizon wrapping the black hole – for a static, far observer. Energy seems to come from the black hole. The black hole is loosing energy – it occurs as a physical decay process. The mass energy content, Mc^2, must be decreasing. Moreover it is diminished to nothing in a finite time!

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[8] Of course, the total entropy in a closed system will not decrease, therefore the observer, who obtains the answer, will inevitably warm up and therefore increase his entropy. This fate of the Maxwell's demon inquiring information on the level of atomic motion was first calculated by Leo Szilard.

To obtain this result easily it is sufficient to consider the Stefan–Boltzmann law of black-body radiation: the energy density $e = \sigma T^4$ (in natural units of $\hbar = c = k_B = 1$) integrated over the total area of the horizon gives the luminosity, the loss of energy in a time unit:

$$\frac{dM}{dt} = -\sigma T^4 A. \tag{7.142}$$

Substituting the corresponding expressions for the Hawking temperature and the effective source area of $A \sim 4\pi R^2$ with R being the Schwarzschild radius of a black hole horizon into this formula we obtain

$$\frac{dM}{dt} = -\frac{\alpha}{M^2} \tag{7.143}$$

with some constant α. The simple differential equation (7.143) is analytically integrable to

$$\frac{1}{3}\left(M^3 - M_0^3\right) = -\alpha t, \tag{7.144}$$

therefore a black hole having a mass of M_0 at the beginning of Hawking radiation will be evaporated away in a finite time of

$$t_0 = \frac{1}{3\alpha} M_0^3. \tag{7.145}$$

This radiation also occurs to be a conversion from a pure quantum mechanical state, a single photon near the horizon (or the Fock vacuum state as well) into an incoherent many photon state, like a black body radiation appears for a far observer. Entropy has been picked up while propagating from close to the event horizon to the detection in flat spacetime far away. This process has to overcompensate the entropy loss by shrinking the horizon of an evaporating black hole.

There were countless speculations about where the entropy may go to, when a black hole is shrinking due to Hawking evaporation. At the end of this process, when the Schwarzschild radius approximates the corresponding Compton wavelength of the black hole mass, quantum gravity must be used to describe the situation. Notably, this happens when, $R = 2GM/c^2 \approx \hbar/Mc$, i.e. by reaching the Planck scale, $M \approx M_P$, $R \approx L_P$. The description of the very end of black hole evaporation is therefore described as the "trans-Planckian" problem [73].

A further, from thermodynamical viewpoint strange property of the black hole evaporation is, that by shrinking the radius the temperature rises, since $k_B T/\hbar c = 1/4\pi R$. This way an evaporating black hole would loose energy, but instead of cooling down in this process, it warms up. It is so far unusual, that in this respect black holes must have negative heat capacity. However, bodies with negative heat capacity cannot be thermodynamically stable; this could be the reason for decay. Being unstable, they also cannot be formed by near-equilibrium, adiabatic processes. They – if they exist – must be remnants of a dynamically dramatic, far from equilibrium epoch of the Universe [74].

7.2.4 Gravity Emerging from Information

In the previous sections, it was demonstrated how the classical concepts of temperature and entropy have emerged from such unexpected corners of physics, like strong gravity and black holes. In particular, gravitational force has been reinterpreted in the language of geometry as effects on the spacetime metric in the theory of general relativity. These effects, under certain circumstances, when the relevant phenomena are bound to a constant acceleration, mimic the effect of finite temperature radiation spectra. The very question is: do they just mimic, or in fact are thermal in a general, but still with classical thermodynamics compatible, sense?

There are two possible logical paths to seek answer to this question. One possibility is to consider mechanisms other than a constant acceleration and the equivalence principle, as it was discussed above. Regarding the diffuseness of energy distribution as a leading effect of a finite temperature, other causes or forms of energy (or wave frequency) dispersion may be accounted for. In particular, one may speculate that if quantum uncertainty of energy and spacetime were considered simultaneously, as it has to be in the framework of quantum gravity, new interpretation channels could be reached also for the Unruh temperature. The back side of this coin, namely a quantum theory emerging from classical gravity in a higher dimensional bulk, has been proposed by t'Hooft.

A further possibility is to reinterpret our classical theories about gravity in terms of thermodynamics, reverting this way the levels of being more elementary: if gravity – in theory – can be derived from an entropy maximum principle instead of deriving entropy for black holes by analogies, as it historically has been done, then we would consider the concept of information (entropy) and noise level (temperature) more elementary than space, time and gravitational force. The latter would be then derived quantities. Such a suggestion in fact has been made, most recently in [75]. We outline the main steps of this chain of thoughts below.

Motivated by the suggestive paper of Erik Verlinde [75] *"On the Origin of Gravity and the Laws of Newton"* and its predecessors [76] we indicate the possible way to derive our classical knowledge on mechanics and gravity from an entropy maximum principle. This is actually the same connection between these concepts as we were discussing so far, but viewed from another corner. Such a change of our viewpoint is sometimes quite refreshing.

The starting point is Bekenstein's original "thought experiment" of dropping a small particle with mass m into a black hole horizon [70]. The particle is kept by a string and is adiabatically slowly lowered towards the horizon. Due to the infinite redshift at the horizon for a far, static observer this process may seem so, that the mass of the black hole would not be increased at all. A thermal gas of such particles could then disappear beyond the horizon reducing entropy for the outside world. This effect must be compensated. Bekenstein argues that in fact already being close to the horizon, as far as a Compton wavelength, $\lambda = \hbar/mc$ only, means to be part of the black hole. This way there is a small, but finite mass increase and consequently there is a small increase of the horizon area.

Let us return to the following problem: We seek for the entropy inside a horizon defined by an extremal Reissner–Nordstrøm solution (now simply in 3+1 space-time dimensions) supported with a cosmological term (cf. problem 7.3). Observing that $M_{\mathrm{P}}L_{\mathrm{P}} = \hbar/c$ is a purely quantum mechanical, while $L_{\mathrm{P}}/M_{\mathrm{P}} = G/c^2$ is a purely gravitational combination of the Planck scales, the formula (7.134) can be written entirely in terms of these scales:

$$\frac{S}{k_{\mathrm{B}}} = 4\pi \iint \delta\left(f(r;M)\right) \frac{\mathrm{d}r}{L_{\mathrm{P}}} \frac{\mathrm{d}M}{M_{\mathrm{P}}}. \tag{7.146}$$

From now on everything is understood in Planck scale and Boltzmann units. The radial metric factor for an extremal RN black hole with cosmological term is given as

$$f(r;M) = \left(1 - \frac{M}{r}\right)^2 - \frac{r^2}{a^2}. \tag{7.147}$$

The horizons are determined by the solution of the fourth order algebraic equation $f(r;M) = 0$ leading to

$$M_0(r) = r(1 \mp r/a). \tag{7.148}$$

The derivative of f with respect to M gives

$$\frac{\partial f}{\partial M} = -\frac{2}{r}\left(1 - \frac{M}{r}\right), \tag{7.149}$$

which at the horizon becomes $\mp 2/a$. The entropy is therefore obtained as

$$S = 4\pi \int \frac{\mathrm{d}r}{\left|\frac{\partial f}{\partial M}\right|} = 2\pi r a. \tag{7.150}$$

This is *not* the (one fourth of the) horizon *area*, but its *perimeter* multiplied by the cosmological length scale a.

Our result is that the entropy associated to such an extremal Reissner–Nordstrøm black hole with cosmological term in physical units is given as

$$S = 2\pi k_{\mathrm{B}} \frac{R}{L_{\mathrm{P}}} \frac{a}{L_{\mathrm{P}}}, \tag{7.151}$$

the Unruh-Planck temperature as

$$k_{\mathrm{B}} T = L_{\mathrm{P}} M_{\mathrm{P}} \frac{g}{2\pi} \tag{7.152}$$

with R being the radius of the event horizon and g the magnitude of acceleration near to this horizon. Conjecturing now that the “cosmological” scale parameter would be responsible for particle mass, one assumes

$$\frac{a}{L_{\mathrm{P}}} = \frac{m}{M_{\mathrm{P}}}. \tag{7.153}$$

This assumption – perhaps surprisingly – leads to a formula in which the Planck scales cancel:

$$TS = mgR. \tag{7.154}$$

In a final step we consider the free energy of a particle with mass m in gravitational field near to such a horizon, $mc^2 - TS$, and interpret its change by the horizon radius as a force acting on the particle:

$$F = \frac{\partial}{\partial R}\left(mc^2 - TS\right) = -mg. \tag{7.155}$$

It is not only the correct gravity effect on a test particle near the horizon, but interpreting in a wider context also Newton's second law derived as a linear force effect stemming from an extremal RN black hole in a de Sitter universe.

A very similar reasoning has been recently given by Erik Verlinde [75]. But his argumentation goes on to connect even Newton's law of gravity and the Einstein–Hilbert theory of gravity with the thermodynamical formulas for black holes. Considering that the force acting on masses is in fact a consequence of a temperature,

$$F = mg = 2\pi \frac{m}{M_{\mathrm{P}}} \frac{k_{\mathrm{B}} T}{L_{\mathrm{P}}}, \tag{7.156}$$

and interpreting the horizon area as just being a playground for

$$N = \frac{A}{L_{\mathrm{P}}^2} \tag{7.157}$$

independent degrees of freedom, the energy associated to the "noise" at the same temperature is given by

$$E = \frac{1}{2} N k_{\mathrm{B}} T. \tag{7.158}$$

By identifying this energy with the total mass causing the black hole, $E = Mc^2$, and calculating with a spherical surface area, $A = 4\pi R^2$ one arrives at the force

$$F = 2\pi \frac{m}{M_{\mathrm{P}}} \frac{2Mc^2}{L_{\mathrm{P}}} \frac{L_{\mathrm{P}}^2}{4\pi R^2} = G\frac{Mm}{R^2}. \tag{7.159}$$

In this interpretation, gravity is an entropic force. This concept holds effective even for deriving the Einstein equations.

7.3 Quark Matter Equation of State from Dual Gravity Models

Certainly, one of the most interesting novel theoretical developments in high energy physics is the application of the so called AdS/CFT conjecture [77,78] for predicting important quantities in strongly coupled field theories, among others most remarkably for strongly coupled quark-gluon plasmas (QGP). There is a growing evidence that such a QGP state is formed in relativistic heavy-ion experiments before the decay into hadrons [79, 80].

The AdS/CFT conjecture is a duality hypothesis between field theories defined in d dimensions and obeying a local internal SU(N) symmetry on the one hand, and a type IIB string theory on a $d+1$-dimensional AdS spacetime together with a $9-d$ dimensional compact manifold on the other hand. For our experienced world $d=4$, this means an $\mathrm{AdS}_5 \times S_5$ manifold. Although this string theory is also not entirely solvable, as well as the strongly coupled field theory describing the particle physics world is not, there are limits which are mutually corresponding to each other by a weak coupling – strong coupling duality. Field theories, including Yang–Mills fields and a corresponding coupling, g_{YM} and an $SU(N)$ symmetry in the large N limit, behave like the classical supergravity approximation to string theory with the coupling constant $\lambda = g_{\mathrm{YM}}^2 N$. This way weakly coupled, almost classical string theory problems are connected to strongly coupled (large g_{YM}^2) field theory, where solutions have been provided by complex numerical calculations on an Euclidean spacetime lattice before this technique. Such problems, better to say mathematical exercises akin to such problems, are now solvable by using equations of classical, higher dimensional supergravity.

This promising conjecture is not yet proved, whatsoever. Also further traps are hidden in differences between the phenomenologically best fitted field theory of strong interactions, quantum chromodynamics (QCD) and supersymmetric Yang–Mills theories. Also the meaning of large N for evaluation of experimental results is mysterious. Yet, this interconnectedness of two fields of theoretical physics is tantalizing, and its use in modern contemporary research seems to assume (but not to prove) deep properties of spacetime and matter. It has a place in a book asking "Is there a temperature?" in energetic events forming the elementary matter.

In this section, we review the classical (anti-)de Sitter solution of the Einstein equations, we outline the most characteristic issues of the evolution of string theory and present the AdS/CFT conjecture. Particular solutions in higher dimensional spaces will be introduced and reference will be taken to comparisons of results to high energy quark matter phenomena, especially to the equation of state of matter consisting of Yang–Mills field excitations. The temperature, used in this context, is on the one side a kind of Unruh-temperature associated to black-hole thermodynamics in a higher dimension, and – by duality – the more "normal" temperature used in four-dimensional field theory calculations as the reciprocal value of the periodicity length of field configurations in imaginary time.

7.3.1 The AdS Spacetime

The static, radial vacuum solution with a cosmological constant λ has the spacetime metric given in (7.61) by replacing $c_1 = 0$. In this case, no horizon is apparent. The AdS spacetime assumes $\lambda > 0$; in this case it is comfortable to denote it as $\lambda = 3/a^2$. Introducing furthermore the abbreviation

$$\mathrm{d}\Omega^2 = \mathrm{d}\theta^2 + \sin^2\theta \mathrm{d}\phi^2 \tag{7.160}$$

for the differential surface element on S^2, the AdS spacetime metric has the following standard form:

$$\mathrm{d}s^2 = -\left(1 + \frac{r^2}{a^2}\right)\mathrm{d}t^2 + \frac{\mathrm{d}r^2}{1 + \frac{r^2}{a^2}} + r^2\mathrm{d}\Omega^2. \tag{7.161}$$

With a real parameter a this metric nowhere has a horizon, nor a coordinate singularity.

There are, however, coordinate transformations, which lead to another, frequently used form of this metric. The basic one is an embedding into the five-dimensional Lorentzian spacetime $R^{(2,3)}$. Here, the quadratic length of an infinitesimal arc is given by

$$\mathrm{d}s^2 = -\mathrm{d}t_1^2 - \mathrm{d}t_2^2 + \mathrm{d}r^2 + r^2\mathrm{d}\Omega^2. \tag{7.162}$$

The embedding of the 4-dimensional AdS spacetime is achieved by satisfying the following hyperbolic equation

$$t_1^2 + t_2^2 - r^2 = a^2. \tag{7.163}$$

We briefly show the isometric equivalence of this four-surface with the standard AdS metric (7.161). The defining equation (7.163) allows for the following parametrization:

$$\begin{aligned} t_1 &= \sqrt{a^2+r^2}\sin\zeta, \\ t_2 &= \sqrt{a^2+r^2}\cos\zeta. \end{aligned} \tag{7.164}$$

This gives rise to the following differentials

$$\begin{aligned} \mathrm{d}t_1 &= \frac{r}{\sqrt{a^2+r^2}}\sin\zeta\,\mathrm{d}r + \sqrt{a^2+r^2}\cos\zeta\,\mathrm{d}\zeta, \\ \mathrm{d}t_2 &= \frac{r}{\sqrt{a^2+r^2}}\cos\zeta\,\mathrm{d}r - \sqrt{a^2+r^2}\sin\zeta\,\mathrm{d}\zeta. \end{aligned} \tag{7.165}$$

The squared sum of these two expressions becomes

$$\mathrm{d}t_1^2 + \mathrm{d}t_2^2 = \frac{r^2}{a^2+r^2}\mathrm{d}r^2 + \left(a^2+r^2\right)\mathrm{d}\zeta^2 \tag{7.166}$$

Substituting this result into the metric expression (7.162) of the embedding five-dimensional spacetime we arrive at

$$\mathrm{d}s^2 = -\left(a^2+r^2\right)\mathrm{d}\zeta^2 + \left(1-\frac{r^2}{a^2+r^2}\right)\mathrm{d}r^2 + r^2\mathrm{d}\Omega^2. \tag{7.167}$$

Now it is easy to realize that the coordinate $t = a\zeta$ becomes the corresponding time coordinate in order to achieve the standard AdS form (7.161). It is amazing to note that the timelike coordinates in the five-dimensional Lorentzian spacetime, in which the hyperboloid is embedded, are now periodic functions of the time coordinate t of the standard AdS vacuum solution:

$$\begin{aligned} t_1 &= \sqrt{a^2+r^2}\,\sin\frac{t}{a}, \\ t_2 &= \sqrt{a^2+r^2}\,\cos\frac{t}{a}. \end{aligned} \tag{7.168}$$

On the (t_1, t_2) brane, a “two-dimensional time-sheet” there are closed trajectories possible; closed timelike paths. The period of time, $\beta = 2\pi a$, can be related to the Unruh temperature $T = g/2\pi$ at $r = 0$ by noting that in the case of constant acceleration g, analyzed in imaginary time, one would have $it_1 = \frac{1}{g}\sinh(igt)$ and hence $g = 1/a$ with $T = g/(2\pi) = 1/(2\pi a) = 1/\beta$. All these strange mathematical coincidences make some to believe that the AdS spacetime has to play an important role in the final theory of quantum gravity: a period in imaginary time as the inverse temperature also occurs in high temperature field theory without gravity effects.

A further important transformation of the standard AdS coordinates leads us to a form ready to explore correspondence with modern string theory; a candidate for being the underlying explanation both for strong gravity objects, like black holes, and quantum behavior, i.e. field theory of interacting quanta. This transformation leads to the so called “conformal” coordinates.

Let us discuss this transformation for the more general case allowing for the presence of a spherical black hole wrapped in a radial horizon at $r = c_1$. In this case, the radius dependent factor occurring in the standard metric is given as $A(r) = 1 - c_1/r^{d-2} + \lambda r^2/3$ [cf. (7.61) for $d = 3$]. The following conformal metric form in d space and 2 timelike dimensions,

$$\mathrm{d}s^2 = \frac{1}{f(z)}\left(-\mathrm{d}z^2 - \mathrm{d}t^2 + \mathrm{d}R^2 + R^2\mathrm{d}\Omega_{d-1}^2\right) \tag{7.169}$$

includes the macroscopic classical spacetime we know for $d = 3$. With an eye on string theory we allow, however, for an arbitrary number of spatial dimensions d.

In order to be compatible to the standard AdS metric form one has to ensure that

$$A(r) = B(R) = \frac{1}{f(z)} \tag{7.170}$$

defining implicitly the $z(r)$ relation which embeds a $d+1$-dimensional spacetime into the conformal metric space (7.169). Furthermore we have $R = r/\sqrt{A(r)}$ for the "angular" part, in order to ensure $R^2 \mathrm{d}\Omega_{d-1}^2 / f(z) = r^2 \mathrm{d}\Omega_{d-1}^2$. Differentiating this relation one observes that

$$\sqrt{A}\,\mathrm{d}R = \left(1 - \frac{rA'}{2A}\right) \mathrm{d}r \tag{7.171}$$

and therefore

$$\mathrm{d}s^2 = -A\mathrm{d}z^2 - A\mathrm{d}t^2 + \left(1 - \frac{rA'}{2A}\right)^2 \mathrm{d}r^2 + r^2 \mathrm{d}\Omega_{d-1}^2. \tag{7.172}$$

Utilizing now the – yet unknown – $z(r)$ relation we obtain $\mathrm{d}z = z'(r)\mathrm{d}r$, and arrive at the following metric on the embedded $d+1$-hypersurface

$$\mathrm{d}s^2 = -A\mathrm{d}t^2 + \left[-A(z')^2 + \left(1 - \frac{rA'}{2A}\right)^2\right] \mathrm{d}r^2 + r^2 \mathrm{d}\Omega_{d-1}^2. \tag{7.173}$$

In order to have the standard form, the coefficient of the term $\mathrm{d}r^2$ in the square bracket in the above formula must be equated to $1/A$. This leaves us with a differential equation for the unknown $z(r)$ function:

$$-A\left(\frac{\mathrm{d}z}{\mathrm{d}r}\right)^2 + \left(1 - \frac{rA'}{2A}\right)^2 = \frac{1}{A}. \tag{7.174}$$

In the case without black hole horizon, $c_1 = 0$, the above equation is analytically solvable. We have $A(r) = 1 + \lambda r^2/3$ and hence $A' = 2\lambda r/3$. This gives rise to

$$1 - \frac{rA'}{2A} = 1 - \frac{\lambda r^2/3}{1 + \lambda r^2/3} = \frac{1}{1 + \lambda r^2/3}. \tag{7.175}$$

Following (7.174) we arrive at

$$\left(\frac{\mathrm{d}z}{\mathrm{d}r}\right)^2 = \frac{1}{1 + \lambda r^2/3}\left[\frac{1}{(1 + \lambda r^2/3)^2} - \frac{1}{1 + \lambda r^2/3}\right]. \tag{7.176}$$

Performing the square root we obtain

$$\frac{dz}{dr} = \frac{r\sqrt{-\lambda/3}}{(1+\lambda r^2/3)^{3/2}}. \tag{7.177}$$

This equation is easily integrable with the result:

$$z = \sqrt{-3/\lambda}\left(1+\lambda r^2/3\right)^{-1/2}. \tag{7.178}$$

Comparing this result with expression for $A(r)$ at $c_1 = 0$ we conclude that the conformal factor in the metric (7.169) has to be

$$f(z) = \frac{1}{A(r)} = -\frac{\lambda}{3}z^2. \tag{7.179}$$

It is interesting to note that while the radial coordinate r runs from zero to infinity, the conformal radial coordinate, R is given by

$$R = \frac{r}{\sqrt{1+\lambda r^2/3}}, \tag{7.180}$$

and is therefore limited between zero and the maximal value $R_{\max} = \sqrt{3/\lambda}$ for a positive cosmological constant, λ.

7.3.2 A Brief History of Strings

We, of course, cannot have a comprehensive introduction into string theory as a subsection in a book about the concept of temperature in extreme physical situations. On the other hand, it cannot be avoided to sketch a faint picture of the main concepts and mathematical language of string theory; otherwise, we would not have a chance to speculate about the whys and hows of applying the (super)gravity analogues to the field theory of the elementary strong interaction. We follow here the summary given in the PhD thesis of William Horowitz [81]. For a more throughout discussion the Reader may consult [82].

Originally, string theory has been developed with the purpose to describe the nuclear “alpha” force, the hadronic strong interaction. After a gigantic detour towards an elementary string theory of everything (i.e. space and time, quantum gravity and all elementary interactions), due to the AdS/CFT correspondence – tacitly including a CFT/QCD correspondence, too – again it is used as a fast lane for obtaining results for QCD matter. Of course, this is not the only research field in contemporary string theory; among many, questions of elementary physical world geometry and quantum physics still belong to this research area.

In the 1960s the phenomenological, special relativistic string model has been created to explain the mass spectrum of hadronic resonances. In fact, it had success in describing a particular property of such spectra, namely the linear dependence of the total angular momentum on the mass squared, $J \propto M^2$. Since the mass of resonances is obtained from scattering measurements via the four-momentum squared of the (mostly binary) decay products, $M^2 = s = (p_1 + p_2)^2$, the linear trend expressed by

$$J = \alpha(s) = \alpha(0) + \alpha' s \tag{7.181}$$

can be well fitted to experimental points. Moreover, the slope of this line, α', looks universal over several meson and baryon resonance families: $\alpha' \approx 1\ \mathrm{GeV}^{-2}$. This can be easily modeled by a string constant, σ, describing the energy per unit length stored in a string: $E = \sigma\ell$. The model of the hadron is then a spinning rod – a maximally stretched string – carrying the relativistic energy

$$E = \int\limits_{-\ell/2}^{\ell/2} \frac{\sigma \mathrm{d}s}{\sqrt{1 - v^2(s)}}. \tag{7.182}$$

Here, $v(s)$ describes the velocity profile of the string while spinning, obviously bounded by the velocity of light. Therefore, $v(-\ell/2) = -1$ and $v(\ell/2) = +1$ in the natural units of light speed $c = 1$. In order to obtain hadronic mass spectrum in this model one minimizes E by constrained total angular momentum,

$$J = \int\limits_{-\ell/2}^{\ell/2} \frac{s v(s)\, \sigma \mathrm{d}s}{\sqrt{1 - v^2(s)}}. \tag{7.183}$$

The minimizing variational condition,

$$\frac{\delta}{\delta v}(E - \omega J) = 0, \tag{7.184}$$

leads to a linear velocity profile, $v(s) = \omega s$. With this solution the total energy and angular momentum are given as

$$\begin{aligned} M = E_{\text{var}} &= \frac{\sigma}{\omega} \int\limits_{-1}^{+1} \frac{\mathrm{d}v}{\sqrt{1 - v^2}} = \frac{\sigma}{\omega}\pi, \\ J = J_{\text{var}} &= \frac{\sigma}{\omega^2} \int\limits_{-1}^{+1} \frac{v^2 \mathrm{d}v}{\sqrt{1 - v^2}} = \frac{\sigma}{\omega^2} \frac{\pi}{2}. \end{aligned} \tag{7.185}$$

This variational solution gives rise to the formula

$$J = \frac{M^2}{2\pi\sigma} \tag{7.186}$$

by eliminating the Lagrange multiplier, ω. The Regge slope parameter, α' is henceforth connected to the string constant in this simple model as $\alpha' = 1/(2\pi\sigma)$.

In the time of the first appearance of the string idea there was a very successful quantum electrodynamics, but understandably a hesitation occurred against to apply it to the strong nuclear force. Further worsened the situation the so called "nuclear democracy": no hadron seemed to be more fundamental than any other. At the beginning even the eightfold way quark model of Gell–Mann was considered as a purely mathematical construct. In the focus of interest were quantities related to scattering experiments, most remarkably the S-matrix. Combined this with asymptotically free, on-shell particles, general properties like causality and unitarity played a leading role. The avoidance of negative probabilities induced the requirement of maximal complex analiticity of the S-matrix.

Partial wave amplitudes, $A_l(s)$, were generalized to analytic functions of complex angular momentum, $A(l,s)$. These complex amplitude functions had well-separated poles, the so called Regge poles. The pattern in the position of these poles, $l = \alpha(s)$, formed the Regge trajectories: These were – stunningly enough – straight lines. Therefore the Regge pole pattern, $l = \alpha(s) = \alpha(0) + \alpha' s$, offered a motivation for the early string theory.

Understandably, the consequences did not remain restricted for these lines on $J - M^2$ plots, but were conducted back to the analiticity studies. From the crossing symmetry of scattering amplitudes depending on the Mandelstam variables, $s = (p_1 + p_2)^2$, $t = (p_3 - p_1)^2$ and $u = (p_4 - p_1)^2$ in a $1 + 2 \to 3 + 4$ binary scattering, it was discovered that the t-channel exchange of Regge poles (so called *reggeons*) dominates the cross sections at high energy $\sqrt{s}$. A typical amplitude in this limit has the form $A(s,t) \sim b(t)s^{\alpha(s)}$. The partial wave expansion of such a form on the other hand shows a series of resonances at integer and half integer values of l (for mesons and baryons, respectively).

Driven by the logic of the evolution of the S-matrix theory a bootstrap model was proposed by Chew, where hadrons are exchanged between hadrons and this process creates the strong interaction. This model contains already the principle of duality: the poles in the s and t channels show an identical picture. Soon, in 1968, a formula has been found for scattering amplitudes, $T = A(s,t) + A(t,u) + A(u,s)$ satisfying all the required properties from duality and analiticity by Veneziano:

$$A(s,t) = \frac{\Gamma(-\alpha(s))\Gamma(-\alpha(t))}{\Gamma(-\alpha(s) - \alpha(t))}. \tag{7.187}$$

It led to linear Regge trajectories. A fully factorized u,s,t-symmetric form,

$$T = \frac{\Gamma(a)\Gamma(b)\Gamma(c)}{\Gamma(a+b)\Gamma(b+c)\Gamma(c+a)} \tag{7.188}$$

with

$$\begin{aligned} a &= -\frac{1}{2}\alpha(s), \\ b &= -\frac{1}{2}\alpha(t), \\ c &= -\frac{1}{2}\alpha(u), \end{aligned} \tag{7.189}$$

has been proposed by Virasoro. Then came a surprise: many-particle generalizations of these formulas proved to be factorizable into a spectrum of one-particle states of infinitely many harmonic oscillators. An underlying quantum theory behind this became a tempting idea. But the devil was hiding in the detail: The oscillator quantum creating and annihilating operators carried Lorentz indices and there were always among them some which created states with a negative norm of the corresponding wave function. These cannot be physical states! Since they appear unwanted in calculations, although they cannot exist physically, they were named *ghosts* by physicists.

Can these unwanted states be removed? Virasoro has found that by some algebraic constraints among the creation and annihilation operators it is possible. Such constraints are called Virasoro conditions today. Then – for the life of a researcher is never easy – another problem occurred: the leading Regge trajectory (largest spin for a given mass squared) had an intercept $\alpha(0) = 1$ indicating the presence of a ground state with negative mass squared. Such an impossible particle – baptized as a *tachyon* – is against all experimental evidences, so far. In addition unitarity of the S-matrix requires that the dimensions of the spacetime would be $d = 26$ instead of the classical four.

Understandably, with the advent of QCD the string model was forgotten. Only a few string theorists continued, stubbornly believing in the idea that simple requirements, like causality, unitarity and analiticity, would suffice to derive a theory of elementary particles. Abandoned as a theory of hadrons, it re-emerged as a theory of elementary strings; more elementary than the particles themselves. Starting in 1974, a reinterpretation of string theory results in this new light has been made: the massless spin 2 particle must be the graviton as an inevitable excitation of elementary strings. This step coupled the field theory and the theory of gravity – at least as a programmatic view. The theory of everything (every known elementary interactions) is free from problems inherent in the point particle picture. It says point particles do not exist, just elementary strings, sweeping sheets in spacetime.

The richness of particle world received a geometrical interpretation: open strings describe gauge bosons, the mediators of forces in conventional field theory, which itself became a low-energy approximation to string theory. The extra dimensions,

$d = 26$ for a bosonic string theory, but $d = 10$ for a supersymmetric string theory handling fermions and bosons in a mathematical democracy, are pointed out by the requirement of unitarity. The string tension of the elementary string theory is set by the Planck mass as being $\alpha' = 1/M_{\mathrm{P}}^2$; almost forty orders of decimal magnitudes smaller than the hadronic string tension.

Before the second "string revolution" in the 1990s, string theory did not seem to carry any relevance to conventional hadronic physics. Supersymmetry (SUSY) and supergravity (SUGRA) have been developed in the late 1970s. Anomaly cancellation has been discovered and superstrings were introduced in the 1980s. Then the idea of heterotic strings and compactification of complicated manifolds in high dimensions (so called Calabi–Yau spaces) led to multiplets partially reminding to experimentally known Standard Model particles. There were, and there are, however much more particles – described as string excitations – than could be accommodated by experimental observations even to date. Elementary string theory is still the cutest and most demanding mathematical act for understanding the foundation of the physical world, but unfortunately the way from this theory to the experienced and measured physical reality is still obscured.

Nevertheless, string theory has produced a few interesting statements, which might be of experimental relevance in the present and the near future already. One of them is a principal bound on shear viscosity of any matter, including the strongly interacting quark–gluon matter produced in relativistic heavy ion collisions. Such predictions are due to a correspondence between the gravity theories and the conventional field theories derived in the framework of the elementary string theory. This correspondence, most notably the AdS/CFT correspondence, influences our view on the origin of hadrons, quarks and gluons, and their interactions. By the virtue of this also the thermal properties of the quark matter inherit a supergravity interpretation, where black hole horizons and the Unruh temperature play a role.

7.3.3 Holography and Higher Dimensional AdS

Certainly one of the most important ideas to treat quantum theory and black holes consistently is the *holographic principle* due to t' Hooft. It is named after the holographic technique to store two dimensional images of three dimensional objects by processing phase information of the light waves. In a general sense on a $d-1$ dimensional hypersurface the full information about a d-dimensional quantum system can be stored. In the context of string theory this means that by the physics on a boundary world the physics in the bulk is determined. The very property of the entropy associated to black hole horizons, i.e. their extensivity in terms of the horizon area instead of the inside volume, is exactly recalling such a behavior.

In order to gain a little insight into the behavior of solutions of string theory we have a closer look on the gravity in higher dimensions. The Newtonian gravity constant becomes G_d in d dimensions and the action (7.24) generalizes to:

$$S = \int d^{\mathrm{d}}x \sqrt{-\det g} \left(\frac{c^3}{16\pi G_d} \mathscr{R} + \mathscr{L} \right) \tag{7.190}$$

The corresponding d-dimensional Planck length satisfies[9]

$$L_{\mathrm{P}}^{d-2} = \frac{\hbar G_d}{c^3}, \tag{7.191}$$

since $S/\hbar$ must be a dimensionless quantity, while $cd^{\mathrm{d}}x$ has the length dimension of d and the Ricci scalar has -2.

The weak gravity (Newtonian) potential is such that its $d-1$-dimensional spatial Laplacean vanishes outside the source. For a radial symmetric problem this means that

$$\Delta_{d-1}\Phi = \frac{1}{r^{d-2}} \frac{\partial}{\partial r} r^{d-2} \frac{\partial}{\partial r} \Phi_d(r) = 0. \tag{7.192}$$

Assuming a power-law behavior, $\Phi(r) \sim r^s$, this equation leads to

$$\Delta_{d-1}\Phi \sim s(s+d-3)r^{s-2} = 0. \tag{7.193}$$

The nontrivial solution for this constraint is $s = 3-d$, so the Newtonian gravity potential in $d-1$ spatial dimensions reads as

$$\Phi(r) = \frac{K_d}{r^{d-3}}. \tag{7.194}$$

The constant can be related to the total mass for example by fitting to an inside solution of a sphere with radius R and constant density. In this case the radial Laplacean is not zero but constant, so the power in (7.193) equals $s = 2$. The constant density integrates to the total mass, i.e.

$$\frac{R^{d-1}}{d-1} \Omega_{d-2} \rho = M \tag{7.195}$$

with Ω_{d-2} being the (d-2)-dimensional spherical surface at unit radius. The solution of the radial Poisson equation,

$$\Delta_{d-1}\Phi(r) = 4\pi G\rho, \tag{7.196}$$

becomes

$$\Phi(r) = \begin{cases} \frac{4\pi GM}{\Omega_{d-2}R^{d-1}} \frac{r^2}{2} \\ \\ -\frac{K_d}{r^{d-3}} \end{cases} \tag{7.197}$$

---

[9] c times the time coordinate has also length dimension.

From the continuity of the radial derivative, $\Phi'(r)$ at $r = R$ one obtains

$$\Phi'(R) = \frac{4\pi GM}{\Omega_{d-2}} R^{2-d} = (d-3) K_d R^{2-d}, \tag{7.198}$$

so

$$K_d = \frac{4\pi GM}{(d-3)\Omega_{d-2}}. \tag{7.199}$$

This potential is the fit of the Schwarzschild vacuum solution to the Einstein equations, so the metric factor, $f(r)$, becomes

$$f(r) = 1 - \left(\frac{R_d}{r}\right)^{d-3} \tag{7.200}$$

with $R_d^{d-3} = 2K_d/c^2$. The Unruh temperature at the Schwarzschild horizon is then given by

$$\frac{k_{\mathrm{B}}T}{\hbar c} = \frac{1}{4\pi} f'(R) = \frac{d-3}{4\pi R_d}. \tag{7.201}$$

Such black holes would – unfortunately – still evaporate by Hawking radiation.

A non-evaporating black hole (with zero Unruh temperature) is represented by an extremal Reissner–Nordstrøm solution. The higher dimensional pendant of the static radial electric field caused by a charge, contributing to the Lagrangian $\mathscr{L}$ and hence acting like a source term in the Einstein equations, is described by a $p+2$ form instead of a 2-form. The point charge is generalized to a charged p-brane in the d-dimensional spacetime. The electric flux then goes through a $d-p-2$-dimensional (spherical) surface and the Gauss law ensures that

$$\int\limits_{S_{d-p-2}} {}^{*}F_{p+2} = Q. \tag{7.202}$$

In the most quoted ten-dimensional bosonic supergravity action, a low energy approximation to string theory, there is in addition a scalar field, called the dilaton. It couples to the curvature term multiplicative. The total action is given by

$$S = \frac{1}{L_{\mathrm{s}}^8} \int d^{10}x \sqrt{-\det g}\, \mathscr{L} \tag{7.203}$$

with the Lagrangian

$$\mathscr{L} = \mathrm{e}^{-2\Phi}\left(\mathscr{R} + 4(\nabla\Phi)^2\right) + \frac{2}{(8-p)!} {}^{*}F_{p+2} \wedge F_{p+2}. \tag{7.204}$$

Here, the ∇ operator acts covariant. This is a ten-dimensional gravity problem with p-brane electromagnetic field contributions and a scalar field behaving like a conformal factor to the Ricci scalar. The ten-dimensional gravity coupling strength is related to the string length parameter, L_{s} as $G_{10} = 8\pi^6 g_{\mathrm{s}}^2 L_{\mathrm{s}}^8$. The string length parameter is actually related to the Regge slope of the string theory by $L_s^2 = \alpha'$ and hence to the string tension $\kappa = 1/2\pi\alpha'$. Finally $g_s = e^{\Phi_v}$ by replacing a constant vacuum expectation value for the dilaton field.

The solution of the corresponding equations yields a metric similar to the Reissner–Nordstrøm one.

$$ds_{10}^2 = -f_+ \frac{c^2 dt^2}{\sqrt{f_-}} + \sqrt{f_-} ds_p^2 + g \frac{d\rho^2}{f_+ f_-} + g\rho^2 d\Omega_{8-p}^2, \tag{7.205}$$

with

$$f_\pm = 1 - \frac{r_\pm^{7-p}}{\rho^{7-p}} \tag{7.206}$$

and

$$g = f_-^{\frac{1}{2} - \frac{5-p}{7-p}}. \tag{7.207}$$

Moreover, ds_p^2 is the flat metric arc length square on the p-brane and $d\Omega_{8-p}^2$ is the angular differential squared in $8-p$ dimensions. With the time coordinate, ct and the distance ρ we have altogether ten dimensions. The roots $r_\pm$ are connected to the scaled mass and charge causing the RN-metric. It is natural that in d spacetime dimensions static and "radial"-symmetric solutions have $d-2$ degrees of freedom left. Since we have a charge living on a p-brane, the remaining space, the out-of-brane world, has $d-2-p$ dimensions. For $d = 10$ it is $8-p$, the dimension of the angular variable in the metric (7.205). The gravitational and the Coulomb potential both are solutions obtained by inverting a "partial" Laplacean operator with a source on a p-brane: the Gauss-theorem measuring the flux of the gradient of such potentials considers then an integral surface scaling like ρ^{d-2-p}. No wonder that the potentials themselves are like $\Phi \sim \rho^{3+p-d}$. In the more familiar framework of classical physics one deals with a $d = 4$-dimensional spacetime and usually with $p = 0$ point charges. There $\Phi \sim \rho^{-1}$ is the form of a static potential. In superstring theory the surmised proper dimensionality is $d = 10$, leading to static potentials like $\Phi \sim \rho^{p-7}$. Accounting for Newtonian gravity and Coulomb's law far from the brane, also the metric must have such factors.

The classical Reissner–Nordstrøm factor now looks like

$$f(\rho) = 1 - \frac{2\tilde{M}}{\rho^a} + \frac{\tilde{Q}^2}{\rho^{2a}} \tag{7.208}$$

with $a = 7-p$.

The horizon condition has a general form of

$$\rho^{2a} f_+(\rho) f_-(\rho) = \left(\rho^a - \alpha r_+^a\right)\left(\rho^a - \beta r_-^a\right) = 0, \tag{7.209}$$

resulting in the following correspondence between the roots of this equation and the physical mass and charge causing the RN-metric under discussion:

$$\begin{aligned} 2\tilde{M} &= \alpha r_+^a + \beta r_-^a, \\ \tilde{Q}^2 &= \alpha\beta\, r_+^a\, r_-^a. \end{aligned} \tag{7.210}$$

The string theory length scales for the mass and the charge are respectively proportional to $\tilde{M} \sim 1/g_s^2 L_s^8$ and $\tilde{Q} \sim 1/g_s L_s^a$. For the RN-metric $\tilde{M}$ and $\tilde{Q}^2$ must have the same physical string dimension, this points out that in order to explain our 4-dimensional spacetime one has to consider $\tilde{M} \sim \tilde{Q}^2 \sim 1/L_s^8 \sim 1/L_s^{2a}$, selecting out a special dimensionality for the charged brane. Namely due to $2a = 2(7-p) = 8$ one obtains $p = 3$.

Let us continue with an extremal RN-solution, $\tilde{M} = \tilde{Q}$ and therefore $r_+ = r_- = R$. In this case the metric simplifies to

$$\mathrm{d}s_{10}^2 = \sqrt{f}\left(-c^2\mathrm{d}t^2 + \mathrm{d}s_p^2\right) + f^{\frac{1}{2}-\frac{5-p}{7-p}}\left(\frac{\mathrm{d}\rho^2}{f^2} + \rho^2\mathrm{d}\Omega_{8-p}^2\right). \tag{7.211}$$

with ρ still being the radial distance from the p-brane and with f_+ and f_- coinciding. We denoted their common square by f,

$$f(\rho) = 1 - \frac{R^{7-p}}{\rho^{7-p}} = 1 - \frac{R^a}{r^a}. \tag{7.212}$$

We recognize the $(p,1)$ Minkowski metric, $\mathrm{d}s_{(p,1)}^2 = -c^2\mathrm{d}t^2 + \mathrm{d}s_p^2$, in the first brackets. This ten-dimensional metric has a more transparent form using the parameter $a = 7-p$,

$$\mathrm{d}s_{10}^2 = \sqrt{f}\mathrm{d}s_{(7-a,1)}^2 + \frac{f^{2/a}}{\sqrt{f}}\left(\frac{\mathrm{d}\rho^2}{f^2} + \rho^2\mathrm{d}\Omega_{a+1}^2\right). \tag{7.213}$$

In our world, $a = 4$ and

$$\mathrm{d}s_{10}^2 = \sqrt{f}\mathrm{d}s_{(3,1)}^2 + \frac{\mathrm{d}\rho^2}{f^2} + \rho^2\mathrm{d}\Omega_5^2 \tag{7.214}$$

with

$$f = 1 - \frac{R^4}{r^4}. \tag{7.215}$$

For getting closer to a more standard AdS form of the metric, let us introduce a new coordinate, measuring the distance from the horizon at $\rho = R$. We define it implicitly by

$$\rho^a = R^a + r^a. \tag{7.216}$$

By the virtue of this we obtain $f = 1 - (R/\rho)^a = (r/\rho)^a$ and $\mathrm{d}\rho = (r/\rho)^{a-1}\mathrm{d}r$. The metric form becomes

$$\mathrm{d}s_{10}^2 = \left(\frac{r}{\rho}\right)^{a/2} \mathrm{d}s_{(7-a,1)}^2 + \left(\frac{r}{\rho}\right)^{-a/2} \mathrm{d}r^2 + \left(\frac{r}{\rho}\right)^{2-a/2} \rho^2 \mathrm{d}\Omega_{a+1}^2. \tag{7.217}$$

In particular for the physically interesting $p = 3$, $a = 4$ case we arrive at

$$\mathrm{d}s_{10}^2 = \frac{r^2}{\rho^2}\mathrm{d}s_{(3,1)}^2 + \frac{\rho^2}{r^2}\mathrm{d}r^2 + \rho^2 \mathrm{d}\Omega_5^2, \tag{7.218}$$

with $\rho^4 = R^4 + r^4$.

Near to the horizon $\rho \approx R$ and the metric can be casted into a form consisting of two flat parts combined in a way already studied earlier by the AdS and Rindler spaces. One writes

$$\mathrm{d}s_{10}^2 \approx \frac{r^2}{R^2}(-c^2\mathrm{d}t^2 + \mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2) + \frac{R^2}{r^2}\mathrm{d}r^2 + R^2\mathrm{d}\Omega_5^2. \tag{7.219}$$

Here, the last term is the contribution of the differential arc on S_5, a 5-dimensional spherical surface, and the rest is isometric to a 5-dimensional AdS spacetime, AdS_5. The latter can be viewed as the metric on a 5-dimensional hyperboloid embedded in 6-dimensional spacetime with signature $(-,-,+,+,+,+)$.

The horizon is at $r = 0$, the acceleration is given by $g/c^2 = -f'(R)/2 = 1/2R$. The Unruh temperature becomes $k_\mathrm{B}T/\hbar c = 1/4\pi R$.

Finally, let us mention some further peculiar features of the choice $p = 3$. The radius of the event horizon satisfies the scaling $R^{7-p} \propto g_\mathrm{s} Q L_\mathrm{s}^{7-p}$. The charge, Q, will be related to the number of color components in the corresponding conformal field theory, $Q \sim N$. The dilaton field is related to the metric scale factor as

$$\mathrm{e}^{-2\Phi} = \frac{1}{g_\mathrm{s}^2} h^{\frac{3-p}{4}}(r). \tag{7.220}$$

It can have a constant value for exactly $p = 3$, when $h(r) = 1 + (R/r)^4$ and $R = 4\pi g_\mathrm{s} N L_\mathrm{s}^4$. This is the case, which is especially interesting: the factor $4\pi g_\mathrm{s} = g_\mathrm{SYM}^2$ is related to a super Yang–Mills field theory coupling, which should be dual to the near-horizon ten-dimensional gravity [77,78]. The weak coupling approach requires $N g_\mathrm{SYM}^2 = (R = L_\mathrm{s})^4 \ll 1$. At the other end, for a strongly coupled super Yang–Mills theory, the horizon is much larger than the string length parameter, $R/L_\mathrm{s} \gg 1$. Similarly, demanding that this size is much larger than the quantum scale of the Planck length, leads to $(R/L_\mathrm{P})^4 \sim N \gg 1$, to the large number of colors (N) limit of Yang–Mills theory. By a duality transformation a strong and a weak string coupling can be interchanged, $g_\mathrm{s} \to 1/g_\mathrm{s}$, but N has to remain large in order not to run into quantum gravity problems while relying on the AdS/CFT correspondence.

7.3.4 Higher Dimensional Gravity and Plasma Equation of State

It is quite intriguing to consider the correspondence between black holes and a high temperature plasma of particles. At very high temperature all particles behave as they were massless (any mass is negligible besides the thermal energy, $mc^2 \ll k_B T$). In such a case, the entropy density must be proportional to $s \sim T^3$ in $d = 3$ spatial dimensions. The $S(T,V) = aVT^3$ relation is a form of the equation of state for a plasma of massless excitations at temperature T in volume V, the coefficient a counting for the number of degrees of freedom. The same relation follows from $e = 3p$, when the energy–momentum tensor of a perfect fluid is traceless, $T_i^{\,i} = 0$. Since this property of T_{ij} is univalent for conformal metrics, the high temperature limit corresponds to this conformal limit.

The interesting mathematical fact is that – in some spacetime dimensions – near a black hole horizon a similar relation can be established between the entropy and the temperature. Moreover even the coefficient counting for the degrees of freedom can be equated between a certain type of near-horizon black hole metric and a special supersymmetric plasma of massless bosons and fermions. We briefly recapitulate here the main arguments, following the work of Gubser, Klebanov, and Peet [83].

Let us start with the equation of state of a plasma of massless particles in volume V at temperature T (we use here units such that $k_B = 1$, $\hbar = 1$ and $c = 1$). The total energy is given by $E = 3aVT^4$, while the total entropy by $S = 4aVT^3$. From the ratio of these two expressions $T = 4E/3S$ and

$$S = 4(aV)^{1/4}(E/3)^{3/4}. \tag{7.221}$$

For a super Yang–Mills theory there are altogether $2\mathcal{N}$ massless particle types: to each half bosons and fermions, respectively. Each massless degree of freedom contributes by a factor of $\pi^2/12$ to the entropy. Considering N copies of branes where strings may end on, the effective number of degrees of freedom becomes $2\mathcal{N}N^2$, therefore one considers

$$a = \frac{\pi^2}{48} 2\mathcal{N}N^2. \tag{7.222}$$

Counting everything together and taking a box of size L as the volume ($V = L^3$) we arrive at

$$\boxed{S = \frac{\pi^2}{6} \mathcal{N}N^2 V T^3} \tag{7.223}$$

or expressed via the microcanonical $S(E)$ form

$$S = \frac{2}{3}\left(\pi^2 2\mathcal{N}N^2\right)^{1/4} (EL)^{3/4}. \tag{7.224}$$

How can a black hole simulate this relation? Or the more elementary $E = \frac{3}{4}TS$ relation? A simple Schwarzschild black hole has an energy $E = M = RM_{\text{P}}/2L_{\text{P}}$ an Unruh temperature of $T = M_{\text{P}}L_{\text{P}}/4\pi R$ and the entropy $S = \pi R^2/L_{\text{P}}^2$ in $c = 1$ units. These values satisfy $E = 2TS$, not the one we are seeking for.

For a Reissner–Nordstrøm black hole $T = \Delta/4\pi r_+^2$ and $S = \pi r_+^2$, so we have $TS = \Delta/4 = \sqrt{\tilde{M}^2 - \tilde{Q}^2}/2$. This is smaller than M, and so is the required plasma energy $3TS/4$.

These coefficients are different for a ten-dimensional black hole, stemming from string theory. In this case the goal is to describe finite temperature, so the Reissner–Nordstrøm solution in the background is not extremal. Since the constancy of the dilaton field singles out $p = 3, a = 4$, we deal with the equation (7.205) for this case:

$$\mathrm{d}s_{10}^2 = -f_+ \frac{c^2 \mathrm{d}t^2}{\sqrt{f_-}} + \sqrt{f_-}\,\mathrm{d}s_3^2 + \frac{\mathrm{d}\rho^2}{f_+ f_-} + \rho^2 \mathrm{d}\Omega_5^2. \tag{7.225}$$

Note that here the factor $g(r) = 1$ becomes trivial. On the other hand no Minkowski spacetime part can be factorized out for non-extremal RN black holes. The product of the factors f_+ and f_- define the horizons

$$f_+ f_- = \left(1 - \frac{r_+^4}{\rho^4}\right)\left(1 - \frac{r_-^4}{\rho^4}\right). \tag{7.226}$$

For the purpose of later simplifications it is useful to introduce the quantity r_0 defined by the relation $r_0^4 = r_+^4 - r_-^4$ and the factor

$$h(r) = 1 - \frac{r_0^4}{r^4}. \tag{7.227}$$

Naturally, r will be a new radial coordinate replacing ρ. We do this by requiring

$$\rho^4 = r_-^4 + r^4. \tag{7.228}$$

This formula leads to $\rho^3 \mathrm{d}\rho = r^3 \mathrm{d}r$ and

$$\begin{aligned} f_+ &= 1 - \frac{r_+^4}{r_-^4 + r^4} = \frac{r^4 - r_0^4}{\rho^4} \\ f_- &= 1 - \frac{r_-^4}{r_-^4 + r^4} = \frac{r^4}{\rho^4}. \end{aligned} \tag{7.229}$$

Substituting these expressions into the metric (7.225) we arrive at

$$\mathrm{d}s_{10}^2 = -\bar{f}(r)\,c^2 \mathrm{d}t^2 + \frac{\mathrm{d}r^2}{\bar{f}(r)} + \frac{r^2}{\rho^2}\mathrm{d}s_3^2 + \rho^2 \mathrm{d}\Omega_5^2 \tag{7.230}$$

with

$$\bar{f}(r) = \frac{r^2}{\rho^2} h(r). \tag{7.231}$$

The horizon in these coordinates is defined by $h(r) = 0$ leading to $r = r_0$. In order to obtain the corresponding Unruh temperature we have to calculate the derivative of the factor $\bar{f}(r)$ responsible for a coordinate singularity at $r = r_0$. Using the definition (7.228), this factor is given by

$$\bar{f}(r) = \frac{1}{\sqrt{r_-^4 + r^4}} \left(r^2 - \frac{r_0^4}{r^2} \right). \tag{7.232}$$

The acceleration at the horizon is given by the derivative of this function at $r = r_0$. One obtains

$$\bar{f}'(r) = \frac{1}{\rho^6} \left((4r_0^4 + 2r_-^4) r + \frac{2r_0^4 r_-^4}{r^3} \right) \tag{7.233}$$

and by the virtue of this result at the horizon the following acceleration reigns

$$\frac{g}{c^2} = \frac{2r_0}{r_+^2}. \tag{7.234}$$

The corresponding Unruh temperature is given by

$$\frac{k_\mathrm{B} T}{\hbar c} = \frac{r_0}{\pi r_+^2}. \tag{7.235}$$

Turning it around, the scale factor at the horizon can be expressed by the temperature as $r_0/R = \pi R T$ with $R = r_+$ and $\hbar = c = k_\mathrm{B} = 1$. Near the horizon $R = r_+ \approx r_- \approx \rho$ holds to leading order.

The entropy is now calculated from the 8-dimensional area spanned by the three coordinates (x, y, z) included in $\mathrm{d}s_3$ and the five other ones incorporated in the $R\,\mathrm{d}\Omega_5$ differential. This includes a normal three-volume, L^3, but each length scaled with the factor r_0/R:

$$A_8 = \Omega_5 R^5 \frac{r_0^3}{R^3} V_3. \tag{7.236}$$

Now considering the string theory correspondence mentioned in the previous subsection one uses the scale $R^4 = 4\pi g_\mathrm{s} L_\mathrm{s}^4 N^2$ and the effective ten-dimensional Newton constant $G_{10} = 8\pi^6 g_\mathrm{s}^2 L_\mathrm{s}^8 = \pi^4 R^8 / 2N^2$. Utilizing this and the expression of the scale factor at the horizon [following from (7.235)] the black hole entropy is given by

$$S_8 = \frac{1}{4G_{10}} A_8 = \frac{\pi^2}{2} N^2 V_3 T^3. \tag{7.237}$$

Comparing this with the entropy of massless string gas [cf. (7.223)], one concludes that the black hole entropy is

$$S_8 = \frac{3}{\mathcal{N}} S_{\mathrm{SYM}}. \tag{7.238}$$

For the $\mathcal{N} = 4$ super Yang–Mills theory this means a factor of $3/4$ less entropy stored inside the 8-dimensional black hole horizon than in the high temperature plasma of four types of fermions and bosons. Since the conjecture between these two theories is the duality, one interprets this result that $1/4$-th of the degrees of freedom "freeze" when going from weakly coupled to strongly coupled super Yang–Mills plasma. As if always the transverse polarization degrees of freedom would survive, and one of the four possibilities, i.e. the longitudinal polarization in our spacetime were confined.

7.3.5 Lower Bound for the Shear Viscosity

Another hot topic of the last decade was a prediction of a lower bound for the shear viscosity of matter in general [84]. The shear viscosity measures the effectivity of momentum transfer between differently moving fluid parts across streamlines. The corresponding dissipative part of the energy–momentum tensor, representing an anisotropic pressure term, is proportional to the gradient of flow velocity to leading order in a linear response model. If the x-component of the flow varies in the y-direction, one has

$$\delta T_{xy} = -\eta \frac{\partial u_x}{\partial y}. \tag{7.239}$$

Physically, the anisotropic pressure part is a force per area, defined as the momentum x-component transfer in y-direction per unit time. Since such a momentum transfer microscopically occurs within a mean free path, related to particle density and (transfer) cross section, $\lambda = 1/n\sigma$, one estimates

$$\delta T_{xy} \approx -n u_y \lambda \frac{\partial p_x}{\partial y} = -\frac{u_y}{\sigma} \frac{\partial p_x}{\partial y}. \tag{7.240}$$

However, for particles with a fixed mass the momentum is proportional to the velocity, so

$$u_y \frac{\partial p_x}{\partial y} = p_y \frac{\partial u_x}{\partial y}. \tag{7.241}$$

Comparing now (7.240, 7.239) and estimating the magnitude of momentum in a thermal fluid with very high temperature, $T \gg m$ one concludes that the shear viscosity coefficient, η is in general related to the cross section as

$$\eta \approx \frac{\langle p_y \rangle}{\sigma} \approx \frac{T}{\sigma}. \tag{7.242}$$

More precisely the shear viscosity coefficient can be obtained in field theory by using the Kubo formula,

$$\eta = \lim_{\omega \to 0} \frac{1}{2\omega} \int \mathrm{d}t\mathrm{d}^3x \, \langle [T_{xy}(\mathbf{x},t), T_{xy}(\mathbf{0},0)] \rangle. \tag{7.243}$$

This formula connects the relaxation of δT_{xy} to the correlator of the equilibrium quantity, T_{xy}. The latter is an operator in the field theoretical treatment, its correlator is obtained from the exchange of the corresponding operators.

In the dual gravity calculation, following [83], one considers a graviton of frequency ω, polarized in the xy-plane as it propagates perpendicular to the black brane. The absorption cross section of the graviton on the brane is described by twice the imaginary part of the retarded Green function – in analogy to plasmon damping. Moreover, the Green function in question has to be the one coupled to the fluctuations of the metric tensor component g_{xy}, which is exactly the energy–momentum tensor component, T_{xy}.[10] This way the absorption cross section in the ten-dimensional theory is given by

$$\sigma_{10}(\omega) = -\frac{16\pi G}{\omega} \mathrm{Im}\, G^{\mathrm{ret}}(\omega), \tag{7.244}$$

which is nothing else than the correlator

$$\sigma_{10}(\omega) = \frac{8\pi G}{\omega} \int \mathrm{d}t\mathrm{d}^3x \, \langle [T_{xy}(\mathbf{x},t), T_{xy}(\mathbf{0},0)] \rangle. \tag{7.245}$$

This way this graviton absorption cross section simply determines the shear viscosity coefficient [cf. (7.243)]:

$$\eta = \frac{\sigma_{10}(0)}{16\pi G_{10}} \tag{7.246}$$

by using $\hbar = c = k_{\mathrm{B}} = 1$ units.

It has been shown by Kovtun, Son and Starinets [84] that $\sigma_{10}(0)$ is calculable from solving the linearized Einstein equations for metric tensor perturbations. It turns out that it cannot be smaller than the horizon area divided by the three-volume:

$$\sigma_{10}(0) \geq A_8/V_3. \tag{7.247}$$

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[10] One should remember that T_{ij} is derived by varying the matter part of the action with the metric tensor.

Comparing this with the entropy of the black hole given in (7.237) one concludes that the shear viscosity is bound from below by the entropy density $s = S_8/V_3$:

$$\eta \geq \frac{1}{4\pi} s. \tag{7.248}$$

Restoring SI units the shear viscosity coefficient to entropy density ratio is bounded from below by $\eta/s \geq \hbar/4\pi k_B$. It was a very exciting moment, when the heavy ion experiment at RHIC presented evidence that the presumed quark matter formed in some of these violent collisions shows flow properties with a shear viscosity very close to this lower bound [80].

However, a caveat was made to this story by some later theoretical discoveries of models, where *this lower bound can yet be undergone*. This may be achieved e.g. by gravity terms nonlinear in the Ricci scalar of the ten-dimensional theory [80]. On the other hand, at finite chemical potential for fermions another energy scale enters into the calculation of the shear viscosity invalidating the naive estimate.

Problems

7.1. Prove that R^2 is flat in polar coordinates. The arc length squared is given as $\mathrm{d}s^2 = \mathrm{d}r^2 + r^2 \mathrm{d}\vartheta^2$. Note that not all Christoffel symbol elements are zero, but the Riemann tensor components.

7.2. Prove that S^2, the surface of the unit sphere, has a constant curvature. The metric tensor is given by $\mathrm{d}s^2 = \mathrm{d}\theta^2 + \sin^2\theta \mathrm{d}\phi^2$.

7.3. Obtain the entropy for an extremal Reissner–Nordstrøm black hole with cosmological constant, $\lambda = -3/a^2 L_P^2$, according to the formula (7.134).

7.4. Prove that (7.184) leads to a linear velocity profile.

7.5. Find the coordinate transformation to embed the metric (7.219) as a five-dimensional hyperboloid surface in six dimensions.

7.6. Prove that the volume of the 5-dimensional spherical hypersurface is $\Omega_5 = \pi^3$.

7.7. Obtain the horizon-entropy for a Reissner–Nordstrøm black hole with fixed charge to mass ratio, $\tilde{Q} = \mu \tilde{M}$ in Planck scale units, in the presence of a de Sitter-type cosmological constant term with $\lambda = -3/a^2$.

Chapter 8
The Temperature in Quantum Field Theory

Imaginary time formalism and the KMS relation, finite temperature Green functions, and Matsubara frequencies. Non-equilibrium Green functions, off-shell effects in the kinetic theory. Stochastic and chaotic quantization.

8.1 Imaginary Time Formalism

In the quantum description of statistical physics, the basic extensive quantities, like the total energy, charge or entropy, are described by Hermitean operators instead of real functions. Hermitean operators do have real eigenvalues, so the expectation values of such operators in a mixture of their eigenstates give back the classical real valued picture. However, a basic condition is that all operators have a common set of eigenvectors; with other words they are commuting. This is the case for a Hamilton operator, H, and a particle counting operator, N, if $[H,N] = HN - NH = 0$. This happens "automatically" if the associated charge carried by the particle is conserved.[1]

The entropy, the partition function and in general the thermal averages are expressed by the help of the *density operator*, ρ. Having a general time-dependent operator,[2] its statistical average is given by

$$\langle A(t) \rangle = \mathrm{Tr}\,(\rho A(t)) . \tag{8.1}$$

For depicting the underlying concept clearly, we restrict ourselves in the followings to the canonical density matrix

$$\rho = \mathrm{e}^{-\beta H} \tag{8.2}$$

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[1] In general, the commutators of two operators in the quantum theory vanish if their predecessors in the classical mechanics have a vanishing Poisson bracket.

[2] This is the so called Heisenberg picture.

T.S. Biró, *Is There a Temperature? Conceptual Challenges at High Energy, Acceleration and Complexity*, Fundamental Theories of Physics 171,
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with H being the Hamilton operator and $\beta = 1/k_{\mathrm{B}}T$ the usual thermal parameter. Since the states in the Schrödinger representation evolve according to the solution of the Schrödinger equation, $i\hbar \mathrm{d}\psi/\mathrm{d}t = H\psi$, the time dependence of operators in the Heisenberg picture is governed by the same Hamiltonian:

$$A(t) = \mathrm{e}^{\frac{i}{\hbar}tH} A(0)\, \mathrm{e}^{-\frac{i}{\hbar}tH}. \tag{8.3}$$

This way the canonical statistical weight and the time evolution factor due to quantum mechanics both occur in an exponential form; in fact these two can be unified by considering a complex time argument, $\tau = t + i\hbar\beta$,

$$\mathrm{e}^{-\beta H}\, \mathrm{e}^{\frac{i}{\hbar}tH} = \mathrm{e}^{\frac{i}{\hbar}\tau H}. \tag{8.4}$$

We note that $\hbar\beta = \hbar/k_{\mathrm{B}}T$ is an inverse frequency according to Planck's law of the black body radiation (cf. Chap. 3). The expectation value (8.1) can be then expressed in an alternative form. First one utilizes the Heisenberg form (8.3) to obtain

$$\langle A(t) \rangle = \mathrm{Tr}\left(\mathrm{e}^{-\beta H} \mathrm{e}^{\frac{i}{\hbar}tH} A(0)\, \mathrm{e}^{-\frac{i}{\hbar}tH} \right). \tag{8.5}$$

This expression equals to

$$\langle A(t) \rangle = \mathrm{Tr}\left(\mathrm{e}^{\frac{i}{\hbar}\tau H} A(0)\, \mathrm{e}^{-\frac{i}{\hbar}\tau H}\, \mathrm{e}^{-\beta H} \right) = \langle A(\tau) \rangle \tag{8.6}$$

It is not only that the thermal expectation value of a general time-dependent quantum operator is the same at another time argument shifted in the imaginary time direction. The above derivation can be repeated for the correlation function with another arbitrary operator, B:

$$C_{AB}(t) := \langle A(t)B(0) \rangle = \langle B(0)A(t + i\hbar\beta) \rangle, \tag{8.7}$$

based on the above. This is the famous *KMS* (Kubo–Martin–Schwinger) relation.

A remarkable consequence of this relation is the following: For bosonic systems the field operators at unequal times [$t \neq 0$ in the KMS formula (8.7)] do commute, so $A(t)B(0) = B(0)A(t)$ at arbitrary nonzero time argument. Therefore

$$\langle B(0)A(t) \rangle = \langle B(0)A(t + i\hbar\beta) \rangle. \tag{8.8}$$

This is possible only with periodic field operators,

$$A(t) = A(t + i\hbar\beta). \tag{8.9}$$

Fermionic field operators at unequal times on the other hand anticommute, therefore $A(t)B(0) = -B(0)A(t)$. This way we obtain

$$\langle B(0)A(t) \rangle = -\langle B(0)A(t + i\hbar\beta) \rangle. \tag{8.10}$$

This relation can be fulfilled only with anti-periodic operators in imaginary time:

$$A(t) = -A(t + i\hbar\beta). \tag{8.11}$$

We note that this result – although derived for the canonical statistical operator only – is valid for all ensembles and even for superstatistical systems, because these can be obtained by integration over the parameter β from the canonical one. Since the KMS relation (8.7) is linear in the statistical operator, it remains valid for this more general case, provided that the expectation value sign $\langle \dots \rangle$ includes the integration over a distribution of β values.

Finally, we demonstrate that the usual treatment of field operators as a mode sum is in accord with quantum statistics due to the KMS relation. A general expansion of a field operator contains quantum annihilation, a_k, and creation, $a_k^\dagger$ operators:

$$\Phi(t) = \sum_k \left(\phi_k a_k \mathrm{e}^{\mathrm{i}\omega_k t} + \phi_k^* a_k^\dagger \mathrm{e}^{-\mathrm{i}\omega_k t} \right), \tag{8.12}$$

assuming that ω_k is the eigenvalue of the Hamiltonian for the mode k. The time-dependent factors,

$$a_k(t) = a_k \mathrm{e}^{\mathrm{i}\omega_k t}, \qquad a_k^\dagger(t) = a_k^\dagger \mathrm{e}^{-\mathrm{i}\omega_k t}, \tag{8.13}$$

define the occupation "number,"

$$n_k(t) = \left\langle a_k^\dagger(t) a_k(0) \right\rangle. \tag{8.14}$$

It describes a complex probability amplitude to re-create a particle with quantum number k at time t which was annihilated at time zero. It is guaranteed to be a real number by the above definition. Due to the KMS relations for bosons and fermions we obtain

$$n_k(t + i\hbar\beta) = \langle a^\dagger(t + i\hbar\beta) a_k(0) \rangle = \left\langle a_k(0) a_k^\dagger(t) \right\rangle = 1 \pm n_k(t) \tag{8.15}$$

according to the elementary commutation relation $a_k^\dagger(t) a_k(0) = 1 \pm a_k(0) a_k^\dagger(t)$. On the other hand

$$a^\dagger(t + i\hbar\beta) = a_k^\dagger(t) \mathrm{e}^{\hbar\beta\omega_k} \tag{8.16}$$

due to (8.13). Putting this together with (8.15) one arrives at

$$\mathrm{e}^{\hbar\beta\omega_k} n_k(t) = 1 \pm n_k(t). \tag{8.17}$$

From here the familiar, time-independent quantum statistical formula for the occupation number of states in equilibrium follows:

$$n_k(t) = \frac{1}{\mathrm{e}^{\beta\hbar\omega_k} \pm 1}. \tag{8.18}$$

8.1.1 Green Function

Field theory at finite temperature is based on the unified treatment of fluctuations and correlations due to quantum effects on the one hand and due to thermal ensemble properties on the other hand. While in the first the non-localisability of the quantum mechanical wave function in ordinary space plays a prominent role, the second – more classical, but also more general – effect rather restricts our dynamical knowledge, by taking into account only statistical properties of some unknown or just unconsidered forces on the observed system or property. Although also quantum effects are sometimes referred to as being "statistical," or "probabilistic," their true nature is unlike the classical statistical physics: Quantum effects do occur in the basic laws of nature, causing that the theory cannot follow exact particle paths singled out by solving a given equation of motion; rather an infinite bundle of interfering paths should be taken into account. This also means that the concept of point particle has only a limited use in field theory.

The propagation of a particle in space and time is in fact a correlation between two events: the creation and the annihilation of the quantum state describing the particle with its physical properties (charge, spin, mass, etc.) and actual state of motion (energy, momentum). Viewing the propagator as a correlation, it is just the basic element in an infinite hierarchy of all possible correlations referring to several spacetime points characterizing an event. Such correlations are called *n-point functions* in general. In particular, the propagator is a two-point function.

All n-point function for an even number, $n = 2m$, can be viewed as a property connected to a quantum transition amplitude involving m particles. This possibility is, however, only theoretical, since very often an m-particle state cannot be disentangled to m separate one-particle states. Not only that there are strong interactions which do not cease to act between such elementary particles, like quarks and gluons, being bound by the *confinement principle*, but also the density of particles can be so high in nature – and for a while in physics experiments – that the individuality cannot be established, not even approximately. Especially it is a delicate question, whether a given elementary particle is "there," whether is it already formed (and when was it formed exactly) in a given reaction. Although zero temperature field theory operates with the concept of *asymptotically free* states, and any interaction is taken into account perturbatively, the real properties of even a single, lonesome particle become definite only after an infinite time.[3] In particular, the physical *dispersion relation*, identifying the particle's rest mass, is encoded in the 2-point function (in the propagator). After calculating the effect of physical interactions this result has to be a meaningful and therefore finite relation between momentum, energy and mass. The procedure to achieve this by starting a theoretical description of fields and their interactions involving "bare" parameters, is called *renormalization*.[4]

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[3] Assumed that all interactions are switched off with a satisfactorily converging rate in time.

[4] This procedure often involves cancelation of infinite quantities, but this is not a prerequisite for renormalization; finite theories also have to be renormalized.

Since the propagator stands for the one of the simplest quantities in field theory reflecting the basic conceptual features, we discuss shortly this quantity for very simple systems, like a harmonic oscillator, in order to elucidate its relations to questions of causality and thermodynamics. We analyze now a harmonic oscillator, its dynamics is described by the following simple differential equation[5]

$$\ddot{x}+\omega_0^2 x = f(t). \tag{8.19}$$

Here, the double dot denotes second derivative with respect to the time argument, and $f(t)$ is the accelerating effect of a generally unknown external force. The eigenfrequency, ω_0 may depend on several parameters, in a field theory most prominently on the wave number vector $\mathbf{k}$. Here, we concentrate on the dynamical behavior in time and its connection to the imaginary time periodicity. The $x(t)$ "response" of the oscillator to the external effect $f(t)$ is described by the Green function:

$$x(t) = \int\limits_{-\infty}^{\infty} G(t,t')f(t')\mathrm{d}t'. \tag{8.20}$$

Let us denote the total structure of the left hand side of (8.19) by $Dx(t)$. This way

$$Dx(t) = D\int\limits_{-\infty}^{\infty} G(t,t')f(t')\mathrm{d}t' = f(t) \tag{8.21}$$

leads to the evolution equation for the Green function, G:

$$DG(t,t') = \delta(t-t'). \tag{8.22}$$

This is a relation involving the Dirac-delta distribution. It can be comprised into a simpler form by Fourier transformation. Replacing

$$G(t,t') = \int\limits_{-\infty}^{\infty} G(\omega)\,\mathrm{e}^{-\mathrm{i}\omega(t-t')}\,\frac{\mathrm{d}\omega}{2\pi} \tag{8.23}$$

into the above equation one concludes that

$$G(\omega) = \frac{1}{\omega_0^2-\omega^2}. \tag{8.24}$$

This result, however, does not fix all the problems. When one likes to obtain the time representation of the Green function, the Fourier transformation meets an expression with two poles, sitting on the real axis at $\omega = \pm\omega_0$. This causes an ambiguity by choosing the integration pathway in the complex ω-plane. This ambiguity is resolved based on the following physical considerations.

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[5] This is an example of the $0+1$-dimensional field theory.

Let us now supplement our model by friction. This force is proportional to the velocity $\dot{x}$ and – at least in the classical context – has a definite sign. The dynamical equation of motion becomes

$$\ddot{x}+2\delta\dot{x}+\omega_0^2 x = f(t). \tag{8.25}$$

After Fourier-expanding $x(t)$ as,

$$x(t)=\int\limits_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-\mathrm{i}\omega t}x(\omega), \tag{8.26}$$

one obtains the equation for the Green function in frequency-representation:

$$\left(-\omega^2-2i\delta\omega+\omega_0^2\right)G(\omega)=1. \tag{8.27}$$

Using this result one realizes that the Green function,

$$G(\omega)=\frac{1}{-\omega^2-2i\delta\omega+\omega_0^2}=\frac{-1}{(\omega-\omega_+)(\omega-\omega_-)}, \tag{8.28}$$

has poles,

$$\omega_\pm=-i\delta\pm\sqrt{\omega_0^2-\delta^2}=-i\delta\pm E, \tag{8.29}$$

moved away from the real ω-axis for finite friction coefficient, δ. In a general – quantum – context, this coefficient can also be a complex parameter. Considering namely a Schrödinger equation for an energy-eigenstate wave function with a time-dependent external disturbance term,

$$i\hbar\frac{\partial}{\partial t}\psi-E\psi=J(t), \tag{8.30}$$

with the energy eigenvalue E, one derives the following oscillator-like equation by the repetition of the time derivation operator:

$$\hbar^2\frac{\partial^2}{\partial t^2}\psi+E^2\psi=-EJ-i\hbar\frac{\partial}{\partial t}J. \tag{8.31}$$

It is alike the oscillator equation (8.19), but with a complex $x(t)=\psi$ and $f(t)=-EJ-\hbar\partial J/\partial t$. In this case, the friction coefficient can also be considered as a complex parameter. As a consequence, the poles of the Green function (8.28) may lie in any of the quadrants on the complex omega plane. Correspondingly four different Green functions can be defined.

The time-dependent propagator is calculated by a Fourier integral from (8.28). By doing so a closed path is used in the complex ω-plane including a large part of the real axis between say $-R$ and $+R$. The path is closed by an arc of a circle with radius R, so on this curve one has $\omega=R\mathrm{e}^{\mathrm{i}\varphi}$ with constant R. And here enters causality into the game. Namely, depending on whether the upper arc or the lower arc can be chosen by the requirement of convergence,

$$\lim_{R\to\infty}\int\limits_0^{\pi}\frac{d\varphi}{2\pi}\,iRe^{i\varphi}\,G(Re^{i\varphi})\,e^{-iRe^{i\varphi}(t-t')}<\infty,\tag{8.32}$$

the real-time propagator, $G(t,t')$, sometimes becomes identically zero. This means that for given arrangements of the time arguments t and t' there is *no correlation* between the external action $f(t)$ and the system's response $x(t)$ to that. In particular, for the harmonic oscillator one determines

$$\int\limits_0^{\pi}\frac{d\varphi}{2\pi}\,iRe^{i\varphi}\,G(Re^{i\varphi})\,e^{-iRe^{i\varphi}(t-t')}=\int\limits_0^{\pi}\frac{d\varphi}{2\pi}\,\frac{-iRe^{i\varphi}e^{-iRe^{i\varphi}(t-t')}}{(Re^{i\varphi}-\omega_+)(Re^{i\varphi}-\omega_-)}\tag{8.33}$$

which for $R\to\infty$ approximates the expression

$$\int\limits_0^{\pi}\frac{d\varphi}{2\pi}\,\frac{1}{R}e^{-i(\varphi+\pi/2+R(t-t')\cos\varphi)}\,e^{R(t-t')\sin\varphi}.\tag{8.34}$$

Here, the decisive factor for convergence is $(t-t')\sin\varphi$; whenever it is negative the integration contribution on the arc vanishes in the $R\to\infty$ limit. In these cases, the value of the integral over the closed semicircular path equals to the one along the real axis. The latter is what we are looking for.

Using the residuum theorem of complex analysis now the contributions to the real-time propagator are collected by residuum contributions from the complex poles of the integrand. By doing so one also has to pay care to the fact that for an upper semicircle one follows a counterclockwise path ($2\pi i$ factor in the residual theorem), while for a lower semicircle an oppositely directed path ($-2\pi i$ factor). Taking this all into account one encounters the following cases:

1. Both poles lie in the lower half plane (the classical solution with $\delta>0$). The lower arc contribution vanishes for $t\geq t'$, since in this case $t-t'\geq 0$ and $\sin\varphi$ is negative, their product is negative. Otherwise, for $t<t'$, the upper arc closes the path of convergent integration. Not having any pole in the upper plane, the propagator itself is zero in such cases; it has nonzero contributions only for $t>t'$. We denote this fact by using the Heaviside function: $G(t,t')=\Theta(t-t')\,(\mathrm{Res}(\omega_+)+\mathrm{Res}(\omega_-))$. This is called the *retarded propagator*, characterized by $\mathrm{Im}\,\omega_\pm<0$. Evaluating the contributions of residua one obtains

$$G^R(t,t')=\Theta(t-t')\,\frac{\sin E(t-t')}{E}\,e^{-\delta(t-t')}$$

with $E = \sqrt{\omega_0^2 - \delta^2}$. It will be of use to introduce the complex factor

$$f(E) = \frac{1}{2iE}\,\mathrm{e}^{\mathrm{i}E(t-t')}. \tag{8.35}$$

Its complex conjugate belongs to the reflected pole, $f^*(E) = f(-E)$. Using also the abbreviation $\Theta = \Theta(t-t')$ and $\bar{\Theta} = \Theta(t'-t)$, the retarded propagator $G^R = G^R(t,t')$ has the following comprised form in the $\delta \to 0^+$ limit:

$$G^R = \Theta\,(f + f^*)\,. \tag{8.36}$$

2. Were it $\delta < 0$ (an imagined anti-friction), we had both poles in the upper half plane. The corresponding *advanced propagator*, $G^A = G^A(t,t')$, vanishes for $t < t'$:
$$G^A = -\bar{\Theta}\,(f + f^*)\,. \tag{8.37}$$
3. In the cases analyzed previously both poles were in retarded (causal) or advanced (anti-causal) positions. They actually can be ordered also in a mixed fashion, when considering quantum theory. Since the energy of a particle, in our simplified analysis the eigenfrequency of the harmonic oscillator, in relativistic theories may also be negative, there is a freedom to interpret negative energy states as the absence of a positive energy particle with opposite momenta and conserved charges. Such holes in the negative energy continuum are then regarded as packets of positive energy antiparticles, which propagate. Considering a causal (retarded) propagation both for positive energy particles and positive energy antiparticles (negative energy holes), one associates a positive friction to the positive energy pole and a negative one to the negative energy pole: $\omega_+ = -i\delta + E$, $\omega_- = i\delta - E$. In this case, the Green function is no more real, it can only be interpreted as a Green function belonging to a complex solution of the oscillator equation of motion. But exactly this is suggested by quantum mechanics. This Green function is called the *Feynman propagator*:
$$G^{\mathrm{F}} = \Theta f^* - \bar{\Theta} f. \tag{8.38}$$
This expression was also taken in the $\delta \to 0^+$ limit.
4. Conversely, an "anti-Feynman" propagator can be defined which is advanced for positive energy particles and antiparticles. In this case the poles are located as $\omega_+ = E + i\delta$ and $\omega_- = -E - i\delta$ (with $\delta > 0$) and one gets
$$\bar{G}^{\mathrm{F}} = \Theta f - \bar{\Theta} f^*. \tag{8.39}$$

Since the identity $\Theta + \bar{\Theta} = \Theta(t-t') + \Theta(t'-t) = 1$ holds, these four versions of propagators are linearly related

$$\bar{G}^{\mathrm{F}} + G^{\mathrm{F}} = G^R + G^A = (f + f^*)(\Theta - \bar{\Theta}). \tag{8.40}$$

It is enlightening to investigate the behavior of these quantities by the *time reversal* operation, i.e. by interchanging t and t'. One obtains $f(t',t) = -f^*(t,t')$ and the trivial interchange between Θ and $\bar{\Theta}$. It follows that the retarded and advanced propagator change their role by time reversal: $G^R(t',t) = G^A(t,t')$ and $G^A(t',t) = G^R(t,t')$. The Feynman propagator and its pendant are invariant against this transformation: $G^{\mathrm{F}}(t',t) = G^{\mathrm{F}}(t,t')$ and $\bar{G}^{\mathrm{F}}(t',t) = \bar{G}^{\mathrm{F}}(t,t')$. Since time reversal is equivalent to change ω to $-\omega$, the reflection of complex poles to the origin clearly reflects the above properties. Complex conjugation on the other hand exchanges only the Feynman propagators among each other, $G^{\mathrm{F}\,*} = \bar{G}^{\mathrm{F}}$. The combined CT-transformation of the above is equivalent to a reflection with respect to the real ω-axis.

One realizes easily that the above expressions for the propagators contain products of $\mathrm{e}^{\pm \mathrm{i}Et}$ factors. They can in fact be viewed as expectation values of differently ordered products of field operators using a second quantized formalism with b quantum annihilation and $b^\dagger$ quantum creation operators. Considering from now on a general (either bosonic or fermionic) field operator,

$$\phi(t) = \frac{1}{\sqrt{2E}} \left(\mathrm{e}^{-\mathrm{i}Et} b + \mathrm{e}^{\mathrm{i}Et} d^\dagger \right), \tag{8.41}$$

we obtain the following ordered expectation values [85]:

$$\begin{aligned} iG^{+-} &= \left\langle \phi(t)\phi(t')^\dagger \right\rangle = -if^* \left\langle bb^\dagger \right\rangle + if \left\langle d^\dagger d \right\rangle \\ \pm iG^{-+} &= \left\langle \phi(t')^\dagger \phi(t) \right\rangle = -if^* \left\langle dd^\dagger \right\rangle + if \left\langle b^\dagger b \right\rangle . \end{aligned} \tag{8.42}$$

Here, transition elements between states containing a different number of quanta are neglected. The upper sign is for bosons the lower sign is for fermions. Upon using the property $bb^\dagger \mp b^\dagger b = 1$ and $dd^\dagger \mp d^\dagger d = 1$, the difference (for fermions the sum) of the above two lines results in the following expectation value for the (anti-)commutator

$$(iG^{+-} - iG^{-+}) = \left\langle \phi(t)\phi(t')^\dagger \mp \phi(t')^\dagger \phi(t) \right\rangle = (-if^* \mp if)\, 1. \tag{8.43}$$

The retarded and advanced propagators can be expressed as the expectation values

$$\begin{aligned} G^R &= \pm i \left\langle \left[\phi(t), \phi(t')^\dagger\right]_\mp \right\rangle \Theta(t-t') = (f \pm f^*)\Theta, \\ G^A &= -i \left\langle \left[\phi(t), \phi(t')^\dagger\right]_\mp \right\rangle \Theta(t'-t) = \mp(f \pm f^*)\bar{\Theta}, \end{aligned} \tag{8.44}$$

denoting the sign in the commutator as an index. This way

$$G^A \mp G^R = \mp(f \pm f^*) = G^{+-} - G^{-+}.$$

The $+$ and $-$ upper index notation is well fit to the Feynman–Keldysh-diagram technique; in any expression by calculating transition amplitudes the products of propagators occur always with these indices fitted to each other.

A general propagator on the other hand has contributions depending on the occupation numbers, $n = \left\langle b^\dagger b \right\rangle$ and $\bar{n} = \left\langle d^\dagger d \right\rangle$. Taking into account the equations (8.42) one arrives at linear expressions:

$$\begin{aligned} G^{+-} &= \bar{n} f - (1 \pm n) f^*, \\ \pm G^{-+} &= (1 \pm \bar{n}) f - n f^*. \end{aligned} \tag{8.45}$$

The determinant of the coefficient matrix is $D = (1 \pm n)(1 \pm \bar{n}) - n\bar{n} = 1 \pm (n + \bar{n})$. These equations are consequent only if $(G^{+-})^* = \mp G^{-+}$ and $n^* = \bar{n}$.

It is customary to introduce time-ordered and anti-ordered expectation values:

$$iG^{--} = \left\langle \mathscr{T} \phi(t)\phi(t')^\dagger \right\rangle = \Theta(t-t') \left\langle \phi(t)\phi(t')^\dagger \right\rangle \pm \Theta(t'-t) \left\langle \phi(t')^\dagger \phi(t) \right\rangle \tag{8.46}$$

being the expectation value of the *time ordered* field operator product and

$$iG^{++} = \left\langle \overline{\mathscr{T}} \phi(t)\phi(t')^\dagger \right\rangle = \mp \Theta(t-t') \left\langle \phi(t')^\dagger \phi(t) \right\rangle + \Theta(t'-t) \left\langle \phi(t)\phi(t')^\dagger \right\rangle \tag{8.47}$$

its reverse, the *anti-time-ordered* product. In the time ordered product, operators belonging to a later time come to the left, those belonging to an earlier time come to the right. In vacuum $n = 0$, and the Feynman propagator is simply the expectation value of the time-ordered product of field operators. Note also that the following identity holds:

$$G^{--} + G^{++} = G^{-+} + G^{+-}. \tag{8.48}$$

Fourier transformation and interchange of the time arguments shows the anti-Hermitean properties of the Keldysh-propagators: $G_{12}^{--} = -G_{21}^{++\,*}$ and $G_{12}^{-+} = -G_{21}^{-+\,*}$, $G_{12}^{+-} = -G_{21}^{+-\,*}$.

8.1.2 Matsubara Frequencies

The equilibrium operators being periodic or anti-periodic in the imaginary time direction, their expectation values, in particular the propagators, also show periodicity. As a consequence their expansion into a Fourier series reveals special properties. Both bosons and fermions are periodic in the length of a double period, 2β. Therefore it is a common property that their series expansion in the imaginary time is given by a Fourier series

$$\begin{aligned} G(\tau) &= \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \mathrm{e}^{-i\tau\omega_n} G_n \\ G_n &= \frac{1}{2\beta} \int_{-\beta}^{\beta} G(\tau) \mathrm{e}^{i\tau\omega_n} \mathrm{d}\tau. \end{aligned} \tag{8.49}$$

Owing to the (anti-)periodicity $G(\tau-\beta)=\pm G(\tau)$, so following the above expansion

$$\sum_n \mathrm{e}^{-i\tau\omega_n}\mathrm{e}^{i\beta\omega_n}G_n=\pm\sum_n \mathrm{e}^{-i\tau\omega_n}G_n. \tag{8.50}$$

Combining it to a quantity which should be zero,

$$\sum_n\left(\mathrm{e}^{i\beta\omega_n}\mp 1\right)\mathrm{e}^{-i\tau\omega_n}G_n=0, \tag{8.51}$$

we conclude that only at certain frequencies can this requirement be fulfilled by arbitrary coefficients, G_n. These special frequencies are the *Matsubara frequencies*. For bosons these are the solutions of

$$\mathrm{e}^{i\beta\omega_n}=1, \tag{8.52}$$

i.e. all integer multiples of $2\pi/\beta$,

$$\omega_n=2n\pi\frac{k_{\mathrm{B}}T}{\hbar}. \tag{8.53}$$

For fermions, described by anti-commuting field operators, the Matsubara frequencies are solutions of

$$\mathrm{e}^{i\beta\omega_n}=-1, \tag{8.54}$$

i.e. all odd integer multiples of π/β,

$$\omega_n=(2n+1)\pi\frac{k_{\mathrm{B}}T}{\hbar}. \tag{8.55}$$

In order to have finite results, the Fourier transform of the propagator, $G_n=G(\omega_n)$, must have poles at these frequencies. The propagator itself then can be written as a sum of such pole contributions, the Matsubara sum:

$$G(x,\tau|0,0)=\int\frac{\mathrm{d}^3k}{(2\pi)^3}\,k_{\mathrm{B}}T\sum_n G(\mathbf{k},\omega_n)\,\mathrm{e}^{\mathbf{ik\cdot x}-\mathrm{i}\omega_n\tau}. \tag{8.56}$$

8.1.3 The Spectral Function

What information is included in the use of propagators about the physics of fields and particles?

Inspecting (8.45), one realizes that the two basic propagators, G^{+-} and G^{-+}, do depend on the thermal distribution of frequency modes, $n(\omega)$. This distribution in equilibrium coincides with either the Bose–Einstein or the Fermi–Dirac distributions – derived by using statistical argumentation in Chap. 3 already. There is, however, a combination which is independent of the occupation, $n(\omega)$, $G^{+-}-G^{-+}$.

Either in the imaginary (complex) time formalism or in the original real time formalism this combination encodes an information about the physical system which is independent of the imaginary time period, β. Let us inspect the Fourier transform of (8.45) with respect to $(t-t')$. The *spectral density* is defined independently of the occupation expectation value, $n(\omega)$, as

$$\rho(\omega) = \pm\left(iG^{+-} - iG^{-+}\right) = iG^R \mp iG^A. \tag{8.57}$$

The spectral density is a function of the mode frequency, ω (and the corresponding energy eigenvalue, $\hbar\omega$). Due to time reversal property of the retarded and advanced propagators in the Fourier representation it is also $\rho(\omega) = -2\,\mathrm{Im}\,G^R(\omega)$. All propagators – both in real and imaginary time – can be expressed with the help of the spectral density, $\rho(\omega)$, the mode occupation functions, $n(\omega)$ and $\bar{n}(\omega)$, and the proper combination of Heaviside functions in the time difference. For most physical systems, showing particle–antiparticle symmetry and being unpolarized, $\bar{n} = n$.

The above definition can easily be extended to involve arbitrary operators, $A(t)$ and $B(t')$. In this case

$$\int\limits_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}\, \mathrm{e}^{\mathrm{i}\omega(t-t')}\, \rho_{AB}(\omega) = \left\langle A(t)B(t') \mp B(t')A(t) \right\rangle. \tag{8.58}$$

The generalized spectral density can be obtained from this formula by inverse Fourier transformation:

$$\rho_{AB}(\omega) = \int\limits_{-\infty}^{\infty} d(t-t')\, \mathrm{e}^{-\mathrm{i}\omega(t-t')} \left\langle A(t)B(t') \mp B(t')A(t) \right\rangle. \tag{8.59}$$

Using the *KMS* relation $\langle A(t)B(t') \rangle = \langle B(t')A(t-i\beta) \rangle$ for obtaining the spectral density we are interested in the following canonical expectation value

$$\left\langle B(t')\,[A(t-i\beta) \mp A(t)] \right\rangle = \frac{1}{Z}\sum_{a,b} \left\langle b|\mathrm{e}^{-\beta H} B(t')|a \right\rangle \langle a|A(t-i\beta) \mp A(t)|b \rangle. \tag{8.60}$$

Here, Z is the partition sum, while a and b denote energy eigenstates. In equilibrium, there is a time shift symmetry and all operators can be expressed by their values at time zero and appropriate exponential factors:

$$\begin{aligned}\left\langle B(t')\,[A(t-i\beta) \mp A(t)] \right\rangle &= \frac{1}{Z}\sum_{a,b} \langle b|B(0)|a \rangle \langle a|A(0)|b \rangle\, \mathrm{e}^{\mathrm{i}(E_a-E_b)(t'-t)} \\ &\times \left[\mathrm{e}^{-\beta E_a} \mp \mathrm{e}^{-\beta E_b}\right].\end{aligned} \tag{8.61}$$

Finally, the Fourier transformation in $(t-t')$ leads to

$$\rho_{AB}(\omega) = \frac{1}{Z}\sum_{a,b} \langle a|A(0)|b\rangle \langle b|B(0)|a\rangle \, 2\pi\delta(E_a - E_b - \omega) \left[\mathrm{e}^{-\beta E_a} \mp \mathrm{e}^{-\beta E_b} \right]. \tag{8.62}$$

Associated to the field operator ϕ as $A = \phi$, $B = \phi^\dagger$ the spectral density is given by

$$\rho(k,\omega) = \frac{1}{Z}\sum_{a,b} 2\pi\delta(E_a - E_b - \omega)\, |\langle a|\phi|b\rangle|^2 \left(\mathrm{e}^{-\beta E_a} \mp \mathrm{e}^{-\beta E_b} \right). \tag{8.63}$$

In general, a and b denote quantum eigenstates of the Hamiltonian, or of $H - \mu N$ in case of the grand-canonical ensemble. The corresponding eigenvalues E_a and E_b, respectively, in this case include the chemical potential μ.

The retarded propagator is given by

$$G^R(\mathbf{k},\omega) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\Omega}{2\pi} \, \frac{\rho(\mathbf{k},\Omega)}{\Omega - (\omega + i\varepsilon)} \tag{8.64}$$

in the $\varepsilon \to 0^+$ limit. The advanced propagator can be obtained by $G^A = G^{R*}$ for time-reversal invariant systems; in particular in thermal equilibrium. The Matsubara sum (8.56) also can be expressed with the spectral density as using

$$G_n = G(\mathbf{k},\omega_n) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\Omega}{2\pi} \, \frac{\rho(\mathbf{k},\Omega)}{\Omega - i\omega_n}. \tag{8.65}$$

8.2 Off Equilibrium Field Theory

The temperature as an inverse of a Lagrange multiplier can be formally introduced into the quantum field theory along the lines described above. What about the temperature, however, as a property of the physical noise? To what extent follow such kinetic equations, like the Boltzmann equation [86, 87], from some particular averaging over evolution equations for the field operator? In this subsection, we outline how an evolution equation for the occupation, $n(\omega)$, and the spectral density, $\rho(\omega)$, i.e. for a general propagator in interacting systems, may follow from operator equations of field theory.

Our starting point is an exact equation for interacting systems relating the exact propagator, the free propagator and the self-energy; the Schwinger–Dyson equation [85]

$$G^R = G_0^R + G_0^R * \Sigma^R * G^R \tag{8.66}$$

with $_0$ indices denoting the propagators of a free particle and by $*$ the convolution of space-time integrals. It can be derived based on the general field equation

$$\Box_1 \Phi_1 = \int\limits_2 \Sigma_{12} \Phi_2 \tag{8.67}$$

denoting the space-time arguments by 1 and 2. The operator $\Box_1$ is a differential operator belonging to the free field equation with respect to the argument $x_1 = (t_1, \mathbf{r}_1)$. Multiplying the field equation by the value $\Phi_2^\dagger$ we obtain an equation for a general propagator G_{12}:

$$\Box_1 G_{12} = \delta_{12} + \int\limits_3 \Sigma_{13} G_{32} = \delta_{12} + \Sigma_{13} * G_{32}. \tag{8.68}$$

This equation can be compared to its time reversal conjugate by interchanging the indices 1 and 2. Since $G_{21} = G_{12}^*$ one arrives at

$$(\Box_1 - \Box_2^*)\, G_{12} = \Sigma_{13} * G_{32} - (\Sigma_{23} * G_{31})^* \tag{8.69}$$

This is the basis of the derivation of a transport equation in a certain approximation. Its stationary solution then ought to describe the equilibrium.

Following [88] we restrict our discussion to real boson fields. We also use the Wigner-transform of the quantities, a Fourier transform in the relative coordinates $x_1 - x_2$:

$$\bar{G} = \mathscr{W} G(x,p) = \int \mathrm{d}\xi\, \mathrm{e}^{\mathrm{i}p\xi} G(x+\xi/2, x-\xi/2). \tag{8.70}$$

As it is shown by solving problem (8.3), the Wigner transform of the convolution $H = \Sigma * G$ can be formally written as being

$$\mathscr{W}(\Sigma * G)(x,p) = \mathrm{e}^{\frac{i}{2}\Delta}\, \mathscr{W}\Sigma(x,p)\, \mathscr{W} G(x',p') \tag{8.71}$$

using the "triangle operator"

$$\Delta = \frac{\partial}{\partial p}\frac{\partial}{\partial x'} - \frac{\partial}{\partial x}\frac{\partial}{\partial p'} \tag{8.72}$$

and taking the result at $x' = x$, $p' = p$. To leading order in the *gradient expansion*, i.e. when the effect of the triangle operator is small compared to the identity, one receives the product of the Wigner transforms. The next to leading order correction on the other hand becomes a Poisson bracket:

$$\mathscr{W}(\Sigma * G)(x,p) \approx \mathscr{W}\Sigma(x,p)\, \mathscr{W} G(x,p) + \frac{i}{2}\{\mathscr{W}\Sigma(x,p), \mathscr{W} G(x,p)\} + \cdots \tag{8.73}$$

An evolution equation for the (say retarded) propagator can be obtained by acting on the Schwinger–Dyson equation by the inverse of the free propagator. This inverse is, however, nothing else than the differential operator in the free field equation. On the other hand this differential operator acts on the Wigner-transform as

$$-\Box_1 G(x_1,x_2) = \left(\frac{1}{2}\frac{\partial}{\partial x} - ip\right)^2 \bar{G}(x,p) \tag{8.74}$$

This leads to the following evolution equation for the Wigner-transform of the retarded propagator

$$\left[p^2 - m^2 - \frac{1}{4}\frac{\partial^2}{\partial x^2} + ip\cdot\frac{\partial}{\partial x}\right]\bar{G}^R = 1 + \bar{\Sigma}\bar{G}^R + \frac{i}{2}\left\{\bar{\Sigma},\bar{G}^R\right\} + \cdots \tag{8.75}$$

Let us try to solve this equation order by order in the gradient expansion. To leading order (LO) we get

$$(p^2 - m^2)\bar{G}^R = 1 + \bar{\Sigma}\bar{G}^R, \tag{8.76}$$

with the solution

$$\bar{G}^R = \frac{1}{p^2 - m^2 - \bar{\Sigma}}. \tag{8.77}$$

The surprising fact is that this solution remains up to two consecutive orders in the gradient expansion. To see this, one has to realize that

$$ip\cdot\frac{\partial}{\partial x}\bar{G}^R = \frac{i}{2}\left\{p^2 - m^2, \bar{G}^R\right\} \tag{8.78}$$

is fulfilled. This way the next to leading order (NLO) terms satisfy

$$\frac{i}{2}\left\{p^2 - m^2 - \bar{\Sigma}, \bar{G}^R\right\} = 0. \tag{8.79}$$

But it is in general true that the Poisson bracket between a quantity and its differentiable function vanishes,

$$\{B, f(B)\} = f'(B)\left(\frac{\partial B}{\partial p}\frac{\partial B}{\partial x} - \frac{\partial B}{\partial x}\frac{\partial B}{\partial p}\right) = 0. \tag{8.80}$$

Similarly, the next-to-next-to-leading order (NNLO) term in the gradient expansion is achieved by a repeated application of the triangle operator:

$$-\frac{1}{4}\frac{\partial^2}{\partial x^2}\bar{G}^R = -\frac{1}{8}\left(\frac{\partial^2\bar{\Sigma}^R}{\partial p^2}\frac{\partial^2\bar{G}^R}{\partial x^2} - \frac{\partial^2\bar{\Sigma}^R}{\partial x^2}\frac{\partial^2\bar{G}^R}{\partial p^2}\right) \tag{8.81}$$

We only need to realize that the similar expression with $p^2 - m^2$ instead of $\bar{\Sigma}^R$ leads to the left hand side of this equation, meaning that the repeated triangle operation of $p^2 - m^2 - \bar{\Sigma}^R$ with $\bar{G}^R$ also vanishes.

In order to connect this derivation to the spectral function and decay width of particle resonances, we split the propagator and the self-energy into their real and imaginary parts. Using $\bar{G}^R = F - iA/2$ and $\bar{\Sigma} = U - i\Gamma/2$ we arrive at

$$F = \frac{p^2 - m^2 - U}{\left(p^2 - m^2 - U\right)^2 + \Gamma^2/4},$$
$$A = \frac{\Gamma}{\left(p^2 - m^2 - U\right)^2 + \Gamma^2/4}. \tag{8.82}$$

The retarded propagator in the Wigner representation is given by

$$\bar{G}^R = \frac{1}{p^2 - m^2 - U + i\Gamma/2}. \tag{8.83}$$

Since the spectral function is $\rho(\omega) = -2\,\mathrm{Im}\,G^R$ the quantity for $A(x,p)$ in (8.82) is the closest to a "local" spectral function. In particular, equilibrium is achieved by a homogeneous state where $\bar{G}^R$ has no x-dependence. The solution for the advanced propagator, G^A, can be obtained by time reversal transformation, equivalent to a change from ω to $-\omega$.

Only the equations for those propagator combinations, which contain the occupation number – in a non-equilibrium theory using the Wigner transforms their common-time dependent pendants, – cannot be derived from the retarded solution. In this case, the Kadanoff–Baym equations (8.69) also carry a more complex form.

What can we tell about some general property of their equilibrium solution, without knowing the details of interaction (the Lagrangian of the field theory)? It is important to observe that all interaction effects, comprised into the self-energy term, Σ, and its convolution with the different causality propagators, i.e. differently time-ordered expectation values of fields, always contains terms alike: Products of occupation number factors for positive and negative frequency at the same common time t, i.e. $n(\omega_i,t)$ and $1 \pm n(\omega_i,t)$ on the one hand, and corresponding exponentials with positive and negative phases. Over the frequency (and other quantum labels) of the interacting partners there will be an integration (summation) by calculating the convolution.

Let us suppose we deal with a general term with N positive and M negative frequencies (or energies, which are the same in $\hbar = 1$ units). Each term in the source side of the Kadanoff–Baym equations contains then factors of the following type under integration over all ω_i-s but the first one:

$$C^{N+M} = \int \ldots \left(G^{(N)} L^{(M)} - L^{(N)} G^{(M)} \right) \ldots \tag{8.84}$$

with the general *gain* and *loss* terms at common-time t and time difference τ:

$$G^{(N)} = \prod_{i=1}^{N} n(\omega_i,t)\; \mathrm{e}^{\sum\limits_{i=1}^{N} \mathrm{i}\omega_i\tau}$$
$$L^{(M)} = \prod_{j=1}^{M} \left(1 \pm n(\omega_j,t)\right)\; \mathrm{e}^{-\sum\limits_{j=1}^{M} \mathrm{i}\omega_j\tau}. \tag{8.85}$$

We realize that each product of $N+M$ Φ and $\Phi^\dagger$ operators contains the terms with positive and negative frequencies in an anti-symmetric fashion balancing the creation and annihilation of the corresponding quanta. This product ansatz is the so called *two-particle independent* (2PI) approximation.

In a detailed balance equilibrium state, all such terms vanish. Such a state, however, physically can be realized only if stationary. In this case, the common-time dependence vanishes, $n(\omega,t) = n(\omega)$. This way the above factors can be integrated over the time t leaving us with Dirac-delta factors for energy conservation:

$$\int\limits_{-\infty}^{\infty} \mathrm{e}^{\sum\limits_{i=1}^{N} \mathrm{i}\omega_i\tau} \, \mathrm{e}^{-\sum\limits_{j=1}^{M} \mathrm{i}\omega_j\tau} \, \mathrm{d}\tau = 2\pi\,\delta\left(\sum_{i=1}^{N}\omega_i - \sum_{j=1}^{M}\omega_j\right). \tag{8.86}$$

Exactly this step is challenged by off-shell effects causing observable time-dependence of the occupation numbers. Neglecting such memory effects for now, the time-integrated interaction terms contain factors of type

$$\begin{aligned} & G^{(N)}L^{(M)} - L^{(N)}G^{(M)} \\ &= \left\{ \prod_{i=1}^{N} n(\omega_i,t) \prod_{j=1}^{M} (1 \pm n(\omega_j,t)) - \prod_{i=1}^{N} (1 \pm n(\omega_i,t)) \prod_{j=1}^{M} n(\omega_j,t) \right\} \\ &\qquad \delta\left(\sum_{i=1}^{N}\omega_i - \sum_{j=1}^{M}\omega_j\right). \end{aligned} \tag{8.87}$$

In general, all such factors are zero if

$$\frac{n(\omega)}{1 \pm n(\omega)} = \mathrm{e}^{\beta(\mu-\omega)}. \tag{8.88}$$

As already shown, this leads to the Bose–Einstein or Fermi–Dirac distribution in equilibrium.

Is it possible to achieve a similar, long term equilibrium state beyond the 2PI picture? There is no detailed answer to this question up to date. One may only speculate, that – relying on the introduction of more general energy composition rules than the addition – one may assume a superstatistical density matrix in the form

$$\rho = \int\limits_{0}^{\infty} w_a(\beta)\mathrm{e}^{-\beta H}\mathrm{d}\beta = \mathrm{e}^{-\bar{\beta}L_a(H)}. \tag{8.89}$$

As a consequence the time-difference integration in equilibrium leads to Dirac-delta conditions on the sum of $L(\omega_i)$-s and the equilibrium energy distribution modifies to

$$\frac{n(\omega)}{1 \pm n(\omega)} = \mathrm{e}^{\beta((\mu-L(\omega)))}. \tag{8.90}$$

8.3 Feynman Path Integral and Canonical Partition Sum

There seems to be an analogy between quantum and statistical physics. A diffusion – or more generally a Fokker–Planck – equation describing evolution of probabilities and phase space occupancy factors in real time on the one hand and the quantum evolution, described by the Schrödinger equation as a diffusion in imaginary time, on the other hand. Similarly, methods developed for solving the diffusion problem by using *path integrals* have been "continued" over, albeit without rigorous mathematical proof, to a general solution of the quantum problem in terms of the Feynman–Hibbs path integral. After a while this habit of denoting theoretical solutions, which at first had been worked out for the non-interacting case only, became a method of "path integral quantization": a recipe to associate a quantum theory once the action of a classical theory is given.

Amazingly, the path integral quantization method uses the classical action as a starting point. This governs then the dynamical evolution in a space of possible quantum states, the Hilbert space. The description of the latter, however, has to be added. It turns out that a certain way of labeling quantum states, based on the coherent state description known from quantum optics, leads the closest to the dynamics of the non-quantum original. This way a phase space point centered description of each quantum state emerges, and the path integration is done over such labels of possible quantum states. And finally, it is just a characteristic, perhaps fortunate circumstance, that for most problems handled in quantum field theory over the half of all degrees of freedom – namely over those labeled by the canonical momentum fields – can be path-integrated analytically. The result emerges from an infinite product of Gaussian integrals and contains the classical action in an exponential form. In a somewhat sloppy, symbolic notation one can write

$$\int \mathscr{D}q\,\mathscr{D}p\,\mathrm{e}^{-\frac{i}{\hbar}\int H\mathrm{d}t} = \int \mathscr{D}q\,\mathrm{e}^{\frac{i}{\hbar}\int L\mathrm{d}t}, \tag{8.91}$$

with $H(p,q)$ being the Hamiltonian and $L = p\dot{q} - H$ the Lagrangian.

The exponential factor containing the time-integral of the Hamiltonian is on the one hand the formal solution of a general, time-dependent Schrödinger equation. On the other hand it becomes the canonical statistical factor, $\mathrm{e}^{-\beta H}$, integral-averaged over an imaginary-time period β. This analogy between real-time and imaginary time quantum-mechanics, as a canonical statistical equilibrium theory, can be extended to all methods applied in solving quantum problems:

$$\int \mathscr{D}q\,\mathscr{D}p\,\mathrm{e}^{-\beta H} = \int \mathscr{D}q\,\mathrm{e}^{-\int_0^\beta L_\mathrm{E}\mathrm{d}\tau}, \tag{8.92}$$

where $L_\mathrm{E} = p\mathrm{d}q/\mathrm{d}\tau + H$ denotes the "Euclidean" version of the Lagrangian, belonging to the use of the imaginary time formalism. In particular, the concept of the inverse temperature as an imaginary time periodicity pioneers some more speculative ideas about the question of emergent quantum theory: Why and how may quantum effects be a consequence of an underlying dynamics?

Since averaging over a noise – based upon an assumed hierarchy of characteristic times – leads to an effective statistical theory, the question arises, whether Nature itself might make use of a similar trick. To the idea of *chaotic quantization* it underlies a concept of "thermal" motion, however this motion evolves in an extra timelike dimension. Combining the temperature of this imaginary noise in this extra time dimension with an elementary time scale, either emerging from a cosmological constant or from an elementary time-lattice spacing – this varies according to the very theory – the unit of the quantum action emerges: $\hbar = aT$ (in $k_{\mathrm{B}} = c = 1$ units). If a lies in the order of Planck length, then T should be in the order of the Planck mass (energy). Of course, this idea is rather speculative at present, no experimental hints about the magnitude of this quantity is known, besides the relative weakness of the force of gravity compared to other elementary interactions. Nevertheless the mechanism is related to the concept of temperature, so it is proper to include a short description of it in this book. The idea of chaotic quantization has been worked out in close collaboration with Profs. Berndt Müller and Sergei Matinyan at the Duke University [89, 90].

Before doing so, however, a sketchy summary about the basics of the path integral method and its connection to statistical physics shall be given in the following subsections.

8.3.1 Path Integral for Diffusion and Quantum Mechanics

The easiest to catch the core idea is to consider a simplified model of a one-dimensional, symmetric diffusion. On an infinite chain of positions (or states) there is a constant probability rate to hop to one of the neighboring ones. The occupation probability of the n-th member of this chain then changes in time according to the following simple master equation, which takes into account the in and out jumps from and to the $n-1$-th and $n+1$-th positions:

$$\dot{P}_n = \lambda\,(P_{n-1} - P_n) + \lambda\,(P_{n+1} - P_n). \tag{8.93}$$

The general solution of this system of infinitely many differential equations is the best to obtain by using a generating function, defined as being

$$\Gamma(z,t) := \sum_n \mathrm{e}^{nz} P_n(t). \tag{8.94}$$

It is straightforward to realize that the z-derivatives of $\Gamma(z,t)$ generate expectation values of n:

$$\Gamma(0,t) = 1, \qquad \left.\frac{\partial \Gamma}{\partial z}\right|_{z=0} = \langle n \rangle, \qquad \left.\frac{\partial^k \Gamma}{\partial z^k}\right|_{z=0} = \left\langle n^k \right\rangle. \tag{8.95}$$

The evolution equation for $\Gamma(z,t)$ is derived replacing the definition (8.94) into (8.93). We get

$$\frac{\partial \Gamma}{\partial t}(z,t) = \lambda \left((e^{z} - 1) + (\mathrm{e}^{-z} - 1) \right) \Gamma(z,t). \tag{8.96}$$

In the general case, λ may depend on the initial position of a jump, n and it may differ for going up or down in the chain, (the latter denoted by μ then). The solution of (8.96) generalizes to

$$\Gamma(z,t) = \mathrm{e}^{tW(z,\frac{\partial}{\partial z})}\, \Gamma(z,0), \tag{8.97}$$

with

$$W\left(z, \frac{\partial}{\partial z}\right) = (\cosh(z) - 1)\,(\lambda + \mu)\left(\frac{\partial}{\partial z}\right) + \sinh(z)\,(\lambda - \mu)\left(\frac{\partial}{\partial z}\right). \tag{8.98}$$

Here, the n-dependence of the jumping rate coefficients is converted to an operator expression formally substituting n by $\frac{\partial}{\partial z}$. The simple symmetric diffusion has the solution for $\mu = \lambda =$ constant:

$$W = 2\lambda(\cosh(z) - 1). \tag{8.99}$$

It is important to realize that not only some expectation values, but also the time-dependent occupation probabilities can be reconstructed from the above solution. Using the notation $s = e^{z}$ the ratio,

$$\frac{\Gamma(z,t)}{\Gamma(z,0)} = \mathrm{e}^{-2\lambda t} \mathrm{e}^{\lambda t(s+1/s)} = \mathrm{e}^{-2\lambda t} \sum_{n=-\infty}^{\infty} s^{n} I_{n}(2\lambda t), \tag{8.100}$$

is recognized as a generating function for the modified Bessel functions, I_n. The probabilities therefore are

$$P_n(t) = \mathrm{e}^{-2\lambda t} \sum_{k} I_{n-k}(2\lambda t) P_k(0). \tag{8.101}$$

Starting with a concentrated distribution, $P_n(0) = \delta_{n,0}$, one has $\Gamma(z,0) = 1$ and the resulting $P_n(t)$ solution reflects the Green function of the discrete diffusion problem:

$$G_{nk}(t,t') = \mathrm{e}^{-2\lambda(t-t')} I_{n-k}\left(2\lambda(t-t')\right) = g_{n-k}(t-t'). \tag{8.102}$$

It is of course not guaranteed that a generating function can readily be recognized as an infinite sum of known analytic expressions. Therefore, the characteristic function method is used, which considers the above logarithmic generating function, Γ, at pure imaginary argument, $z = i\vartheta$. In this case the generating function is periodic,

$$\tilde{\Gamma}(\vartheta,t) := \sum_{n=-\infty}^{\infty} \mathrm{e}^{in\vartheta} P_n(t) = \tilde{\Gamma}(\vartheta + 2k\pi, t) \tag{8.103}$$

with arbitrary integer, k. The occupation probabilities in this case can be obtained by Fourier analysis:

$$P_n(t) = \frac{1}{2\pi} \int_{-\pi}^{+\pi} \tilde{\Gamma}(\vartheta,t)\, \mathrm{e}^{-\mathrm{i}n\vartheta} \mathrm{d}\vartheta. \tag{8.104}$$

This simple model can be utilized when considering the problem of continuous diffusion. In the diffusion equation,

$$\frac{\partial c}{\partial t} = \lambda \frac{\partial^2 c}{\partial x^2}, \tag{8.105}$$

we model the concentration variable c by discrete values

$$c(x,t) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} P_n(t) \bigg|_{x=n\varepsilon}. \tag{8.106}$$

The corresponding discrete master equation to leading order in ε becomes

$$\dot{P}_n(t) = \frac{\lambda}{\varepsilon^2} (P_{n+1} + P_{n-1} - 2P_n). \tag{8.107}$$

On the other hand the concentration can be viewed as a sum

$$c(x,t) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \sum_n \delta_{n,x/\varepsilon} P_n(t), \tag{8.108}$$

where the Kronecker-delta has an integral representation:

$$\delta_{n,x/\varepsilon} = \int_{-\pi}^{+\pi} \frac{\mathrm{d}\vartheta}{2\pi} \mathrm{e}^{\mathrm{i}(n-x/\varepsilon)\vartheta}. \tag{8.109}$$

Putting this together and changing the integration variable to $k = \vartheta/\varepsilon$ (and caring for the fact that in the small ε limit the integration borders tend to infinity) we obtain

$$c(x,t) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}k}{2\pi} \mathrm{e}^{-\mathrm{i}k(x-x')} \lim_{\varepsilon \to 0} \frac{\tilde{\Gamma}(k\varepsilon,t)}{\tilde{\Gamma}(k\varepsilon,0)} c(x',0). \tag{8.110}$$

The complex logarithmic generating function ratio, determining the Green function, with the effective hopping probability rate being λ/ε^2, tends to

$$\frac{\tilde{\Gamma}(k\varepsilon,t)}{\tilde{\Gamma}(k\varepsilon,0)} = \mathrm{e}^{\frac{2\lambda t}{\varepsilon^2}(\cos(k\varepsilon)-1)} \longrightarrow \mathrm{e}^{-\lambda t k^2}. \tag{8.111}$$

As a consequence the Green function of the free diffusion is Gaussian

$$G(x,x',t,t') = \int_{-\infty}^{+\infty} \frac{\mathrm{d}k}{2\pi}\, \mathrm{e}^{-\mathrm{i}k(x-x')}\, \mathrm{e}^{-\lambda(t-t')k^2} = \frac{1}{\sqrt{4\pi\lambda(t-t')}}\, \mathrm{e}^{-\frac{(x-x')^2}{4\lambda(t-t')}}. \tag{8.112}$$

The Green function of diffusion, $G(x,x',t,t')$, is a particular conditional probability: the probability to find the diffusing particle at time t' in the position x' when it was surely (with 100% probability) in the position x at the time t'. The path integral is a particular view of this probability; as it were composed from *alternative paths* to get from x' to x while the time passes from t' to t. The basic idea to single out a given diffusion path is fixing it by given control points and then to consider the limit of a continuous observation. The one-path-probability is approximated by the series of restrictions of passing all the points $x_i = \varepsilon n_i$ at times t_i:

$$P_1(\{n_i\}) := \prod_{i=1}^{N+1} P_{n_i}(t_i) \tag{8.113}$$

in the discrete model with $N+1$ observations. The total conditional probability of a diffusion from somewhere to somewhere else is combined as a sum over independent alternatives for the arrangements of the N intermediate observations. This can be labeled by the set of all physically possible values of n_i, and one sums over all possible configurations of these labels:

$$Z := \sum_{\{n_i\}} P_1(\{n_i\}). \tag{8.114}$$

This formula reminds to that of the partition sum in spin models, and in fact this analogy is helpful by numerical calculations of path integrals.

In the continuum limit of the above model, the sum over configurations of intermediate positions becomes an infinite dimensional integral, the *path integral*. From the scaling between the discrete model and the continuous diffusion problem one finds easily out that the proper scaling of distances and time intervals should be like ε and ε^2, respectively. This way the transition probability from one observational point to the next one along a diffusion path becomes

$$\Delta_i P = P(x_i, x_{i+1}; t_i, t_{i+1}) = \mathscr{P}\left(x_{i+1} - x_i, \varepsilon^2\right), \tag{8.115}$$

reflecting translational invariance. The one-path-probability is a $(N+1)$-fold product of such terms. Each such step is in itself a diffusion – this self-similarity helps to obtain the path integral. Using the result with the logarithmic generator function at imaginary argument for the free diffusion one writes

$$\Delta_i P = \int_{-\infty}^{\infty} \frac{\mathrm{d}k_i}{2\pi}\, \mathrm{e}^{-\mathrm{i}k_i(x_{i+1}-x_i)}\, \tilde{\Gamma}(k_i\varepsilon, \varepsilon^2). \tag{8.116}$$

Substituting the formula (8.99) for free diffusion one obtains

$$\Delta_i P = \int\limits_{-\infty}^{\infty} \frac{\mathrm{d}k_i}{2\pi}\, \mathrm{e}^{-\mathrm{i}k_i(x_{i+1}-x_i)+2\lambda(\cos(k_i\varepsilon)-1)}. \tag{8.117}$$

Finally, for small ε, in the continuum limit, we expand the cosine function and arrive at

$$\Delta_i P = \int\limits_{-\infty}^{\infty} \frac{\mathrm{d}k_i}{2\pi}\, \mathrm{e}^{-\varepsilon^2\left(\mathrm{i}k_i\frac{x_{i+1}-x_i}{\varepsilon^2}+\lambda k_i^2\right)}. \tag{8.118}$$

Taking into account that in the same limit the first term in the exponent approximates the derivative of the function $x(t)$ describing the path,

$$\lim_{\varepsilon\to 0}\frac{x_{i+1}-x_i}{\varepsilon^2} = \frac{\mathrm{d}x}{\mathrm{d}t}, \tag{8.119}$$

the product of such terms along a single diffusion path is then given as follows:

$$P_1 = \prod_{i=1}^{N+1}\int\limits_{-\infty}^{\infty} \frac{\mathrm{d}k_i}{2\pi}\, \mathrm{e}^{-\varepsilon^2\left(\mathrm{i}k_i\frac{\mathrm{d}x}{\mathrm{d}t}+\lambda k_i^2\right)}. \tag{8.120}$$

This is an $(N+1)$-fold Gaussian integral, and as such can be factorized. This reflects the self-similarity of diffusion. On the other hand it can be viewed as an $(N+1)$-dimensional integral over the exponent of the sum of alike terms,

$$P_1 = \left(\prod_{i=1}^{N+1}\int\limits_{-\infty}^{\infty} \frac{\mathrm{d}k_i}{2\pi}\right) \mathrm{e}^{-\varepsilon^2\sum\limits_{i=1}^{N+1}\left(\mathrm{i}k_i\frac{\mathrm{d}x}{\mathrm{d}t}+\lambda k_i^2\right)}, \tag{8.121}$$

where in turn the sum in the exponent is an approximation of a time integral. In the $N\to\infty$, $\varepsilon\to 0$ limit the density of observation points grows. One keeps, however, the time interval finite, so $t=(N+1)\varepsilon^2$ is fixed. In this sense, the k_i variables approach a continuous set of a curve, $k(\tau)$, labeled by a continuous time-variable $0<\tau<t$. The infinite dimensional integral in the above formula will be reminded by a special notation, that of the path integral measure:

$$P_1 = \int \mathscr{D}[k(\tau)]\; \mathrm{e}^{-\int\limits_0^t \mathrm{d}\tau\left(\mathrm{i}k\frac{\mathrm{d}x}{\mathrm{d}t}+\lambda k^2\right)} \tag{8.122}$$

All the integrals Gaussian in k_i can be carried out analytically. Their result are exponential factors with $\frac{\mathrm{d}x}{\mathrm{d}t}^2$ in the exponent:

$$P_1 = \left(4\pi\varepsilon^2\lambda\right)^{-(N+1)/2}\, \mathrm{e}^{-\sum\limits_{i=1}^{N+1}\left(\frac{\mathrm{d}x_i}{\mathrm{d}t}\right)^2}, \tag{8.123}$$

where the $x_i(t)$ points represent the diffusion path. The sum over all alternative paths then also becomes a path integral:

$$Z = \sum_{\{n_i\}} P_1 = \int \mathscr{D}[x(\tau)] \; \mathrm{e}^{-\frac{1}{4\lambda}\int\limits_0^t \mathrm{d}\tau \left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2} . \tag{8.124}$$

This computational technique can be extended to problems when the particle does not propagates freely, when it interacts. Then an absorption factor is associated to each observation point and the Green function with absorption factor $A(x,t)$ becomes

$$G_A(x,t|x_0,t_0) = \int\limits_{(x_0,t_0)}^{(x,t)} \mathscr{D}[x(\tau)] \; \mathrm{e}^{-\int\limits_0^t \mathrm{d}\tau \left(\frac{1}{4\lambda}\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 + A(x,\tau)\right)} . \tag{8.125}$$

The integral in the exponent already reminds us to the structure of a Lagrangian composed from a kinetic energy term, proportional to the square of the time-derivative of the variable describing the position of a particle, and from another term depending on the position. In fact, generalizing the above approach to imaginary time, one formally solves a Schrödinger equation instead of the diffusion problem. Then the square of the τ-derivative picks up a minus sign, and the τ-integration an overall imaginary unit, i. The absorption factor will belong to the potential energy term in the Schrödinger equation, $A = V(x)$. The Green function is given as the path integral

$$G_A(x,t|x_0,t_0) = \int\limits_{(x_0,t_0)}^{(x,t)} \mathscr{D}[x(\tau)] \; \mathrm{e}^{\frac{i}{\hbar}\int\limits_0^t \mathrm{d}\tau \left(\frac{1}{4\lambda}\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 - V(x)\right)} . \tag{8.126}$$

Interpreting finally $1/4\lambda = m/2$ as the proper factor, the path integral formally includes the classical action of the motion:

$$G_A(x,t|x_0,t_0) = \int\limits_{(x_0,t_0)}^{(x,t)} \mathscr{D}[x(\tau)] \; \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S}, \tag{8.127}$$

with

$$S = \int\limits_0^t \mathrm{d}\tau \left(\frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 - V(x) \right) . \tag{8.128}$$

This is the Feynman–Hibbs path integral, describing the Green function solution of a general Schrödinger equation.

8.3.2 Path Integral over Coherent States

The Feynman–Hibbs path integral, originally formulated in the coordinate space (Schrödinger) representation, has been generalized to a more abstract description of quantum dynamics. All path integrals represent quantum mechanical transition amplitudes, which determine the probabilities of the corresponding processes. Such an amplitude is a path integral, whenever the intermediate states are continuously indexed and the possible alternative transition processes are continuous paths in the index space. Differentiability, however, in the general case is not given for these paths.

Coherent states span a subspace in Hilbert space, consisting of continuously indexed states. Let the set of indices be $\mathscr{L}$ and the Hilbert space $\mathscr{H}$; then a coherent state, $|\ell\rangle \in \mathscr{H}$, is represented by an index element, $\ell \in \mathscr{L}$, if the following conditions are met:

1. The index is continuous, i.e.
$$\| \, |\ell\rangle - |\ell'\rangle \, \| \to 0, \qquad \text{for} \qquad |\ell - \ell'| \to 0, \tag{8.129}$$
with the corresponding norms in the Hilbert- and index space.
2. The index representation is complete, i.e. the unity operator is spanned by an integral in the index space:
$$1 = \int_{\mathscr{L}} |\ell\rangle\langle\ell| \, \delta\ell, \tag{8.130}$$
with $\delta\ell$ being a proper integral measure.

We give some examples for coherent states in the above general sense. Elements in a Fock space define the following general index state:

$$|\ell\rangle = \sum_n |n\rangle \, \langle n|\ell\rangle. \tag{8.131}$$

The completeness for continuously indexed states is fulfilled, i.e.

$$\int |\ell\rangle \, \langle\ell| \, \delta\ell = \sum_{n,m} |n\rangle \, \langle m| \int \langle n|\ell\rangle \, \langle\ell|m\rangle \, \delta\ell = 1, \tag{8.132}$$

if the following is true:

$$\int \langle n|\ell\rangle \, \langle\ell|m\rangle \, \delta\ell = \langle n|m\rangle. \tag{8.133}$$

The overlap of a coherent state with a general state, $|\psi\rangle$, the coherent wave function is given by

$$\Psi(\ell) = \langle\ell|\psi\rangle = \sum_n \langle\ell|n\rangle\langle n|\psi\rangle = \langle 0|\hat{U}^\dagger \, [\ell] \, |\psi\rangle. \tag{8.134}$$

and herewith represented by elements of l^2.

Eigenstates of the coordinate operator, $\hat{x}|x\rangle = x|x\rangle$ can also be used as basis. In this case we need to fulfill

$$\int \langle x|\ell\rangle\langle\ell|y\rangle\,\delta\ell = \delta(x-y), \tag{8.135}$$

and the wave functions are elements of L^2:

$$\Psi(\ell) = \langle\ell|\psi\rangle = \int \langle\ell|x\rangle\langle x|\psi\rangle \mathrm{d}x. \tag{8.136}$$

In general, for a complex functional of the index,

$$\Phi(\ell) = \langle\ell|\Phi\rangle, \tag{8.137}$$

the completeness equation (8.130) ensures that it is normalizable:

$$\langle\Phi|\Phi\rangle = \int |\langle\ell|\Phi\rangle|^2\,\delta\ell < \infty. \tag{8.138}$$

Also, the group property of coherent states, i.e.

$$\langle\ell'|\ell''\rangle = \int \langle\ell'|\ell\rangle\langle\ell|\ell'\rangle\,\delta\ell \tag{8.139}$$

is a consequence of the completeness. Orthogonality, however, is not demanded for coherent states. Therefore from the group property it follows the linear dependency:

$$|\ell'\rangle = \int |\ell\rangle\langle\ell|\ell'\rangle\,\delta\ell. \tag{8.140}$$

Many authors call therefore the coherent state basis overcomplete.

Particular coherent states (mostly used in optics) are built on a Fock space generated by bosonic creating and annihilating operators, $a^\dagger$ and a. Besides the bosonic commutator relation, $\left[a,a^\dagger\right] = 1$ is fulfilled, there exists a lowest state defined by $a|0>= 0$ (this is the empty state). Successive application of the creation operators lead to n-fold occupied quantum states:

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle. \tag{8.141}$$

They span a Fock space: $\{|n\rangle\} \subset \mathscr{H}$ for n running over all non-negative integers. It is straightforward to create states, indexed by a complex number, $z \in \mathscr{C}$,

$$|z\rangle = \exp\left(za^\dagger - z^*a\right)\,|0\rangle. \tag{8.142}$$

Since $(a+a^\dagger)$ is Hermitean, while $(a-a^\dagger)$ is anti-hermitean and $(z+z^*)$ is real, while $(z-z^*)$ is pure imaginary, the operator expression in the exponent is anti-hermitean (or i times hermitean), so the state $|z\rangle$ is made from the lowest state by a unitary transformation. Therefore its norm is unity: $\langle z|z\rangle = 1$.

For alternative forms of the canonical coherent state we note the operator identity

$$e^{A+B} = e^{-\frac{1}{2}[A,B]}\, e^{A}\, e^{B} \tag{8.143}$$

if the commutator, $[A,B]$, commutes with both A and B. (This is a special case of the Baker–Campbell–Hausdorff formula.) For the operators $A = za^{\dagger}$ and $B = -z^{*}a$ this is fulfilled, so one derives

$$|z\rangle = e^{-\frac{1}{2}|z|^2}\, e^{za^{\dagger}}\, e^{-z^{*}a}\, |0\rangle. \tag{8.144}$$

Now, since the action of the operator a on the vacuum state is zero, the last factor can be replaced by the unity. Using the recursive action of $a^{\dagger}$ one arrives at the alternative form:

$$|z\rangle = e^{-\frac{1}{2}|z|^2}\, e^{za^{\dagger}}\, |0\rangle = e^{-\frac{1}{2}|z|^2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle. \tag{8.145}$$

Viewing by this, a canonical (optical) coherent state is a mixture of all n-quantum states with a fixed complex factor z.

In this representation is the easiest to derive its most cited property:

$$a|z\rangle = e^{-\frac{1}{2}|z|^2} \sum_{n=1}^{\infty} \frac{z^n}{\sqrt{n!}} \sqrt{n} |n-1\rangle = z|z\rangle. \tag{8.146}$$

i.e. that a coherent state is an eigenstate to the annihilation operator with the eigenvalue equal to the complex index z. This result can be used to show that a coherent state is a minimal uncertainty state. One just needs to inspect

$$\langle z|a^{\dagger}a|z\rangle = z^{*}z = \langle z|a^{\dagger}|z\rangle\, \langle z|a|z\rangle. \tag{8.147}$$

There is always an overlap between two different canonical coherent states, but this diminishes with the distance of indices. Using the formula (8.145) it is easy to get that

$$\langle z_2|z_1\rangle = e^{-\frac{1}{2}|z_1|^2}\, e^{-\frac{1}{2}|z_2|^2}\, e^{z_2^{*}z_1}, \tag{8.148}$$

whose absolute value is given by

$$|\langle z_2|z_1\rangle| = e^{-\frac{1}{2}|z_1-z_2|^2}. \tag{8.149}$$

The (over)completeness is fulfilled by the “natural” integration measure on the complex plane

$$1 = \int |z\rangle\, \langle z|\, \frac{d^2 z}{\pi}. \tag{8.150}$$

It is relatively simple to relate canonical coherent states to the classical phase space. Considering harmonic quantum oscillators associated to the creation and annihilation operators, the hermitean generalized coordinate and momentum operators are given as linear combinations:

$$\hat{Q} = \sqrt{\frac{\hbar}{2\omega}}(a + a^\dagger), \qquad \hat{P} = i\sqrt{\frac{\hbar\omega}{2}}(a^\dagger - a). \tag{8.151}$$

The Heisenberg commutation relation, $\left[\hat{Q}, \hat{P}\right] = i\hbar$ is fulfilled independent of the value of ω. The integration measure in the complex z-plane becomes the phase space integral,

$$\frac{\mathrm{d}^2 z}{\pi} = \frac{\mathrm{d}q\mathrm{d}p}{2\pi\hbar}, \tag{8.152}$$

after the identification

$$z = \sqrt{\frac{\omega}{2\hbar}}q + \frac{i}{\sqrt{2\hbar\omega}}p. \tag{8.153}$$

The combination $(za^\dagger - z^* a)$ becomes $\frac{i}{\hbar}(p\hat{Q} - q\hat{P})$, and herewith the coherent state can be indexed by real phase space points as

$$|z\rangle = |p, q\rangle = \hat{U}\,[p, q]\,|0\rangle, \tag{8.154}$$

with the unitary Weyl operator

$$\hat{U}\,[p, q] = \mathrm{e}^{\frac{i}{\hbar}(p\hat{Q} - q\hat{P})}. \tag{8.155}$$

The Weyl operator acts as a shift operator in the sense that

$$\hat{U}^\dagger \hat{Q} \hat{U} = \hat{Q} + q\hat{1}, \qquad \hat{U}^\dagger \hat{P} \hat{U} = \hat{P} + p\hat{1}. \tag{8.156}$$

It is interesting to note that the operator identity (8.143) leads both to the following commutator–eigenvalue equations,

$$\left[\hat{Q}, \hat{U}\right] = q\hat{U}, \qquad \left[\hat{P}, \hat{U}\right] = p\hat{U}, \tag{8.157}$$

and to the symplectic structure of classical Hamiltonian dynamics:

$$\frac{1}{2}(\hat{Q}\hat{U} + \hat{U}\hat{Q}) = \frac{\hbar}{i}\frac{\partial}{\partial p}\hat{U}, \qquad \frac{1}{2}(\hat{P}\hat{U} + \hat{U}\hat{P}) = -\frac{\hbar}{i}\frac{\partial}{\partial q}\hat{U}. \tag{8.158}$$

For an arbitrary operator combination $\hat{A} = A(\hat{Q}, \hat{P})$ we get

$$\hat{A}\,\hat{U} = A\left(\frac{q}{2} + \frac{\hbar}{i}\frac{\partial}{\partial p}, \frac{p}{2} - \frac{\hbar}{i}\frac{\partial}{\partial q}\right)\hat{U} \tag{8.159}$$

and

$$\hat{U}\hat{A} = A\left(-\frac{q}{2} + \frac{\hbar}{i}\frac{\partial}{\partial p}, -\frac{p}{2} - \frac{\hbar}{i}\frac{\partial}{\partial q}\right)\hat{U}. \tag{8.160}$$

Due to the completeness any such operator has an integral representation, too:

$$\hat{A} = \int \mathrm{tr}\left(U^\dagger [p,q]\hat{A}\right) \hat{U}[p,q] \, \frac{\mathrm{d}p\mathrm{d}q}{2\pi\hbar} \tag{8.161}$$

The unitary transformations described by the Weyl operator constitute a fast-Abelean group:

$$\hat{U}[p_2,q_2]\,\hat{U}[p_1,q_1] = \mathrm{e}^{\frac{i}{2\hbar}(q_1p_2-q_2p_1)}\,\hat{U}[p_2+p_1,q_2+q_1]\,. \tag{8.162}$$

It is interesting to study the coordinate space representation of the Weyl operator; it becomes related to the Wigner function. The states $|\alpha\rangle$ and $|\beta\rangle$ are described by the complex valued wave functions, $\alpha(x)$ and $\beta(x)$ in this representation. The general matrix element of the Weyl operator becomes

$$U_{\alpha\beta} = \langle\alpha|\hat{U}[p,q]|\beta\rangle = \int \alpha^*(x)\langle x|\mathrm{e}^{\frac{i}{\hbar}(p\hat{Q}-q\hat{P})}|y\rangle\beta(y)\,\mathrm{d}x\mathrm{d}y. \tag{8.163}$$

Using again (8.143) the operator $\hat{U}$ can be expressed as

$$\hat{U}[p,q] = \mathrm{e}^{-\frac{i}{2\hbar}pq}\,\mathrm{e}^{\frac{i}{\hbar}p\hat{Q}}\,\mathrm{e}^{-\frac{i}{\hbar}q\hat{P}}. \tag{8.164}$$

Since the actions of the respective operators on coordinate eigenstates are given as

$$\langle x|\hat{Q} = x\langle x|, \qquad \hat{P}|y\rangle = \frac{\hbar}{i}\frac{\partial}{\partial y}|y\rangle, \tag{8.165}$$

we have

$$\langle x|\hat{U}[p,q]|y\rangle = \mathrm{e}^{-\frac{i}{2\hbar}pq}\,\mathrm{e}^{\frac{i}{\hbar}px}\,\mathrm{e}^{-q\frac{\partial}{\partial y}}\langle x|y\rangle. \tag{8.166}$$

Using now $\langle x|y\rangle = \delta(x-y)$, partial integration and the variable substitution $x' = x - q/2$ in (8.163) we obtain

$$U_{\alpha\beta}(p,q) = \mathrm{e}^{-\frac{i}{\hbar}pq}\int \alpha^*\left(x-\frac{q}{2}\right)\mathrm{e}^{\frac{i}{\hbar}px}\,\beta\left(x+\frac{q}{2}\right)\mathrm{d}x \tag{8.167}$$

This expression differs from the well-known Wigner function just in the Fourier transformed variable:

$$W_{\alpha\beta}(p,x) = \int \mathrm{e}^{\frac{i}{\hbar}pq}\,\alpha^*\left(x-\frac{q}{2}\right)\beta\left(x+\frac{q}{2}\right)\mathrm{d}q. \tag{8.168}$$

Both quantities are Fourier transforms of the density matrix in coordinate representation,

$$\rho_{\alpha\beta}(x,y) = \alpha^*(x)\beta(y). \tag{8.169}$$

The Husimi function is given as the expectation value of the density matrix in a coherent state:

$$H_{\alpha\beta} = \langle 0|\hat{U}^\dagger[p,q]\,\hat{\rho}\,\hat{U}[p,q]|0\rangle = \int\langle p,q|\alpha^*\left(x-\frac{q}{2}\right)\beta\left(x+\frac{q}{2}\right)|p,q\rangle. \tag{8.170}$$

The latter is a positive semi-definite function, it is often interpreted as a probability distribution. Exactly this defines the Wehrl-entropy:

$$S_{\mathrm{W}} = -\int H_{\alpha\beta}(p,q)\,\ln H_{\alpha\beta}(p,q)\,\frac{\mathrm{d}q\mathrm{d}p}{2\pi\hbar}. \tag{8.171}$$

8.3.2.1 Coherent Path Integrals

A coherent state $|\ell\rangle$ is represented by a point in the index space $\mathscr{L}$. During the time evolution of quantum systems under the action of a conservative Hamiltonian, $\hat{H}$, the state remains a coherent state, its evolution is described by a path $\ell(t)$. The quantum mechanical transition amplitude between a state ℓ' in time t' and a state ℓ'' in time t'' is given as

$$G = \langle \ell'', t'' | \ell', t' \rangle = \langle \ell'' | \mathrm{e}^{-\frac{i}{\hbar}(t''-t')\hat{H}} | \ell' \rangle. \tag{8.172}$$

Since coherent states span an overcomplete system, actually all transition amplitudes can be described by paths going over coherent states inside the time interval.

The usual construction of path integrals (cf. Sect. 8.5) replaces the exponential evolution operator by a product of ones belonging to short times. Considering uniform timesteps of $\varepsilon = (t''-t')/(N+1)$, the factorization can be done for Hamiltonians satisfying

$$\|\hat{H}^N |\ell\rangle\|^2 \leq ab^N (2N)! \tag{8.173}$$

for large enough N. In the $\varepsilon \longrightarrow 0$ limit – by keeping $(t''-t')$ finite – The exponential factors are linearized:

$$G = \lim_{N\longrightarrow\infty} \langle \ell'' | \left(1 - \frac{i\varepsilon}{\hbar}\hat{H} \right)^{N+1} | \ell' \rangle. \tag{8.174}$$

This formula is factorized alongside of reference points ℓ_n, starting with $\ell_0 = \ell'$ and ending in $\ell_{N+1} = \ell''$, by inserting $1 = \int |\ell_n\rangle \langle \ell_n | \delta\ell_n$ between each linear factor:

$$G = \lim_{N\longrightarrow\infty} \int \prod_{n=0}^{N} \langle \ell_{n+1} | \left(1 - \frac{i\varepsilon}{\hbar}\hat{H} \right) | \ell_n \rangle \prod_{n=1}^{N} \delta\ell_n. \tag{8.175}$$

Now the transition matrix elements of the Hamiltonian are to be evaluated between two coherent states:

$$H(\ell_a, \ell_b) = \frac{\langle \ell_a | \hat{H} | \ell_b \rangle}{\langle \ell_a | \ell_b \rangle}. \tag{8.176}$$

Giving examples, for a free Hamiltonian, $\hat{H} = aa^\dagger$, it consists of a vacuum part and a normal ordered part: $H(z_a, z_b) = 1 + z_a^* z_b$. For an anharmonic interaction term among canonical coherent states, $\hat{H} = (a + a^\dagger)^4$ more nontrivial contributions occur: $H(z_a, z_b) = 3 + 6(q_a + q_b)^2 + (q_a + q_b)^4$. The rules are the same as for Gaussian wave pockets.

The path integral for the transition amplitude can be written as

$$G = \lim_{N\to\infty} \int \prod_{n=0}^{N} \langle \ell_{n+1} | \ell_n \rangle \, \mathrm{e}^{-\frac{i\varepsilon}{\hbar} H(\ell_{n+1},\ell_n)} \prod_{n=1}^{N} \delta \ell_n \tag{8.177}$$

up to order ε. Now the continuity property in the index space ensures that $H(\ell_{n+1},\ell_n)$ can be replaced by $H_n = H(\ell_n,\ell_n)$ to leading order in ε. Then the N-fold integral over the control points ℓ_n becomes a path integral with the measure $\mathscr{D}\ell(t)$ in the usual limit. The overlap between neighboring states alongside the path can also be written in exponential form to leading order:

$$\langle \ell_{n+1} | \ell_n \rangle = 1 - \langle \ell_{n+1} | \ell_{n+1} - \ell_n \rangle = \mathrm{e}^{-\langle \ell_{n+1} | \mathrm{d}\ell_{n+1} \rangle}, \tag{8.178}$$

so at the end we arrive at

$$G = \int \mathscr{D}\ell \, \mathrm{e}^{-\int_{\ell'}^{\ell''} \langle \ell(t) | \mathrm{d}\ell(t) \rangle - \frac{i}{\hbar} \int_{t'}^{t''} H(\ell(t)) \mathrm{d}t} . \tag{8.179}$$

Working with normalized coherent states, $H(\ell(t)) = \langle \ell(t) | \hat{H} | \ell(t) \rangle$. In coordinate representation, this becomes a Gaussian smeared Hamiltonian, the Gaussian effective potential.

Note also that the first integral term in the exponential was written without reference to the time variable; this is a phase factor akin to the Berry phase in classical chaos studies. Nevertheless, whenever $\ell(t)$ is a differentiable path and $\dot{\ell}(t) = \mathrm{d}\ell/\mathrm{d}t$ is calculable at least at the control points ℓ_n, the whole exponential can be written as one time integral – similar to that of the classical diffusion problem (Sect. 8.3). This way the partial time derivation operator and the Hamilton operator act together as

$$G = \int \mathscr{D}\ell \, \mathrm{e}^{\frac{i}{\hbar} \int_{t'}^{t''} \langle \ell(t) | i\hbar \frac{\partial}{\partial t} - \hat{H} | \ell(t) \rangle} . \tag{8.180}$$

Here, one recognizes the operator of the time dependent Schrödinger equation ordered to zero, whose expectation value is taken alongside the coherent state path $\ell(t)$.

8.3.2.2 Path Integrals in the Phase Space

In the phase space notation, the time dependent path over coherent states is fabricated from the ground state by applying the Weyl-operator with time dependent phase space parameters:

$$|\ell(t)\rangle = \hat{U}\,[p(t), q(t)]\,|0\rangle. \tag{8.181}$$

The time derivative of this coherent state path can be obtained as

$$|\dot{\ell}(t)\rangle \,=\, \lim_{\tau\to 0}\left(\hat{U}\left[p+\tau\dot{p},q+\tau\dot{q}\right]-\hat{U}\left[p,q\right]\right)|0\rangle. \tag{8.182}$$

In order to calculate this quantity we use the factorized form of the Weyl operator:

$$\hat{U}_t = \mathrm{e}^{\frac{i}{2\hbar}pq}\,\mathrm{e}^{-\frac{i}{\hbar}q\hat{P}}\,\mathrm{e}^{\frac{i}{\hbar}p\hat{Q}}. \tag{8.183}$$

For a small time difference τ, the left and right factors are linear giving

$$\hat{U}_{t+\tau} = \left(1+\frac{i\tau}{2\hbar}\frac{\partial}{\partial t}pq\right)\left(1-\frac{i\tau}{\hbar}\dot{q}\hat{P}\right)U_t\left(1+\frac{i\tau}{\hbar}\dot{p}\hat{Q}\right). \tag{8.184}$$

This leads to the following parametric derivative of the Weyl operator:

$$\frac{\partial}{\partial t}\hat{U} \,=\, \frac{i}{2\hbar}\left(\dot{p}q+p\dot{q}\right)\hat{U} \,-\, \frac{i}{\hbar}\dot{q}\hat{P}\hat{U} \,+\, \frac{i}{\hbar}\dot{p}\hat{U}\hat{Q}. \tag{8.185}$$

The Berry phase factor becomes the ground state expectation value of the Mauer–Cartan form of the fast-Abelean Weyl group

$$\langle\ell|\mathrm{d}\ell\rangle = \langle 0|U^{\dagger}\mathrm{d}U|0\rangle, \tag{8.186}$$

and using the above equation (8.185) we arrive at

$$\langle\ell|\dot{\ell}\rangle \,=\, \frac{i}{2\hbar}\left(\dot{p}q+p\dot{q}\right)\langle 0|\hat{U}^{\dagger}\hat{U}|0\rangle \,-\, \frac{i}{\hbar}\dot{q}\langle 0|\hat{U}^{\dagger}\hat{P}\hat{U}|0\rangle \,+\, \frac{i}{\hbar}\dot{p}\langle 0|\hat{U}^{\dagger}\hat{U}\hat{Q}|0\rangle. \tag{8.187}$$

Using now that $\hat{U}^{\dagger}\hat{U}=1$ and $\hat{U}^{\dagger}\hat{P}\hat{U}=\hat{P}+p\hat{1}$, one obtains

$$i\hbar\langle\ell|\dot{\ell}\rangle \,=\, p\dot{q}-\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}(pq) \tag{8.188}$$

for a zero-centered, $\langle 0|\hat{Q}|0\rangle=0$, and translation invariant ground state: $\langle 0|\hat{P}|0\rangle=0$. After neglecting the integral of the total time-derivative term, it recovers the familiar Hamiltonian action principle:

$$G = \int\mathscr{D}p\mathscr{D}q\,\mathrm{e}^{\frac{i}{\hbar}\int\limits_{t'}^{t''}(p\dot{q}-H(p,q))\mathrm{d}t}. \tag{8.189}$$

For particular forms of the Gaussian effective potential, i.e. for $H(p,q)=p^2/2+V(q)$, the path integral over $p(t)$ is Gaussian and therefore can be carried out exactly. In this case one obtains the Feynman–Hibbs formula for the path integral:

$$G = \int\mathscr{D}q\,\mathrm{e}^{\frac{i}{\hbar}\int\limits_{t'}^{t''}L(\dot{q},q)\mathrm{d}t} \tag{8.190}$$

with

$$L(\dot{q},q)=\frac{1}{2}\dot{q}^2-V(q). \tag{8.191}$$

8.3.3 Canonical Partition: Paths in Euclidean Time

The correspondence between imaginary-time quantum mechanics and statistical physics also occurs in the relation of path integrals to the canonical partition function. The formal definition (for in the thermodynamical limit additive Hamiltonians),

$$Z=\mathrm{tr}\,\mathrm{e}^{-\beta H}=\sum_n \mathrm{e}^{-\beta E_n} \tag{8.192}$$

expresses the canonical partition function with the help of the eigenvalues of the Hamiltonian. Since the Hamiltonian is the generator of the infinitesimal time shifts, such a state is stationary by definition. On the other hand the Feynman path-integral for transition from an initial state at time t_a to the *same state* at time t_b but irrespective of the fact that which state it were also includes a summation over this initial-end-state, x:

$$Z_{QM}=\mathrm{tr}\,\mathrm{e}^{-i(t_b-t_a)H/\hbar}. \tag{8.193}$$

In coordinate basis, we have $x_a=x_b=x$ and sum over all starting points of possible closed evolution paths in a continuous labeling of the Hilbert space. One writes

$$Z=\int_{-\infty}^{\infty}\mathrm{d}x\,\langle x|\mathrm{e}^{-\beta H}|x\rangle=\int_{-\infty}^{\infty}\mathrm{d}x\,\langle x,t_b|x,t_a\rangle\big|_{t_b-t_a=-i\hbar\beta}\,, \tag{8.194}$$

recognizing that the statistical canonical partition function is in fact formally a path integral over closed paths quantum-evolving in imaginary time for a period length of $i\hbar\beta$.

The discretization of such paths for observation points in the imaginary time can as well be done as it was demonstrated for the free diffusion problem, previously. Taking imaginary time steps of $\varepsilon=\hbar\beta/(N+1)$ one goes over a closed chain (path) of states:

$$Z=\prod_{n=1}^{N+1}\left(\int_{-\infty}^{\infty}\mathrm{d}x_n\right)\langle x_{N+1}|\mathrm{e}^{-\varepsilon H/\hbar}|x_N\rangle\ldots\langle x_1|\mathrm{e}^{-\varepsilon H/\hbar}|x_{N+1}\rangle. \tag{8.195}$$

Representing the overlap of states in a plane wave basis one uses the approximation

$$\langle||\rangle\approx\int_{-\infty}^{\infty}\frac{\mathrm{d}p_n}{2\pi}\,\mathrm{e}^{ip_n(x_n-x_{n-1})/\hbar-\varepsilon H/\hbar}. \tag{8.196}$$

By the virtue of this the partition function gains a phase space representation,

$$Z = \prod_{n=1}^{N+1} \left(\int_{-\infty}^{\infty} \mathrm{d}x_n \int_{-\infty}^{\infty} \frac{\mathrm{d}p_n}{2\pi} \right) \mathrm{e}^{-S_N/\hbar} \tag{8.197}$$

with the discretized action

$$S_N = \sum_{n=1}^{N+1} \left(-ip_n(x_n - x_{n-1}) + \varepsilon H(x_n, p_n) \right) \tag{8.198}$$

In the usual path integral limit, the latter becomes the classical action integrated, however, in the real time, τ:

$$S_\infty = \int_0^{\hbar\beta} \mathrm{d}\tau \left[-ip(\tau) \frac{\mathrm{d}x(\tau)}{\mathrm{d}\tau} + H\left(p(\tau), x(\tau)\right) \right], \tag{8.199}$$

and the canonical partition function is represented as a path integral

$$Z = \int \mathscr{D}[x(\tau)] \, \frac{\mathscr{D}[p(\tau)]}{2\pi\hbar} \, \mathrm{e}^{-S/\hbar} \tag{8.200}$$

Based on this representation of the canonical partition function one can easily obtain the diagonal elements of the statistical density matrix,

$$\rho(x_a, x_a) = \frac{1}{Z} \langle x_a | \mathrm{e}^{-\beta H} | x_a \rangle. \tag{8.201}$$

It is normalized and in a basis of energy eigenstates it reads as

$$\rho(x_a, x_a) = \frac{\sum_n |\psi_n(x_a)|^2 \, \mathrm{e}^{-\beta E_n}}{\sum_n \mathrm{e}^{-\beta E_n}}. \tag{8.202}$$

At the absolute zero temperature the smallest energy eigenvalue dominates the sums both in the numerator and denominator. As a consequence the density matrix diagonal element becomes the absolute value squared of the ground state wave function – interpreted as a probability to be found at x_a by the Copenhagen interpretation of quantum mechanics:

$$\lim_{T \to 0} \rho(x_a, x_a) = |\psi_0(x_a)|^2. \tag{8.203}$$

On the other hand, at high enough temperature, i.e. when the thermal excitation scale dominates over the quantum scale, $k_\mathrm{B}T \gg \hbar/t \sim E_0$, the partition function (8.200) approaches the classical partition function:

$$\lim_{T \to \infty} Z = \int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi\hbar} \, \mathrm{e}^{-\beta H(p,x)}. \tag{8.204}$$

Here, several approximations occur: (1) the integral over a short imaginary period gives space to a multiplication with the interval length, $\hbar\beta$, canceling this way the dependence on the Planck constant and (2) the "kinetic" contribution averages out close to zero. For free oscillators at a general temperature, $T = k_{\mathrm{B}}/\beta$, the partition function path integral leads back to the formula of the Bose distribution [91].

8.4 Quantization due to Higher-Dimensional Chaotic Dynamics

The idea of chaotic quantization was in part motivated by the frustration stemming from the experience that gravity is resisting theoretical intentions to be quantized. String theory, while it approaches the problem on the basis of quantum field theory, not only requires ten space-time dimensions to be consistent and predicts yet undiscovered super-partners to known elementary particles, but also calls upon the additional concept of compactification.

Chaotic quantization realizes an opposite strategy, starting with classical gauge field theory which due to its own Hamiltonian dynamics is chaotic. It evolves ergodically – enough time given – in field-configuration phase space and this process leads in the long-time limit to a stationary distribution sampling from lower dimensional sub-configurations. These, as result of the higher dimensional *classical* dynamics, are distributed as the lower dimensional *quantum* field theory requires in the imaginary time formalism. The chaotic quantization is a particular form of the stochastic quantization [92], it works self-contained, driven by its inner dynamics, not requiring any assumption of an external heat bath or noise. We outline its main ideas by presenting an example of a strongly coupled electrodynamics on a lattice, which is a classically chaotic system. What follows is based on common work with Berndt Müller and Sergei Matinyan at the Duke University, NC, USA.

As a working example we take a 5-dimensional lattice on which a classical, pure U(1) gauge theory resides. This simple group still shows chaotic dynamics at strong coupling, being equivalent to the large amplitude motion of many coupled pendulums. Although in the continuum limit U(1) is not chaotic, since all anharmonic terms in the expansion of cosine functions are neglected, at finite lattice spacing its classical dynamics is chaotic. This was numerically demonstrated in the 3-dimensional case.

The conjecture between the 5-dimensional classical theory with chaotic dynamics and the 4-dimensional quantum field theory can be comprised into a simple formula between the "normal" (4-dimensional) Planck constant and two physical characteristics of the higher dimensional theory, its temperature and lattice spacing:

$$\hbar = aT \tag{8.205}$$

Usually, such a formula is read in an opposite direction, automatically relating a Planck mass ($M_{\mathrm{P}} = T$) with a Planck length ($L_{\mathrm{P}} = a$). Our philosophy here, however, views $\hbar$ as a constant of nature factorized to two other, underlying properties of the (in the present theory 5-dimensional) world. An enlightening analogy of this situation is given by the classical electrodynamics formula factorizing another constant of nature, c, the speed of light:

$$1/c^2 = \varepsilon_0 \mu_0. \tag{8.206}$$

Taking $c =$ constant as a postulate, we arrive at the theory of special relativity. One derives the laws of Lorentz transformation in the framework of mechanics without making any reference to electric or magnetic fields.[6] Maxwell theory on the other hand, as a classical field theory regards ε_0 and μ_0 as independent properties of the physical vacuum, as dielectric constant and magnetic permeability. Light waves are solutions of Maxwell theory and the speed of light is calculable. The relation between nowadays Quantum Field Theory and the conjectured underlying classical field theory is analogous to this. Furthermore, just as ether does not need to exist for Maxwell theory to work, the five dimensional lattice also may prove to be just a theoretical construct without measurability. The fixed length, a, may also stem from another mechanism as in fact having a space-time lattice at the Planck length.

8.4.1 Chaos in Gauge Theory

First non-abelian then also abelian gauge theories has been studied with respect to chaotic behavior [93]. In the eighties model systems, with a few, selected degrees of freedom with long wavelength has been studied. The most characteristic results stem from SU(2) Yang–Mills theory, considering two $k = 0$ modes of different polarization and color. We denote the spatially constant, scaled vector potential components as $x = gA_1^{(2)}(t)$ and $y = gA_2^{(1)}(t)$. The SU(2)-colored electric field has two, the magnetic field only one non-vanishing component (in the Hamiltonian gauge annulling the scalar potentials):

$$E_1^{(2)} = \dot{A}_1^{(2)}, \quad E_2^{(1)} = \dot{A}_2^{(1)}, \quad B_3^{(3)} = gA_1^{(2)}A_2^{(1)}. \tag{8.207}$$

Since these are space-homogeneous, the Hamiltonian,

$$H = \frac{V}{2} \sum_{i,a} \left(E_i^a E_i^a + B_i^a B_i^a \right), \tag{8.208}$$

summed over polarization indices $i = 1,2,3$ and color indices $a = 1,2,3$, leads to the model-Hamiltonian

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[6] This has been first demonstrated by Albert Einstein.

$$H' = \frac{g^2}{V} H = \frac{1}{2}\left(\dot{x}^2 + \dot{y}^2\right) + \frac{1}{2} x^2 y^2. \tag{8.209}$$

This describes a classically chaotic system with a null-measure of regular periodic orbits. The turning points of the classical motion lie on $H' =$ constant hyperboles, defocusing parallel trajectories. Figure 8.1 demonstrates the gradual dispersion of nearby configurations eventually covering the allowed configuration space uniformly. This is in accordance with the general mechanism, how chaotic motion fills phase space regions with a pace dictated by the sum of all positive Lyapunov exponents, the exponential rate of the divergence of nearby phase space points. Viewing this process by a fixed resolution, information is lost and this defines a rate for entropy generation (the so-called Kolmogorov–Sinai entropy). The time integral between the totally ordered initial state then estimates the final, maximal entropy at uniform coverage. Now, since the Hamiltonian motion is energy-conserving, each constant $H' = g^2 H/V$ predestines a region in the phase space to be covered at the end. At a fixed resolution, i.e. at a given size of classical phase space cells, this reveals a microcanonical equation of state, $S(E)$.

Numerical studies on lattices followed in the 1990s. Mainly the gauge groups U(1), SU(2) and SU(3) has been studied, all showed chaotic behavior. The scaling of the leading Lyapunov exponent with the scaled total energy of the classical lattice, $a\lambda_{\text{max}} \sim ag^2 H$ for non-abelian gauge groups, as well as the extensivity of the Lyapunov spectrum and the Kolmogorov–Sinai (KS) entropy – related to the ergodization speed – were studied. Interpreting the KS-entropy as the physical entropy of the lattice gauge system even an attempt can be done to extract a classical equation of state.

A basic interest lies in the investigation whether classically chaotic systems and configurations are also special for the quantum pendant. Correlation between chaos and confinement has been observed in SU(2) and U(1) lattices comparing quantum Monte Carlo results and classical Hamiltonian dynamics in $3+1$ dimensions. For the U(1) group in the strong coupling phase a strong tendency could have been observed between the presence of magnetic monopole anti-monopole pairs and the chaotic behavior.

8.4.2 *Higher Dimensional Plasma Physics*

The main point of the stochastic quantization, namely generating field configurations distributed according to Boltzmann weights,

$$\mathscr{P} = \exp\left(-\beta S_E[A']\right) \tag{8.210}$$

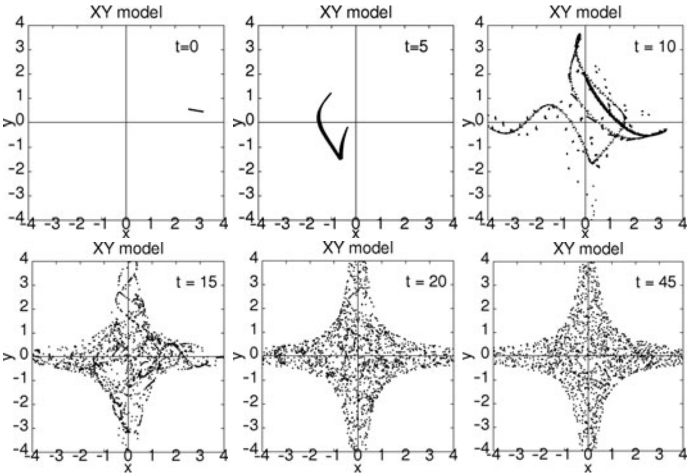

Fig. 8.1 Time evolution of initially adjacent trajectories in the *xy*-model. One hundred initially adjacent points eventually scatter over the whole classically allowed phase space. These figures demonstrate the case $H' = \dot{x}^2 + \dot{y}^2 + x^2y^2 = 1$

for pure gauge theories, where the original vector potential variable, A is rescaled to $A' = gA$ and as a consequence $\beta = 1/g^2\hbar$ due to the scaling of the action $S[A] = S[gA]/g^2$. These Boltzmann weights occur in Feynman path integrals when calculating expectation values in quantum field theory. At the same time they can be regarded as a stationary distribution of a corresponding Fokker–Planck equation,

$$\sigma_5 \frac{\partial}{\partial t_5}\mathscr{P} = \int \mathrm{d}^4x \, \frac{\delta}{\delta A}\left(\frac{1}{\beta}\frac{\delta}{\delta A}\mathscr{P} + \frac{\delta S}{\delta A}\mathscr{P}\right). \tag{8.211}$$

Formally, $1/\beta$ can be interpreted as a temperature of the five dimensional system, T_5. The Fokker–Planck equation is equivalent to the solution of the corresponding Langevin equation,

$$\ddot{A} + \frac{\delta S}{\delta A} = J, \tag{8.212}$$

where the source current density is split to a dissipative term (like ohmic resistance) and to a fluctuative (noise) term:

$$J = -\sigma\dot{A} + \zeta. \tag{8.213}$$

This noise is usually treated simplified, as a Gaussian white noise with zero mean and a correlation sharply localized in space and time:

$$\langle \zeta(x_1)\zeta(x_2)\rangle = 2\sigma T \delta^4(x_1 - x_2). \tag{8.214}$$

In the infrared limit, the low frequency components dominate the relevant vector potential configurations, the radiative term $\ddot{A}$ can be neglected besides the dissipative term $\sigma\dot{A}$. The typical frequency is small, $\omega \ll \sigma$, the typical time is large, $\tau \gg 1/\sigma$. The effective model to electrodynamics is a Langevin plasma described by

$$\sigma\dot{A} + \frac{\delta S}{\delta A} = \zeta. \tag{8.215}$$

This equation is analogous to the well-known Brownian motion, so are the mean features of its solution: the action S after long enough time is distributed around its ergodic limit of $k_{\mathrm{B}}T/2$ per degree of freedom, and initial correlations decay exponentially with the characteristic time of the corresponding damping constant, $t_{\mathrm{char}} = 1/\gamma = \sigma/|k|^2$. The long time average of such correlations with the initial value are interpreted in the lower dimensional field theory as propagators.

This analogy with plasma physics in the continuum limit led us to detailed investigations of dynamical time scales: the thermal ($\hbar/T$), electric ($\sqrt{\hbar}/gT$) and magnetic screening length ($1/g^2T$) in a usual, three dimensional plasma depend on the temperature, on the Planck constant and on the coupling constant of the original gauge theory, g. In the long time limit, the plasma dynamics leads to distributions simulating a dimensionally reduced, three dimensional field theory with the effective coupling $g_3 = g^2T$. It can happen only for pure gauge theories, with mass scale invariance. The magnetic part of the energy is identical with a lower dimensional Maxwell or Yang–Mills action:

$$\frac{1}{2}B_iB_i = -\frac{1}{4}F_{ij}F^{ij}. \tag{8.216}$$

The effective approach with white noise and Langevin equation is valid for the long-time behavior, $t \gg 1/g^2T$. Table 8.1 summarizes the most important features of traditional plasma physics, in the third column showing the corresponding formulas for classical lattices. Since most of the time-constants in plasma physics are coefficients in a linear response approach, they can be calculated on a classical lattice as well as in quantum field theory. Here no Planck constant occurs, but the lattice spacing plays a basic role. These two approaches coincide if the universal relation $\hbar = aT$ is assumed.

These calculations can be repeated in arbitrary number of Euclidean dimensions, including the $4+1$-dimensional case of traditional stochastic quantization. Table 8.2 shows the characteristic results for d-dimensional plasmas and $d+1$-dimensional lattices with classical Hamiltonian dynamics.

Table 8.1 Scales in plasma physics and on the lattice show a universal scaling: $\hbar = aT$

	3-dim QFT plasma	$3+1$ class. lattice
d_m	$1/g^2T$	$1/g^2T$
d_e	$\sqrt{\hbar}/gT$	$\sqrt{a/g^2T}$
ω^2	$g^2T^2/\hbar$	g^2T/a
γ	g^2T	g^2T
σ	$T/\hbar(\log)$	$1/a(\log)$
$d_m \gg d_e$	$g^2\hbar \ll 1$	$a \ll 1/g^2T$

Table 8.2 Scales in plasma physics and on the lattice in arbitrary dimensions

	d dim. QFT plasma	d+1 class. lattice
d_m	$\frac{\hbar}{G^2} = \frac{\hbar^{d-3}}{g^2 T^{d-2}}$	$\frac{a}{G^2} = \frac{a^{d-3}}{g^2 T}$
d_e	$\frac{\hbar}{GT} = \frac{\hbar^{d/2-1}}{g T^{(d-1)/2}}$	$\frac{a}{G} = \frac{a^{d/2-1}}{g\sqrt{T}}$
σ	$\frac{d_{\mathrm{e}}^{d-5}}{g^2 T}$	$\frac{d_{\mathrm{e}}^{d-5}}{g^2 T}$
g_d^2	$\frac{g^2 T}{\hbar}$	$\frac{g^2}{a}$
$G^2 \ll 1$	$g^2 T^{d-3} \hbar^{4-d}$	$g^2 T a^{4-d}$

All formulas coincide if $\hbar = aT$. Here, g is the original coupling, G the weak parameter signaling the infrared limit and g_{d} the effective coupling of the dimensionally reduced theory

8.4.3 U(1) Lattice Model

In this section, we report about numerical simulations on a U(1) lattice gauge system both in 4 and 5 dimensions. The former was simulated by quantum Monte Carlo techniques in order to reproduce long known standard results, the latter independently by $4+1$-dimensional classical Hamiltonian dynamics known to be chaotic from our former studies. In both cases, regular (rather small, 4^4) lattices are considered.

In order to appreciate the computational complexity one faces to, we review briefly basic formulas and techniques of lattice gauge theory calculations. For more advanced information on lattice gauge theories one may consult [94, 95].

In these models of continuum field theory (both in the classical and quantized version), lattice links starting at point x and pointing in the μ direction are associated with phases, $A_\mu(x)$ of unimodular complex numbers – elements of U(1) – $U = \exp(\mathrm{i} g a A_\mu(x))$, while the lattice action is constructed from phase sums around elementary plaquettes, upon using lattice forward derivatives ($a\partial_\mu f = f(x + ae_\mu) - f(x)$). The plaquette phase sums satisfy

$$F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x), \tag{8.217}$$

and determine the lattice action

$$S = \frac{1}{g^2} \sum_x \sum_{\mu>\nu} (1 - \cos(g a^2 F_{\mu\nu})). \tag{8.218}$$

Here, the summation runs over all lattice plaquettes in planes each characterized by a pair of two (ordered and different) direction indices, $\mu > \nu$, and attached with its corner to the site x. In the continuum limit $a \to 0$, the action of the classical electrodynamics is recovered. Quantum Monte Carlo algorithms produce and sample U lattice link values (so called configurations) which are weighted by a Boltzmann type factor

$$w = \mathrm{e}^{-S/\hbar}. \tag{8.219}$$

This corresponds to the evaluation of Feynman path integrals in quantum field theory in the imaginary time formalism.

The classical Hamiltonian approach on the other hand uses the Hamiltonian split to electric and magnetic parts,

$$H = \sum_{x,\mu} \frac{a}{2g^2} |\dot{U}|^2 + E^{\text{magn}}[U]. \tag{8.220}$$

Here, the magnetic contribution to the total Hamiltonian,

$$E^{\text{magn}}[U] = \frac{1}{g^2 a} \sum_x \sum_{i<j} \left(1 - \cos(g a^2 F_{ij})\right), \tag{8.221}$$

is a sum over plaquettes lying in spatio-spatial (hyper)planes. This sum is formally equivalent to the Euclidean action of the same lattice gauge theory in one dimension lower. This self-similarity of pure gauge actions is an essential ingredient for the particular mechanism of chaotic quantization we are pursuing now.

We present results of numerical simulations of a five dimensional classical Hamiltonian U(1) lattice system and compare its evolution in the 5-th coordinate with traditional quantum Monte Carlo generated configurations on a four dimensional lattice, using the four dimensional U(1) lattice action. In the classical Hamiltonian approach the evolution of the U configurations proceeds in a 5-th dimension, often called “fictitious” time when it has been used as a method for stochastic quantization. The important difference is, that so far always an external heat bath or a white noise for solving Langevin type equations has been added to the evolution; we consider here pure classical Hamiltonian dynamics with no other source of noise or fluctuations.

As by construction $aE_5^{\text{magn}} = S_4$ (since the dimensionless plaquette sum or average over the 4-dimensional (sub)lattice is either $ag^2E_5^{\text{magn}}$ when used in the Hamiltonian simulation or $g^2\hbar(S_4/\hbar)$ when used in quantum Monte Carlo algorithms), the conjecture

$$E_5^{\text{magn}}/T = S_4/\hbar \tag{8.222}$$

is literally equivalent to $\hbar = aT$ (1), as we have argued earlier on the basis of plasma physics considerations.

Now we demonstrate the validity of the relation (8.222) by numerical computation. Figure 8.2 shows the absolute value square of the lattice-averaged Polyakov line (the standard order parameter of lattice gauge theory) values – averaged over many quantum Monte Carlo configurations (full squares) as a function of the 4-dimensional lattice plaquette sum per plaquette g^2S_4. On the same plot the same order parameter is shown as a function of the partial plaquette sum corresponding to the magnetic energy $ag^2E_5^{\text{magn}}$ after Hamiltonian equilibration on the classical 4-dimensional lattice, averaged over many points alongside a single evolution trajectory at consecutive 5-th coordinate times (open diamonds). That these two sets of points belong to the same (in the Coulomb plasma phase linear) scaling law, supports our main conjecture.

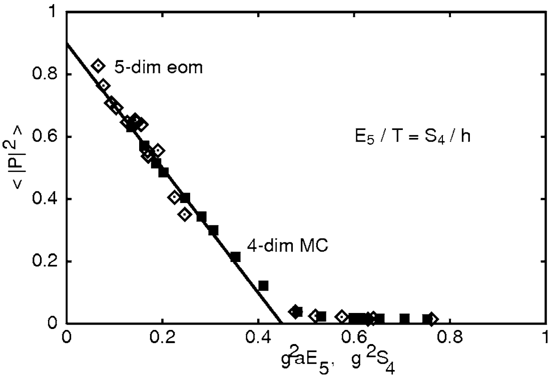

Fig. 8.2 The order parameter, the absolute value square of the Polyakov line averaged over the lattice and over many configurations is plotted against the 4-dimensional plaquette sum in the classical Hamiltonian (*open diamonds*) and in the quantum Monte Carlo (*full squares*) simulations, respectively. The scaling of these results coincides if $E_5/T = S_4/\hbar$

The reason that we do not plot the Polyakov line as usual, as a function of inverse coupling, is that different couplings belong to the 4 and to the 5-dimensional simulation once $\hbar = aT$ is valid. In fact, the lines fitted to our simulation points do not coincide *unless* we assume (8.222).

In order to offer a possibly more direct insight into the relation of 4-dimensional quantum and 5-dimensional classical lattice U(1) theories we plot several points on the complex Polyakov-line plane, both from 4-dimensional quantum Monte Carlo (right column) and from 5-dimensional classical Hamiltonian evolution (left column, actually one single trajectory is plotted). The left and right parts of Fig. 8.3 belong to different inverse couplings for the 4- and 5-dimensional cases, the correspondence is made by selecting out pairs of simulations satisfying (8.222). The 5-dimensional coupling actually does not play any important role; only the scaled energy content of the configuration is related to it. Once it is given, the equipartition happens due to the very same Hamiltonian evolution initially (not shown in the figure). It governs the chaotic trajectory, covering the same region of configurations as the one generated by quantum Monte Carlo codes.

Now the correspondence between classical and quantum configurations is excellent, both for the magnitude and for the phase of Polyakov lines. Some initial points in the middle of the rings for overcritical couplings $\beta_4 = 1/g_4^2 \geq 1$ are irrelevant; they stem from an initial MC heating phase. The classical Hamiltonian evolution also had an initial phase, equilibrating electric and magnetic field energy (in 5 dimensions their ratio is however not 1:1 but 2:3).

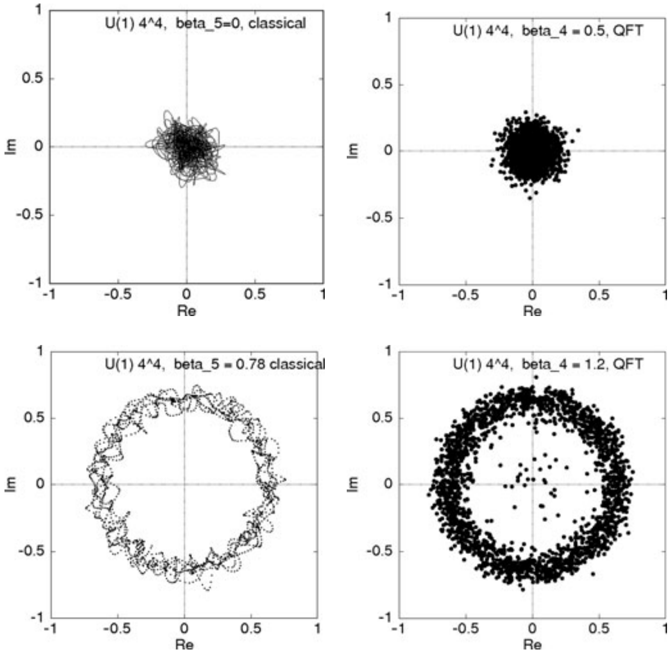

Fig. 8.3 Complex Polyakov line values from 4-dimensional quantum Monte Carlo simulation (*right column*) and from 5-dimensional classical Hamiltonian equation of motion (*left column*) at $aE_5^{\mathrm{mag}} = S_4$

By studying 4-dimensional U(1) lattice gauge theory, it is demonstrated that the mechanism of chaotic quantization – conjectured earlier on the basis of non-abelian plasma physics – works in the practice for lattice gauge theory in 5-dimensional classical form. The correspondence to the traditional 4-dimensional quantum Monte Carlo simulations is given by the general formula $\hbar = aT$, a formula encoding physical properties of the higher dimensional lattice and field configurations into the Planck constant. This fact underlines the hope for a unified classical field theory of gravity and standard particle physics, in particular for an explanation of standard model parameters via the mechanism of chaotic quantization, as well as for getting closer to an insight on the origin of Planck's constant.

Finally, we would like to address the question whether factorizing the Planck constant would not mean to construct a hidden parameter theory. It is not necessarily the case, since none of the laws of experimental quantum physics seem to be violated by our results: the higher dimensional classical dynamics acts as Euclidean quantum field theory in 4 dimensions in all respects. On the other hand the impossibility of a hidden parameter is proved for local actions in a strict manner, while the existence of a higher dimension allows for subtle non-local effects in the 4 dimensions of the physical experience.

Of course, as anything referring to the Planck scale, the theory of chaotic quantization seems to be speculative at the first glance. What is – at least in principle – better than in the case of fundamental string theory, that the autocorrelation time-scale, $\tau \sim \sigma/k^2$ may be effective at scales other, than the Planck length. From the known experimental fact of the relative weakness of gravity coupling compared to standard quantum field theories (QFT) $g_{\mathrm{grav}}^2 \ll g_{\mathrm{QFT}}^2$, we conclude that the time scales beyond which a phenomenon occurs to be quantum, and for shorter time observations not, separates gravity from the rest of the standard particle physics:

$$\tau_{\mathrm{grav}} \ll \tau_{\mathrm{observ}} \ll \tau_{\mathrm{QFT}}.$$

As a consequence, gravity behaves classically while the other three known interactions according to quantum field theory.

Problems

8.1. Obtain the parity of the canonical spectral function by expressing $\rho_{AB}(-\omega)$.

8.2. Calculate the following sum rule for the canonical spectral function:

$$R = \int \frac{\mathrm{d}\omega}{2\pi}\, \rho_{AB}(\omega).$$

8.3. Obtain an operator formula for the Wigner transform of a convolution.

8.4. Consider the $\ddot{x} + 2\Gamma\dot{x} + k^2 x = f(t)$ oscillator within a white noise environment, $\langle f(t) \rangle = 0$, and $\langle f(t)f(t') \rangle = 4\Gamma T \delta(t-t')/V$. What is the correlator in the real-time, $\langle x(t)x(t') \rangle$, and in the frequency representation, $\langle \tilde{x}(\omega)\tilde{x}(\omega') \rangle$, in the infrared $(k \to 0)$ limit?

Afterword

A physics book never ends. The cause of this fact lies only partially in the finiteness of the number of pages a book may include; also, the number of exciting questions tends to grow steadily. It is like a very fine network, ramified in a rather complex fashion. Writing about one or the other problem, its solution, the development of logical concepts and conceptual ideas, very often receives echoes from unexpected corners. Resonating to an idea there are some others, and then yet some further burring questions emerge. This process never ends, so the end of a book must be set *artificially* – no other way exists.

In the present book about challenges to the concept of temperature and some related quantities, like heat and entropy, dissipation an information, equilibrium, and motion, we have brought just a few highlights to attention. In order to lay foundations for the understanding of the nature of these challenges we started with a review of the measurement and interpretation of temperature – as it has been laid down in classical thermodynamics. Already at this level it should have been clear that the temperature as a concept and as a mathematical quantity has several connections, it plays different roles in different parts of theoretical physics. It occurs as an empirical, but yet universal scale associated to thermal equilibrium. It is derived from a Lagrange multiplier used in counting for the energy conservation. Sometimes it takes the form related to a derivative of the entropy–energy function; but sometimes a more general form. Moreover it can be related to statistical parameters of the internal (originally atomic) motion; in a more general setup to a width property of unknown dynamical agents – cited as "noise" for brevity. All these facets sit on the same diamond: These roles and definitions are interrelated.

The first – long known – challenge to this picture emerges from considering systems with a sufficiently small number of degrees of freedom. In such cases the equivalence between the different statistical ensembles is not working, the finite number corrections can be appreciable. In a way in a small, or just "mesoscopic" closed system the entropy maximum with a given energy leads to equilibrium distributions resembling a spread of the inverse temperature parameter. Akin to this

T.S. Biró, *Is There a Temperature? Conceptual Challenges at High Energy, Acceleration and Complexity*, Fundamental Theories of Physics 171,
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phenomenon is the idea of superstatistics, which assumes a probability distribution of different temperatures on the top of the canonical description. As a dynamical model, coupled stochastic evolution equations in a characteristic time-hierarchy approximation can explain such effects. Leaving the canonical paradigm of equilibrium distributions exponentially falling in the energy, the question arises towards a possible generalization of the Gibbsean–Boltzmannian thermodynamics. We have presented a particular approach to this by analyzing abstract composition rules and their infinite repetitions. We have put an emphasis on indicating the possibility of this type of generalizations everywhere in the discussion of the classical laws of thermodynamics.

Classical thermodynamics is particularly challenged by the motion at relativistic speed. While some aspects can be treated by exchanging the energy-momentum relation of particles only, some other – like local and causal dissipation – need a treatment in the framework of relativistic hydrodynamics. Surprisingly, a classical debate about the correct relativistic transformation formula for the absolute temperature – already started by Planck and Einstein – can also be transparently analyzed in this framework.

High acceleration offers a further challenge on thermal concepts. The Unruh effect, by the virtue of which a constant acceleration of a monochromatic wave is observed by a far static observer as a black body radiation at a temperature proportional to the acceleration – is most shocking. In relation with this an entropy can be associated to event horizons around black holes and the zeroth, first and second law of thermodynamics can be demonstrated. Moreover other horizons, namely a cosmological horizon, also behaves mathematically a similar way: a thermal looking environment is created by non-trivial spacetime structures. This concept is carried over to higher dimensional gravity theories describing – by the duality principle – plasmas of strongly interacting matter.

Finally, we have discussed the formal use of the inverse temperature in field theory, where it becomes a period length in the imaginary time direction. This sounds quite abstract and mathematical. However, it does describe the proper thermal statistics for free bosons and fermions, relating the different sign in the basic formula to the different commutation property of the fundamental field operators. Furthermore, it opens up the possibility to treat the kinetic theory of heat and temperature on the level of elementary quantum fields – possibly including quantum effects like off-shellness (uncertainty) of particle states. We have shed a little light on the basics of this. For closing this presentation we took reference to the path integral formalism and the stochastic quantization method used in field theory: an intriguing, albeit speculative analogy between a higher dimensional classical chaotic field theory and the usual quantum field theory has been outlined. This study uncovered a further possible role, which the temperature may play; it might be a factor in producing Planck's constant.

We could have written, however, much more about.[1] Without any preference let us see here a list of omitted topics: We left out the discussion of continuum thermodynamics, the problems with very slowly flowing material, like glasses or spin glasses. From the field of material science the behavior of lattice faults, the time evolution of dislocations and other deformations could have added some new aspects to our perspective on near-equilibrium and far-equilibrium physics. The statistical behavior of granular matter, different type of sandbox and avalanche models, or the phenomenon of percolation and fragmentation – both on the solid state and on the nuclear level – including jet-fragmentation as a particular type of hadronization in high-energy collisions, also could have been mentioned.

Outgrowing from statistical studies of such self-similar dynamical systems the "self-organizing criticality" and chaotic dynamics in general may have been touched upon. Also the relatively recent development on the theory of random networks and graphs with the power-law stationary distributions of node connectivity (causing the "small-world" effect) would have been a delicacy to discuss. To support the need for a novel, presumably non-extensive approach to thermodynamics, models and calculations from the field of econophysics, magnetic systems, earthquakes, climate changes or game theory and other social models would have served excellent. Finally – in relation to the field theoretical treatment of thermal phenomena – also a number of further speculations about an emerging quantum theory would have been exciting to cite.

At the end we may summarize the contemporary challenges to the concept of temperature as follows: The relevance of independent statistics expressed in factorizing marginal probabilities and the exclusive presence of short range interactions cannot be guaranteed in a number of physical phenomena. Most characteristically a too low number of degrees of freedom, or a time hierarchy between processes establishing detailed balance in some, but failing to achieve such a state in other variables, create physical situations, where a generalization of the classical thermodynamics is desired. Motion of whole bodies with relativistic speed or high acceleration also challenges the belief that the temperature would be an intuitive, easily comprehensible quantity in theoretical physics. Finally, entanglement between statistical and quantum effects in a really dynamical situation for drastic, short-time evolution offers a possibility to re-think the interpretation of temperature in a fundamental way: can it be related to the very structure of space and time? May it be behind the very existence of quantum effects?

As to the question in the title of this book: *There is a temperature*. It is an unexpectedly useful concept even in problems far from the realm of the classical thermodynamics. However, one has to be careful in relying on its classical derivation; under given circumstances a generalization is necessary. It cannot just be used the same way as in the classical context, the different physical roles, the variable called "temperature" plays, all have to be carefully considered.

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[1] In fact, originally we did have some plans to include more topics.

Solutions

Problems of Chap. 2

2.1 Convert by heart (and fast) the following temperature values between the Celsius and Fahrenheit scales: 36°C, 27°C, 22°C, 100°C, 32°F, 64°F, 80°F, 71°F, 451°F.

Temperatures given in Celsius grades have to be interpreted in groups of nine, then shifted by +2 and re-interpreted as 16°F each. This way 36°C $\rightarrow 4 \rightarrow 6 \rightarrow$ 96°F and 27°C $\rightarrow 3 \rightarrow 5 \rightarrow$ 80°F. 22°C is not readily dividable by 9, but it is 5 less than 27°C. Since 5°C is equivalent to about 9°F, it follows that 22°C is about $80-9=71$°F. 100°C is about 99°C meaning 11 in nonal system. Adding 2 it makes 13×16°F, which is about 160 plus three times 16 (about 50). This way 100°C makes about 210°F.

32, 64, and 80 are multiples of 16 by 2, 4, and 5 respectively. The corresponding centigrades are then multiples of 9 by 0, 2 and 3, giving 0, 18 and 27°C, respectively. 71°F is 9 less than 80, so it is about 5 less than 27 in centigrades, i.e. 22°C. Finally, 451°F is about $480-32$ meaning $30-2=28$ groups of 16. Shifting to centigrades it is $28-2=26$ groups of 9 resulting in $9 \times 26 = 260 - 26 = 234$°C.

2.2 Derive Kirchhoff's law from the equality of intensities of emitted and absorbed radiation between two bodies in equilibrium.

Two bodies, labeled as 1 and 2, radiate and absorb energy. Let the intensity of the energy current arriving to body 2 from body 1 be denoted by I^+, the opposite (and in equilibrium equal) intensity by I^-. The respective emissivity coefficients are ε_1 and ε_2, the absorptivity coefficients A_1 and A_2. The $1-A_i$ $(i=1,2)$ part of the incoming radiations are reflected, these currents contribute to the total infalling intensities on the respective bodies.

The intensities are hence related as

$$I^+ = \varepsilon_1 + (1-A_1)I^-,$$

and

$$I^- = \varepsilon_2 + (1 - A_2) I^+.$$

In equilibrium, $I^+ = I^- = I$ and the above system of linear equations leads to

$$\frac{\varepsilon_1}{A_1} = \frac{\varepsilon_2}{A_2} = I.$$

This proves that the ratio ε/A is independent of the material quality of the bodies equilibrating by radiation. This is the essence of Kirchhoff's law.

2.3 Using Wien's law determine the wavelengths of maximal intensity for the Sun's surface, for a light bulb, for the human body and for the cosmic microwave background.

Following Wien's law the wavelength of intensity maximum is at $\hbar\omega/k_BT = 3$ giving $\lambda = h/3k_BT \approx 2.897\,\mathrm{mm\,K}$. This relates roughly $T = 1{,}000\,\mathrm{K}$ to $\lambda = 3\,\mu\mathrm{m}$. The visible surface of the Sun has a temperature around $T = 6{,}000\,\mathrm{K}$, resulting in $\lambda = 500\,\mathrm{nm}$. In fact, biologically evolved eyes on the Earth are most sensitive near to this wavelength. A common light bulb glows at the temperature $T = 1{,}500\,\mathrm{K}$. The corresponding wavelength is $\lambda = 2{,}000\,\mathrm{nm}$, giving more power in the infrared than in the visible spectrum. Warm blood animal bodies maintain a temperature around 36°C, about 300 K. The radiation power is maximal at $\lambda = 10\,\mu\mathrm{m}$, well in the infrared range. This fact is utilized by "night seeing" devices. Finally, the cosmic microwave background has a temperature of around 3 K. The corresponding wavelength is $\lambda = 1\,\mathrm{mm}$.

2.4 What is the average energy carried by a photon in thermal radiation according to Planck's law, according to Wien's law and according to a Raleigh-Jeans law cut at the maximal frequency of Wien's formula?

The differential frequency distribution of photons is described by Planck's law (and by its low- and high-frequency limits in case of Raleigh-Jeans and Wien, respectively):

$$f(\omega)\mathrm{d}\omega = \frac{\omega^2 \mathrm{d}\omega}{\mathrm{e}^{\hbar\omega/k_BT} - 1} \longrightarrow \begin{cases} \frac{k_BT}{\hbar}\,\omega \mathrm{d}\omega \\ \omega^2 \mathrm{e}^{-\hbar\omega/k_BT} \mathrm{d}\omega \end{cases}$$

The maximal intensity according to Wien's displacement law is at $\omega_{\max} = 3k_BT/\hbar$. The average frequency is given by

$$\bar{\omega} = \frac{\int\limits_0^\infty \omega f(\omega)\mathrm{d}\omega}{\int\limits_0^\infty f(\omega)\mathrm{d}\omega}.$$

Expanding Planck's formula as a geometrical series,

$$\frac{1}{e^x - 1} = \sum_{n=1}^{\infty} e^{-nx},$$

we deal with a series of integrals with powers and exponentials of ω. The generic integral looks like

$$\sum_{n=1}^{\infty} \int_0^{\infty} x^k e^{-nx} dx = \sum_{n=1}^{\infty} \frac{k!}{n^{k+1}} = k!\zeta(k+1),$$

containing Riemann's zeta function $\zeta(k)$. The average frequency by the Planck's law becomes

$$\bar{\omega} = \frac{k_B T}{\hbar} \frac{3!\zeta(4)}{2!\zeta(3)} \approx 3T \frac{k_B}{\hbar} \frac{1.0823}{1.2021}.$$

In $k_B = c = \hbar = 1$ units $\bar{\omega} \approx 2.7T$.

Wien's approximation keeps the $n = 1$ term from the series only by using the exponential Boltzmann factor instead of Planck's law. The average frequency is equal to the one where the intensity is maximal, according to his displacement law:

$$\bar{\omega}_W = \frac{k_B T}{\hbar} \frac{3!}{2!} = 3T \frac{k_B}{\hbar}.$$

Finally, the Raleigh–Jeans formula cannot be integrated up to infinite frequencies, the integrals being divergent (this is called the "ultraviolet catastrophe"). Making the cut instead at $x_{\max} = \hbar\omega_{\max}/k_B T = 3$ one obtains

$$\bar{\omega}_{RJ} = \frac{k_B T}{\hbar} \frac{\int_0^{x_{\max}} x^2 dx}{\int_0^{x_{\max}} x dx} = \frac{2}{3}\omega_{\max},$$

resulting in $\bar{\omega} = 2k_B T/\hbar$.

Problems of Chap. 3

3.1 Prove the two leading orders in the Stirling formula for $\ln N!$.

Due to the recursive property of factorial, $(N+1)! = (N+1)N!$, its logarithm, $S_N = \ln N!$ satisfies

$$S_{N+1} - S_N = \ln(N+1).$$

Comparing this with the rule for $(N-1)$ and subtracting we get

$$S_{N+1}+S_{N-1}-2S_N=\ln\left(1+\frac{1}{N}\right)\approx\frac{1}{N}$$

in the large N limit. Considering now the $N\to\infty$ limit the above recursion formula can be approximated by a differential equation

$$\frac{\mathrm{d}^2S}{\mathrm{d}x^2}=\frac{1}{x}.$$

The solution of this equation with the conditions $S(0)=0$, $S'(0)=0$ is

$$S(x)=x\,(\ln x-1)\,,$$

leading to the large N estimate we were after.

3.2 Determine the occupation probabilities for three states having zero, one and two quanta of the energy ε by excluding all other states. The average energy is fixed to be $\bar{\varepsilon}$.

Following the general discussion of the canonical BG distribution the probabilities are given as

$$w_n=\frac{\mathrm{e}^{-\beta\varepsilon_n}}{\sum_n \mathrm{e}^{-\beta\varepsilon_n}}.$$

In the present case, we have $n=0,1$ and 2 states only with the energies $\varepsilon_0=0$, $\varepsilon_1=\varepsilon$ and $\varepsilon_2=2\varepsilon$. This leads to the following relation between the average energy and the temperature $k_{\mathrm{B}}T=1/\beta$:

$$\bar{\varepsilon}=\varepsilon\,\frac{\mathrm{e}^{-\beta\varepsilon}+2\mathrm{e}^{-2\beta\varepsilon}}{1+\mathrm{e}^{-\beta\varepsilon}+\mathrm{e}^{-2\beta\varepsilon}}.$$

The temperature can be obtained by inverting this relation.

Formally, for $\bar{\varepsilon}>\varepsilon$ the solution is at negative absolute temperature ($\beta<0$) reflecting the so called “inverse population” of energy levels. Clearly, such a value can only be reached if the double energy states are populated more than the ones with single quantum. In fact all probability ratios

$$\frac{w_{n+1}}{w_n}=\mathrm{e}^{-\beta\varepsilon},$$

are less than one for β being positive and more than one for β negative. The average energy per the energy quantum, $\bar{\varepsilon}/\varepsilon$, is exactly one at $\beta=0$, i.e. at infinite temperature.

3.3 Determine the grand-canonical equilibrium distribution for a fractionally fermionic-bosonic system: maximum the fraction qN can be in an indistinguishable state of K states.

The number of distinguishable macrostates is given by

$$W = \binom{K+qN}{N}.$$

The entropy per level function in the $K \to \infty$ limit with fixed $N/K = p$ (in $k_B = 1$ units) becomes

$$\sigma(p) = (1+qp)\ln(1+qp) - p\ln p - (1+(q-1)p)\ln(1+(q-1)p).$$

Its derivative with respect to p equals to $\ln x = (\varepsilon - \mu)/T$. We obtain

$$\frac{(1+qp)^q}{p(1+(q-1)p)^{q-1}} = x.$$

This means $(1+p)/p = x$ for $q = 1$ leading to the Bose, and $(1-p)/p = x$ for $q = 0$ leading to the Fermi distribution. It is interesting that for $q = 1/2$ not the Boltzmann distribution emerges, but

$$\frac{(1+p/2)^{1/2}}{p(1-p/2)^{-1/2}} = \frac{\sqrt{1-p^2/4}}{p} = x$$

leading to

$$p = \frac{1}{\sqrt{x^2+1/4}}.$$

The BG distribution would be $p = 1/x$, in fact for large x any of the q-on formulas leads to this result. We note that at $x = 1$ the Fermi surface is located where $\varepsilon = \mu$. The $p = 1$ value at $x = 1$ is achieved for $q^* \approx 0.5628$.

3.4 Prove the generalized Markov inequality (3.52).

The partial measure of x values satisfying the constraint $f(x) \geq t$ is given by

$$P_f(t) = \int\limits_{f(x)\geq t} \mathrm{d}\mu(x).$$

Multiplying this integral by $g(t)$ and using its monotonic rising property, under the above constraint $g(f(x)) \geq g(t)$ is fulfilled. We estimate

$$\int\limits_{f(x)\geq t} g(t)\,\mathrm{d}\mu(x) \leq \int\limits_{f(x)\geq t} g(f(x))\,\mathrm{d}\mu(x).$$

Now, since both the PDF, $\mathrm{d}\mu(x) = p(x)\mathrm{d}x$, and the test function, $g(t)$ are non-negative, the restricted integral on the right hand side is smaller or equal to the integral over all possible values of x:

$$\int\limits_{f(x)\geq t} g(f(x))\,\mathrm{d}\mu(x) \leq \int\limits_{x\in X} g(f(x))\,\mathrm{d}\mu(x).$$

A division by $g(t) \neq 0$ delivers the Markov inequality

$$P_f(t) \leq \frac{1}{g(t)} \int\limits_{x\in X} g(f(x))\,\mathrm{d}\mu(x) = \frac{\langle g(f(x)) \rangle}{g(t)}.$$

3.5 What is the distribution of energy differences in an ideal Maxwell–Boltzmann gas?

Using scaled variables, $x = E/k_{\mathrm{B}}T$, the MB distribution in terms of individual energies is an Euler–Gamma distribution with the power $n = 3/2$. The distribution of a given difference, $x = x_1 - x_2$, is defined with the help of Dirac's delta function:

$$P(x) = \int \mathrm{d}x_1 \int \mathrm{d}x_2\; w(x_1)\, w(x_2)\, \delta(x_1 - x_2 - x).$$

Making use of the Fourier expansion of the Dirac delta one obtains

$$P(x) = \int\limits_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi}\, \mathrm{e}^{-\mathrm{i}kx} \left\langle \mathrm{e}^{\mathrm{i}kx_1} \right\rangle \left\langle \mathrm{e}^{-\mathrm{i}kx_2} \right\rangle.$$

The individual energy distributions, $w(x_i)$ are given by

$$w(x_i) = \frac{1}{\Gamma(n)} x_i^{n-1} \mathrm{e}^{-x_i},$$

so their characteristic function is

$$\left\langle \mathrm{e}^{\mathrm{i}kx_i} \right\rangle = \frac{1}{\Gamma(n)} \int\limits_{0}^{\infty} x_i^{n-1} \mathrm{e}^{-x_i} \mathrm{e}^{\mathrm{i}kx_i} \mathrm{d}x_i = \frac{1}{(ik-1)^n}.$$

The distribution of differences is hence given by the Fourier integral

$$P(x) = \int\limits_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi}\, \mathrm{e}^{-\mathrm{i}kx} \frac{1}{(1+k^2)^n}.$$

The result of this integration for $n = 3/2$ is

$$P(x) = \frac{1}{\pi}\, |x|\; K_1(|x|),$$

with the K_1 Bessel function (Fig. 1). As it can be inspected on the figure below, the most probable is to find two molecules with the same energy in an MB gas. The 50% level of the integrated probability is for energy differences less than $0.941 k_B T$, indicated by the vertical dotted lines.

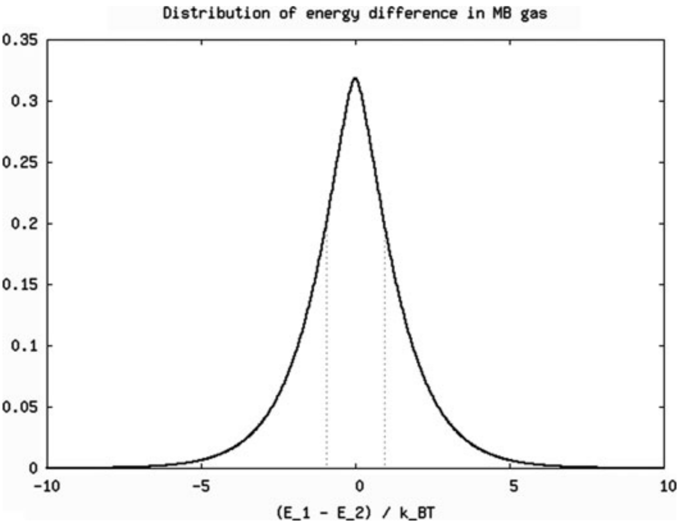

Fig. 1 The distribution of scaled energy difference, $x = (E_1 - E_2)/k_B T$, in a Maxwell–Boltzmann ideal gas. The 50% integrated probability is between the *vertical dotted lines*

3.6 The Jensen inequality,

$$\prod_{i=1}^{\mathcal{N}} a_i^{p_i} \leq \sum_{i=1}^{\mathcal{N}} p_i a_i$$

for all $a_i > 0$, $p_i \in [0, 1]$ and $\sum_i p_i = 1$ is the generalization of the traditional inequality between the geometric and arithmetic means. Prove this inequality. What does it say for the information entropy?

First, we consider the $\mathcal{N} = 2$ case. Let it be $p_1 = p$, $p_2 = 1 - p$ and

$$\frac{a_1}{a_2} = (1+x)^{1/p}.$$

We assume $a_1 > a_2$, otherwise exchange the roles of indices and p with $1 - p$. Due to this assumption $x > 0$ and by construction $1/p \geq 1$. The Jensen inequality for $\mathcal{N} = 2$ states that

$$a_1^{p_1} a_2^{p_2} = (1+x)a_2 \leq p_1 a_1 + p_2 a_2 = p(1+x)^{1/p} a_2 + (1-p)a_2.$$

Dividing this by $a_2 > 0$ and denoting $w = 1/p$ one obtains

$$1 + x \leq p(1+x)^w + 1 - p$$

which after rearrangement and division by $p > 0$ becomes

$$1 + wx \leq (1+x)^w.$$

This is true for any $w > 1$ and $x > 0$, so the original inequality is also true.

Now we generalize the $\mathscr{N} = 2$ result for arbitrary $\mathscr{N}$ by induction. Denoting the generalized geometrical mean of $\mathscr{N}$ a_i values by $G_{\mathscr{N}}$ and the arithmetic mean by $A_{\mathscr{N}}$ we prove the Jensen inequality for $\mathscr{N}$ factors while assuming that it is true for $\mathscr{N} - 1$ and for 2. The geometrical mean can be written as

$$G_{\mathscr{N}} = a_{\mathscr{N}}^{p_{\mathscr{N}}} \times G_{\mathscr{N}-1}^{1-p_{\mathscr{N}}},$$

since

$$\sum_{i=1}^{\mathscr{N}-1} p_i = 1 - p_{\mathscr{N}},$$

and in order to satisfy the normalization in the expression for

$$G_{\mathscr{N}-1} = \prod_{i=1}^{\mathscr{N}-1} a_i^{\tilde{p}_i}$$

the scaled powers,

$$\tilde{p}_i = \frac{p_i}{1 - p_{\mathscr{N}}},$$

have to be used. The above expression for $G_{\mathscr{N}}$ itself is a generalized geometrical mean for two factors, so according to our previous proof

$$G_{\mathscr{N}} \leq p_{\mathscr{N}} a_{\mathscr{N}} + (1 - p_{\mathscr{N}}) G_{\mathscr{N}-1}.$$

In this the term, $G_{\mathscr{N}-1}$ can be further estimated from above by the inductive assumption that the Jensen inequality is valid for $\mathscr{N} - 1$. This leads to

$$G_{\mathscr{N}} \leq p_{\mathscr{N}} a_{\mathscr{N}} + (1 - p_{\mathscr{N}}) \sum_{i=1}^{\mathscr{N}-1} \tilde{p}_i a_i,$$

what in turn – using the scaling factor in the definition of the $\tilde{p}_i$ – simply equals to the generalized arithmetic mean of $\mathscr{N}$ factors. Therefore,

$$G_{\mathscr{N}} \leq \sum_{i=1}^{\mathscr{N}} p_i a_i = A_{\mathscr{N}},$$

completing the proof.

Taking the logarithm of the Jensen inequality one achieves

$$\sum_{i=1}^{\mathcal{N}} p_i \ln a_i \leq \ln \sum_{i=1}^{\mathcal{N}} p_i a_i .$$

Applying this formula for the special case $a_i = 1/p_i$ the following estimate arises

$$\varsigma = \sum_{i=1}^{\mathcal{N}} p_i \ln \frac{1}{p_i} \leq \ln \sum_{i=1}^{\mathcal{N}} p_i \frac{1}{p_i} = \ln \mathcal{N} .$$

Finally, this means $\varsigma \leq \ln \mathcal{N}$, the equality being fulfilled when all a_i terms are the same. In case of the BG entropy formula it means equipartition.

3.7 Second Law and Life

By thermal equilibration between two subsystems the colder heats up and the warmer body cools down until a common temperature is achieved. How is it possible then, that on the Earth, while steadily gaining energy from the hotter Sun, entropy is virtually reduced by the spontaneous evolution of highly improbable – as highly correlated – structures, shortly named Life.

The key to the solution is to observe that three bodies are involved: the Sun, the Earth and Space. Denoting the reciprocal temperatures by $\beta_i = 1/T_i$ and the energies by E_i, the Second Law demands that

$$\mathrm{d}S = \beta_1 \mathrm{d}E_1 + \beta_2 \mathrm{d}E_2 + \beta_3 \mathrm{d}E_3 \geq 0,$$

while the system is energetically closed for these three bodies:

$$\mathrm{d}E_1 + \mathrm{d}E_2 + \mathrm{d}E_3 = 0.$$

Owing to the fact that the Sun cools, the outer Space takes energy, while the Earth cools or has constant energy, $\mathrm{d}E_1 < 0$, $\mathrm{d}E_2 \leq 0$ and $\mathrm{d}E_3 > 0$. Introducing the parameter λ with values between zero and one, we have $\mathrm{d}E_1 = -\lambda \mathrm{d}E_3$ and $\mathrm{d}E_2 = -(1-\lambda)\mathrm{d}E_3$. The total entropy balance,

$$\mathrm{d}S = (-\lambda\beta_1 - (1-\lambda)\beta_2 + \beta_3)\, \mathrm{d}E_3 \geq 0,$$

translates to the following inequality:

$$(\beta_3 - \beta_2) + \lambda\,(\beta_2 - \beta_1) \geq 0.$$

This is fulfilled for arbitrary positive λ if $\beta_3 > \beta_2 > \beta_1$, or expressed by the absolute temperatures if $T_3 < T_2 < T_1$. In this setting $\mathrm{d}S_2 = \beta_2 \mathrm{d}E_2 \leq 0$, so the reduction of Earth's entropy is perfectly in accordance with the Second Law of Thermodynamics.

Problems of Chap. 4

4.1 Prove the rule for the Pascal triangle,

$$\binom{k}{n} = \binom{k-1}{n} + \binom{k-1}{n-1}.$$

It can be proved by using the definition of the binomial coefficient. One has

$$\binom{k}{n} = \frac{k!}{n!(k-n)!} = \frac{k}{n(k-n)}\,\frac{(k-1)!}{(n-1)!(k-1-n)!}$$

The first factor can be split as a sum

$$\frac{k}{n(k-n)} = \frac{1}{n} + \frac{1}{k-n}$$

whence

$$\binom{k}{n} = \left(\frac{1}{n} + \frac{1}{k-n}\right)\frac{(k-1)!}{(n-1)!(k-1-n)!} = \binom{k-1}{n} + \binom{k-1}{n-1}.$$

The Pascal triangle rule also can be proved by considering the identity

$$(a+b)^k = (a+b)^{k-1}(a+b)$$

and the expansion

$$(a+b)^k = \sum_{n=0}^{k} w_{n,k} a^n b^{k-n},$$

denoting the binomial coefficient “k over n” by $w_{n,k}$. Considering now

$$\sum_{n=0}^{k-1} w_{n,k-1} a^n b^{k-1-n}(a+b) = \sum_{n=0}^{k-1} w_{n,k-1} a^{n+1} b^{k-1-n} + \sum_{n=0}^{k-1} w_{n,k-1} a^n b^{k-n}$$

one redefines the running index from n to $n-1$ in the first sum and obtains

$$\sum_{n=0}^{k-1} w_{n,k-1} a^n b^{k-1-n}(a+b) = \sum_{n=1}^{k} w_{n-1,k-1} a^n b^{k-n} + \sum_{n=0}^{k-1} w_{n,k-1} a^n b^{k-n}.$$

Comparing finally the general coefficients of the terms $a^n b^{k-n}$ one concludes that

$$w_{n,k} = w_{n,k-1} + w_{n-1,k-1}.$$

4.2 What is the Pascal triangle-like recursion rule for the probabilities in the Bernoulli distribution?

The formula for the Bernoulli distribution is given as

$$P_{n,k} = \binom{k}{n} f^n (1-f)^{k-n}.$$

Using the Pascal triangle rule it splits to a sum

$$\binom{k}{n} f^n (1-f)^{k-n} = \left(\binom{k-1}{n} + \binom{k-1}{n-1} \right) f^n (1-f)^{k-n}$$

therefore

$$P_{n,k} = (1-f)P_{n,k-1} + fP_{n-1,k-1}.$$

This is a weighted Pascal rule with the average hole and particle occupation rates.

4.3 What is the Pascal triangle-like recursion rule for the probabilities in the hypergeometric distribution?

We transform the hypergeometric probability times the normalization factor:

$$\binom{K}{N} P_{n,k,N,K} = \binom{k}{n}\binom{K-k}{N-n} = \left(\binom{k-1}{n} + \binom{k-1}{n-1} \right) \binom{K-k}{N-n}.$$

The two summands can be reinterpreted as

$$\binom{k-1}{n}\binom{K-k}{N-n} + \binom{k-1}{n-1}\binom{K-k}{N-n} =$$

$$\binom{K-1}{N} P_{n,k-1,N,K-1} + \binom{K-1}{N-1} P_{n-1,k-1,N-1,K-1}.$$

Finally, one observes that

$$\frac{\binom{K-1}{N}}{\binom{K}{N}} = \frac{\frac{(K-1)!}{N!(K-1-N)!}}{\frac{K!}{N!(K-N)!}} = \frac{K-N}{K} = 1 - \bar{f}$$

and

$$\frac{\binom{K-1}{N-1}}{\binom{K}{N}} = \frac{\frac{(K-1)!}{(N-1)!(K-N)!}}{\frac{K!}{N!(K-N)!}} = \frac{N}{K} = \bar{f}.$$

Using this information we conclude that

$$P_{n,k,N,K} = (1-\bar{f})P_{n,k-1,N,K-1} + \bar{f}P_{n-1,k-1,N-1,K-1}.$$

4.4 What is the recursion rule for the probabilities in the bosonic Bernoulli distribution?

The bosonic Bernoulli probability is

$$B_{n,k} = \binom{k+n}{n} f^n (1+f)^{-n-k-1}.$$

Using Pascal's rule it is split as

$$B_{n,k} = \binom{k-1+n}{n} f^n (1+f)^{-n-k-1} + \binom{k+n-1}{n-1} f^n (1+f)^{-n-k-1}.$$

The terms are reinterpreted:

$$B_{n,k} = \frac{1}{1+f} B_{n,k-1} + \frac{f}{1+f} B_{n-1,k}.$$

Note that the last term is also on the k-th level, not on the $(k-1)$-th. It means that an actual element is the weighted sum of the left in the same row and the right one above. Since for bosons $n > k$ is possible, the probabilities fill infinite stripes instead of a triangle.

4.5 Derive the generating function $Z(\gamma)$ for the bosonic occupation probability, given in (4.50).

The generating function is defined by

$$Z(\gamma) = \langle \mathrm{e}^{\gamma n} \rangle = \sum_{n=0}^{\infty} B_{n,k} \mathrm{e}^{n\gamma},$$

with the distribution

$$B_{n,k} = \binom{k+n}{n} f^n (1+f)^{-n-k-1}.$$

This gives rise to the infinite sum representation

$$Z(\gamma) = (1+f)^{-k-1} \sum_{n=0}^{\infty} \frac{(k+n)!}{k!} \frac{x^n}{n!}$$

with $x = f\mathrm{e}^{\gamma}/(1+f)$. We compare this sum with the Taylor expansion

$$(1-x)^{-k-1} = 1 + (k+1)x + \frac{1}{2}(k+1)(k+2)x^2 + \cdots$$

and realize that this is the same infinite sum. Therefore,

$$Z(\gamma) = (1+f)^{-k-1}\left(1-\frac{f}{1+f}\mathrm{e}^{\gamma}\right)^{-k-1} = (1+f-f\mathrm{e}^{\gamma})^{-k-1}.$$

4.6 Determine the double generating function,

$$Z_P(\gamma,\alpha,f) = \sum_{n=0}^{\infty}\sum_{k=0}^{\infty} P_n(k;f)\mathrm{e}^{\gamma n}\,\mathrm{e}^{\alpha k}$$

for the negative binomial distribution $P_n(k;f)$. It plays the role of the partition function in the pressure ensemble.

We use the integral representation

$$P_n(k;f) = \int_0^{\infty} \frac{(xf)^n}{n!}\mathrm{e}^{-xf}\,\frac{x^k}{k!}\mathrm{e}^{-x}\,\mathrm{d}x$$

to obtain

$$Z_P(\gamma,\alpha,f) = \int_0^{\infty}\sum_{n=0}^{\infty}\frac{(xf\mathrm{e}^{\gamma})^n}{n!}\mathrm{e}^{-xf}\,\sum_{k=0}^{\infty}\frac{(x\mathrm{e}^{\alpha})^k}{k!}\mathrm{e}^{-x}\,\mathrm{d}x.$$

Carrying out the summations, both lead to a respective exponential:

$$Z_P(\gamma,\alpha,f) = \int_0^{\infty} \mathrm{e}^{xf(\mathrm{e}^{\gamma}-1)}\,\mathrm{e}^{x(\mathrm{e}^{\alpha}-1))}\,\mathrm{d}x.$$

It remains a simple integral of the exponential function. The final result is given by

$$Z_P(\gamma,\alpha,f) = \frac{1}{(1-\mathrm{e}^{\alpha})+f(1-\mathrm{e}^{\gamma})}.$$

4.7 Find a transformation formula between the fermionic and bosonic type Bernoulli distributions.

The transformation formula relies on the following property of the negative binomial:

$$\binom{k+n}{n} = (-1)^n\binom{-k-1}{n}.$$

Applying this to the bosonic Bernoulli distribution,

$$B_n(k,f) = \binom{k+n}{n} f^n (1+f)^{-k-n-1},$$

one gets

$$B_n(k,f) = \binom{-k-1}{n}(-f)^n(1-(-f))^{(-k-1)-n} = F_n(-k-1,-f).$$

Is is easy to see that the inverse transformation is given by

$$F_n(k,f) = B_n(-k-1,-f).$$

So the transformation $k \to -k-1$, $f \to -f$ interchanges the bosonic and fermionic Bernoulli distributions.

It is another question that what can be the physical meaning of a negative number of slots for a positive number of quanta, and a negative average occupancy rate. Inspecting the formulas (4.36) for fermions and (4.48) for bosons distributed in respective subsystems of slots, the above negative binomial formula leads to the transformation property:

$$B_n(k;N,K) = F_n(-k-1;N,-K-2), \qquad F_n(k;N,K) = B_n(-k-1;N,-K-2).$$

The transformations $k \to -k-1$ and $K \to -K-2$ transform these two distributions into each other. We note that the expressions $k(k+1)$ and $K(K+2)$ are *invariants* of this statistically "supersymmetric" transformation. The negative number of slots can be interpreted as an "over-occupation," as a waiting queue for slots.

4.8 Estimate the magnitude of energy fluctuations near to thermal equilibrium for the non-extensively modified black body radiation, described by the equation of state

$$S(E,V) = \frac{4}{3}\sigma^{1/4} V \left(\frac{L(E)}{V}\right)^{3/4}.$$

Assuming $L(E) = \frac{1}{a}\ln(1+aE)$ with a small parameter $a > 0$, how do these fluctuations behave with a?

Following the general recipe presented in Chap. 4 we obtain the first and second derivatives of the entropy function.

$$\frac{\partial S}{\partial V} = \frac{1}{3}\sigma^{1/4}\left(\frac{L(E)}{V}\right)^{3/4} = \frac{p}{T}$$

defines the pressure in equilibrium, while from

$$\frac{\partial S}{\partial E} = \sigma^{1/4}\left(\frac{L(E)}{V}\right)^{-1/4} L'(E) = \frac{L'(E)}{T}$$

we obtain the temperature, $T = (L(E)/\sigma V)^{1/4}$. It follows

$$L(E) = \sigma V T^4,$$

and

$$p = \frac{1}{3}\sigma T^4 = \frac{1}{3}\frac{L(E)}{V}.$$

In this approach, the role of energy density is played by $\varepsilon = L(E)/V$.

We use the above relations to simplify expressions occurring in the second derivatives. With respect to the volume we obtain

$$\frac{\partial^2 S}{\partial V^2} = -\frac{3}{4V}\frac{p}{T} = -\frac{L(E)}{4V^2 T}.$$

The mixed second derivative becomes

$$\frac{\partial^2 S}{\partial V \partial E} = \frac{1}{4V}\frac{\partial S}{\partial E} = \frac{L'(E)}{4VT},$$

and the second derivative with respect to the energy

$$\frac{\partial^2 S}{\partial E^2} = \frac{1}{T}\left(L''(E) - \frac{L'(E)L'(E)}{4L(E)} \right).$$

Utilizing all these second derivatives the coefficient "metric" tensor in the expansion of the entropy around its maximum becomes

$$g = \frac{1}{T}\begin{pmatrix} -L'' + L'L'/4L, & -L'/4V \\ -L'/4V, & L/4V^2 \end{pmatrix}$$

Its determinant is

$$\det g = -\frac{LL''}{4V^2 T^2}$$

and the inverse matrix is given by

$$g^{-1} = T\begin{pmatrix} -1/L'', & -VL'/LL'' \\ -VL'/LL'', & 4V^2/L - V^2 L'L'/L^2 L'' \end{pmatrix}$$

This gives rise to the following expectation values for squared fluctuations:

$$\left\langle \Delta E^2 \right\rangle = -\frac{T}{L''(E)},$$

$$\left\langle \Delta E \Delta V \right\rangle = -V \frac{T}{L''(E)} \frac{L'(E)}{L(E)},$$

$$\left\langle \Delta V^2 \right\rangle = 4\frac{TV^2}{L(E)} - V^2 T \frac{L'(E)L'(E)}{L(E)L''(E)}.$$

We note that energy density $\varepsilon = L(E)/V$ has the fluctuation

$$\Delta\varepsilon = \Delta \frac{L(E)}{V} = \frac{1}{V}\left(L'(E)\Delta E - \varepsilon \Delta V \right).$$

With the help of this relation we obtain

$$\left\langle \Delta\varepsilon^2 \right\rangle = \frac{4T}{V}\varepsilon.$$

The characteristic fluctuations in the energy density scale like the inverse square root of the total volume V at a given temperature.

For the special energy function given,

$$L(E) = \frac{1}{a}\ln(1+aE) = V\varepsilon$$

and we have

$$L'(E) = \frac{1}{1+aE}$$

and

$$L''(E) = -\frac{a}{(1+aE)^2}.$$

This gives rise to the following expectation values

$$\left\langle \Delta E^2 \right\rangle = \frac{T}{a}\mathrm{e}^{2a\varepsilon V},$$

$$\left\langle \Delta E \Delta V \right\rangle = \frac{T}{a\varepsilon}\mathrm{e}^{a\varepsilon V},$$

$$\left\langle \Delta V^2 \right\rangle = \frac{T}{a\varepsilon^2}\left(1+4a\varepsilon V\right).$$

Expressed in this form one realizes, that the squared energy fluctuations at a given temperature, and consequently at a given energy density ε, grow more rapidly than linear with the volume. This exponential growth is due to the use of the particular formula for $L(E)$. Finally, we note that for too large fluctuations the Gaussian approximation utilized here is no more sufficient, so the above results are only approximate.

Problems of Chap. 5

5.1 Derive the general result (5.17) by executing the integration (5.16) and substituting into the formula (5.15). What can one tell about the limits $D \to 0$ and $C \to 0$?

The first key step is to observe that the linear expression $K_1(p)$ contains the derivative of the second order form $K_2'(p) = 2(Cp - B)$:

$$K_1(p) = F - Gp = -\frac{G}{2C}K_2'(p) + F - \frac{B}{C}G.$$

we use the abbreviation $\alpha = BG/C - F$. The argument of the exponential in (5.15) becomes

$$L(p) = \int_0^p \mathrm{d}q \, \frac{K_1(q)}{K_2(q)} = -\alpha \int_0^p \frac{\mathrm{d}q}{K_2(q)} - \frac{G}{2C} \int_0^p \mathrm{d}q \, \frac{K_2'(q)}{K_2(q)}.$$

It is straightforward to evaluate the second integral, the first we denote by $I(p)$. By doing so we have

$$L(p) = -\alpha I(p) - \frac{G}{2C} \ln \frac{K_2(p)}{K_2(0)},$$

and using (5.15) the stationary detailed balance distribution

$$f(p) = f(0) \left(1 - \frac{2B}{D} p + \frac{C}{D} p^2\right)^{-1-G/2C} \mathrm{e}^{-\alpha I(p)}.$$

We are left with task to evaluate

$$I(p) = \int_0^p \frac{\mathrm{d}q}{K_2(q)}.$$

In order to achieve this, one considers the zeros of $K_2(p)$. From

$$K_2(p) = D - 2Bp + Cp^2 = c(p - p_+)(p - p_-)$$

follows

$$p_\pm = \frac{B \pm i\vartheta}{C}$$

with $\vartheta = \sqrt{DC - B^2}$. The integral $I(p)$ with these notations becomes

$$I(p) = \int_0^p \frac{C dq}{(Cq - p_+)(Cq - p_-)} = \frac{1}{2i\vartheta} \ln \frac{1 - p/p_+}{1 - p/p_-}.$$

This expression contains the logarithm of a ratio between a complex number and its complex conjugate. This way it is an angle whose tangent is the ratio of the imaginary to the real part. As an intermediate step we obtain

$$\frac{p}{p_\pm} = \frac{Cp}{B \pm i\vartheta} = \frac{Cp}{B^2 + \vartheta^2}(B \mp i\vartheta) = \frac{p}{D}(B \mp i\vartheta).$$

Using this we obtain

$$I(p) = \frac{1}{2i\vartheta} \ln \frac{D - Bp + i\vartheta p}{D - Bp - i\vartheta p} = \frac{2i\varphi}{2i\vartheta},$$

with

$$\tan\varphi = \frac{\vartheta p}{D - Bp}.$$

Our final result is hence

$$I(p) = \frac{1}{\vartheta} \operatorname{atn} \frac{\vartheta p}{D - Bp},$$

and the stationary distribution

$$f(p) = f(0) \left(1 - \frac{2B}{D} p + \frac{C}{D} p^2\right)^{-1-G/2C} \mathrm{e}^{-\frac{\alpha}{\vartheta} \operatorname{atn} \frac{\vartheta p}{D-Bp}}.$$

With no cross correlation $B = 0$, and the above result simplifies to

$$f(p) = f(0) \left(1 + \frac{C}{D} p^2\right)^{-1-G/2C} \mathrm{e}^{\frac{F}{D} \frac{\sqrt{D}}{\sqrt{C}} \operatorname{atn}(p \frac{\sqrt{C}}{\sqrt{D}})}.$$

With vanishing mean value of the additive noise (no driving force) one has $F = 0$ and the stationary distribution is a pure cut power-law:

$$f(p) = f(0) \left(1 + \frac{C}{D} p^2\right)^{-1-G/2C}.$$

The $C \to 0$ limit of this expression, upon using Euler's formula, is the classical Gaussian

$$f(p) = f(0) \mathrm{e}^{-\frac{G}{2D} \frac{p^2}{2m}}.$$

The $\vartheta = 0$ is the degenerate case. The two roots of the second order expression $K_2(p)$ coincide and the inverse tangent function can be approximated by its argument. The stationary distribution is given by

$$f(p) = f(0) \left(1 - \frac{p}{p_m}\right)^{-2-G/C} \mathrm{e}^{\frac{F - Gp_m}{Dp_m} \frac{p}{p_m - p}},$$

with $p_m = \sqrt{D/C}$. Only the values $p \le p_m$ and $F \le Gp_m$ are meaningful in this case. At $p = p_m$ the probability density $f(p)$ becomes zero.

5.2 Consider the expectation value of the Taylor expansion with a Gauss-distributed deviation. What could be the next term continuing the construction recipe for Fisher's entropy?

We use a normal Gauss-distributed variable, z:

$$P(z) = \frac{1}{\kappa\sqrt{2\pi}} \mathrm{e}^{-z^2/2\kappa^2}.$$

The odd powers of z have vanishing expectation value, $\langle z^{2k+1} \rangle = 0$, while the even powers amount to $\langle z^{2k} \rangle = (2k-1)!!\kappa^{2k}$. Here, the double exclamation mark denotes the product of odd numbers only. The expectation value of the exponential function, represented by its infinite Taylor series, contains only contributions with even power:

$$\left\langle e^{\beta z} \right\rangle = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle z^n \rangle = \sum_{k=0}^{\infty} \frac{(2k-1)!!}{(2k)!} \beta^{2k} \kappa^{2k}.$$

Considering now that the factorial product of numbers up to $2k$ contains all the odd numbers up to $(2k-1)$ and k times the factor of 2 besides the numbers from 1 to k, one realizes that $(2k)! = 2^k (2k-1)!!k!$. Substituting this relation into the above one arrives at the short and elegant result,

$$\left\langle e^{\beta z} \right\rangle = e^{\beta^2 \kappa^2 /2}.$$

As a last step we apply this result to the Taylor expansion formula and obtain

$$\langle f(a+z) \rangle = \left\langle e^{z \frac{\partial}{\partial a}} f(a) \right\rangle = e^{\frac{\kappa^2}{2} \frac{\partial^2}{\partial a^2}} f(a).$$

The leading terms of this Gauss-averaged Taylor expansion are

$$\langle f(a+z) \rangle \approx f(a) + \frac{\kappa^2}{2} \frac{\partial^2}{\partial a^2} f + \frac{\kappa^4}{8} \frac{\partial^4}{\partial a^4} f.$$

Applying this result to the construction of Fisher entropy from the BGS formula, the fourth order term,

$$S_4 = \frac{\kappa^4}{8} \int f \, \nabla^4 (-\ln f) \, d\Gamma,$$

becomes quite involved when expanded in terms of ∇f. Therefore, it has no high value for a practical use.

5.3 What is the asymptotic rule to Einstein's velocity addition rule:

$$u \oplus v = \frac{u+v}{1+uv/c^2}?$$

The asymptotic rule to Einstein's velocity addition formula is itself. One way to prove this is to check associativity:

$$h(h(u,v),w) = \frac{h(u,v)+w}{1+wh(u,v)/c^2} = \frac{\frac{u+v}{1+uv/c^2} + w}{1 + w\frac{u+v}{c^2+uv}}.$$

After multiplying numerator and denominator by $(c^2 + uv)$ this fraction becomes

$$h(h(u,v),w) = \frac{c^2(u+v+w)+uvw}{c^2+uv+wu+wv}.$$

In this form, u, v and w are arranged symmetrically, so this expression could have been derived by starting with any permutation of them. This means that

$$h(h(u,v),w) = u \oplus v \oplus w = h(u,h(v,w)).$$

Another way is to utilize the scaling equation for asymptotic rules: We have $h_2'(u,0) = 1 - u^2/c^2$ and therefore the formal logarithm is given by

$$L(u) = \int_0^u \frac{\mathrm{d}z}{1 - z^2/c^2} = c\,\mathrm{Arth}\frac{u}{c}.$$

This quantity is the rapidity, additive by Lorentz-transformations. The asymptotic rule is given by

$$\varphi(u,v) = L^{-1}\left(L(u) + L(v)\right) = \frac{u+v}{1 + uv/c^2},$$

which is the original Einstein-rule.

5.4 Is the following rule associative?

$$x \oplus y = x + y + \frac{a}{\frac{1}{x} + \frac{1}{y}}$$

The non-additive part can easily be casted into the form

$$\frac{a}{\frac{1}{x} + \frac{1}{y}} = a\frac{xy}{x+y}.$$

Since for the rule $h(x,y) = x + y + axy/(x+y)$ the derivative $h_2'(x,0) = 1 + a$ is constant, the asymptotic rule is the simple addition, $\varphi(x,y) = x + y$. It differs from the original rule, so that one is not associative.

5.5 Obtain the formal particle–hole correspondence for the deformed Fermi and Bose distributions:

$$f_a(x) = \frac{1}{e_a(x) + 1}, \qquad \text{and} \qquad g_a(x) = \frac{1}{e_a(x) - 1}.$$

What replaces the known results, $f_0(-x) = 1 - f_0(x)$ and $-g_0(-x) = 1 + g_0(x)$ for general values of the parameter a?

Since $1/e_a(x) = e_{-a}(-x)$, one obtains

$$1 - f_a(x) = \frac{e_a(x)}{e_a(x) + 1} = \frac{1}{e_{-a}(-x) + 1} = f_{-a}(-x)$$

for the extension of the Fermi distribution and

$$1+g_a(x)=\frac{e_a(x)}{e_a(x)-1}=\frac{1}{1-e_{-a}(-x)}=-g_{-a}(-x)$$

for that of the Bose distribution. The known results for $a=0$ generalize so that besides the $x\longrightarrow -x$ replacement also $a\longrightarrow -a$ is required.

5.6 What is the canonical energy distribution with an additive energy and the following entropy composition rule?

$$S_{12}=S_1\sqrt{1+a^2S_2^2}+S_2\sqrt{1+a^2S_1^2}.$$

The composition rule $h(x,y)=x\sqrt{1+a^2y^2}+y\sqrt{1+a^2x^2}$ is of Kaniadakis type, the corresponding formal logarithm is given by $L_a(x)=\frac{1}{a}\text{Arsh}(ax)$. The entropy is therefore given as

$$S=\sum_i w_i\frac{1}{a}\sinh\left(a\ln\frac{1}{w_i}\right)=\frac{1}{2a}\sum_i\left(w_i^{1-a}-w_i^{1+a}\right).$$

The canonical maximization problem,

$$S-\alpha\sum_i w_i-\beta\sum_i w_iE_i=\max.$$

leads to the following equation for the probability w_i of having energy E_i:

$$\frac{1}{2a}\left[(1-a)w_i^{-a}-(1+a)w_i^{a}\right]=\alpha+\beta E_i.$$

This is a second order algebraic equation for w_i^a, which should be a quantity less than one for $a>0$. Denoting $\alpha+\beta E_i$ by X, this solution is given by

$$w_i=\left(\frac{\sqrt{1-a^2+a^2X^2}-aX}{1+a}\right)^{1/a}.$$

For large energies it is power-law:

$$\lim_{X\to\infty}w_i=\left(\frac{1-a}{2aX}\right)^{1/a}=KX^{-1/a}.$$

5.7 Obtain the canonical energy distribution for the following class of pairwise energy composition rule:

$$E_1\oplus E_2=E_1+E_2+\frac{a}{2}(E_1+E_2)^2.$$

The energy composition rule

$$h(x,y) = x + y + \frac{a}{2}\,(x+y)^2$$

leads to $h_2'(x,0) = 1 + ax$. This way the asymptotic rule is the Tsallis rule, $\varphi(x,y) = x + y + axy$, and the canonical entropy maximization principle becomes

$$\sum_i w_i \ln\frac{1}{w_i} - \alpha \sum_i w_i - \beta \sum_i w_i \frac{1}{a} \ln(1 + aE_i) = \max.$$

Its derivative with respect to w_i leads to

$$-\ln w_i - 1 - \alpha - \frac{\beta}{a} \ln(1 + aE_i) = 0,$$

resulting in a power-law tailed energy distribution

$$w_i = K\,(1 + aE_i)^{-\beta/a}$$

with an appropriate constant factor K.

5.8 Verify that the Rényi entropy is additive for factorizing probabilities.

The Rényi entropy,

$$S = \frac{1}{1-q} \ln \sum_i w_i^q,$$

applied to factorizing (uncorrelated) joint probabilities, $p_{ij} = w_i v_j$ gives

$$S_{12} = \frac{1}{1-q} \ln \sum_i \sum_j p_{ij}^q = \frac{1}{1-q} \ln \left(\sum_i w_i^q \right) \left(\sum_j v_j^q \right),$$

which is additive due to the same property of the natural logarithm, ln.

5.9 Construct a composition rule which does not have a thermodynamical limit.

It is sufficient to consider a composition rule with divergent $h_2'(x,0)$, e.g. $h(x,y) = x + y + a\ln(xy)$ for this purpose. In such a case the formal logarithm degenerates to zero and no asymptotic rule can be obtained by the standard procedure. However, using a small y value instead of zero, the calculation still can be done, and it leads to the addition as asymptotic rule in this case. Another possibility would be to consider a rule which cannot be differentiated with respect to y, e.g. $h(x,y) = \mathrm{sign}(x-y)$.

5.10 Compare the Rényi and Tsallis entropy formulas for binary events, $p_1 = p$, $p_2 = 1 - p$. Discuss the location and value of maximum and the convexity (Fig. 2).

The Tsallis entropy with the parameter $a = 1 - q$ is given as

$$S_{\mathrm{T}} = \frac{1}{a} \left(p^{1-a} + (1-p)^{1-a} - 1 \right).$$

Here, we use $k_{\mathrm{B}} = 1$ units. The first derivative with respect to p,

$$\frac{\partial S_{\mathrm{T}}}{\partial p} = \frac{1-a}{a}\left(p^{-a} - (1-p)^{-a}\right),$$

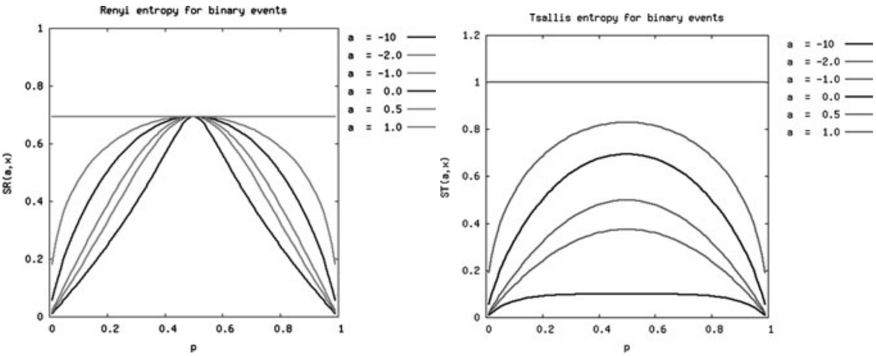

Fig. 2 The Rényi (*left*) and Tsallis (*right*) entropy formula applied to binary events. The Rényi entropy is additive and its maximal value is always 1 bit ($k_{\mathrm{B}} \ln 2$). The Tsallis entropy is convex for all sensible values of the entanglement-deformity parameter, $a < 1$, while the Rényi entropy shows this property only for $a \in (-1, 1)$. (The *curves* from the top to the bottom belong to $a = 1$, 0.5, 0, -1, -2 and -10)

vanishes at $p = 1 - p = 1/2$. The extremal value of the Tsallis entropy depends on the parameter a:

$$S_{\mathrm{T}}^{\mathrm{extr}} = \frac{1}{a}\left(2^{a-1} + 2^{a-1} - 1\right) = \frac{2^a - 1}{a}.$$

Its second derivative,

$$\frac{\partial^2 S_{\mathrm{T}}}{\partial p^2} = (a-1)\left(p^{-a-1} + (1-p)^{-a-1}\right),$$

is negative for every $p \in (0,1)$ provided $a < 1$ ($q > 0$).

The Rényi entropy can be obtained as the formal logarithm of the Tsallis one,

$$S_{\mathrm{R}} = \frac{1}{a}\ln\left(1 + aS_{\mathrm{T}}\right).$$

The first derivative,

$$\frac{\partial S_{\mathrm{R}}}{\partial p} = \frac{1}{1 + aS_{\mathrm{T}}}\frac{\partial S_{\mathrm{T}}}{\partial p}$$

vanishes at the same probability, $p = 1/2$, where S_{T} did. Its extremal value is given as

$$S_{\mathrm{R}}^{\mathrm{ext}} = \ln 2$$

independently of the parameter a. The second derivative has two contributions

$$\frac{\partial^2 S_\mathrm{R}}{\partial p^2} = -\frac{a}{(1+aS_\mathrm{T})^2}\left(\frac{\partial S_\mathrm{T}}{\partial p}\right)^2 + \frac{1}{1+aS_\mathrm{T}}\,\frac{\partial^2 S_\mathrm{T}}{\partial p^2}.$$

After some algebra it can be casted into the following form

$$\frac{\partial^2 S_\mathrm{R}}{\partial p^2} = \frac{(a-1)p^{-a}(1-p)^{-a}}{(1+aS_\mathrm{T})^2}$$

$$\times \quad \left[\frac{1}{a}\left(\left(\frac{p}{1-p}\right)^a + \left(\frac{1-p}{p}\right)^a - 2\right) + \left(\frac{p}{1-p} + \frac{1-p}{p} + 2\right)\right].$$

For further simplification it is useful to introduce a new variable, by $p = re^t$ and $1-p = r\mathrm{e}^{-t}$. Due to the normalization $2r\cosh(t) = 1$. On the other hand

$$\left(\frac{p}{1-p}\right)^n + \left(\frac{1-p}{p}\right)^n \pm 2 = \left(\mathrm{e}^{nt} \pm \mathrm{e}^{-nt}\right)^2.$$

This leads to the final result

$$\frac{\partial^2 S_\mathrm{R}}{\partial p^2} = \frac{4(a-1)\cosh^2(t)}{\cosh^2((a-1)t)}\left[\frac{\sinh^2(at)}{a} + \cosh^2(t)\right]$$

with

$$t = \frac{1}{2}\ln\frac{p}{1-p}.$$

For $a > 1$ this expression is positive, the entropy would have a minimum, not a maximum. This property is shared by the Tsallis entropy. For having a maximum $a < 1$ ($q > 0$) is required. On the other hand for $a < -1$ ($q > 2$) there are probabilities for which the Rényi entropy may not be convex, $S''_\mathrm{R} > 0$ occurs. This depends on the sign of the expression in the square brackets above. Setting $a = -n$ the inflection points, $t = \pm t_i$, satisfy

$$\cosh(t_i) = \frac{1}{\sqrt{n}}\sinh(nt_i).$$

This is a transcendent equation with no analytic solution, but numerically it is easy to handle. For large n (large positive $q = n+1$) the inflection points shrink towards the equipartition point $t = 0$, as $t \sim \pm\ln n/2(n-1)$.

5.11 Calculate the pressure for a massless ideal Boltzmann gas with canonical Tsallis–Pareto energy distribution with no chemical potential.

The pressure,

$$p = \frac{1}{\beta}\frac{\partial}{\partial V}\ln Z,$$

for an ideal massless Bose gas is given by

$$p = -\frac{\gamma}{2\pi^2} \int_0^\infty E^2 \mathrm{d}E \, \ln\left(1 - e_{-a}(-\beta E)\right)$$

with γ being a degeneracy factor. After considering $E^2 = (E^3/3)'$ and partial integration one obtains

$$p = \frac{\gamma}{6\pi^2} \int_0^\infty E^3 \mathrm{d}E \, \frac{1}{1 + a\beta E} \frac{1}{e_a(\beta E) - 1}.$$

Now, denoting βE by x and $1/\beta$ by T, we expand the generalized Bose factor and use the fact that $e_a(x) = (1 + ax)^{1/a}$. In this case

$$n_a(x) = \frac{1}{(1 + ax)^{1/a} - 1} = \sum_{n=1}^{\infty} (1 + ax)^{-n/a}$$

and we get

$$p = \frac{\gamma}{6\pi^2} T^4 \sum_{n=1}^{\infty} \int_0^\infty x^3 \mathrm{d}x \, (1 + ax)^{-(1+n/a)}.$$

The integrals can be evaluated by the substitution $t = 1 + ax$ leading to

$$I_\nu = \int_0^\infty \mathrm{d}x x^3 (1 + ax)^{-\nu} = a^{-4} \int_1^\infty \mathrm{d}t \, (t - 1)^3 t^{-\nu}.$$

It is easy to show that such an integral results in

$$I_\nu = \frac{1}{a^4} \left(\frac{1}{\nu - 4} - \frac{3}{\nu - 3} + \frac{3}{\nu - 2} - \frac{1}{\nu - 1} \right).$$

Applying this result for $\nu = 1 + n/a$ finally we arrive at the pressure formula

$$p = \frac{\gamma}{\pi^2} T^4 \sum_{n=1}^{\infty} \frac{1}{n(n - a)(n - 2a)(n - 3a)}.$$

For $a = 0$ the well-known Riemann zeta coefficient $\pi^4/90$ emerges, for a general value of the deformity parameter a the infinite sum can be expressed by incomplete Euler-gamma functions. For positive values of a (more high-energy particles than the pure exponential formula would yield) the pressure is enhanced.

Problems of Chap. 6

6.1 Express temperature transformation in rapidity variables.

By the definitions $w_i = \tanh\alpha_i$ and $v_i = \tanh\beta_i$ the equilibrium conditions read

$$\alpha_1 + \beta_1 = \alpha_2 + \beta_2$$

and

$$T_1 \cosh\alpha_1 = T_2 \cosh\alpha_2.$$

The relative rapidity of the moving bodies is $\zeta = \beta_2 - \beta_1 = \alpha_1 - \alpha_2$ so the temperature shown by the thermometer becomes

$$T_1 = T_2 \frac{\cosh\alpha_2}{\cosh(\alpha_2 + \zeta)}.$$

6.2 Can it be that $T_1/T_2 \leq |w_1/w_2|$? What does it mean for the measured value T_1?

Following the results of the previous problem (6.1) the required inequality is given as

$$\frac{T_1}{T_2} = \frac{\cosh\alpha_2}{\cosh\alpha_1} \leq \left|\frac{\tanh\alpha_1}{\tanh\alpha_2}\right| = \frac{|\sinh\alpha_1|}{\cosh\alpha_1} \frac{\cosh\alpha_2}{|\sinh\alpha_2|}.$$

This is fulfilled if $|\alpha_1| \geq |\alpha_2|$ and it has the consequence that $T_1 \leq T_2$.

6.3 At what special values of the relative velocity can it be $T_1 = 2T_2$?

Using the transformation formula we have

$$\frac{T_1}{T_2} = \frac{\sqrt{1-v^2}}{1+w_2 v} = 2.$$

Its square leads to the following second order equation for the relative velocity, v:

$$(1+4w_2^2)v^2 + 8w_2 v + 3 = 0.$$

The solutions are

$$v = -\frac{1}{1+4w_2^2}\left(-4w_2 \pm \sqrt{4w_2^2 - 3}\right).$$

Real solutions are possible as long as $w_2^2 \geq 3/4$. The extreme values of v are achieved by $w_2 = \pm 1$. The possible relative velocities leading to the above temperature ratio are $3/5 \leq v \leq 1$ and $-1 \leq v \leq -3/5$. Relative velocities with a magnitude smaller than $3/5 = 0.6$ cannot lead to such a temperature ratio in equilibrium.

Problems of Chap. 7

7.1 Prove that R^2 is flat in polar coordinates. The arc length squared is given as $\mathrm{d}s^2 = \mathrm{d}r^2 + r^2\mathrm{d}\vartheta^2$. Note that not all Christoffel symbol elements are zero, but the Riemann tensor components.

From the metric formula, $\mathrm{d}s^2 = \mathrm{d}r^2 + r^2\mathrm{d}\vartheta^2$ the following Lorentzian one-forms can be recognized: $\omega^1 = \mathrm{d}r$ and $\omega^2 = r\mathrm{d}\vartheta$. Their Cartan derivatives are $\mathrm{d}\omega^1 = 0$ and $\mathrm{d}\omega^2 = \mathrm{d}r \wedge \mathrm{d}\vartheta = \frac{1}{r}\omega^1 \wedge \omega^2$. This means that some of the composition coefficients are nonzero: ${c_{12}}^2 = -1/r$ and ${c_{21}}^2 = 1/r$. Since $\eta_{ij} = \delta_{ij}$ is the diagonal unit matrix, we also have $c_{122} = -1/r$ and $c_{212} = 1/r$. The antisymmetric two-index collection becomes

$$\Omega_{12} = \frac{1}{2}\left(c_{12a} + c_{1a2} - c_{2a1}\right)\omega^a = -\frac{1}{r}\omega^2 = -\mathrm{d}\vartheta.$$

This way ${\Omega^1}_2 = -\mathrm{d}\vartheta$ and the curvature two-from vanishes:

$${R^1}_2 = \mathrm{d}{\Omega^1}_2 = 0.$$

7.2 Prove that S^2, the surface of the unit sphere, has a constant curvature. The metric tensor is given by $\mathrm{d}s^2 = \mathrm{d}\theta^2 + \sin^2\theta\mathrm{d}\phi^2$.

From $\mathrm{d}s^2 = \mathrm{d}\theta^2 + \sin^2\theta\mathrm{d}\phi^2$ the basis one-forms are: $\omega^1 = \mathrm{d}\theta$ and $\omega^2 = \sin\theta\mathrm{d}\phi$. Their derivatives, $\mathrm{d}\omega^1 = 0$ and

$$\mathrm{d}\omega^2 = \cos\theta\mathrm{d}\theta \wedge \mathrm{d}\phi = \mathrm{ctg}\theta\ \omega^1 \wedge \omega^2$$

reveal a nonzero entry to the Christoffel symbols. We have $c_{122} = -\mathrm{ctg}\theta$ and $c_{212} = \mathrm{ctg}\theta$, all the other coefficients are zero. The antisymmetric one-form matrix is given as

$$\Omega_{12} = \frac{1}{2}\left(c_{12a} + c_{1a2} - c_{2a1}\right)\omega^a = c_{122}\omega^2 = -\mathrm{ctg}\theta\sin\theta\mathrm{d}\phi.$$

It simplifies to ${\Omega^1}_2 = \Omega_{12} = -\cos\theta\mathrm{d}\phi$. The curvature two-form becomes

$${R^1}_2 = \mathrm{d}{\Omega^1}_2 = \sin\theta\mathrm{d}\theta \wedge \mathrm{d}\phi = \omega^1 \wedge \omega^2.$$

This way some entries of the Riemann tensor are nonzero: ${R^1}_{212} = 1$, ${R^1}_{221} = -1$, ${R^2}_{112} = -1$ and ${R^2}_{121} = 1$. The Ricci tensor is diagonal, $\mathscr{R}_{ij} = \delta_{ij}$ (it is always proportional to the unity matrix for two-dimensional surfaces and hence the Einstein tensor vanishes in such cases). The scalar curvature is $\mathscr{R} = 2$ belonging to unit radii of the main circles in the general formula $\mathscr{R} = 2/r_1r_2$.

7.4 Prove that (7.184) leads to a linear velocity profile.

Combining (7.184) with the relativistic formulas for the energy and angular momentum carried by the spinning string we have the following variational problem:

$$\sigma \frac{\delta}{\delta v} \int\limits_{-\ell/2}^{+\ell/2} \frac{1-\omega s v(s)}{\sqrt{1-v^2(s)}} \, \mathrm{d}s = 0.$$

This is an $L(s, v(s))$ type Lagrangian problem, so the Euler-Lagrange equations simply end up with

$$\frac{\partial L}{\partial v} = -\frac{\omega s}{\sqrt{1-v^2}} + \frac{1-\omega s v}{(1-v^2)^{3/2}} v = 0.$$

This leads quickly to the result $v = \omega s$.

7.3 Obtain the entropy for an extremal Reissner–Nordstrøm black hole with cosmological constant, $\lambda = -3/a^2 L_{\mathrm{P}}^2$, according to the formula (7.134).

Observing that $M_{\mathrm{P}} L_{\mathrm{P}} = \hbar/c$ is a purely quantum mechanical, while $L_{\mathrm{P}}/M_{\mathrm{P}} = G/c^2$ is a purely gravitational combination of the Planck scales, the formula (7.134) can be written entirely in terms of these scales:

$$\frac{S}{k_{\mathrm{B}}} = 4\pi \int\int \delta\left(f(r;M)\right) \frac{\mathrm{d}r}{L_{\mathrm{P}}} \frac{\mathrm{d}M}{M_{\mathrm{P}}}.$$

From now on everything is understood in Planck scale and Boltzmann units. The radial metric factor for an extremal RN black hole with AdS term is given by

$$f(r;M) = \left(1 - \frac{M}{r}\right)^2 - \frac{r^2}{a^2}.$$

The horizons are determined by the solution of the fourth order algebraic equation $f(r;M) = 0$ leading to

$$M_0(r) = r(1 \mp r/a).$$

The derivative of f with respect to M gives

$$\frac{\partial f}{\partial M} = -\frac{2}{r}\left(1 - \frac{M}{r}\right),$$

which at the horizon becomes $\mp 2/a$. The entropy is therefore obtained as

$$S = 4\pi \int \frac{\mathrm{d}r}{\left|\frac{\partial f}{\partial M}\right|} = 2\pi r a.$$

This is *not* the (one fourth of the) horizon *area*, but its *perimeter* multiplied by the AdS scale a.

7.5 Find the coordinate transformation to embed the metric (7.219) as a five-dimensional hyperboloid surface in six dimensions.

Using $c = 1$ units the goal is to induce the 5-dimensional metric

$$\mathrm{d}s_5^2 = \frac{r^2}{R^2}\mathrm{d}s_4^2 + \frac{R^2}{r^2}\mathrm{d}r^2$$

with

$$\mathrm{d}s_4^2 = -\mathrm{d}t^2 + \mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^4$$

being flat Minkowskian. The embedding space is flat

$$\mathrm{d}s_6^2 = -\mathrm{d}t_1^2 - \mathrm{d}t_2^2 + \mathrm{d}x_1^2 + \mathrm{d}x_2^2 + \mathrm{d}x_3^2 + \mathrm{d}x_4^2.$$

We use the variable $s_4^2 = -t^2 + x^2 + y^2 + z^2$ and the light cone variables $x_1 - t_1 = r$, $x_1 + t_1 = u$. By using the scaling factor r/R we set $t_2 = tr/R, x_2 = xr/R, x_3 = yr/R$ and $x_4 = zr/R$. This way we have two sub-hyperboles,

$$-t_2^2 + x_2^2 + x_3^2 + x_4^2 = (rs_4/R)^2$$

and

$$-t_1^2 + x_1^2 = ru.$$

The equation for the hyperboloid in the 6-dimensional flat spacetime becomes

$$s_6^2 = x_1^2 + x_2^2 + x_3^2 + x_4^2 - t_1^2 - t_2^2 \; = \; ru + \frac{r^2}{R^2}\, s_4^2.$$

By the same assumptions the subspace metrics are given by

$$-\mathrm{d}t_2^2 + \mathrm{d}x_2^2 + \mathrm{d}x_3^2 + \mathrm{d}x_4^2 = [\mathrm{d}(s_4 r/R)]^2$$

and

$$-\mathrm{d}t_1^2 + \mathrm{d}x_1^2 = \mathrm{d}r\mathrm{d}u.$$

Noting the scaled four-distance by $w = s_4 r/R$ we have

$$\mathrm{d}s_6^2 = \mathrm{d}r\mathrm{d}u + \mathrm{d}w^2$$

which we restrict onto the hyperboloid defined by

$$s_6^2 = ru + w^2.$$

From this we express

$$u = \frac{1}{r}\left(s_6^2 - w^2\right)$$

yielding the differential

$$du = -\frac{dr}{r^2}\left(s_6^2 - w^2\right) - \frac{2w}{r}dw.$$

This way the 6-dimensional metric restricted to the hyperboloid becomes

$$ds_6^2 = dw^2 - \left(s_6^2 - w^2\right)\frac{dr^2}{r^2} - \frac{2w}{r}dwdr.$$

On the other hand ds_5^2 can also be expressed in terms of w and r. One gets

$$ds_5^2 = \left(rd\frac{w}{r}\right)^2 + \frac{R^2}{r^2}dr^2.$$

This expression equals to

$$ds_5^2 = \left(dw - \frac{w}{r}dr\right)^2 + \frac{R^2}{r^2}dr^2 = dw^2 - \frac{2w}{r}dwdr + \frac{w^2+R^2}{r^2}dr^2.$$

Clearly, with the choice $s_6^2 = -R^2$ the two metrics are equivalent. In conclusion, the embedded hyperboloid interpretation is equivalent to using scaled 4-dimensional spacetime coordinates and taking r as a light cone coordinate in a $1+1$-dimensional additive spacetime.

7.6 Prove that the volume of the 5-dimensional spherical hypersurface is $\Omega_5 = \pi^3$.

The volume of S_n is the surface of a sphere with unit radius embedded in $n+1$ dimensions. It can be written as a product of angular integrals, each factor containing a higher power of $\sin\vartheta_i$ than the previous one:

$$\Omega_{n+1} = I_n \Omega_n$$

with

$$I_n = \int_0^\pi \sin^{n-1}\vartheta \, d\vartheta.$$

The starting points are given by $I_1 = \pi$ and $I_2 = 2$, the rest can be obtained by a recursion formula. Such a formula is easily derived by noting that $(\sin\vartheta\cos\vartheta)' = 1 - 2\sin^2\vartheta$. In this case

$$I_{n-1} - 2I_{n+1} = \int_0^\pi (\sin\vartheta\cos\vartheta)' \sin^{n-2}\vartheta \, d\vartheta.$$

After partial integration it becomes

$$I_{n-1} - 2I_{n+1} = -(n-2)\int_0^\pi \sin\vartheta\cos\vartheta \, \sin^{n-3}\vartheta \, \cos\vartheta \, d\vartheta,$$

which upon using $\cos^2\vartheta = 1 - \sin^2\vartheta$ can be casted into the simple result

$$I_{n-1} - 2I_{n+1} = (n-2)\left(I_{n+1} - I_{n-1}\right).$$

The resolution of this linear equation is the simple recursion formula

$$I_{n+1} \;=\; \left(1 - \frac{1}{n}\right) I_{n-1}.$$

With the starting points we have $I_1 = \pi, I_2 = 2, I_3 = \pi/2, I_4 = 4/3, I_5 = 3\pi/8$ and therefore $\Omega_1 = 2\pi, \Omega_2 = 4\pi, \Omega_3 = 2\pi^2, \Omega_4 = 8\pi^2/3$ and $\Omega_5 = \pi^3$.

7.7 Obtain the horizon-entropy for a Reissner–Nordstrøm black hole with fixed charge to mass ratio, $\tilde{Q} = \mu\tilde{M}$ in Planck scale units, in the presence of a de Sitter-type cosmological constant term with $\lambda = -3/a^2$.

The radial function describing the horizon in Planck units is given by

$$f(r) = 1 - \frac{2M}{r} + \frac{\mu^2 M^2}{r^2} - \frac{r^2}{a^2} = 0.$$

Resolving this second order expression for M, one easily obtains

$$M_\pm(r) = \frac{r}{\mu^2}\left(1 \pm \sqrt{1 - \mu^2 + \frac{\mu^2 r^2}{a^2}}\right).$$

The derivative of f with respect to M is linear in M:

$$\frac{\partial f}{\partial M} = -\frac{2}{r} + 2\frac{\mu^2}{r^2}M,$$

which replacing $M_\pm(r)$ from the horizon condition becomes at the horizon

$$\left.\frac{\partial f}{\partial M}\right|_{M=M_\pm(r)} = \pm\frac{2}{r}\sqrt{1 - \mu^2 + \frac{\mu^2 r^2}{a^2}}.$$

The horizon-entropy in Planck scale units is given by the following integral

$$S = 2\pi \int \frac{r\,\mathrm{d}r}{\sqrt{1 - \mu^2 + \frac{\mu^2 r^2}{a^2}}}.$$

This integral can be evaluated analytically with the result:

$$S = 2\pi\left(\frac{a^2}{\mu^2}\sqrt{1 - \mu^2 + \frac{\mu^2 r^2}{a^2}} - K(a,\mu)\right).$$

The integration constant, $K(a,\mu)$ can be obtained from the requirement that at zero horizon area or zero horizon radius, $r = 0$ the entropy should be zero. This way we finally obtain:

$$S = 2\pi \frac{a^2}{\mu^2} \left(\sqrt{1-\mu^2+\frac{\mu^2 r^2}{a^2}} - \sqrt{1-\mu^2} \right).$$

For $\mu/a \to 0$ one gets back

$$\lim_{\mu/a \to 0} S = \frac{\pi r^2}{\sqrt{1-\mu^2}} \geq \frac{1}{4} A,$$

and for an extremal black hole with $\mu = 1$

$$S(1,a) = 2\pi a r.$$

Both particular cases have been discussed in Chap. 7.

Problems of Chap. 8

8.1 Obtain the parity of the canonical spectral function by expressing $\rho_{AB}(-\omega)$.

Using the definition with $-\omega$ one has

$$\rho_{AB}(-\omega) = \frac{1}{Z} \sum_{a,b} \langle a|A(0)|b \rangle \langle b|B(0)|a \rangle \, 2\pi\delta(E_a - E_b + \omega) \left[\mathrm{e}^{-\beta E_a} \mp \mathrm{e}^{-\beta E_b} \right].$$

In this formula we exchange the summation labels a and b and arrive at

$$\rho_{AB}(-\omega) = \frac{1}{Z} \sum_{a,b} \langle b|A(0)|a \rangle \langle a|B(0)|b \rangle \, 2\pi\delta(E_b - E_a + \omega) \left[\mathrm{e}^{-\beta E_b} \mp \mathrm{e}^{-\beta E_a} \right].$$

Now we use that the Dirac-delta is an even functional of its argument and factorize the ∓ 1 out of the square bracket term. We also interchange the order of the transition matrix elements $\langle b|A(0)|a \rangle$ and $\langle a|B(0)|a \rangle$. By doing so we get

$$\rho_{AB}(-\omega) = \mp \frac{1}{Z} \sum_{a,b} \langle a|B(0)|b \rangle \langle b|A(0)|a \rangle \, 2\pi\delta(E_a - E_b - \omega) \left[\mathrm{e}^{-\beta E_a} \mp \mathrm{e}^{-\beta E_b} \right].$$

In this form, the final result is easy to recognize:

$$\rho_{AB}(-\omega) = \mp \rho_{BA}(\omega).$$

8.2 Calculate the following sum rule for the canonical spectral function:

$$R = \int \frac{\mathrm{d}\omega}{2\pi} \rho_{AB}(\omega).$$

The ω-integration "consumes" the Dirac-delta and one arrives at

$$R = \frac{1}{Z} \sum_{a,b} \langle a|A(0)|b\rangle \langle b|B(0)|a\rangle \left[\mathrm{e}^{-\beta E_a} \mp \mathrm{e}^{-\beta E_b}\right].$$

This expression is equal to the canonical expectation value

$$R = \langle A(0)B(0) \mp B(0)A(0)\rangle .$$

In particular, for the creation and annihilation operator this integral is $R = 1$.

8.3 Obtain an operator formula for the Wigner transform of a convolution.

We use the notation $x_1 = x + \frac{\xi}{2}$, $x_2 = x - \frac{\xi}{2}$ for the coordinates. Let H be the convolution of F and G, then its Wigner transform is given by

$$\bar{H}(x,p) = \int \mathrm{d}\xi \mathrm{e}^{\mathrm{i}p\xi} H\left(x + \frac{\xi}{2}, x - \frac{\xi}{2}\right) = \int \mathrm{d}\xi \mathrm{e}^{\mathrm{i}p\xi} \int \mathrm{d}z F\left(x + \frac{\xi}{2}, z\right) G\left(z, x - \frac{\xi}{2}\right).$$

We introduce the quantity ε by using $z = x + \varepsilon = x - \frac{\xi}{2} + (\varepsilon + \frac{\xi}{2}) = x + \frac{\xi}{2} + (\varepsilon - \frac{\xi}{2})$. This way we obtain

$$\bar{H}(x,p) = \int \mathrm{d}z \mathrm{d}\xi \mathrm{e}^{\mathrm{i}p\xi} F\left(x + \frac{\xi}{2}, x - \frac{\xi}{2} + \left(\varepsilon + \frac{\xi}{2}\right)\right) G\left(x + \frac{\xi}{2} + \left(\varepsilon - \frac{\xi}{2}\right), x - \frac{\xi}{2}\right).$$

This formula can be rewritten by using the exponential form of the Taylor expansion for a shifted argument as

$$\bar{H}(x,p) = \int \mathrm{d}z \mathrm{d}\xi \mathrm{e}^{\mathrm{i}p\xi} \left[\mathrm{e}^{(\varepsilon + \frac{\xi}{2})\frac{\partial}{\partial x_2}} F(x_1, x_2)\right] \left[\mathrm{e}^{(\varepsilon - \frac{\xi}{2})\frac{\partial}{\partial x_1'}} G(x_1', x_2')\right]$$

taken at $x' = x$ at the end. As the next step we express the functions $F(x_1, x_2)$ and $G(x_1', x_2')$ from their respective Wigner transforms:

$$\bar{H}(x,p) = \int \left[\mathrm{e}^{(\varepsilon + \frac{\xi}{2})\frac{\partial}{\partial x_2}} \mathrm{e}^{-\mathrm{i}q(x_1 - x_2)} \bar{F}\left(\frac{x_1 + x_2}{2}, q\right)\right]$$

$$\times \left[\mathrm{e}^{(\varepsilon - \frac{\xi}{2})\frac{\partial}{\partial x_1'}} \mathrm{e}^{-\mathrm{i}r(x_1' - x_2')} \bar{G}\left(\frac{x_1' + x_2'}{2}, r\right)\right]$$

with the multiple integral

$$\int \cdots = \int \mathrm{d}z\mathrm{d}\xi \, \frac{\mathrm{d}q}{2\pi} \frac{\mathrm{d}r}{2\pi} \, \mathrm{e}^{\mathrm{i}p\xi} \cdots$$

Replacing x_1 and x_2 by their respective definitions it is equivalently written in the form

$$\bar{H}(x,p) = \int \left[\mathrm{e}^{(\varepsilon+\frac{\xi}{2})(iq+\frac{1}{2}\frac{\partial}{\partial x})} \mathrm{e}^{-\mathrm{i}q\xi} \bar{F}(x,q) \right] \left[\mathrm{e}^{(\varepsilon-\frac{\xi}{2}')(-ir+\frac{1}{2}\frac{\partial}{\partial x'})} \mathrm{e}^{-\mathrm{i}r\xi'} \bar{G}(x',r) \right]$$

taken at $x' = x$ and $\xi' = \xi$. Collecting now alike terms in the exponents (containing and not containing derivatives, respectively) we arrive at

$$\bar{H}(x,p) = \int \left[\mathrm{e}^{\mathrm{i}q(\varepsilon-\frac{\xi}{2})} \, \mathrm{e}^{(\varepsilon+\frac{\xi}{2})(\frac{1}{2}\frac{\partial}{\partial x})} \bar{F}(x,q) \right] \left[\mathrm{e}^{-\mathrm{i}r(\varepsilon+\frac{\xi}{2}')} \, \mathrm{e}^{(\varepsilon-\frac{\xi}{2}')(\frac{1}{2}\frac{\partial}{\partial x'})} \mathrm{e}^{-\mathrm{i}r\xi'} \bar{G}(x',r) \right]$$

It is purposeful to write $q = p + a$ and $r = p' + b$, and taking the result at $p' = p$ at the end. This way the exponential factors can be re-arranged and the integrations over z, q and r are replaced by those over ε, a and b:

$$\bar{H}(x,p) = \int \mathrm{e}^{\mathrm{i}\varepsilon\left(a-b+\frac{1}{2i}(\frac{\partial}{\partial x}+\frac{\partial}{\partial x'})\right)} \, \mathrm{e}^{\mathrm{i}\xi\left(-\frac{a+b}{2}+\frac{1}{4i}(\frac{\partial}{\partial x}-\frac{\partial}{\partial x'})\right)} \, \bar{F}(x,p+a)\bar{G}(x',p'+b).$$

Now $\int = \int \mathrm{d}\xi \mathrm{d}\varepsilon \frac{\mathrm{d}a}{2\pi}\frac{\mathrm{d}b}{2\pi}$, and at the end $x' = x$ and $p' = p$ are taken. The shifted momentum arguments $p+a$ and $p'+b$ are also Taylor-expanded,

$$\bar{F}(x,p+a)\bar{G}(x',p'+b) = \mathrm{e}^{a\frac{\partial}{\partial p}+b\frac{\partial}{\partial p'}} \bar{F}(x,p)\bar{G}(x',p'),$$

to have

$$\bar{H}(x,p) = \int \mathrm{e}^{\mathrm{i}a\left(\varepsilon-\frac{\xi}{2}+\frac{1}{i}\frac{\partial}{\partial p}\right)} \, \mathrm{e}^{\mathrm{i}b\left(-\varepsilon-\frac{\xi}{2}+\frac{1}{i}\frac{\partial}{\partial p'}\right)} \, \mathrm{e}^{\mathrm{i}\frac{\varepsilon}{2}\left(\frac{\partial}{\partial x}+\frac{\partial}{\partial x'}\right)} \, \mathrm{e}^{\mathrm{i}\frac{\xi}{4}\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial x'}\right)} \, \bar{F}(x,p)\bar{G}(x',p').$$

The last important step is to recognize that the integration over a and b leads to the following equivalence

$$\varepsilon - \frac{\xi}{2} = -\frac{1}{i}\frac{\partial}{\partial p}$$

and

$$\varepsilon + \frac{\xi}{2} = \frac{1}{i}\frac{\partial}{\partial p'}.$$

Using these relations the leftover exponent is given as

$$\hat{\nabla} = \frac{1}{2}\left[\left(\varepsilon+\frac{\xi}{2}\right)\frac{\partial}{\partial x} + \left(\varepsilon-\frac{\xi}{2}\right)\frac{\partial}{\partial x'} \right] = \frac{1}{2i}\left[\frac{\partial}{\partial p'}\frac{\partial}{\partial x} - \frac{\partial}{\partial p}\frac{\partial}{\partial x'} \right].$$

Using this "triangle" operator notation the Wigner transform of the convolution is given by

$$\bar{H}(x,p) = \mathrm{e}^{\hat{\nabla}}\,\bar{F}(x,p)\,\bar{G}(x',p')\Big|_{x'=x,\,p'=p}$$

The two leading orders of its expansion, if the effect of $\hat{\nabla}$ is small compared to the identity (the so called "gradient – expansion"), are given by

$$\bar{H}(x,p) \approx \bar{F}(x,p)\,\bar{G}(x,p) + \frac{1}{2i}\left\{\bar{F},\bar{G}\right\}$$

where

$$\left\{\bar{F},\bar{G}\right\} = \frac{\partial\bar{F}}{\partial x}\frac{\partial\bar{G}}{\partial p} - \frac{\partial\bar{F}}{\partial p}\frac{\partial\bar{G}}{\partial x}$$

is the Poisson bracket.

8.4 Consider the $\ddot{x}+2\Gamma\dot{x}+k^2x = f(t)$ oscillator within a white noise environment, $\langle f(t)\rangle = 0$, and $\langle f(t)f(t')\rangle = 4\Gamma T\delta(t-t')/V$. What is the correlator in the real-time, $\langle x(t)x(t')\rangle$, and in the frequency representation, $\langle\tilde{x}(\omega)\tilde{x}(\omega')\rangle$, in the infrared $(k\to 0)$ limit?

Fourier transformation with respect to the time, t, leads to

$$\left(-\omega^2+2i\Gamma\omega+k^2\right)\tilde{x}(\omega) = \tilde{f}(\omega).$$

The correlator for the Fourier-transform of the white noise can easily be obtained as being

$$\left\langle \tilde{f}(\omega)\tilde{f}(\omega')\right\rangle = \frac{4\Gamma T}{V}2\pi\delta(\omega+\omega').$$

The real-time correlator becomes

$$G(t-t',k) = \left\langle x(t)x(t')\right\rangle = \int\frac{\mathrm{d}\omega}{2\pi}\frac{\mathrm{d}\omega'}{2\pi}\,\mathrm{e}^{\mathrm{i}(\omega t+\omega' t')}\left\langle \tilde{x}(\omega)\tilde{x}(\omega')\right\rangle.$$

Due to the Dirac-delta factor in the white-noise correlation in the frequency-representation this simplifies to

$$\left\langle x(t)x(t')\right\rangle = \int\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{\mathrm{i}\omega(t-t')}\left\langle \tilde{x}(\omega)\tilde{x}(-\omega)\right\rangle.$$

The particular x-correlator in the frequency-representation, which we need here, is given by

$$\left\langle \tilde{x}(\omega)\tilde{x}(-\omega)\right\rangle = \frac{4\Gamma T/V}{(-\omega^2+2i\Gamma\omega+k^2)\,(-\omega^2-2i\Gamma\omega+k^2)}.$$

The denominator can be re-factorized as follows: Since

$$\begin{aligned}\left(-\omega^2+2i\Gamma\omega+k^2\right)\left(-\omega^2-2i\Gamma\omega+k^2\right) &= \left(\omega^2-k^2\right)^2+4\Gamma^2\omega^2\\ &= \left(\omega^2+2\Gamma^2-k^2\right)^2+4\Gamma^2\left(k^2-\Gamma^2\right),\end{aligned}$$

the final factors are

$$\omega^2 + 2\Gamma^2 - k^2 + 2i\Gamma\sqrt{k^2 - \Gamma^2}$$

and its conjugate version with $-\Gamma$ instead of Γ.

For small values of k the square root is purely imaginary and we arrive at

$$\frac{1}{(-\omega^2 + 2i\Gamma\omega + k^2)\,(-\omega^2 - 2i\Gamma\omega + k^2)} \approx \frac{1}{4\Gamma^2}\left(\frac{1}{\omega^2 + k^4/4\Gamma^2} - \frac{1}{\omega^2 + 4\Gamma^2}\right).$$

This way the static infrared correlator becomes

$$G(\omega = 0, k \ll \Gamma) \approx \frac{4\Gamma T}{V}\,\frac{1}{k^4}$$

describing a linear (confining) potential between heavy and static sources. In fact the stochastic background model of confinement used to be popular in the 1980s. On the other hand the real-time correlator features two damping factors according to the above result, $\gamma_1 = 2\Gamma$ and $\gamma_2 = k^2/2\Gamma$. In the infrared limit $k \to 0$ this means a very slow forgetting:

$$G(t - t', k \ll \Gamma) = \frac{T}{Vk^2}\mathrm{e}^{-k^2|t-t'|/2\Gamma} - \frac{T}{4\Gamma^2 V}\mathrm{e}^{-2\Gamma|t-t'|}.$$

the $\gamma_2 = k^2/2\Gamma$ damping factor occurs in the discussion of chaotic quantization, too.

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Index