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# Quantum Foundations, Probability and Information



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# Quantum Foundations, Probability and Information



*Editors* Andrei Khrennikov International Center for Mathematical Modeling in Physics and Cognitive Science Linnaeus University Växiö, Sweden

Bourama Toni Department of Mathematics Howard University Washington, DC, USA

National Research University of Information Technologies Mechanics and Optics (ITMO) St. Petersburg, Russia

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## Preface

The last 20 years were characterized by tremendous development of the fields of quantum probability and information. The *quantum information revolution* has also renewed the interest in the foundations of quantum theory (philosophical and mathematical), to the extent that fundamental concepts are now reconsidered in terms of a new information-theoretical perspective [1-9]. This recent revolutionary transformation of quantum physics toward information physics also stimulated the development of novel mathematical models and methods.

This book is composed of contributions by leading experts in quantum foundations, especially from informational, probabilistic, and mathematical perspectives, and it presents their expert viewpoints on a number of foundational problems as well as novel mathematical models of quantum and subquantum phenomena. The mathematical content of the book is very rich and multidisciplinary: theory of partial differential equations of quantum field theory (derivation, modification, properties of solutions), differential geometry (including Riemann and Weyl geometries), oscillatory processes and vibrations, probability theory and its interpretations (especially the subjective one), classical versus quantum Bayesian inference, update of probabilities, Turing machines and random generators, action-reaction models, Feynman integrals for quickly growing potential functions, theory of open quantum systems, quantum master equation, quantum Markovian processes, mathematical modeling of decoherence in quantum and classical frameworks, Bell's inequality and its probabilistic structure, mathematical models of theories of hidden variables, theory of cellular automata, quantum versus classical entropy, measures of quantum information, theory of complexity and optimization, quantum theory of classification, clustering based on the Hilbert space framework, and representation of information by density operators. Some of these chapters are quite speculative, but the complexity (physical, mathematical, and philosophical) of the problems under study justifies such speculative considerations. Some of them depart far from the mainstream of quantum physical studies. This is up to the reader whether to accept or to reject such novel but sometimes controversial arguments and mathematical models of the authors. Other chapters are devoted to the fundamental problems of the conventional quantum theory including its mathematical formalism. We trust that these contributions would be useful for experts in the corresponding areas of quantum theory. In this preface a few such contributions will be discussed in more detail.

One cluster of related chapters in this book concerns quantum and classical field theory and oscillatory processes. These are the contributions of A. Akhmeteli, "The Dirac Equation as One Fourth-Order Equation for One Function: A General, Manifestly Covariant Form"; B.R. La Cour, C.I. Ostrove, M.J. Starkey, and G.E. Ott, "Quantum Decoherence Emulated in a Classical Device"; S.A. Rashkovskiy, "Classical-Field Theory of the Photoelectric Effect"; and H. Yau, "Temporal Vibrations in a Quantized Field."

Some of these studies go beyond the conventional quantum theory. For example, Rashkovskiy claims that he can show that all properties of the photoelectric effect can be completely described within the framework of classical field theory without any quantization; in particular, three well-known laws of the photoelectric effect are derived without quantization of light and atom.

The chapter of C. Lopez, "The Action Reaction Principle in Quantum Mechanics," reminds the reader that the action–reaction principle is not automatically fulfilled in the standard formulation of quantum mechanics. An extended phase space can be considered where the formulation is consistent. In an extended spin phase space, there is a new quantum state, isotropic. Using this new state the composite singlet becomes separable instead of entangled. The perfect anticorrelation between both particles of the singlet appears in the subquantum states.

The chapter of C. Baladrón and A. Khrennikov, "At the Crossroads of Three Seemingly Divergent Approaches to Quantum Mechanics," considers quantum mechanics from the Darwinian evolutionary perspective. Several concepts stemming from three apparently divergent approaches to quantum mechanics, i.e., Bohmian mechanics, QBism, and time-symmetric quantum mechanics, are interwoven in an information-theoretic Darwinian scheme applied to fundamental physical systems that might shed light on some long-standing quantum mechanical conundrums. Here quantum systems are treated as endowed with individual Turing machines and random generators. Such systems have predictive power explaining nonlocal correlations and violation of Bell's inequality. The problem of nonlocality, probabilistic structure of quantum correlation functions, and violation of Bell's inequality is also studied in the chapters of H. Geurdes, "A Computational Proof of Locality in Entanglement," and G.N. Mardari, "Local Realism Without Hidden Variables." Closely related problems are discussed in the chapter of D.J. Ben Daniel, "Implications of Einstein-Weyl Causality on Quantum Mechanics."

The chapter of A. Baumeler, J. Degorre, and S. Wolf, "Bell Correlations and the Common Future," starts with the reminder that Reichenbach's principle states that in a causal structure, correlations of classical information can stem from a common cause in the common past or a direct influence from one of the events in correlation to the other. The difficulty of explaining Bell correlations through a mechanism in that spirit can be read as questioning either the principle or even its basis: causality. In the former case, the principle can be replaced by its quantum version, accepting as a common cause an entangled state, leaving the phenomenon as mysterious as

ever on the classical level (on which, after all, it occurs). If, more radically, the causal structure is questioned in principle, closed space–time curves may become possible that, as is argued in the present note, can give rise to nonlocal correlations if to-be-correlated pieces of classical information meet in the common future—which they need to if the correlation is to be detected in the first place. The result is a view resembling Brassard and Raymond-Robichaud's parallel-lives variant of Hermann's and Everett's relative state formalism, avoiding "multiple realities."

The chapter of E.N. Dzhafarov, "Replacing Nothing with Something Special: Contextuality-by-Default and Dummy Measurements," presents quantum contextuality (playing the fundamental role in modern quantum information theory) in the rigorous probabilistic framework. This approach is also closely related to aforementioned problems: violation of the Bell-type inequalities and theories of hidden variables. The object of contextuality analysis is a set of random variables, each of which is uniquely labeled by a content and a context. In the measurement terminology, the content is that which the random variable measures, whereas the context describes the conditions under which this content is measured (in particular, the set of other contents being measured together with this one). Such a set of random variables is deemed noncontextual or contextual depending on whether the distributions of the context-sharing random variables are or are not compatible with certain distributions imposed on the content-sharing random variables. In the traditional approaches, contextuality is either restricted to only consistently connected systems (those in which any two content-sharing random variables have the same distribution) or else all inconsistently connected systems (those not having this property) are considered contextual. In the Contextuality by Default theory, an inconsistently connected system may or may not be contextual.

An important biological application of quantum theory is presented in the chapter of Y. Mitome, S. Iriyama, K. Sato, and I.V. Volivich, "Efficient Energy Transfer in Network Model of Photosynthesis." G. Jaeger critically analyzes computerlike models of nature in his contribution "Clockwork Rebooted: Is the Universe a Computer?" A. Khrennikov in his chapter "External Observer Reflections on QBism, Its Possible Modifications, and Novel Applications" critically discusses development of QBism from its early days and the first sound presentations at the Växjö conferences early this century to the flourishing modern theory. This is the collection of very personal recollections of the author about his longterm debates with the creator of the subjective probability approach to quantum mechanics, Christopher Fuchs. The chapter of S. Kak, "Epistemic View of Quantum Communication," is devoted to the foundational problems of quantum information theory and especially quantum communications.

The team of researchers (theoreticians and experimenters), J. Marton, S. Bartalucci, A. Bassi, M. Bazzi, S. Bertolucci, C. Berucci, M. Bragadireanu, M. Cargnelli, A. Clozza, C. Curceanu, L. De Paolis, S. Di Matteo, S. Donadi, J.-P. Egger, C. Guaraldo, M. Iliescu, M. Laubenstein, E. Milotti, A. Pichler, D. Pietreanu, K. Piscicchia, A. Scordo, H. Shi, D. Sirghi, F. Sirghi, L. Sperandio, O. Vazquez-Doce, E. Widmann, and J. Zmeskal, present the recent experimental study, "Underground Test of Quantum Mechanics: The VIP2 Experiment," where they investigate possible violations of standard quantum mechanics predictions. They tested with high precision the *Pauli Exclusion Principle (PEP) and the collapse of the wave function (collapse models)*. Included here is the novel method of searching for possible small violations of PEP for electrons, through the search for anomalous X-ray transitions in copper atoms, produced by fresh electrons (brought inside the copper bar by circulating current) which can have the probability to undergo Pauli-forbidden transition to the level already occupied by two electrons. Also therein is described the VIP2 (VIolation of PEP) experiment taking data at the Gran Sasso underground laboratories. From the mathematical side, this study is based on advanced statistical analysis for occurrence of events having very small probabilities.

H. Mohameden and H. Ouerdiane have written the chapter, "Feynman Integrals for a New Class of Time-Dependent Exponentially Growing Potentials," devoted to the rigorous mathematical study about justification of the method of the path integral. This is a complex mathematical problem which has been studied by many authors, mathematicians, and physicists. And this chapter is the important contribution to this area of research on the boundary between pure mathematics and quantum physics.

The chapter of E. Santucci and G. Sergioli, "Classification Problem in a Quantum Framework," is devoted to application of the methods of quantum theory to classification problems. One of the important outputs of this study is the design of the novel method of presentation of information by density matrices. The main aim of this study is to provide a quantum counterpart of the well-known minimum-distance classifier named nearest mean classifier (NMC). In particular, this chapter contains the review about previous works in this area.

The chapter of N. Watanabe, "On Complexity for Open System Dynamics," represents in detail measures of quantum entropy and information, especially the achievements of the school of M. Ohya at Tokyo University of Science.

We hope that the reader will enjoy this book, which will be useful to experts working in quantum physics and quantum probability and information theory, ranging from theoreticians, experimenters, and mathematicians to philosophers.

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## Contributors

Andrey Akhmeteli LTASolid Inc., Houston, TX, USA

**Carlos Baladrón** Departamento de Física Teórica, Atómica y Óptica, Universidad de Valladolid, Valladolid, Spain

S. Bartalucci LNF-INFN, Frascati, Italy

**A. Bassi** Dipartimento di Fisica, Universita di Trieste and INFN Sezione di Trieste, Trieste, Italy

**Ämin Baumeler** Faculty of Informatics, Università della Svizzera italiana, Lugano, Switzerland

Facoltà indipendente di Gandria, Lunga scala, Gandria, Switzerland

M. Bazzi LNF-INFN, Frascati, Italy

D. J. BenDaniel Johnson School, Cornell University, Ithaca, NY, USA

S. Bertolucci CERN, Meyrin, Switzerland

C. Berucci Stefan Meyer Institute, Vienna, Austria

**M. Bragadireanu** Horia Hulubei National Institute of Physics and Nuclear Engineering, Bucharest, Magurele, Romania

M. Cargnelli Stefan Meyer Institute, Vienna, Austria

A. Clozza LNF-INFN, Frascati, Italy

C. Curceanu LNF-INFN, Frascati, Italy

Museo Storico della Fisica e Centro Studi e Ricerche Enrico Fermi, Roma, Italy

L. De Paolis LNF-INFN, Frascati, Italy

**Julien Degorre** Faculty of Informatics, Università della Svizzera italiana, Lugano, Switzerland

Facoltà indipendente di Gandria, Lunga scala, Gandria, Switzerland

**S. Di Matteo** Institut de Physique UMR CNRS-UR1 6251, Universite de Rennes 1, Rennes, France

S. Donadi Dipartimento di Fisica, Universita di Trieste and INFN Sezione di Trieste, Trieste, Italy

Ehtibar N. Dzhafarov Purdue University, West Lafayette, IN, USA

J.-P. Egger Institut de Physique, Universite de Neuchatel, Neuchatel, Switzerland

Han Geurdes Geurdes Datascience, Den Haag, Netherlands

C. Guaraldo LNF-INFN, Frascati, Italy

M. Iliescu LNF-INFN, Frascati, Italy

Satoshi Iriyama Tokyo University of Science, Tokyo, Japan

**Gregg Jaeger** Quantum Communication and Measurement Laboratory, Department of Electrical and Computer Engineering and Division of Natural Science and Mathematics, Boston University, Boston, MA, USA

**Subhash Kak** School of Electrical and Computer Engineering, Oklahoma State University, Stillwater, OK, USA

Andrei Khrennikov International Center for Mathematical Modeling in Physics and Cognitive Science, Linnaeus University, Växjö, Sweden

National Research University of Information Technologies, Mechanics and Optics (ITMO), St. Petersburg, Russia

**Brian R. La Cour** Applied Research Laboratories, The University of Texas at Austin, Austin, TX, USA

**M. Laubenstein** INFN, Laboratori Nazionali del Gran Sasso, Assergi, L'Aquila AQ, Italy

Carlos López UAH, Madrid, Spain

Ghenadie N. Mardari Open Worlds Research, Sparks, MD, USA

Johann Marton Stefan Meyer Institute, Vienna, Austria

**E. Milotti** Dipartimento di Fisica, Universita di Trieste and INFN Sezione di Trieste, Trieste, Italy

Yuta Mitome Tokyo University of Science, Tokyo, Japan

Hammah Mohameden Department of Mathematics, Faculty of Sciences of Tunis, University of Tunis El-Manar, Tunis, Tunisia

**Corey I. Ostrove** Applied Research Laboratories, The University of Texas at Austin, Austin, TX, USA

**Granville E. Ott** Applied Research Laboratories, The University of Texas at Austin, Austin, TX, USA

Habib Ouerdiane Department of Mathematics, Faculty of Sciences of Tunis, University of Tunis El-Manar, Tunis, Tunisia

A. Pichler Stefan Meyer Institute, Vienna, Austria

D. Pietreanu LNF-INFN, Frascati, Italy

K. Piscicchia LNF-INFN, Frascati, Italy

Museo Storico della Fisica e Centro Studi e Ricerche Enrico Fermi, Roma, Italy

**Sergey A. Rashkovskiy** Institute for Problems in Mechanics of the Russian Academy of Sciences, Moscow, Russia

Tomsk State University, Tomsk, Russia

Enrica Santucci University of Cagliari, Cagliari, Italy

Keiko Sato Tokyo University of Science, Tokyo, Japan

A. Scordo LNF-INFN, Frascati, Italy

Giuseppe Sergioli University of Cagliari, Cagliari, Italy

H. Shi LNF-INFN, Frascati, Italy

D. Sirghi LNF-INFN, Frascati, Italy

F. Sirghi LNF-INFN, Frascati, Italy

L. Sperandio LNF-INFN, Frascati, Italy

**Michael J. Starkey** Applied Research Laboratories, The University of Texas at Austin, Austin, TX, USA

**O. Vazquez-Doce** Excellence Cluster Universe, Technische Universität München, Garching, Germany

Igor V. Volivich Steklow Mathematical Institute, Moskva, Russia

Noboru Watanabe Tokyo University of Science, Noda City, Chiba, Japan

E. Widmann Stefan Meyer Institute, Vienna, Austria

Stefan Wolf Faculty of Informatics, Università della Svizzera italiana, Lugano, Switzerland

Facoltà indipendente di Gandria, Lunga scala, Gandria, Switzerland

Hou Yau FDNL Research, Daly City, CA, USA

J. Zmeskal Stefan Meyer Institute, Vienna, Austria

# The Dirac Equation as One Fourth-Order Equation for One Function: A General, Manifestly Covariant Form



Andrey Akhmeteli

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#### 1 Introduction

The Dirac equation "remains a cornerstone of physics to this day" [12]. It is crucial for such diverse areas as high-energy physics and quantum chemistry (e.g., it is required to explain the properties of the ubiquitous lead-acid batteries [1]).

Dirac sought an equation of the first order in time [8]. To this end, he had to introduce a four-component spinor function. Feynman and Gell-Mann [9] argued that the wave function does not have to have four complex components and showed that the Dirac equation is equivalent to a second-order equation for a two-component function. It was shown recently ([2]; see also [5], pp. 24–25) that, surprisingly, in a general case, three out of four complex components of the Dirac spinor can be algebraically eliminated from the Dirac equation in an arbitrary electromagnetic field. Therefore, the Dirac equation is generally equivalent to a fourth-order partial differential equation for just one component, which can be made real (at least locally) by a gauge transform. However, this result was derived for a specific (chiral) representation of  $\gamma$ -matrices and for a specific component. In this article, the fourth-order equation for one function, which is equivalent to the Dirac equation, is derived for an arbitrary set of  $\gamma$ -matrices satisfying the standard hermiticity conditions and for an arbitrary component that is also a component of the right-handed or

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A. Akhmeteli (🖂)

the left-handed part of the Dirac spinor function. The resulting equation is also manifestly relativistically covariant, unlike that of Ref. [2]. This nontrivial result adds to the immense beauty of the Dirac equation and belongs in textbooks. It is important both for foundations of quantum theory (see [3, 4]) and for numerous applications of the Dirac equation.

# 2 Algebraic Elimination of Components from the Dirac Equation in a General Form

Let us start with the Dirac equation in the following form:

$$(i\partial - A)\psi = \psi, \tag{1}$$

where, e.g.,  $A = A_{\mu}\gamma^{\mu}$  (the Feynman slash notation). For the sake of simplicity, a system of units  $\hbar = c = m = 1$  is used, and the electric charge *e* is included in  $A_{\mu}$  ( $eA_{\mu} \rightarrow A_{\mu}$ ). The metric tensor used to raise and lower indices is [10]

$$g_{\mu\nu} = g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, g^{\nu}_{\mu} = \delta^{\nu}_{\mu}.$$

Multiplying both sides of Eq. (1) by  $(i\partial - A)$  from the left and using notation

$$\sigma^{\mu\nu} = \frac{i}{2} [\gamma^{\mu}, \gamma^{\nu}], \qquad (2)$$

$$F^{\mu\nu} = A^{\nu,\mu} - A^{\mu,\nu} = \begin{pmatrix} 0 & -E^1 & -E^2 & -E^3 \\ E^1 & 0 & -H^3 & H^2 \\ E^2 & H^3 & 0 & -H^1 \\ E^3 & -H^2 & H^1 & 0 \end{pmatrix},$$
(3)

we obtain:

$$\psi = (i\gamma^{\nu}\partial_{\nu} - A_{\nu}\gamma^{\nu})(i\gamma^{\mu}\partial_{\mu} - A_{\mu}\gamma^{\mu})\psi =$$

$$(-\gamma^{\nu}\gamma^{\mu}\partial_{\nu}\partial_{\mu} - iA_{\nu}\gamma^{\nu}\gamma^{\mu}\partial_{\mu} - i\gamma^{\nu}A_{\mu}\gamma^{\mu}\partial_{\nu} - i\gamma^{\nu}\gamma^{\mu}A_{\mu,\nu} + A_{\nu}A_{\mu}\gamma^{\nu}\gamma^{\mu})\psi =$$

$$(-\frac{1}{2}(\gamma^{\nu}\gamma^{\mu} + \gamma^{\mu}\gamma^{\nu})\partial_{\nu}\partial_{\mu} - iA_{\nu}\gamma^{\nu}\gamma^{\mu}\partial_{\mu} - i\gamma^{\mu}A_{\nu}\gamma^{\nu}\partial_{\mu} - i\gamma^{\nu}\gamma^{\mu}A_{\mu,\nu} +$$

$$\frac{1}{2}(A_{\nu}A_{\mu}\gamma^{\nu}\gamma^{\mu} + A_{\mu}A_{\nu}\gamma^{\mu}\gamma^{\nu}))\psi =$$

The Dirac Equation as One Fourth-Order Equation for One Function: A...

$$(-g^{\mu\nu}\partial_{\nu}\partial_{\mu} - 2iA_{\nu}g^{\mu\nu}\partial_{\mu} - \frac{i}{2}(\gamma^{\nu}\gamma^{\mu}A_{\mu,\nu} + \gamma^{\mu}\gamma^{\nu}A_{\nu,\mu}) + A_{\nu}A_{\mu}g^{\mu\nu})\psi = (-\partial^{\mu}\partial_{\mu} - 2iA^{\mu}\partial_{\mu} - \frac{i}{2}(\gamma^{\nu}\gamma^{\mu}A_{\mu,\nu} + (2g^{\mu\nu} - \gamma^{\nu}\gamma^{\mu})A_{\nu,\mu}) + A^{\mu}A_{\mu})\psi = (-\partial^{\mu}\partial_{\mu} - 2iA^{\mu}\partial_{\mu} - \frac{i}{2}(\gamma^{\nu}\gamma^{\mu}(A_{\mu,\nu} - A_{\nu,\mu}) + 2A^{\mu}_{,\mu}) + A^{\mu}A_{\mu})\psi = (-\partial^{\mu}\partial_{\mu} - 2iA^{\mu}\partial_{\mu} - \frac{i}{4}(\gamma^{\nu}\gamma^{\mu} - \gamma^{\mu}\gamma^{\nu})F_{\nu\mu} - iA^{\mu}_{,\mu} + A^{\mu}A_{\mu})\psi = (-\partial^{\mu}\partial_{\mu} - 2iA^{\mu}\partial_{\mu} - \frac{i}{4}(\gamma^{\nu}\gamma^{\mu} - \gamma^{\mu}\gamma^{\nu})F_{\nu\mu} - iA^{\mu}_{,\mu} + A^{\mu}A_{\mu})\psi = (-\partial^{\mu}\partial_{\mu} - 2iA^{\mu}\partial_{\mu} - \frac{i}{4}(\gamma^{\nu}\gamma^{\mu} - \gamma^{\mu}\gamma^{\nu})F_{\nu\mu} - iA^{\mu}_{,\mu} + A^{\mu}A_{\mu})\psi =$$
(4)

(A similar equation can be found in the original article by Dirac [8]. Feynman and Gell-Mann [9] used a similar equation to eliminate two out of four components of the Dirac spinor function). We obtain:

$$(\Box' + F)\psi = 0, (5)$$

where the modified d'Alembertian  $\Box'$  is defined as follows:

$$\Box' = \partial^{\mu}\partial_{\mu} + 2iA^{\mu}\partial_{\mu} + iA^{\mu}_{,\mu} - A^{\mu}A_{\mu} + 1 = -(i\partial_{\mu} - A_{\mu})(i\partial^{\mu} - A^{\mu}) + 1, \quad (6)$$

and

$$F = \frac{1}{2} F_{\nu\mu} \sigma^{\nu\mu}.$$
 (7)

Let us note that  $\Box'$  and *F* are manifestly relativistically covariant.

We assume that the set of  $\gamma$ -matrices satisfies the standard hermiticity conditions [10]:

$$\gamma^{\mu\dagger} = \gamma^0 \gamma^\mu \gamma^0, \, \gamma^{5\dagger} = \gamma^5. \tag{8}$$

Then a charge conjugation matrix C can be chosen in such a way [7, 11] that

$$C\gamma^{\mu}C^{-1} = -\gamma^{\mu T}, C\gamma^{5}C^{-1} = \gamma^{5T}, C\sigma^{\mu\nu}C^{-1} = -\sigma^{\mu\nu T},$$
(9)

$$C^{T} = C^{\dagger} = -C, CC^{\dagger} = C^{\dagger}C = I, C^{2} = -I,$$
 (10)

where the superscript T denotes transposition, and I is the unit matrix.

Let us choose a component of the Dirac spinor  $\psi$  in the form  $\overline{\xi}\psi$ , where  $\xi$  is a constant spinor (so it does not depend on the spacetime coordinates  $x = (x^0, x^1, x^2, x^3)$ , and  $\partial_{\mu}\xi \equiv 0$ ), and multiply both sides of Eq. (5) by  $\overline{\xi}$  from the left:

$$\Box'(\bar{\xi}\psi) + \bar{\xi}F\psi = 0. \tag{11}$$

To derive an equation for only one component  $\bar{\xi}\psi$ , we need to express  $\bar{\xi}F\psi$  via  $\bar{\xi}\psi$ , but the author cannot do this for an arbitrary spinor  $\xi$  (or prove that this cannot be done). Therefore, to simplify this task, we demand that  $\xi$  is an eigenvector of  $\gamma^5$  (in other words,  $\xi$  is either right-handed or left-handed). This condition is Lorentzinvariant. Indeed, Dirac spinors  $\chi$  transform under a Lorentz transformation as follows:

$$\chi' = \Lambda \chi, \tag{12}$$

where matrix  $\Lambda$  is non-singular and commutes with  $\gamma^5$  if the Lorentz transformation is proper and anticommutes otherwise [6]. Therefore, if  $\xi$  is an eigenvector of  $\gamma^5$ , then  $\xi'$  is also an eigenvector of  $\gamma^5$ , although not necessarily with the same eigenvalue.

Eigenvalues of  $\gamma^5$  equal either +1 or -1, so  $\gamma^5 \xi = \pm \xi$ . The linear subspace of eigenvectors of  $\gamma^5$  with the same eigenvalue as  $\xi$  is two-dimensional, so we can choose another constant spinor  $\eta$  that is an eigenvector of  $\gamma^5$  with the same eigenvalue as  $\xi$  in such a way that  $\xi$  and  $\eta$  are linearly independent. This choice is Lorentz-covariant, as matrix  $\Lambda$  in Eq. (12) is non-singular.

Obviously, we can derive an equation similar to (11) for  $\eta$ :

$$\Box'(\bar{\eta}\psi) + \bar{\eta}F\psi = 0. \tag{13}$$

If  $\gamma^5 \xi = \pm \xi$ , then  $\overline{\xi} = \xi^{\dagger} \gamma^0$  is a left eigenvector of  $\gamma^5$  with an eigenvalue  $\mp 1$ , as

$$\bar{\xi}\gamma^5 = \xi^{\dagger}\gamma^0\gamma^5 = -\xi^{\dagger}\gamma^5\gamma^0 = -(\gamma^5\xi)^{\dagger}\gamma^0 = \mp\bar{\xi}.$$
(14)

The same is true for spinors  $\bar{\eta} = \eta^{\dagger} \gamma^0$  (the proof is identical to that in (14)),  $\bar{\xi} F$ , and  $\bar{\eta} F$ , as  $\gamma^5$  commutes with  $\sigma^{\mu\nu}$  [10]. As the subspace of left eigenvectors of  $\gamma^5$  with an eigenvalue  $\mp 1$  is two-dimensional and includes spinors  $\bar{\xi} F$ ,  $\bar{\eta} F$ ,  $\bar{\xi}$ , and  $\bar{\eta}$ , where the two latter spinors are linearly independent (otherwise spinors  $\xi$  and  $\eta$  would not be linearly independent), there exist such a = a(x), b = b(x), a' = a'(x), b' = b'(x) that

$$\bar{\xi}F = a\bar{\xi} + b\bar{\eta},\tag{15}$$

$$\bar{\eta}F = a'\bar{\xi} + b'\bar{\eta}.\tag{16}$$

The Dirac Equation as One Fourth-Order Equation for One Function: A...

For each spinor  $\chi$ , the charge conjugated spinor

$$\chi^c = C \bar{\chi}^T \tag{17}$$

can be defined, and it has the same transformation properties under Lorentz transformations as  $\chi$  [11]. We have

$$\bar{\chi}\chi^c = \bar{\chi}C\bar{\chi}^T = (\bar{\chi})_{\alpha}C_{\alpha\beta}(\bar{\chi})_{\beta} = 0,$$
(18)

as  $(\bar{\chi})_{\alpha}(\bar{\chi})_{\beta}$  and  $C_{\alpha\beta}$  are, respectively, symmetric and antisymmetric (see Eq. (10)) with respect to transposition of  $\alpha$  and  $\beta$ .

Let us multiply Eqs. (15) and (16) by  $\xi^c$  and  $\eta^c$  from the right:

$$\begin{split} \bar{\xi}F\xi^c &= a(\bar{\xi}\xi^c) + b(\bar{\eta}\xi^c) = b(\bar{\eta}\xi^c),\\ \bar{\xi}F\eta^c &= a(\bar{\xi}\eta^c) + b(\bar{\eta}\eta^c) = a(\bar{\xi}\eta^c),\\ \bar{\eta}F\xi^c &= a'(\bar{\xi}\xi^c) + b'(\bar{\eta}\xi^c) = b'(\bar{\eta}\xi^c),\\ \bar{\eta}F\eta^c &= a'(\bar{\xi}\eta^c) + b'(\bar{\eta}\eta^c) = a'(\bar{\xi}\eta^c), \end{split}$$

so

$$a = \frac{\bar{\xi}F\eta^c}{\bar{\xi}\eta^c}, b = \frac{\bar{\xi}F\xi^c}{\bar{\eta}\xi^c}, a' = \frac{\bar{\eta}F\eta^c}{\bar{\xi}\eta^c}, b' = \frac{\bar{\eta}F\xi^c}{\bar{\eta}\xi^c}.$$
(19)

Let us note that

$$\bar{\xi}\eta^c = \bar{\xi}C\bar{\eta}^T = (\bar{\xi})_{\alpha}C_{\alpha\beta}(\bar{\eta})_{\beta} = -(\bar{\eta})_{\beta}C_{\beta\alpha}(\bar{\xi})_{\alpha} = -\bar{\eta}\xi^c$$
(20)

and

$$\bar{\xi}F\eta^c = \bar{\xi}FC\bar{\eta}^T = (\bar{\xi}FC\bar{\eta}^T)^T = \bar{\eta}C^TF^T\bar{\xi}^T = \bar{\eta}FC\bar{\xi}^T = \bar{\eta}F\xi^c, \qquad (21)$$

as

$$\sigma_{\mu\nu}C = -C\sigma_{\mu\nu}^T \tag{22}$$

(see Eqs. (9), (10)). Therefore,

$$b' = -a. \tag{23}$$

Equations (11), (13), (15), and (16) yield

$$\Box'(\bar{\xi}\psi) + a(\bar{\xi}\psi) + b(\bar{\eta}\psi) = 0,$$
$$\Box'(\bar{\eta}\psi) + a'(\bar{\xi}\psi) + b'(\bar{\eta}\psi) = \Box'(\bar{\eta}\psi) + a'(\bar{\xi}\psi) - a(\bar{\eta}\psi) = 0,$$

so

$$\bar{\eta}\psi = -b^{-1}(\Box'(\bar{\xi}\psi) + a(\bar{\xi}\psi)) \tag{24}$$

and

$$(\Box' - a)(-b^{-1})(\Box' + a)(\bar{\xi}\psi) + a'(\bar{\xi}\psi) = 0$$
(25)

or

$$((\Box' - a)b^{-1}(\Box' + a) - a')(\bar{\xi}\psi) = 0.$$
 (26)

Substituting the expressions for a, b, a' from Eq. (19) and using Eq. (20), we finally obtain:

$$(((\bar{\xi}\eta^{c})\Box' - \bar{\xi}F\eta^{c})(\bar{\xi}F\xi^{c})^{-1}((\bar{\xi}\eta^{c})\Box' + \bar{\xi}F\eta^{c}) + \bar{\eta}F\eta^{c})(\bar{\xi}\psi) = 0.$$
(27)

This equation looks more complex than equation (21) of Ref. [2], but it is much more general and manifestly relativistically covariant.

#### **3** Equivalency to the Dirac Equation

Let us first prove that a different choice of  $\eta$  yields an equivalent equation. As the subspace of eigenvectors of  $\gamma^5$  with the same eigenvalue as  $\xi$  is two-dimensional, the different choice  $\eta'$  can be expressed as follows:

$$\eta' = \sigma \eta + \tau \xi, \tag{28}$$

where  $\sigma$  and  $\tau$  are constant and  $\sigma \neq 0$ , as otherwise  $\eta'$  and  $\xi$  would not be linearly independent. We need to substitute  $\eta$  in the operator acting on  $\bar{\xi}\psi$  in Eq. (27) with the expression for  $\eta'$  from Eq. (28), but let us first note that

$$\bar{\xi}\eta^{\prime c} = \bar{\xi}(\sigma^*\eta^c + \tau^*\xi^c) = \sigma^*(\bar{\xi}\eta^c), \tag{29}$$

$$\bar{\xi}F\eta^{\prime c} = \sigma^*(\bar{\xi}F\eta^c) + \tau^*(\bar{\xi}F\xi^c), \tag{30}$$

$$\bar{\eta'}F\eta'^{c} = (\sigma^{*})^{2}(\bar{\eta}F\eta^{c}) + 2\sigma^{*}\tau^{*}(\bar{\xi}F\eta^{c}) + (\tau^{*})^{2}(\bar{\xi}F\xi^{c})$$
(31)

(we used Eqs. (18), (21)). The substitution then yields

$$((\bar{\xi}\eta'^{c})\Box' - \bar{\xi}F\eta'^{c})(\bar{\xi}F\xi^{c})^{-1}((\bar{\xi}\eta'^{c})\Box' + \bar{\xi}F\eta'^{c}) + \eta'F\eta'^{c} =$$
(32)  
$$(\sigma^{*}(\bar{\xi}\eta^{c})\Box' - \sigma^{*}(\bar{\xi}F\eta^{c}) - \tau^{*}(\bar{\xi}F\xi^{c}))(\bar{\xi}F\xi^{c})^{-1}(\sigma^{*}(\bar{\xi}\eta^{c})\Box' +$$
$$\sigma^{*}(\bar{\xi}F\eta^{c}) + \tau^{*}(\bar{\xi}F\xi^{c})) +$$
$$(\sigma^{*})^{2}(\bar{\eta}F\eta^{c}) + 2\sigma^{*}\tau^{*}(\bar{\xi}F\eta^{c}) + (\tau^{*})^{2}(\bar{\xi}F\xi^{c}) =$$

$$\begin{split} (\sigma^*)^2 ((\bar{\xi}\eta^c)\Box' - \bar{\xi}F\eta^c) (\bar{\xi}F\xi^c)^{-1} ((\bar{\xi}\eta^c)\Box' + \bar{\xi}F\eta^c) - \sigma^*\tau^* ((\bar{\xi}\eta^c)\Box' + \bar{\xi}F\eta^c) + \\ \sigma^*\tau^* ((\bar{\xi}\eta^c)\Box' - \bar{\xi}F\eta^c) - (\tau^*)^2 (\bar{\xi}F\xi^c) + (\sigma^*)^2 (\bar{\eta}F\eta^c) + \\ 2\sigma^*\tau^* (\bar{\xi}F\eta^c) + (\tau^*)^2 (\bar{\xi}F\xi^c) = \\ (\sigma^*)^2 (((\bar{\xi}\eta^c)\Box' - \bar{\xi}F\eta^c) (\bar{\xi}F\xi^c)^{-1} ((\bar{\xi}\eta^c)\Box' + \bar{\xi}F\eta^c) + \bar{\eta}F\eta^c). \end{split}$$

Thus, the operator after the substitution coincides with the original one up to a constant factor, so Eq. (27) does not depend on the choice of  $\eta$ .

This equation for one component  $\bar{\xi}\psi$  is generally equivalent to the Dirac equation (if  $\bar{\xi}F\xi^c \neq 0$ ): on the one hand, it was derived from the Dirac equation, and on the other hand, the Dirac spinor  $\psi$  can be restored if its component  $\bar{\xi}\psi$  is known (a more precise definition of the equivalency is provided below, after Eq. (50)). Let us demonstrate that.

If  $\xi \psi$  is known, another component,  $\bar{\eta}\psi$ , can be determined using Eq. (24). Then  $\psi$  can be expressed as a sum of a right-handed and a left-handed spinors  $\psi_+$  and  $\psi_-$ , where  $\gamma^5 \psi_{\pm} = \pm \psi_{\pm}$ :

$$\psi = \psi_+ + \psi_-, \tag{33}$$

$$\psi_{\pm} = \frac{1}{2} (1 \pm \gamma^5) \psi.$$
 (34)

Then  $\psi_{\mp}$  can be expressed as a linear combination of  $\xi^c$  and  $\eta^c$  (one can show that these two spinors are also eigenvectors of  $\gamma^5$  with an eigenvalue  $\mp 1$  and are linearly independent, and the subspace of eigenvectors of  $\gamma^5$  with an eigenvalue  $\mp 1$  is two-dimensional):

$$\psi_{\mp} = u\xi^c + v\eta^c, \tag{35}$$

where u = u(x) and v = v(x).

Let us note that, e.g.,

$$\bar{\xi}\psi = \bar{\xi}\psi_{\pm} + \bar{\xi}\psi_{\mp} = \bar{\xi}\psi_{\mp},\tag{36}$$

as

$$\bar{\xi}\psi_{\pm} = \frac{1}{2}\bar{\xi}(1\pm\gamma^5)\psi = 0$$
(37)

 $(\bar{\xi} \text{ is a left eigenvector of } \gamma^5 \text{ with an eigenvalue } \mp 1)$ . Therefore, we can multiply Eq. (35) by  $\bar{\xi}$  and  $\bar{\eta}$  from the left:

$$\bar{\xi}\psi = \bar{\xi}\psi_{\mp} = u(\bar{\xi}\xi^c) + v(\bar{\xi}\eta^c) = v(\bar{\xi}\eta^c),$$
  
$$\bar{\eta}\psi = \bar{\eta}\psi_{\mp} = u(\bar{\eta}\xi^c) + v(\bar{\eta}\eta^c) = u(\bar{\eta}\xi^c)$$
(38)

(we took into account Eq. (18)).

Thus,  $\psi_{\mp}$  can be expressed via components  $\bar{\xi}\psi$  and  $\bar{\eta}\psi$  as follows:

$$\psi_{\mp} = \frac{(\bar{\xi}\psi)\eta^c - (\bar{\eta}\psi)\xi^c}{\bar{\xi}\eta^c} \tag{39}$$

(note Eq. (20)). When  $\psi_{\mp}$  is found in this way,  $\psi_{\pm}$  can be found using the Dirac equation (1):

$$(i\partial - A)\psi_{\mp} = \frac{1}{2}(i\partial - A)(1 \mp \gamma^5)\psi = \frac{1}{2}(1 \pm \gamma^5)(i\partial - A)\psi = \psi_{\pm}; \quad (40)$$

thus, the Dirac spinor can be fully restored if component  $\bar{\xi}\psi$  is known.

Let us explicitly prove that the expression for  $\psi_{\mp}$  (Eq. (39)) and, therefore, the expression for  $\psi$  (Eq. (33)) do not depend on the choice of  $\eta$ . We have from Eqs. (19), (20), (24):

$$\bar{\eta}\psi = (\bar{\xi}F\xi^{c})^{-1}((\bar{\xi}\eta^{c})\Box' + \bar{\xi}F\eta^{c})(\bar{\xi}\psi);$$
(41)

therefore, we obtain from Eq. (39):

$$\psi_{\mp} = (\bar{\xi}\eta^c)^{-1} ((\bar{\xi}\psi)\eta^c - (\bar{\xi}F\xi^c)^{-1} ((\bar{\xi}\eta^c)\Box' + \bar{\xi}F\eta^c)(\bar{\xi}\psi)\xi^c).$$
(42)

Substituting  $\eta$  in Eq. (42) with  $\eta'$  (see Eq. (28)), we obtain, using Eqs. (29), (30):

$$\psi_{\mp} = (\sigma^* \bar{\xi} \eta^c)^{-1} \times ((\bar{\xi} \psi)(\sigma^* \eta^c + \tau^* \xi^c) - (\bar{\xi} F \xi^c)^{-1}(\sigma^* (\bar{\xi} \eta^c) \Box' + \sigma^* (\bar{\xi} F \eta^c) + \tau^* (\bar{\xi} F \xi^c))(\bar{\xi} \psi) \xi^c) = (\bar{\xi} \eta^c)^{-1} ((\bar{\xi} \psi) \eta^c - (\bar{\xi} F \xi^c)^{-1} ((\bar{\xi} \eta^c) \Box' + \bar{\xi} F \eta^c)(\bar{\xi} \psi) \xi^c).$$
(43)

Therefore, the expression for  $\psi$  defined by Eqs. (33), (39), (40) does not depend on the choice of  $\eta$ .

Let us prove that  $\psi$  defined by Eqs. (33), (39), (40) satisfies the Dirac equation (1). This is not quite obvious as the set of solutions of Eq. (5) used to derive Eq. (27) is broader than the set of solutions of the Dirac equation (additional solutions appeared as a result of multiplication by  $(i\partial - A)$ ; as a result, Eq. (5) does not require the right-handed and left-handed parts of a solution to be related—cf. [9]). To prove that  $\psi$  satisfies the Dirac equation, it is sufficient to prove that

$$(i\partial - A)\psi_{\pm} = \psi_{\mp}, \tag{44}$$

as that would imply that

$$(i\partial - A)\psi = (i\partial - A)(\psi_{\pm} + \psi_{\mp}) = \psi_{\mp} + \psi_{\pm} = \psi$$
(45)

(note Eq. (40)). Equation (44) is equivalent to the following equation:

$$(i\partial - A)(i\partial - A)\psi_{\pm} = \psi_{\pm} \tag{46}$$

(again, note Eq. (40)) or

$$(\Box' + F)\psi_{\mp} = 0 \tag{47}$$

(cf. Eqs. (4), (5)). As  $\Box' + F$  commutes with  $\gamma^5$ ,  $(\Box' + F)\psi_{\mp}$  is an eigenvector of  $\gamma^5$  with the same eigenvalue  $\mp 1$  as  $\psi_{\mp}$ ; thus, it can be presented as a linear combination of  $\eta^c$  and  $\xi^c$ . Therefore, to prove Eq. (47), it is sufficient to prove that the coefficients in the linear combination vanish or, equivalently, that

$$\bar{\xi}(\Box' + F)\psi_{\mp} = \bar{\eta}(\Box' + F)\psi_{\mp} = 0$$
(48)

(cf. Eqs. (38)). Using Eqs. (15), (16), (18)–(20), (24), (39), we obtain:

$$\bar{\xi}(\Box' + F)\psi_{\mp} = (\bar{\xi}\Box' + a\bar{\xi} + b\bar{\eta})((\bar{\xi}\psi)\eta^{c} - (\bar{\eta}\psi)\xi^{c})(\bar{\xi}\eta^{c})^{-1} = 
(\Box'(\bar{\xi}\psi)(\bar{\xi}\eta^{c}) + a(\bar{\xi}\psi)(\bar{\xi}\eta^{c}) - b(\bar{\eta}\psi)(\bar{\eta}\xi^{c}))(\bar{\xi}\eta^{c})^{-1} = \Box'(\bar{\xi}\psi) + 
a(\bar{\xi}\psi) + b(\bar{\eta}\psi) = 0$$
(49)

and

$$\bar{\eta}(\Box' + F)\psi_{\mp} = (\bar{\eta}\Box' + a'\bar{\xi} + b'\bar{\eta})((\bar{\xi}\psi)\eta^{c} - (\bar{\eta}\psi)\xi^{c})(\bar{\xi}\eta^{c})^{-1} = (-\Box'(\bar{\eta}\psi)(\bar{\eta}\xi^{c}) + a'(\bar{\xi}\psi)(\bar{\xi}\eta^{c}) - b'(\bar{\eta}\psi)(\bar{\eta}\xi^{c}))(\bar{\xi}\eta^{c})^{-1} = \Box'(\bar{\eta}\psi) + a'(\bar{\xi}\psi) + b'(\bar{\eta}\psi) = 0$$
(50)

(note Eqs. (23), (26)).

We can summarize the above as follows. Equation (27) for one component  $\bar{\xi}\psi$  is equivalent to the Dirac equation (provided that we know  $\xi$  and that the component of electromagnetic field  $\bar{\xi}F\xi^c$  does not vanish identically) in the following sense: the Dirac equation implies Eq. (27), and the latter implies the Dirac equation for the Dirac spinor restored from its component  $\bar{\xi}\psi$  using Eqs. (19), (24), (33), (39), (40).

To give a physical interpretation to Eq. (27), we need to define the current. The latter equals (up to a constant factor):

$$j^{\mu} = \bar{\psi}\gamma^{\mu}\psi = \overline{\psi_{\pm}}\gamma^{\mu}\psi_{\pm} + \overline{\psi_{\mp}}\gamma^{\mu}\psi_{\mp}, \qquad (51)$$

as one can show that, e.g.,  $\overline{\psi_{\pm}}\gamma^{\mu}\psi_{\mp} = 0$ . Thus, the current can be expressed via component  $\overline{\xi}\psi$  using Eqs. (19), (24), (39), (40), (51).

Let us note that Eq. (26) or (27) reduce to the equation derived in Ref. [2] in a specific case. In the chiral representation of  $\gamma$ -matrices [10]

$$\gamma^{0} = \begin{pmatrix} 0 & -I \\ -I & 0 \end{pmatrix}, \gamma^{i} = \begin{pmatrix} 0 & \sigma^{i} \\ -\sigma^{i} & 0 \end{pmatrix}, \gamma^{5} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, C = \begin{pmatrix} -i\sigma^{2} & 0 \\ 0 & i\sigma^{2} \end{pmatrix},$$
(52)

where index *i* runs from 1 to 3 and  $\sigma^i$  are the Pauli matrices. One can obtain:

$$F = \begin{pmatrix} iF^3 & iF^1 + F^2 & 0 & 0\\ iF^1 - F^2 & -iF^3 & 0 & 0\\ 0 & 0 & -iF^{3*} & -iF^{1*} - F^{2*}\\ 0 & 0 & -iF^{1*} + F^{2*} & iF^{3*} \end{pmatrix},$$
 (53)

where  $F^i = E^i + i H^i$ ; electric field  $E^i$  and magnetic field  $H^i$  are defined by Eq. (3). Let us choose

$$\xi = \begin{pmatrix} 0 \\ 0 \\ -1 \\ 0 \end{pmatrix}, \eta = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix},$$
(54)

then, if  $\psi$  has components

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}, \tag{55}$$

one obtains  $\bar{\xi}\psi = \psi_1$ ,  $a = iF^3$ ,  $b = -iF^1 - F^2$ ,  $a' = -iF^1 + F^2$ , and Eq. (26) acquires the same form as in Ref. [2]:

$$\left(\left(\Box' - iF^{3}\right)\left(iF^{1} + F^{2}\right)^{-1}\left(\Box' + iF^{3}\right) - iF^{1} + F^{2}\right)\psi_{1} = 0.$$
 (56)

#### 4 Conclusion

Building on the results of Ref. [2], we have derived the manifestly covariant fourthorder/one-function equivalent of the Dirac equation for the general case of an arbitrary set of  $\gamma$ -matrices (satisfying the standard hermiticity conditions) and an arbitrary component of the form  $\bar{\xi}\psi$  (where  $\psi$  is the four-component spinor function of the Dirac equation and  $\xi$  is an arbitrary fixed right eigenvector of  $\gamma^5$ ). This fundamental result should be useful for numerous applications of the Dirac equation. Acknowledgements The author is grateful to V.G. Bagrov, A.V. Gavrilin, A.Yu. Kamenshchik, P.W. Morgan, nightlight, R. Sverdlov, and H. Westman for their interest in this work and valuable remarks.

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# At the Crossroads of Three Seemingly Divergent Approaches to Quantum Mechanics



Carlos Baladrón and Andrei Khrennikov

#### 1 Introduction

One of the clearest characterizations of the origin for the discomfort and difficulties caused to scientists by the advent of quantum mechanics was formulated by Schrödinger in his book "*Nature and the Greeks*" [1], namely, that the two incontestable columns on which the edifice of science was based since Ancient Greece were shaken by quantum mechanics. These two basic principles were: (1) nature is understandable and (2) it admits a description independent of the observer. In a more explicit manner, in order to describe and explain certain quantum mechanical experiments, the observer faces, as pointed out by Mückenheim [2], the dilemma of having to reject one—or at least a percentage of it—out of the following three principles<sup>1</sup>: realism, causality, and locality. Classical physics has been consistently and commonly associated with them.

C. Baladrón (🖂)

A. Khrennikov

<sup>&</sup>lt;sup>1</sup>In more precise terms, following Mückenheim [2], these three principles would respectively read: (1) The principle of realism or the possibility of defining precisely an outside real world independently of the observer; (2) The principle of cause and effect or the existence of a definite direction for the arrow of time; and (3) The principle of locality (or separability) or the existence of a limit velocity for the propagation of any interaction. See Jaeger [3, 4] for a profound discussion on the meaning of these three concepts.

Departamento de Física Teórica, Atómica y Óptica, Universidad de Valladolid, Valladolid, Spain e-mail: baladron@cpd.uva.es

International Center for Mathematical Modeling in Physics and Cognitive Science, Linnaeus University, Växjö, Sweden

National Research University of Information Technologies, Mechanics and Optics (ITMO), St. Petersburg, Russia e-mail: andrei.khrennikov@lnu.se

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**Fig. 1** A three-axis representation of the qualitative strength of locality, causality, and realism that is present in an interpretation of quantum mechanics. The strength of every property decreases as the distance from the origin of coordinates increases along the axis. Six different approaches defined in the main text are placed in their corresponding locations according to the explanations therein. The solid curved arrows correspond to the cycle of connections established in the article that starts in BM and finishes in DAQM

A representation in terms of the way in which the interpretations<sup>2</sup> of quantum mechanics tackle this dilemma might help to visualize the differences among interpretations in order to connect them and ultimately to achieve a satisfactory consensus for the long-lasting interpretational conundrums of quantum mechanics.

A representation of this type, in which a number of well-known examples representing a broad range of interpretations have been included, is outlined in Fig. 1. Every coordinate axis reflects the qualitative strength of realism, causality, or locality that is present in an interpretation of quantum mechanics with the only purpose of establishing relations among such interpretations. Initially, three central interpretations<sup>3</sup> have been located in the scheme. Every one of them is quite near an axis of the reference system. This means that every interpretation does not mainly comply with one of the three mentioned principles while mostly satisfying the other two (see Fig. 1). In short, Bohmian Mechanics (BM) [6], sticking to a realist description, is manifestly nonlocal. QBism [7], which in some sense inherits the Copenhagen interpretation tradition, is subjective. And Time-Symmetric Quantum Mechanics (TSQM) [8] does not satisfy the principle of causality by admitting backward in time causation.

<sup>&</sup>lt;sup>2</sup>See Jaeger [3] for an analysis of the role and main kinds of interpretation in quantum mechanics. <sup>3</sup>In a deeper sense, these three so-called interpretations can be considered as three different approaches to quantum mechanics, not merely as interpretations—e.g., see Styer et al. [5] for a discussion on the term interpretation applied to the de Broglie-Bohm theory.

As already mentioned, the representation in Fig. 1 is only a coarse-grained visualization of the differences among interpretations with the ultimate goal of establishing links and possible tracks in order to connect them.

One of the central tenets of this article is that most interpretations of quantum mechanics have something interesting to show about the conceptual difficulties of this discipline, therefore that the comparative analysis of quite different—even seemingly divergent—interpretations might shed some light on the endemic interpretational issues of this subject.

In Sect. 2, the connections among BM, QBism, and TSQM are analyzed. In Sect. 3, a theory that explores these connections from an information-theoretic Darwinian framework is expounded. Finally, in Sect. 4 the conclusion is drawn.

#### 2 Analysis of the Connections Among BM, QBism, and TSQM

There is not a general agreement on which of the three above-mentioned principles is more fundamental to a physical description of nature. In the end, it certainly depends on the philosophical leanings, and a justification supporting an ordering in detriment of the others can always be constructed.

However, the ideal solution would be to stick to all three of them. In our symbolic representation, it means to be located at the origin of coordinates. There are some theories that can be situated at that point (see Fig. 1)—Superdeterminism<sup>4</sup>—or near it—Many-Worlds Interpretation<sup>5</sup> (MWI). These interesting and imaginative options are not free of criticism and difficulties. Therefore, new perspectives still seem necessary in order to make further progress.

The standpoint in this article declared in a telegraphic statement is that the world would be diluted if there were no clear ontology, it would be difficult to pursue science if there were no cause-and-effect relationship, and magic would seem to

<sup>&</sup>lt;sup>4</sup>Superdeterminism [9, 10] is a theory that profits from revising the concept of free will—in short, the freedom of observers to choose their particular experimental setup. This elusive concept was implicitly taken for granted in Bell's theorem [11] which enables the circumvention of its implications by reconsidering free will. See Plotnitsky [12] for Bohr's point of view about the notion of free will. See also O'Connor [13] and Baladrón [14] for an ampler discussion on the concept of free will and the difficulties related to the compatibility of free will and physical theories (compatibilism).

<sup>&</sup>lt;sup>5</sup>In short, MWI [15] rejects the projection postulate of quantum mechanics. The wave function entirely evolves subject to the Schrödinger equation. Most conceptual difficulties of quantum mechanics disappear, but at the price of enlarging reality from the usual three-dimensional physical space to the configuration space in which the wave function is defined, since all the branches of the wave function now have a real existence supposedly in different mutually unobservable worlds—although, in principle, it can be argued that quantum interference is an indirect proof of their existence. A prescription on the way in which observations occur in every world has to be included.

crawl more easily into a nonlocal scenario. Although not one of these assertions is satisfactory for a description of nature, the difficulties are arguably less imposing as one progresses along the statement, i.e. the absence of realism seems more difficult to admit than the lack of causality, however crucial the latter might be from a rational perspective. In the end, nature will probably happen to be the way it is and not the way of the observer's desires. In saying this, there is already implicitly some controversy. Perhaps nature is even more difficult to understand than quantum mechanics in its present status. Notwithstanding, it seems worth exploring all the possibilities of finding a description of nature that preserves the innermost concepts of classical rationality.

The aim of this article, as previously mentioned, is to contribute to the solution of the interpretative problem of quantum mechanics by trying to build some bridges among apparently divergent approaches that might lead to new insight on nature.

These three different approaches to quantum mechanics—BM, QBism, and TSQM—might be connected by slightly reshaping some of their characteristics, but keeping their essentials. The result is a new perspective on quantum mechanics that will be summarized in Sect. 3 in which the weirdness of quantum mechanics—i.e., those features detaching quantum mechanics from a classical rational description of nature that sticks to realism, causality, and locality as basic properties—is explained under this standpoint.

Bearing this in mind, let us start by BM, which offers a clear realist ontology including the position X(t) of a particle at any time t as a characteristic of the particle's state. The trajectory of a particle in physical space is continuous in time. Usually, in BM the wave function  $\psi$  of the system is also included in the ontology as a real object. However, some variants of BM consider  $\psi$  as non-real, just as an information tool. We follow this variant. In addition, the wave function in BM can be considered to contain active information [16], i.e. information for the system about the surrounding systems. Now the speed of the particle dX/dt is determined by the wave function  $\psi$  that acts as pilot wave of the particle through the guiding equation [6] that for a particle without spin reads:

$$\frac{dX}{dt} = \frac{\nabla S\left(X\right)}{m} \tag{1}$$

where  $\nabla$  is the nabla operator, *m* the mass of the particle, and *S* the phase of the wave function in the polar representation,  $\psi = Re^{iS/\hbar}$ ,  $\hbar$  being the Planck constant divided by  $2\pi$ . As analyzed by Goldstein [17], the wave function as pilot wave may be interpreted as having a nomological character, i.e. acting as a law of motion in strong analogy with the role played by the Hamiltonian in classical mechanics.

The concept of information is central to the three approaches, but from a different point of view. The wave function in QBism represents the subjective beliefs of the observer about the results that can be expected when certain operations are performed on the system under study. And in TSQM two states of a system—one in the past and the other in the future—influence the result for a certain measurement made on the system. The result of the measurement is explained in terms of forward and backward in time causation.

The connection among the approaches may be established assuming that every fundamental physical system—that is characterized as in BM by its position X(t) at any time in physical space—is a microscopic agent—extension of the QBist concept of observer—with the capacity to process information, including the property of anticipating the configurations of its surrounding systems. The capacity to process information in the system recalls the double part played by the wave function in BM, first as repository of the information about the surrounding systems, and second as nomological element—pilot wave—that determines the behavior of the system through the guiding equation. In addition, the capacity of processing information characteristic of TSQM with anticipation, calculating the possible future configurations of the surrounding systems, and recovering the natural causal order, but at the same time retaining locality in the physical space. The result is an interpretation that lies much closer to the origin of coordinates in the three-axis representation of Fig. 1.

# **3** Information-Theoretic Darwinian Approach to Quantum Mechanics (DAQM)

Information from different perspectives is the common thread from which the connections among BM, QBism, and TSQM have been interwoven in Sect. 2. As mentioned above, the role of the wave function in BM resembles that of an information processor that computes the actions to be performed by the particle from the input data (information about the surrounding systems).

The information-theoretic Darwinian approach to quantum mechanics (DAQM) [18–21] explores the possibilities of supplementing a fundamental physical system with a classical Turing machine [22]—in short, an information processor. This classical Turing machine can be considered in a certain sense as a generalization of the wave function—the pilot wave in BM. Thus, a fundamental physical system in DAQM is characterized by its position X(t) at any time—as in BM, the system follows a continuous trajectory—and the program stored on its classical Turing machine that determines the behavior of the system. In DAQM there are not universal laws, but evolving algorithms that control the behavior of every physical system, i.e. the emission of a carrier<sup>6</sup> of energy and momentum is determined at every run of the program. In physical space the conservation of energy and momentum is assumed as a general principle.

<sup>&</sup>lt;sup>6</sup>These carriers would convey information about the position of the emitter.

The central problem now is how to implement in real-time quantum behavior for a system by means of a program on a classical Turing machine<sup>7</sup>. DAQM analyzes the possibility that Darwinian evolution under natural selection acting on these systems, characterized as microscopic agents, could generate quantum behavior starting from a state of minimal information at time t = 0, provided that a randomizer was incorporated to the classical Turing machine of every system—in this way the physical systems become generalized Darwinian systems [25] with the properties of variation, selection, and retention.<sup>8</sup>

Darwinian natural selection in the long run would plausibly tend to optimize the flows of information between a system and its environment. It is true that Darwinism does not necessarily bring about optimal results—see Baladrón and Khrennikov [21] and the references therein for a discussion on this question in the framework of DAQM, however optimization could adequately describe the final physical stage assuming that physical evolution would have already come to an end by exhausting the complexity of fundamental physical systems. DAQM studies the possibility that in this scenario, from this optimization criterion, quantum behavior might be generated as the fittest strategy for a system to survive.

Several studies support the interest of DAQM. First, quantum information biology (QIB) [26, 27] analyzes some experiments at different scales in which the quantum formalism adequately describes the behavior of mesoscopic and macroscopic biological systems. Second, some experiments [28, 29] in which a liquid drop bouncing on a liquid bath presents quantum-like behavior by interacting with the surface waves caused by itself on the liquid. Third, some computer simulations [30] showing the possibility that evolution might find some mechanisms to transform exponential time problems into polynomial time ones<sup>9</sup>. Finally, some possible astronomical and cosmological tests proposed to check Bohm-like theories by Valentini [31] could be adapted to check DAQM.

DAQM is a realist—the system has a definite position X(t) at any time, local since nonlocality is restrained to the information space maintaining locality for all the interactions and influences in the physical space, thanks to the anticipation block hypothetically developed in the program by Darwinian evolution,

<sup>&</sup>lt;sup>7</sup>According to Deutsch [23], based on the present knowledge of nature it is consistent to assert that quantum theory is compatible with the Church-Turing principle [23], i.e. that any finite physical system can be simulated by means of a quantum Turing machine. However, the kind of problems that a quantum Turing machine can solve are the same as those solved by a classical Turing machine, the only difference being the efficiency [24], i.e. the time needed for the computation to halt with a solution. DAQM aims to show that this efficiency might be supplied by Darwinian natural selection.

<sup>&</sup>lt;sup>8</sup>These properties that characterize a generalized Darwinian system [25] can be succinctly defined in the following way: variation as the introduction of novelty in the system that in DAQM is supplied by a read-and-write operation error rate during the execution of the program on the Turing machine; selection as the increased rate of persistence or survival for certain systems in the population due to their improved behavioral capabilities through positive variations; and retention as the capacity of storing, preserving or passing on information about adaptations.

<sup>&</sup>lt;sup>9</sup>Notice the quantum-like efficiency trait.

and quasi-causal—since randomness that is intrinsic to the theory persists as an optimization procedure after reaching the quantum equilibrium scenario—theory. Therefore, DAQM would be placed near the origin of coordinates in Fig. 1.

The price to pay by DAQM is the introduction of a classical Turing machine i.e., an information processor—associated with every elementary physical system and the presence of an intrinsic randomness in matter reflected in the attachment of a randomizer to every elementary physical system. The Turing machine might be considered as reflecting an intrinsic complexity in matter [32], as a generalization of the fact already recognized by quantum mechanics when requiring a wave function to characterize a physical system.

The constitution and characterization of a fundamental system in DAQM fits well with the famous saying of Peres [33] about quantum mechanics: "Unperformed experiments have no results." In DAQM, there are no defined properties or magnitudes in a fundamental physical system prior to an experiment, beyond the well-defined position and basic parameters in physical space. Any result obtained when performing an experiment on such a system has to be previously calculated as an output by the information processor of the system and critically depends on the context (experimental set-up) of the measurement. Any magnitude, in the end, has to be related to positions of systems and apparatuses as in BM.

Darwinism has already been applied to analyze some fundamental problems in several fields of physics [34, 35]. The possibility of a universe in which the laws of physics might evolve has also previously been considered—e.g., see Smolin [36] and the references therein, and it is the subject of a deep analysis in some promising studies within a general physical framework [36]. There are also some works— e.g., see Lloyd [37]—that explore the idea of a universe considered as a quantum computer.

In the present study, the universe is described as a set of interacting fundamental physical systems, every one of them formed by bare matter in physical space that is supplemented with a probabilistic classical Turing machine in information space. Darwinian natural selection acting on these systems would plausibly bring about the emergence of quantum behavior as an optimal strategy for the stability of systems. One of the crucial elements in this process would be the generation of the anticipation module in the program that rules the behavior of every system and that would allow the system to calculate the possible future configurations of the surrounding systems as mentioned in Sect. 2. In DAQM, quantum information could admit a description in terms of the optimization process of past, present, and anticipated classical information flows.

The constitution assumed for a physical system in DAQM also renders natural the emergence of complexity in the universe from a simple initial state for matter and information. In addition, the appearance of biological systems could be implied as a consequence of the unifying information-theoretic Darwinian scheme acting on physical and biological systems alike [21], biological systems being the result of certain physical compounds governed by the network of interconnected probabilistic classical Turing machines of their constituents. In biological Darwinism the increase of complexity as a general trend in the long term is mostly accepted, although it is not exempt of criticism—e.g., see Baladrón and Khrennikov [20, 21] and the references therein. In this respect, the role of entanglement in the development of complex biological systems might be crucial and it probably constitutes one of the most challenging questions to be addressed by biophysics in the future.

#### 4 Conclusion

The comparative analysis of different quantum mechanical interpretations suggests new ways to face the deeply rooted interpretational problem. This kind of analysis might contribute to a possible future consensus in the interpretation of quantum mechanics. The comparison put forth in this article among three different approaches to quantum mechanics has oriented the development of an informationtheoretic Darwinian approach from which quantum mechanics could emerge as a realist, quasi-causal, and local theory that would code an optimal strategy for the stability of physical systems. In addition DAQM presents a unifying informationtheoretic scheme for physical and biological systems that might contribute to a deeper understanding of nature.

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# **Implications of Einstein-Weyl Causality on Quantum Mechanics**



D. J. BenDaniel

#### 1 Introduction

A fundamental physical principle that has consequences for the topology of spacetime is the principle of Einstein-Weyl causality. Borchers and Sen have rigorously investigated its mathematical consequences and have shown that a denumerable space-time would be admitted [6]. They then proved that the notion of causality could be effectively extended to discontinuua but were still left with an experimentally unresolvable question regarding the nature of the physical line E, e.g., whether E = R, the real line of mathematics [1]. Alternatively, their initial result opens the possibility of a constructible mathematical foundation; this would describe a spacetime that, while it is denumerable, nevertheless allows physical functions and all their derivatives to be continuous. This paper has three parts. We first introduce such a constructible foundation and show it contains polynomial functions which are homeomorphic with a dense, denumerable metric space  $R^*$ . Other uniformly continuous functions can then be effectively obtained by computational iteration. Secondly, postulating a Lagrangian for fields in a compactified space-time, we obtain a general field description of which the Schrödinger equation is a special case. Therefore, the theory predicts that  $E = R^*$  and quantum mechanics provides an empirical corroboration. Thirdly, from these results, we find that this space-time is relational (in the sense that it is vanishingly small if and only if all physical fields are vanishingly small), and we suggest other possible physical implications of these results.

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D. J. BenDaniel (🖂)

Johnson School, Cornell University, Ithaca, NY, USA e-mail: djb16@cornell.edu
# 2 Theory

We propose the axioms in Table 1. The formulae for these axioms are given in the Appendix. The first six axioms are the set theory of Zermelo-Fraenkel (ZF) without the power set axiom and with the axiom schema of subsets (aka separation) deleted from the axioms of regularity and replacement. Because of the deletion of the axiom schema of subsets, a minimal  $\omega^*$ , usually denoted by  $\omega$  and called the set of all finite ordinals, cannot be shown to exist in this theory; instead this set theory is uniformly dependent on  $\omega^*$ , and then all the finite ordinals as well as infinitely many infinite ordinals are included in  $\omega^*$ . These infinite ordinals are equinumerous with  $\omega^*$ ; a finite ordinal is any member of  $\omega^*$  that is not infinite. All sets of finite ordinals are finite.

The constructibility axiom requires some explanation. By constructible sets, we mean sets that are generated sequentially by some process, one after the other, so that the process well-orders the sets. Gödel has shown that an axiom asserting that all sets are constructible can be consistently adjoined to ZF [4], giving a theory usually called ZFC<sup>+</sup>. No more than countably many constructible subsets of  $\omega$  can be shown to exist in ZFC<sup>+</sup> [3]. This remarkable result will hold for  $\omega^*$  in a theory ZF minus the axiom schema of subsets and the power set axiom and plus an axiom asserting that the subsets of  $\omega^*$  are constructible. The constructibility axiom allows creation of a set of constructible subsets of  $\omega^*$  and, in addition, provides a distance measure, giving a metric space  $R^*$ . The members of  $R^*$  mirror the binimals (i.e., binary decimals) forming a dense, denumerable space. We shall refer to this theory as T.

We can now introduce two essential definitions. First, recall the definition of "rational numbers" as the set of ratios, in ZF called Q, of any two members of the set  $\omega$ . In T, we can likewise, using the axiom of unions, establish for  $\omega^*$  the set of ratios of any two of its members. This will become an "enlargement" of the rational numbers, and we shall call this enlargement  $Q^*$ . Two members of  $Q^*$  are called "identical" if their ratio is 1. We employ the symbol " $\equiv$ " for "is identical to." Next, a member y of  $Q^*$  "equal" to 0, letting y signify the member and employing the

Extensionality	Two sets with just the same members are equal
Pairs	For every two sets, there is a set that contains just them
Union	For every set of sets, there is a set with just all their members
Infinity	There are infinite ordinals $\omega^*$ (i.e., sets are transitive and well-ordered by $\in$ -relation)
Replacement	Replacing the members of a set one-for-one creates a set (i.e., bijective replacement)
Regularity	Every non-empty set has a minimal member (i.e., "weak" regularity)
$\omega^*$ -Constructibility	The subsets of $\omega^*$ are constructible

symbol "=" to signify equality, is defined by  $y = 0 \leftrightarrow \forall k [y < 1/k]$ , where k is a finite ordinal. A member of  $Q^*$  that is not equal to 0 and not "infinite" is "finite". Obviously,  $y \equiv 0 \rightarrow y = 0$ .

An *equality-preserving* bijective mapping  $\phi(x, u)$  between  $x \in R^*$  and  $u \in R^*$  such that

$$\forall x_1, x_2, u_1, u_2[\phi(x_1, u_1) \land \phi(x_2, u_2) \to (x_1 - x_2 = 0 \leftrightarrow u_1 - u_2 = 0)] \quad (1)$$

creates pieces which are homeomorphic to  $R^*$ . Note that the range of these pieces vanishes if and only if the domain vanishes.

If the functions u(x) of  $x \in R^*$  and all their derivatives are homeomorphic to  $R^*$ , consistent with the empirical fact that physical functions and their derivatives are continuous in space-time, then u(x) is a power series, and furthermore, since there is no axiom of subsets in the set-theoretical foundation, the series is finite, i.e., a polynomial. (Note: Differentials are definable in T, so derivatives of polynomials, and their inverse integrals, can be obtained term by term.) We assume u(x), if not constant, is a continuously connected sequence of equality-preserving bijective mappings with range  $u(x) \neq 0 \leftrightarrow domain u(x) \neq 0$ .

Infinite power series, such as sin(x), do not formally exist in this theory but can always be approximated as closely as required for physics by a sum of polynomials of sufficiently high degree obtained by an iteration of:

$$\int_{a}^{b} \left[ p\left(\frac{du}{dx}\right)^{2} - qu^{2} \right] dx = \lambda \int_{a}^{b} ru^{2} dx$$
(2)

where  $\lambda$  is minimized subject to:

$$\int_{a}^{b} ru^{2} dx = \text{const}$$
(3)

where:

$$a \neq b, \quad u\left(\frac{du}{dx}\right) = 0$$
 (4)

at *a* and *b*; *p*, *q*, and *r* are functions of the variable *x*. Letting *n* denote the *n*th iteration,  $\forall k \exists n [\lambda_{n-1} - \lambda_n < 1/k]$  where *k* is a finite ordinal. So, a polynomial such that, say,  $1/k < 10^{-50}$  is effectively a Sturm-Liouville "eigenfunction." These can be decomposed, since they are polynomials, into bijective equality-preserving pieces obeying the boundary conditions. As a bridge to physics, let  $x_1$  be space and  $x_2$  be time. We now postulate the following integral expression for a one-dimensional string  $\Psi = u_1(x_1)u_2(x_2)$ :

$$\int \left[ \left( \frac{\partial \Psi}{\partial x_1} \right)^2 - \left( \frac{\partial \Psi}{\partial x_2} \right)^2 \right] dx_1 dx_2 \equiv 0$$
(5)

The eigenvalues  $\lambda_{1m}$  are determined by the spatial boundary conditions. For each eigenstate *m*, we can use this integral expression constrained by the indicial relation  $\lambda_{1m} \equiv \lambda_{2m}$  to obtain the eigenfunctions  $u_{1m}$  and  $u_{2m}$ .

A more general expression in finitely many space-like and time-like dimensions can likewise be produced. Let  $u_{\ell mi}(x_i)$  and  $u_{\ell mj}(x_j)$  be eigenfunctions with nonnegative eigenvalues  $\lambda_{\ell mi}$  and  $\lambda_{\ell mj}$ , respectively. We define a "field" as a sum of eigenstates:

$$\underline{\Psi}_{m} = \sum_{\ell} \Psi_{\ell m} \underline{i_{\ell}}, \Psi_{\ell m} = C \prod_{i} u_{\ell m i} \prod_{j} u_{\ell m j}$$
(6)

with the postulate: for every eigenstate m, the Lagrangian form for the field equations in a compactified space-time is identically 0. Let ds represent  $\prod_i r_i dx_i$  and  $d\tau$  represent  $\prod_i r_j dx_j$ . Then for all m,

$$\int \sum_{\ell i} \frac{1}{r_i} \left[ P_{\ell m i} \left( \frac{\partial \Psi_{\ell m}}{\partial x_i} \right)^2 - Q_{\ell m i} \Psi_{\ell m}^2 \right] ds d\tau$$

$$-\int \sum_{\ell j} \frac{1}{r_j} \left[ P_{\ell m j} \left( \frac{\partial \Psi_{\ell m}}{\partial x_j} \right)^2 - Q_{\ell m j} \Psi_{\ell m}^2 \right] ds d\tau \equiv 0$$
(7)

In this integral expression, the *P*, *Q*, and *R* can be functions of any of the  $x_i$  and  $x_j$ , thus of any  $\Psi_{\ell m}$  as well. As seen in the case of a one-dimensional string, these  $\Psi_m$  can in principle be obtained by iterations constrained by an indicial relation,  $\sum_{\ell i} \lambda_{\ell m i} \equiv \sum_{\ell j} \lambda_{\ell m j}$  for each *m*. We see that the postulate asserts a fundamental identity of the magnitudes of the two components of the integral.

A proof in T that the sum over all the eigenstates of each component has only discrete values in the case of the Schrödinger equation will now be shown. Let expressions (8) and (9) both be represented by  $\alpha$ , since they are identical:

$$\sum_{\ell m i} \int \frac{1}{r_i} \left[ P_{\ell m i} \left( \frac{\partial \Psi_{\ell m}}{\partial x_i} \right)^2 - Q_{\ell m i} \Psi_{\ell m}^2 \right] ds d\tau \tag{8}$$

$$\sum_{\ell m j} \int \frac{1}{r_j} \left[ P_{\ell m j} \left( \frac{\partial \Psi_{\ell m}}{\partial x_j} \right)^2 - Q_{\ell m j} \Psi_{\ell m}^2 \right] ds d\tau \tag{9}$$

- 1. We assume that  $Q_{\ell m j} = 0$  and  $P_{\ell m j}$  is nonnegative, that domain  $\Psi \neq 0$ , and that  $\alpha(\Psi)$  is nonnegative and closed to addition.
- 2. Since  $\Psi$  is a function on  $R^{*n}$ , we recall that if  $\neg \operatorname{range} \Psi \equiv 0$ , then  $\operatorname{range} \Psi \neq 0$   $\leftrightarrow \operatorname{domain} \Psi \neq 0$ . Accordingly, we obtain: if  $\operatorname{range} \Psi \equiv 0$ , then  $\alpha(\Psi) \equiv 0$  and if  $\neg \operatorname{range} \Psi \equiv 0$ , then  $\alpha(\Psi) \neq 0$ .
- 3. *Therefore*  $\alpha(\Psi)$  *has only discrete values*  $\alpha(\Psi) \equiv n\kappa$ , where *n* is any finite ordinal and  $\kappa$  is some unit which must be determined empirically.

With this result and without any additional physical postulates, we can now obtain the time term of the Schrödinger equation.

Let  $\ell = 1, 2, r_t = P_{1mt} = P_{2mt} = 1, Q_{1mt} = Q_{2mt} = 0, \tau = \omega_m t$ , and we normalize  $\Psi$  as follows:

$$\Psi_m = \sqrt{(C/2\pi)} \prod_i u_{im}(x_i) [u_{1m}(\tau) + \mathbf{i} \cdot u_{2m}(\tau)]$$
(10)

where  $\mathbf{i} = \sqrt{-1}$  with

$$\int \sum_{m} \prod_{i} u_{im}^2 ds (u_{1m}^2 + u_{2m}^2) \equiv 1$$
(11)

We can then employ:

$$\frac{du_{1m}}{d\tau} = -u_{2m} \quad \text{and} \quad \frac{du_{2m}}{d\tau} = u_{1m} \tag{12}$$

or

$$\frac{du_{1m}}{d\tau} = u_{2m} \quad \text{and} \quad \frac{du_{2m}}{d\tau} = -u_{1m} \tag{13}$$

For the minimal nonvanishing field,  $\alpha$  has its least finite value  $\kappa$ . Thus,

$$(C/2\pi) \sum_{m} \oint \int \left[ \left( \frac{du_{1m}}{d\tau} \right)^2 + \left( \frac{du_{2m}}{d\tau} \right)^2 \right]$$
$$\prod_{i} u_{im}^2(x_i) ds d\tau \equiv C \equiv \kappa$$
(14)

Substituting the Planck constant h for  $\kappa$ , this can now be put into the familiar Lagrangian form for the time term in the Schrödinger equation:

$$\frac{h}{2\mathbf{i}}\sum_{m}\oint\int\left[\Psi_{m}^{*}\left(\frac{\partial\Psi_{m}}{\partial t}\right)-\left(\frac{\partial\Psi_{m}^{*}}{\partial t}\right)\Psi_{m}\right]dsdt$$
(15)

Since the Schrödinger equation is well confirmed by experiment, this can be considered an empirical determination of  $\kappa$ .

We can now show a link between quantum theory and space-time.

1. Assume  $\exists \Psi \neg$  range  $\Psi \equiv 0$  and domain  $\Psi$  is all of space-time. With this we have all of space-time  $\neq 0 \rightarrow \exists \Psi$  domain  $\Psi \neq 0$ . Since domain  $\Psi \neq 0 \leftrightarrow$  range  $\Psi \neq 0$  and range  $\Psi \neq 0 \rightarrow \alpha(\Psi) \neq 0$ , we obtain: all of space-time  $\neq 0 \rightarrow \exists \Psi$  $\alpha(\Psi) \neq 0$ 

- 2. Also, if all of space-time = 0, the upper and lower limits of all the integrals in the computation of  $\alpha(\Psi)$  are equal so that all of space-time =  $0 \rightarrow \forall \Psi \alpha(\Psi) = 0$ .
- 3. Therefore all of space-time  $\neq 0 \leftrightarrow \exists \Psi \alpha(\Psi) \neq 0$ . We have thus shown that this denumerable space-time is relational in the sense that it is vanishingly small if and only if all fields are vanishingly small.
- 4. Furthermore, since we have shown for quantized fields  $\alpha(\Psi) \equiv nh$ , it follows that all of space-time  $\neq 0 \leftrightarrow \exists \Psi \ \alpha(\Psi) \geq h$ .  $\alpha(\Psi) \geq h$  is the uncertainty principle. Thus space-time can be vanishingly small only in the absence of any quantized fields.

#### 3 Conclusions

Returning to Einstein-Weyl causality, Borchers and Sen have rigorously investigated its mathematical implications, regarded as a partial order, for the underlying spaces. This partial order was axiomatized by them and proven to admit  $O^2$  as an ordered space. In subsequent papers, they then showed that the notion of causality could be extended effectively to discontinuua but were left with an unresolved question regarding the fundamental nature of the physical line E, e.g., whether E = R, the real line of mathematics. We have viewed their results as an insight into a possible space-time which is denumerable but will still support physical functions and their derivatives. This suggested an investigation into a nonstandard constructible foundation T. We have here shown that T indeed provides a dense, denumerable metric space  $R^*$  that can support polynomial functions and that eigenfunctions governing physical fields can then be effectively obtained by an iterative computation. From this approach, we have derived the Schrödinger equation. Thus the theory proposes that  $E = R^*$  and that quantum mechanics provides an empirical corroboration of this theoretical prediction. It is difficult to see how this theory can be experimentally falsified.

Finally, the Schrödinger equation is obtained in this constructible theory without reference to the statistical interpretation of the wave function, which, it can be argued, may be inferred from the equation itself and a requirement that quantum mechanics will reduce to its classical limit [5]. Philosophically, this suggests that the Schrödinger equation could be considered conceptually cumulative with prior physics. If so, it would resolve a long-standing controversy.

In addition, though we do not have the opportunity here to discuss these points, we note that:

- The proposed theory does not have impredicative sets. This possibly suggests that this foundation allows no physical antinomies. That can be intuitively satisfying since, were there physical antinomies, the universe would tear itself apart.
- Dyson [2] argued that the QED perturbation series cannot converge to a limit without a catastrophically unstable vacuum state and hence the series must be divergent. However, in this constructible theory, there is no induction theorem;

thus, no series limit is reached and an unstable vacuum state is not created. This is a seminal example of the avoidance of infinities in this theory.

• This theory may have some bearing on Wigner's metaphysical question regarding the apparent unreasonable effectiveness of mathematics in physics [7]. The Schrödinger equation along with the denumerability of space-time and its relational nature all arise here as a direct consequence of an axiomatic foundation and its mathematical implications.

#### Appendix: $ZF - Subsets - Power Set + \omega^*$ -Constructibility

*Extensionality* Two sets with just the same members are equal.  $\forall x \forall y \ (\forall z \ (z \in x \leftrightarrow z \in y) \to x = y)$  *Pairs.* For every two sets, there is a set that contains just them.  $\forall x \forall y \exists z \ (\forall w w \in z \leftrightarrow w = x \lor w = y)$  *Union.* For every set of sets, there is a set with just all their members.  $\forall x \exists y \forall z \ (z \in y \leftrightarrow \exists u \ (z \in u \land u \in x))$  *Infinity.* There are infinite ordinals  $\omega^*$  (i.e., sets are transitive and well-ordered by  $\in$ -relation).  $\exists \omega^* (O \in \omega^* \land \forall x \ (x \in \omega^* \to x \cup \{x\} \in \omega^*))$  *Replacement.* Replacing members of a set one-for-one creates a set (i.e., "bijective" replacement). Let  $\phi(x, y)$  a formula in which x and y are free,  $\forall z \forall x \in z \forall y (\phi(x, y) \land \forall u \in z \forall v (\phi(u, v) \to u = x \leftrightarrow y = v)) \to \exists r \forall t \ (t \in r \leftrightarrow \exists s \in z \phi(s, t))$  *Regularity.* Every non-empty set has a minimal member (i.e., "weak" regularity).  $\forall x (\exists yy \in x \to \exists y(y \in x \land \forall z \neg (z \in x \land z \in y)))\omega^*$ -*Constructibility.* All subsets of  $\omega^*$  are constructible.  $\forall \omega^* \exists S[(\omega^*, O) \in S \land \forall y \neq 0 \forall z[(y, z) \in S \leftrightarrow ((y - m_y) \cup m_y, z \cup \{z\}) \in S]]$ , where the minimal element of y is  $m_y$ .

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# The Action Reaction Principle in Quantum Mechanics



**Carlos López** 

# 1 Incompleteness of QM

The action reaction principle (ARP) is not automatically fulfilled in the standard formulation of Quantum Mechanics (SQM) [1, 2]. Some simple academic examples follow showing this fact.

*Example 1* Two systems  $\mathscr{S}_I$  (with associated Hilbert space  $\mathscr{H}_I$ ) and  $\mathscr{S}_{II}$  (with Hilbert space  $\mathscr{H}_{II}$ ) are in initial states  $|a>_I$  and  $|c>_{II}$ , eigenstates of magnitudes A (of  $\mathscr{S}_I$ ) and C (of  $\mathscr{S}_{II}$ ), respectively. The state  $|c>_{II}$  can be expressed as  $|c>_{II}=\sum_j z_j|d_j>_{II}$  in a basis of eigenstates of a non-commuting magnitude D of  $\mathscr{S}_{II}$ ,  $[C, D] \neq 0$ . A Hamiltonian of interaction  $H(A, D) = \kappa AD$  is switched on. More precisely,  $H(A, D) = \kappa A \otimes D$  acts on the product Hilbert space  $\mathscr{H}_I \times \mathscr{H}_{II}$  of the composite. The time evolution of the composite system is

$$|a>_I \otimes \sum_j z_j e^{-i\kappa a d_j t/\hbar} |d_j>_{II}$$

This academic example violates the ARP because  $\mathscr{S}_{II}$  evolves under the interaction while  $\mathscr{S}_I$  remains stationary. A bigger Hilbert space for system  $\mathscr{S}_I$  should contain additional degrees of freedom giving account of some evolution, according to the ARP.

*Example 2* Along the measurement of magnitude A on a system  $\mathscr{S}$  with initial eigenstate  $|a\rangle$ , there is trivial projection of state, output state  $|a\rangle$ , while the

C. López (🖂)

UAH, Madrid, Spain

e-mail: carlos.lopez@uah.es

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apparatus pointer's state changes. Again, some change of state in a bigger Hilbert space for  $\mathcal{S}$  should happen.

As these academic examples prove, the ARP is not automatically fulfilled in SQM. We do not expect the ARP being violated in real interactions. An alternative formulation of QM where the ARP is automatically fulfilled (even for academic examples) seems desirable; bigger Hilbert spaces are possible and perfectly consistent. See in [3] a formulation of Quantum Mechanics in the phase space, that is, with distributions of amplitude  $\Lambda(q, p)$ . In these extended Hilbert spaces, there are simultaneously non-commuting variables, as q and p, but as far as the canonical commutation rules are fulfilled, the formalism is consistent. Notice that many properties of a system with a given Hamiltonian are prescribed by the commutation rules between operators representing physical magnitudes. With regard to the predicted distributions of probability, the rule is to project the distribution of amplitude (marginal amplitudes) onto a Hilbert space of SQM and to apply there the usual Born rule.

The ARP also predicts some (yet unobserved) reaction in detectors for indirect measurements, when some virtual path is discarded because of negative detection.

*Example 3* Particles can follow two or more spatially divergent *virtual* paths, e.g., in an interferometer. An initial state  $|\Psi \rangle (t_0)$  splits, as through a Stern–Gerlach apparatus or a beam splitter, and it evolves to the state

$$|\Psi > (t_{int}) = U(t_{int}, t_0)|\Psi > (t_0) = z_1|x_1 > +z_2|x_2 >$$

where  $x_j$  is the spatial position, at time  $t_{int}$ , of the wave packet following the *j*th trajectory,  $z_j | x_j >$  is the corresponding state's component, and  $U(t_{int}, t_0)$  represents the unitary evolution; other quantum numbers are omitted. An appropriate experimental set up can rejoin these paths around a final position  $x_f$  at  $t_f$ , for a final state  $|\Psi > (t_f) = U(t_f, t_{int})|\Psi > (t_{int})$  where both components are superposed and interfere. If, in another run, a particle detector  $D^{(1)}$  is placed at  $x_1$ , either the particle is detected (and blocked), or it arrives to  $x_f$  following path 2. The state of the composite is  $|\Psi > (t_{int}) \otimes |D_0^{(1)} >$  right before the system/detector interaction, being  $|D_0^{(1)} >$  the ready-to-measure state of the pointer. After interaction the composite evolves to the entangled state

$$z_1|x_1 > \otimes |D_p^{(1)} > +z_2|x_2 > \otimes |D_n^{(1)} > ,$$

 $|D_p^{(1)} > (|D_n^{(1)} >)$  state of the pointer for positive (negative) detection. In case of negative detection and applying the projection rule, we obtain the composite state  $|x_2 > \otimes |D_n^{(1)} >$ , with the particle localized around  $x_2$ . Because of the interaction (negative detection), the state of the particle has changed,  $|x_2 > \neq |\Psi > (t_{int})$ , so that  $|D_n^{(1)} > \neq |D_0^{(1)} >$  according to the ARP. However, when using a particle detector, its macroscopic state does not change. Appropriately designed devices should show an observable reaction, possibly when looking for some wave like

entity. The corpuscular entity is, with certainty, around  $x_2$ , not around  $x_1$  (otherwise it would have been detected); therefore, it is spatially separated from  $x_1$ , and it cannot interact with the detector. Another entity must follow path 1 and interact with  $D^{(1)}$ .

Elementary particles could be composites of a corpuscular subsystem and a distributed field, both entities interacting along the evolution. This proposal is essentially the so-called double field solution [4–7], with a real field accompanying the corpuscular system, different from the distribution of amplitude which is a computational tool of the theory. Also, the quantum potential of Bohm's formalism [8] needs an accompanying system in order to preserve de ARP.

#### 2 Extended Phase Space for QM

The most general phase space for a spinless point particle is the path integral formalism [9]. In the set of paths allowed by the context, there is a distribution of amplitude

$$| path > \rightarrow exp\left(\frac{i}{\hbar}S[ path]\right)$$

The distribution of amplitude in the position representation is obtained through the calculation of the marginal amplitudes

$$\Psi(q) = \sum exp\left(\frac{i}{\hbar}S[path_q]\right)$$

where  $path_q$  are all paths with final position q and  $\sum$  represents the path integral. Similarly, in the momentum representation

$$\xi(p) = \sum exp\left(\frac{i}{\hbar}S[path_p]\right)$$

with  $path_p$  all paths with final momentum p.

We can formally consider intermediate projections, by considering subsets of paths with final position and momentum (q, p), for a marginal distribution

$$\Lambda(q, p) = \sum exp\left(\frac{i}{\hbar}S[path_{q,p}]\right)$$

 $path_{q,p}$  all paths with final position and momentum (q, p). From  $\Lambda(q, p)$  we find the SQM amplitude through an additional projection, for example, integral along momentum p to get the position representation

$$\Psi(q) = \int dp \Lambda(q, p)$$

Technically there is an additional factor making this integral a Fourier projection (see [3] for details). As far as the representations of magnitudes, position, and momentum

$$Q = q + \frac{1}{2}\hbar\partial_p \quad P = p - \frac{1}{2}\hbar\partial_q$$

fulfil the canonical commutation rules  $[Q, P] = i\hbar$ , the formalism is consistent.

In the two-slit experiment, we can group paths allowed by the context, from the left and right slit onto the final screen, into subsets of paths with definite initial slit, say slit L, and final position at the screen q to get

$$\Psi_L(q) = \sum exp\left(\frac{i}{\hbar}S[path_{L,q}]\right)$$

where now  $path_{L,q}$  are all paths from *L* to *q*. States |L, q> and |R, q> project onto the SQM state |q>, and we find the marginal amplitude  $\Psi(q) = \Psi_L(q) + \Psi_R(q)$ where both components are superposed and interfere. If we previously measure the slit variable, the two wave components suffer some random phase shift, and the statistical interference disappears.

We can use the extended formalism to obtain formal distributions of amplitude as follows: given that the final position is q, the (unobserved) probability that the initial slit is L becomes

$$P(L|q) = \frac{|\Psi_L(q)|^2}{|\Psi_L(q)|^2 + |\Psi_R(q)|^2}$$

Generically, an extended phase space contains coordinates of non-commuting magnitudes, and the SQM distribution of probability is found in two steps, first a projection onto a space with commuting magnitudes (SQM) and second application of Born rule. Fibres of this projection allow to calculate unobservable conditional distributions of probability.

#### **3** Extended Spin Phase Space

We can consider a discretization of the path into elementary steps  $\Delta_j q$ , and associate *elementary* phases  $\frac{i}{\hbar}L(q_j, \frac{\Delta_j q}{\Lambda t})\Delta t$  to them. Then, the total phase along the path is

$$\frac{i}{\hbar}S[path] = \sum_{\Delta_j q} \frac{i}{\hbar}L(q_j, \frac{\Delta_j q}{\Delta t}) \Delta t$$

An analogous formalism is presented next for spin variables.

Let us define a generic spin state [1, 10]  $(s_1, s_2, \ldots, s_N)$  for a finite number of directions  $\{\mathbf{n}_1, \mathbf{n}_2, \dots, \mathbf{n}_N\}$ ,  $\mathbf{n}_k$  unit vectors and  $s_k \in \{+, -\}$ , spin up or down in direction  $\mathbf{n}_k$ . The particle has well-defined spin values in all the considered directions (a finite set for easy), but there are *spin wave* components for all spin states allowed by the context, with a distribution of amplitude to be defined next. This hypothesis is similar to the two-slit experiment with the corpuscular particle following one specific slit but the associated wave following both. These spin waves can superpose and interfere (as in the two-slit experiment). The distribution of amplitude is a mathematical tool that encodes this property of superposition and interference. This is why there is not as distribution of probability in the spin phase space, we would be ignoring the wave subsystem. In the two-slit experiment, the distribution of probability P(q) is not obtained by addition of two independent distributions  $P_L(q)$  and  $P_R(q)$ , one for each slit. The marginal amplitude of probability  $\Psi_L(q) + \Psi_R(q)$  determines the diffraction pattern. As in the path integral formalism or in the two-slit experiment, marginal amplitudes through projections from the extended spin phase space will reproduce the usual distributions in SQM.

Let us consider the quaternion

$$\mathbf{N}[\mathbf{n}] = (\mathbf{n} \cdot \mathbf{i})\mathbf{I} + (\mathbf{n} \cdot \mathbf{j})\mathbf{J} + (\mathbf{n} \cdot \mathbf{k})\mathbf{K}$$

with null real part, associated to a unit vector **n**. **i**, **j** and **k** are the three unit vectors of a Cartesian system of coordinates; **I**, **J** and **K** are the three imaginary quaternions, IJ = K, etc. Each spin state  $(s_1, \ldots, s_N)$  will have an associated amplitude *Z*, sum of elementary amplitudes  $s_j N_j$ ,  $N_j \equiv N[n_j]$ ,

$$Z(s_1,\ldots,s_N)\equiv\sum_j s_j\mathbf{N}_j\,.$$

Notice the analogy with the phases in the path integral formalism,  $s_j N_j$  playing the role of  $\frac{i}{\hbar}L(q_j, \Delta_j q/\Delta t)\Delta t$  and  $Z(s_1, \ldots, s_N)$  the role of  $\frac{i}{\hbar}S[path]$ . In the path integral formalism, the context determines which paths must be taken into account. For example, in the two-slit experiment, all paths with end point in the first screen out of the slits are discarded. Only paths going through one or the other slit and with end point at the final screen are considered when computing the distribution of probability along the final screen. Similarly, the context determines which spin states must be taken into account.

#### 3.1 Standard Spin States in SQM

In the two-dimensional (spin 1/2) Hilbert space of SQM, each state (vector or ray) has a well-defined spin in some direction, i.e., it is an eigenstate of some spin

operator. In a preparation procedure using a Stern–Gerlach apparatus, the particle follows one of the two output virtual paths, and the other path is discarded; therefore, the spin wave components associated with the discarded path are suppressed. If the spin value in direction  $\mathbf{n}_1$  is  $+_1$  with certainty, all amplitudes  $Z(+_1, s - 2, ..., s_N)$  are considered, while all amplitudes  $Z(-_1, s - 2, ..., s_N)$  are discarded. We can now project the state, computing the marginal amplitudes, onto two-dimensional Hilbert spaces generated by  $|+_k\rangle$  and  $|-_k\rangle$ . For k = 1 we get

$$Z(+_1) = \sum_{s_2,...,s_N} Z(+_1, s - 2, ..., s_N) = 2^{N-1} \mathbf{N}_1$$

and

$$Z(-1) = 0$$

because all amplitudes  $Z(-1, s_2, ..., s_N)$  have been discarded by the context. This determines the distribution of probability  $P(+_1) = 1$ ,  $P(-_1) = 0$  as expected. For k = 2 (all  $k \neq 1$  are similar), we find

$$Z(s_2) = \sum_{s_3,...,s_N} Z(+_1, s - 2, ..., s_N) = 2^{N-2} (\mathbf{N}_1 + s_2 \mathbf{N}_2)$$

with associated distribution of probability

$$P(s_2) = \frac{|\mathbf{N}_1 + s_2 \mathbf{N}_2|^2}{|\mathbf{N}_1 + \mathbf{N}_2|^2 + |\mathbf{N}_1 - \mathbf{N}_2|^2}$$

which becomes the correct SQM distribution of probability

$$\frac{1}{2}(1+s_2\mathbf{n}_1\cdot\mathbf{n}_2)\,.$$

#### 3.2 New Isotropic State

In SQM there is not an isotropic state, with probabilities  $P(s_k) = \frac{1}{2}$  for all *k*. But this should be the individual quantum state of each particle of the composite singlet. This individual state can be represented in the extended formalism by including all spin wave components. All generic spin states are allowed by the context. We find in this case the projections

$$Z_{isotropic}(s_i) = 2^{N-1} s_i \mathbf{N}_i$$

for both  $s_j \in \{+, -\}$ . The associated distributions of probability are now  $P(s_j) = \frac{1}{2}$ , and the corresponding state is isotropic. One lesson of the former analysis is that **new** quantum states can appear in an extended formalism, states without representation in SQM. The amplitude for this new isotropic state can now be used to represent the composite singlet.

#### 4 The Singlet State

The isotropic spin state allows a local, separable representation of the singlet. Each particle  $\alpha$  and  $\beta$  is in the individual isotropic state, which agrees with the even probabilities of spin up and down in arbitrary directions. The correlation between simultaneous measurements over  $\alpha$  and  $\beta$  of a jointly generated pair is obtained by correlating each (subquantum) states  $(s_1, s_2, \ldots, s_N)_{\beta} = -(s_1, s_2, \ldots, s_N)_{\alpha}$ , i.e., imposing perfect anticorrelation for measurements in a common arbitrary direction. In this way, we measure  $s_1^{\alpha}$  along  $\mathbf{n}_1$  and  $s_2^{\beta}$  along  $\mathbf{n}_2$ . This last measurement over particle  $\beta$  allows to know (without direct measurement) the hidden but deterministic value  $s_2^{\alpha} = -s_2^{\beta}$  of the corpuscular component of particle  $\alpha$ . For the joint distribution of probability  $P(s_1^{\alpha}, s_2^{\alpha}) = P(s_1^{\alpha}, -s_2^{\beta})$ , we use the general procedure, projection, and Born rule. First, the marginal amplitude

$$Z_{isotropic}(s_1^{\alpha}, s_2^{\alpha}) = 2^{N-2}(s_1^{\alpha}\mathbf{N}_1 + s_2^{\alpha}\mathbf{N}_2)$$

is obtained by addition of all other variables  $s_3$  to  $s_N$ . Second

$$P(s_1^{\alpha}, s_2^{\alpha}) = \frac{|s_1^{\alpha} \mathbf{N}_1 + s_2^{\alpha} \mathbf{N}_2|^2}{\sum_{s_1', s_2'} |s_1'^{\alpha} \mathbf{N}_1 + s_2'^{\alpha} \mathbf{N}_2|^2}$$

reproduces the SQM result

$$P(s_1^{\alpha}, s_2^{\beta}) = P(s_1^{\alpha}, s_2^{\alpha} = -s_2^{\beta}) =$$
  
=  $\frac{1}{2}(1 + s_1^{\alpha}s_2^{\alpha}\mathbf{n}_1 \cdot \mathbf{n}_2) =$   
=  $\frac{1}{2}(1 - s_1^{\alpha}s_2^{\beta}\mathbf{n}_1 \cdot \mathbf{n}_2)$ 

Obviously, the superposition and interference obtained with marginal amplitudes of probability cannot be reproduced with a global distribution of probability and its marginal probabilities. Bell's type theorems do not apply because there is an explicit contextual character in the algorithm and the result depends on the spin wave components present and their superposition and interference, as in the two-slit experiment.

# 5 Summary

An extended phase space for an alternative formulation of Quantum Mechanics is needed in order to recover the action reaction principle. This formalism is consistent and allows to project the generalized quantum states into standard quantum states of SQM, where Born rule is applied to obtain the usual distributions of probability. In the case of spin degrees of freedom, a phase space of generic spin states is defined where the distribution of amplitude takes values in the imaginary quaternions. Standard SQM spin states are reproduced and a new isotropic state defined. Using the quantum isotropic spin state, the singlet state of a composite becomes disentangled, each particle having its independent description. The perfect (anti)correlation appears between the subquantum states at the generation event. Typical interference in the calculation of marginal amplitudes determines the standard distributions of probability. The contextual character of the algorithm cannot be reproduced with a global distribution of probability; Bell's theorems do not apply.

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# **Replacing Nothing with Something Special: Contextuality-by-Default and Dummy Measurements**



Ehtibar N. Dzhafarov

Replacing "nothing" with "something" chosen for its special properties is one of the main ways a mathematical theory develops. One speaks of "nothing" when one chooses no elements from a set, adds no number to a total, or leaves a function unchanged; but a more sophisticated way of speaking of these "nothings" would be to take an empty subset of the set, to add a zero to the total, and to apply an identity operator to the function. As a rule, these "somethings" provide not only greater convenience, but also a greater insight. Mature set theory cannot be constructed without empty sets, nor can algebra be developed without neutral elements of operations. One faces an analogous situation in the theory of contextuality: "nothing" here means that certain things are not measured in certain contexts, and the "special somethings" to replace these "nothings" are deterministic random variables.

Contextuality analysis applies to systems of random variables  $R_q^c$  representing the outcomes of measuring a *content* q (property, object, thing, question, sensory stimulus) in a *context* c (circumstances, conditions, setup). An example is the matrix below, with three contents and four contexts:

$R_1^1$	$R_2^1$		c = 1
$R_{1}^{2}$	$R_2^2$	•	c = 2
$R_{1}^{3}$	•	$R_{3}^{3}$	<i>c</i> = 3
	$R_2^4$	$R_3^4$	<i>c</i> = 4
q = 1	q = 2	q = 3	$\mathcal{R}$

E. N. Dzhafarov (🖂)

Purdue University, West Lafayette, IN, USA e-mail: ehtibar@purdue.edu

© Springer International Publishing AG, part of Springer Nature 2018 A. Khrennikov, B. Toni (eds.), *Quantum Foundations, Probability and Information*, STEAM-H: Science, Technology, Engineering, Agriculture, Mathematics & Health, https://doi.org/10.1007/978-3-319-74971-6\_5 The rules such a matrix obeys are: (i) all random variables in the same column have the same set of values (and sigma-algebras); (ii) all random variables within a row are *jointly distributed*; (iii) random variables in different rows are not jointly distributed (are *stochastically unrelated* to each other) [6, 7, 10]. The system is considered *noncontextual* if the joint distributions of the random variables within the rows are compatible with the joint distributions imposed on the random variable within each column (the compatibility meaning that both the observed row-wise distributions and the imposed column-wise ones can be viewed as marginals of a single probability distribution imposed on the entire system). Otherwise the system is *contextual*.

We will use the system  $\mathcal{R}$  throughout to illustrate our points, but the three points we make below hold for all systems of random variables indexed by contents and contexts.

As we see in the matrix, not every content is measured in every context, there are cells with "nothing" in them. It is natural to posit, however, that for a random variable being undefined is logically equivalent to being defined as always attaining a value labeled "undefined." If so, we can fill in the empty cells with deterministic random variables,

$R_1^1$	$R_2^1$	$U_3^1 \equiv u$	c = 1
$R_{1}^{2}$	$R_{2}^{2}$	$U_3^2 \equiv u$	c = 2
$R_{1}^{3}$	$U_2^3 \equiv u$	$R_{3}^{3}$	<i>c</i> = 3
$U_1^4 \equiv u$	$R_2^4$	$R_3^4$	c = 4
q = 1	q = 2	q = 3	$\mathcal{R}'$

where *u* is interpreted as "undefined," and  $U \equiv u$  means that random variable *U* equals *u* with probability 1. In order to comply with the rule (i) above, this value *u* then should be added to the set of possible values of all other random variables, as attained by each of them with probability zero.

The first point of this note is that a well-designed contextuality theory should allow the addition of these deterministic U's to any system without changing whether the system is contextual or noncontextual. One can even implement the addition of the deterministic U's empirically, e.g., by setting the procedure/device measuring q = 3 in contexts c = 3 and c = 4 to produce a fixed outcome interpreted as "undefined" in contexts c = 1 and c = 2.

The second point of this note is that this desideratum cannot be satisfied if one confines contextuality analysis to consistently connected systems only, the systems in which all measurements of the same content (e.g.,  $R_1^1$ ,  $R_1^2$ , and  $R_1^3$  in  $\mathcal{R}$ ) have the same distribution [10]. With the exception of the Contextuality-By-Default theory, discussed below, and of Khrennikov's conditionalization approach [3, 12], this constraint is common in studies of quantum contextuality [1, 2, 4, 14, 15] (see [5, 8, 9, 13] for detailed discussions). Thus, if  $R_1^1$ ,  $R_1^2$ , and  $R_1^3$  in  $\mathcal{R}$  do not have one and the same distribution (i.e., the system is inconsistently connected),

then, from the traditional point of view, either the notion of contextuality is not applicable to  $\mathcal{R}$ , or the system is considered contextual "automatically." In [6–8, 10] we provide several arguments against the necessity and desirability of the consistent connectedness constraint, and the present note adds one more. Namely, if one agrees that the transition from  $\mathcal{R}$  to  $\mathcal{R}'$  is a mere relabeling, one should consider it a flaw that in the traditional understanding of contextuality this transition has dramatic consequences: by adding the deterministic *U*'s to a consistently connected and noncontextual  $\mathcal{R}$ , one would "automatically" render it contextual or else unanalyzable in contextuality terms.

The third point of this note is that the desideratum in question is satisfied in the *Contextuality-By-Default* (CbD) theory [6, 8–10]: adding the deterministic U's to  $\mathcal{R}$  does not change the *degree of contextuality* computed in accordance with CbD. Moreover, the fixed value u in  $\mathcal{R}'$  can be replaced with any other fixed values, and different fixed values can be chosen in different cells:

$R_1^1$	$R_2^1$	$Z_3^1 \equiv z_3^1$	c = 1
$R_{1}^{2}$	$R_{2}^{2}$	$Z_3^2 \equiv z_3^2$	c = 2
$R_{1}^{3}$	$Z_2^3 \equiv z_2^3$	$R_{3}^{3}$	<i>c</i> = 3
$Z_1^4 \equiv z_1^4$	$R_2^4$	$R_3^4$	<i>c</i> = 4
q = 1	q = 2	q = 3	$\mathcal{R}^*$

Since the choice is arbitrary, one can always avoid the necessity of adding, with zero probabilities, the values  $z_q^c$  to the set of possible values of all  $R_q^{c'}$ , in the same column. One can instead choose  $z_q^c$  to be one of these possible values (no matter which). Let, e.g.,  $R_3^3$  (hence also  $R_3^4$ ) in  $\mathcal{R}$  be a binary random variable with values +1/-1; then,  $Z_3^1$  can be chosen either as  $Z_3^1 \equiv 1$  or  $Z_3^1 \equiv -1$ .

The rest of the note demonstrates our third point. (Non)contextuality of the system  $\mathcal{R}$  in the CbD theory is understood as follows.

(a) First we introduce a certain *statement* C that can be formulated for any pair of jointly distributed random variables. This statement should be chosen so that, for any column in  $\mathcal{R}$ , say,  $\{R_1^1, R_1^2, R_1^3\}$  for q = 1, there is one and only one set of corresponding and jointly distributed random variables,  $(T_1^1, T_1^2, T_1^3)$ , such that (1) each of the *T*'s is distributed as the corresponding *R* and (2) any two of the *T*'s in  $(T_1^1, T_1^2, T_1^3)$  satisfy the statement C. This unique triple  $(T_1^1, T_1^2, T_1^3)$  is called the C-coupling of  $\{R_1^1, R_1^2, R_1^3\}$ , and the C-couplings for other columns of  $\mathcal{R}$  are defined analogously. Note that any part of the C-coupling of a set of random variables is the unique C-coupling of the corresponding subset of these random variables. In CbD, assuming all random variables in  $\mathcal{R}$  are binary, the role of C is played by the statement "the two random variables are equal to each other with maximal possible probability." If the measurements are not dichotomous, then the system has to be dichotomized,

as detailed in [11]. We need not go into these details, however, because we can make our point on a higher level of abstraction, for any **C** with the just stipulated properties.

(b) The system R is considered C-noncontextual if there is a random variable (vector) S with jointly distributed components corresponding to the components of R,

$S_{1}^{1}$	$S_{2}^{1}$	•	c = 1
$S_{1}^{2}$	$S_{2}^{2}$		c = 2
$S_{1}^{3}$	•	$S_{3}^{3}$	<i>c</i> = 3
•	$S_2^4$	$S_{3}^{4}$	<i>c</i> = 4
q = 1	q = 2	q = 3	S

such that its rows are distributed as the corresponding rows of  $\mathcal{R}$  and its columns are distributed as the C-couplings of the corresponding columns of  $\mathcal{R}$ . Otherwise, if such an *S* does not exist, the system is C-contextual. The intuition behind this definition is that the system is C-contextual if the distributions of the random variables within contexts prevent the random variables measuring one and the same content in different contexts from being coupled in compliance with C.

(c) If the system  $\mathcal{R}$  is C-contextual, the degree of its contextuality is computed in the following way. The random variable S above is characterized by the probability masses

$$p\left(s_{1}^{1}, s_{2}^{1}, s_{1}^{2}, s_{2}^{2}, s_{1}^{3}, s_{3}^{3}, s_{2}^{4}, s_{3}^{4}\right)$$

assigned to every value  $(S_1^1 = s_1^1, S_2^1 = s_2^1, \dots, S_3^4 = s_3^4)$  of *S*. We redefine *S* into a *quasi-random variable* if we replace these probability masses with arbitrary real numbers

$$q\left(s_{1}^{1}, s_{2}^{1}, s_{1}^{2}, s_{2}^{2}, s_{1}^{3}, s_{3}^{3}, s_{2}^{4}, s_{3}^{4}\right)$$

summing to 1. We require that this *quasi-probability distribution* satisfies the same properties as the distribution of *S* in (B), namely, that it agrees with the distributions of the rows of  $\mathcal{R}$  and with the distributions of the C-couplings of its columns. Thus, the agreement with the first row distribution means that, for any  $R_1^1 = r_1^1$ ,  $R_2^1 = r_2^1$ , we should have

$$\sum_{s_1^2, s_2^2, s_1^3, s_3^3, s_2^4, s_3^4} q\left(r_1^1, r_2^1, s_1^2, s_2^2, s_1^3, s_3^3, s_2^4, s_3^4\right)$$

$$= \Pr\left[R_1^1 = r_1^1, R_2^1 = r_2^1\right].$$
(1)

The agreement with the distribution of the C-coupling  $(T_1^1, T_1^2, T_1^3)$  for the first column means that, for any  $R_1^1 = r_1^1$ ,  $R_1^2 = r_1^2$ ,  $R_1^3 = r_1^3$ , we should have

$$\sum_{s_2^1, s_2^2, s_3^3, s_2^4, s_3^4} q\left(r_1^1, s_2^1, r_1^2, s_2^2, r_1^3, s_3^3, s_2^4, s_3^4\right)$$
  
=  $\Pr\left[T_1^1 = r_1^1, T_1^2 = r_1^2, T_1^3 = r_1^3\right].$  (2)

Such quasi-random variables *S* always exist, and among them one can always find (generally non-uniquely) ones whose total variation is minimal [7]. The total variation is defined as

$$V[S] = \sum_{s_1^1, s_2^1, s_1^2, s_2^2, s_1^3, s_3^3, s_2^4, s_3^4} \left| q\left(s_1^1, s_2^1, s_1^2, s_2^2, s_1^3, s_3^3, s_2^4, s_3^4\right) \right|.$$
(3)

The quantity min V[S] - 1 can be taken as a principled and universal measure of the *degree of contextuality*. If this quantity equals 0, which is the smallest possible value for V[S]-1, then all quasi-probability masses q are nonnegative, and  $S^*$  is a proper random variable. The system then is C-noncontextual.

It is easy now to see the truth of our claim that  $\mathcal{R}^*$  has the same degree of contextuality as  $\mathcal{R}$ . On the right-hand side of (1),

$$\Pr \left[ R_1^1 = r_1^1, R_2^1 = r_2^1 \right]$$
$$= \Pr \left[ R_1^1 = r_1^1, R_2^1 = r_2^1, Z_3^1 = z_3^1 \right]$$

because  $Z_3^1 \equiv z_3^1$ . The same reasoning applies to other rows of  $\mathcal{R}^*$ . On the righthand side of (2), for any  $\dot{Z}_1^4 \equiv z_1^4$ ,

$$\Pr\left[T_1^1 = r_1^1, T_1^2 = r_1^2, T_1^3 = r_1^3\right]$$
$$= \Pr\left[T_1^1 = r_1^1, T_1^2 = r_1^2, T_1^3 = r_1^3, \dot{Z}_1^4 = z_1^4\right]$$

Now,  $(T_1^1, T_1^2, T_1^3, \dot{Z}_1^4)$  is the C-coupling of  $\{R_1^1, R_1^2, R_1^3, Z_1^4\}$ . Indeed, the C-coupling  $(\dot{T}_1^1, \dot{T}_1^2, \dot{T}_1^3, \dot{Z}_1^4)$  of  $\{R_1^1, R_1^2, R_1^3, Z_1^4\}$  exists and is unique. The part  $(\dot{T}_1^1, \dot{T}_1^2, \dot{T}_1^3)$  is then the unique C-coupling of  $\{R_1^1, R_1^2, R_1^3\}$ , whence  $(\dot{T}_1^1, \dot{T}_1^2, \dot{T}_1^3) = (T_1^1, T_1^2, T_1^3)$ . The same reasoning applies to other columns of  $\mathcal{R}^*$ . So the right-hand sides in the equations exemplified by (1) and (2) do not change when  $\mathcal{R}$  is replaced with  $\mathcal{R}^*$ . Since, under this replacement, the left-hand sides of these equations do not change either, except that each quasi-probability value

$$q\left(s_1^1, s_2^1, s_1^2, s_2^2, s_1^3, s_3^3, s_2^4, s_3^4\right)$$

in them is bijectively renamed into

$$q\left(s_1^1, s_2^1, \, z_3^1, \, s_1^2, \, s_2^2, \, z_3^2, \, s_1^3, \, z_2^3, \, s_3^3, \, z_1^4, \, s_2^4, \, s_3^4\right),$$

the set of the quasi-probability distributions solving (1) and (2) (and similar equations) in  $\mathcal{R}^*$  remains the same as in  $\mathcal{R}$ , and the minimum value of V[S] in (3) therefore remains unchanged.

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# A Computational Proof of Locality in Entanglement



Han Geurdes

# 1 Introduction

# 1.1 Tabula Rasa

In introductory courses of quantum mechanics, the foundation of quantum theory is a difficult topic. A general presentation of quantum mechanical interpretations can be found in [1]. In a good but somewhat older textbook such as *Merzbacher* [2], the probability interpretation is flatly introduced as a doctrine. Given the wave function  $\psi(\mathbf{r}, t)$ , the doctrine is that the probability to find a particle in a volume  $d^3r$  around a point  $\mathbf{r}$  in  $\mathbb{R}^3$ , at time t, is equal to  $|\psi(\mathbf{r}, t)|^2 d^3r$ . Here,  $|\psi(\mathbf{r}, t)|^2 = \psi^*(\mathbf{r}, t)\psi(\mathbf{r}, t)$ . The approach of Hameka follows, page 20, a similar procedure [3] as does the textbook, page 73, of Rae [4].

It remains a mystery why nature has two different types of probability. It also is a mystery how the one type of probability transforms to the other and why addition of relativity bars the possibility of a wave interpretation of the wave function [5].

An even bigger mystery in quantum theory is entanglement. Perhaps some explanation is at its place here. Entanglement is the translation of the term "Verschränkung" introduced by Schrödinger. It means that there are pure states of a compound system which yield stronger correlations in the joint probability distribution of measuring results on the subsystems than those which can arise from correlations between individual states of the subsystems [6].

H. Geurdes (⊠)

Geurdes Datascience, Den Haag, Netherlands

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## 1.2 Bell's Work

In the debate of the foundation of quantum theory, Bell's theorem [7] is considered an important milestone. In order to study Einstein's incompleteness criticism [8], Bell formulated an expression for the correlation between distant spin measurements. With this formulation, it was possible to answer Einstein's question of completeness with an experiment. It is important to note the following. The experimenters using Bell's correlation formula did not "look under the hood" for extra parameters. They employed classical statistics in spin measurement experiments without much physics theory about hidden variables. The key element is that Bell's theorem exploits the fundamental difference between measure theoretic probability and quantum probability.

Einstein's criticism initially did not include the spin. The reformulation of Einstein's criticism [8] into the entanglement between spins was provided by David Bohm [9] and [10]. For the ease of the argument, let us say that Einstein argued for extra hidden parameters to explain spin correlation. Einstein insisted that the A wing of the experiment is independent of what is done in the B wing and vice versa [11]. Funny enough, here we also can ask a naive question. Namely, how far does Einstein think A and B should be separated for this independence to occur?

The restriction of locality was introduced because in theory the correlation is independent of the distance between the sites of measurement. The Einsteinian locality concept—however see also the previous naive questions—can be tested with the use of the Clauser-Horne-Shimony-Holt (CHSH) inequality. The inequality is derived [12] from Bell's correlation formula [7], E(a, b). Bell's formula reads:

$$E(a,b) = \int d\lambda \rho_{\lambda} A_{\lambda}(a) B_{\lambda}(b)$$
(1.1)

In Eq. (1.1), the (classical) probability density of the hidden variables,  $\lambda$ , is  $\rho_{\lambda} \geq 0$ . So,  $\int d\lambda \rho_{\lambda} = 1$ . The local effect of the  $\lambda$ , e.g., an array  $(\lambda_1, \lambda_2)$ , can be accomplished if, e.g.,  $\lambda_1$  is assigned and related to the *A* wing and  $\lambda_2$  to the *B* wing of the experiment. Furthermore, the measurement functions  $A_{\lambda}(a)$  and  $B_{\lambda}(b)$  both project in  $\{-1, 1\}$  to represent binary spin variables (e.g., up=1, down=-1 along an arbitrary *z*-axis). The *a* and *b* represent unit parameter vectors. Given (1.1) we can study the following four terms:

$$S = E(1, 1) - E(1, 2) - E(2, 1) - E(2, 2)$$
(1.2)

The CHSH inequality  $S \le 2$  can be derived from (1.2). See [12] and, e.g., [11]. So for an E(a, b) in the form (1.1), we have by necessity  $S \le 2$ . However, note that S > 2 is possible with  $E(a, b) = a \cdot b$  for certain proper (a, b) combinations of setting parameter vectors. To be sure, the labels 1 and 2 in (1.2) refer to a and b vectors that can be set in the experiment. For example, 1 on the A side, operated by Alice, is  $a^{(1)} = (a_1^{(1)}, a_2^{(1)}, a_3^{(1)})$ , etc., with  $||a^{(1)}||^2 = a^{(1)} \cdot a^{(1)} = 1$ . The  $|| \cdot ||$  is

the Euclidean norm. Similarly, looking at A, the 2 is associated to  $a^{(2)}$ . Moreover, for B we have  $b^{(1)}$  and  $b^{(2)}$ . Below, a numerical example of  $S \le 2$  violating setting combinations will be given.

Before entering into more details, the author would like to note that we can look upon a CHSH experiment as the question if measure theoretic *or* quantum probability is ruling entanglement.

#### **1.3** Correlation in Experiment

Here we answer the question how to obtain in experiment the *E* values to be used in (1.2). It is technically still impossible to measure directly the E(a, b) for a single pair. The correlation is therefore derived from counting measurement results. The results enter the raw product moment correlation [13] to approximate the correlation E(a, b). This is an "averaged over many pairs" correlation. Again, the naive student could respond like: wait a minute, things in quantum theory are already not always what they look like, so how do you know that one pair correlation can be compared to the next and be averaged in experiment? We don't, but we do it anyway.

Suppose we measure *N* spin pairs. After the last measurement in the series, the correlation E(a, b) is in the experiment of [14] computed approximately. Using the Kronecker delta  $\delta_{s,r}$ , we count the number of times  $S_{A,n}(a_n) = S_{B,n}(b_n)$  and the number of times  $S_{A,n}(a_n) = -S_{B,n}(b_n)$ , i.e.:

$$N(= | a, b) = \sum_{n=1}^{N} \delta_{S_{A,n}(a), S_{B,n}(b)} \delta_{a_n, a} \delta_{b_n, b},$$
(1.3)

and

$$N(\neq | a, b) = \sum_{n=1}^{N} \delta_{S_{A,n}(a), -S_{B,n}(b)} \delta_{a_n, a} \delta_{b_n, b}.$$
 (1.4)

Hence, we obtain the expression of the correlation

$$E(a,b) = \frac{N(=|a,b) - N(\neq |a,b)}{N(=|a,b) + N(\neq |a,b)}$$
(1.5)

This type of computation of E is also employed in the algorithm and its presented proof of concept in Appendix.

It must be noted that if the researcher employs the inequality  $S \le 2$ , defined in (1.2), to see in experiment if *E* in (1.5) gives  $S \le 2$ , then implicitly, Bell's definition of correlation (1.1) is employed. Hence, a measure theoretic probability is tested in experiment. It is one where  $E(a, b) = a \cdot b$  is considered impossible by definition. However, see [15].

#### 2 Preliminaries in the Computer Design

Peres [11] formulates it thus: "....., a hidden variable theory which would predict individual events must violate the canons of special relativity...." Furthermore, the program must mimic an important experiment in the test of locality performed by Weihs [14]. Note that Weihs's experiment is related to the work of Aspect [16]. In Weihs's experiment, strict locality conditions were closely approximated, and a violation S > 2 was observed for violating setting combinations of a and b with a quantum correlation  $a \cdot b$ .

In [17], however, the present author already showed that there is a nonzero probability that a local hidden variables model may violate the CHSH. Objections to the probability loophole claim in [17] were raised in [18] but were answered in [19]. The main point is that the employed probability density remains fixed during the trials. The matter of a possible defective Bell formula was further developed in [15].

It must be noted that the author of [18] acts as though a random model occurs in [17]. However, if  $p_1$  and  $p_2$  are random numbers between 0 and 1 and  $r = p_1 + p_2$ , then the *model* to compute r is fixed, i.e., a + operation, despite the fact that the inputs  $p_1$  and  $p_2$  are random and the outcome r is therefore also random. The present paper completes the rejection of what has been claimed in [18] and observes the nontheatrical requirements of [13].

#### 2.1 Settings

On the A side, Alice has  $1 \equiv \frac{1}{\sqrt{2}}(1, 0, 1)$  and  $2 \equiv (\frac{-1}{2}, \frac{1}{\sqrt{2}}, \frac{1}{2})$  at her disposal. On the B side, Bob has  $1 \equiv (1, 0, 0)$  and  $2 \equiv (0, 0, -1)$ . For the ease of the argument we inspect,  $E(a, b) = a \cdot b$ . A simple computation then shows that for a quantum outcome, we would see  $E(1, 1) = 1/\sqrt{2}$ ,  $E(1, 2) = -1/\sqrt{2}$  while E(2, 1) = -1/2 and E(2, 2) = -1/2. Hence, looking at (1.2), for a quantum value,  $S = 1 + \sqrt{2} > 2$  is expected in an experiment. The setting parameters *a* and *b* are given a value when the A- and B-wing particles leave the source. In flight, we allow B (Bob) to change his setting.

#### 2.2 Information Hiding

We note that information hiding between Alice and Bob is the algorithmic realization of strict locality. Furthermore, in the computer simulation, A doesn't know anything about B and vice versa. All computations are "encapsulated," i.e., local, despite the fact that in the proof of concept (POC), they occur in a single loop (viz., Appendix). In the POC, both the A section (Alice) and the B section (Bob) make use of the produced discrete variables created in the source section. This is the computational equivalent of S sending entangled particles to A and B.

#### 2.3 Notation

In the formalism of the algorithm presented below, there are *no* measures in the sense of measure theoretical distributions. We are dealing with arrays of variables, variables as entries of those arrays, and functions of those variables. Most of the variables and functions project into  $\{-1, 1\}$ . The setting array variables project into  $\{1, 2\}$ . Index variables, most of the time denoted with, e.g., *n*, *m*, *k*, are integer positive numbers, i.e.,  $n \in \{0, 1, ..., N\}$ , with  $N \in \mathbb{N}(N \ge 1)$ .

#### **3** Design of the Algorithm Based on a Local Model

#### 3.1 Random Sources

In the first place, let us introduce random sources to represent random selection of setting. We look at the randomness from the point of view of creating an algorithm. If there are *N* trials, i.e., particle pairs, in the experiment, then, e.g., two independent random sources can be seen as two arrays with index running from 1 to *N*. If  $\mathcal{N}_N = (1, 2, 3, ..., N)$ , then we, initially, define three random source arrays:

$$\frac{\mathcal{R}_{AS} = \text{sample}(\mathcal{N}_N)}{\mathcal{R}_B = \text{sample}(\mathcal{N}_N)}$$

$$\mathcal{R}_C = \text{sample}(\mathcal{N}_N)$$
(3.1)

Technically, the map  $\mathcal{N}_N \mapsto \underline{\mathcal{R}}$  is 1-1 but randomized. As an example, suppose we have  $\mathcal{N}_5 = (2, 3, 5, 1, 4)$  and so  $\mathcal{N}_{5,1} = 2$ . Then in the first trial n = 1, the  $\mathcal{N}_{5,1}$ -th element of another array, e.g., q = (0.1, 0.4, -0.9, 1.2, 1.0), is randomly selected; hence, q(n = 1) = 0.4. In the second trial, looking at  $\mathcal{N}_5$ , we see  $\mathcal{N}_{5,2} = 3$  so q(n = 2) = -0.9, etc. Note that this two-array procedure is similar to rolling a five-sided dice. If, e.g.,  $\mathcal{N}_5$  is replaced by  $\mathcal{M}_{10}$  and multiples are allowed, such as in  $\mathcal{M}_{10} = (2, 3, 5, 1, 4, 4, 5, 1, 3, 3)$ , this q "dice" will in 10 turns show three times the side with -0.9.

In this way, a random source  $\underline{\mathcal{R}}$  can be employed in a program and be looked upon as a physical factor giving rise to randomness. In a certain sense, it refers to 'tHoofts [20] deterministic law hidden inside "randomness." The "freely tossing of a coin" is now replaced with "freely randomizing" the  $\underline{\mathcal{R}}_X$  by filling it with sample( $\mathcal{N}_N$ ). There can be no fundamental objection to this particular two-array form of randomizing.

#### 3.2 Design Time Settings

Experimentalists may claim the construction of their measuring instruments. Hence, servers in the experiment may be tuned in design time. There is no fundamental reason to reject design time to the designer of a computer experiment. There is also no reason in physics theory to reject the denial of access of the observers Alice and Bob to information put in the system by the designer during design time.

Because there is a flow of particles between the S and the A, this sharing, i.e.,  $\underline{\mathcal{R}}_A = \underline{\mathcal{R}}_S = \underline{\mathcal{R}}_{AS}$ , cannot be prevented at run time in a real experiment. The latter is reflected in the infrastructure of servers in the numerical experiment. The  $\{a_n\}_{n=1}^N$  in the experiment are based on the <u>a</u> array and the  $\underline{\mathcal{R}}_A$ . For instance, <u>a</u> = (1, 2, 1, 2, 1, 2, ...). In design time, the designer is allowed to introduce a spin-like variable  $\sigma_n \in \{-1, 1\}$  in the S computer. In the sequence of trials, the variable  $\sigma_n$  is selected from  $\underline{\sigma} = (-1, 1, -1, 1, -1, 1, ...)$ .

We may note that, in case of  $\underline{\mathcal{R}}_A = \underline{\mathcal{R}}_S$ , then *because of*  $\underline{\mathcal{R}}_A = \underline{\mathcal{R}}_S$ , the relation  $a_n = 1 + \frac{1}{2}(1 + \sigma_n)$  occurs on the A side of the experiment. The setting  $a_n$  can be either 1 or 2 and is already presented in terms of selection unit parameter vectors in  $\mathbb{R}^3$ .

Note that the variable  $\sigma_n$  can be sent to Bob and to Alice without any additional information conveying its meaning. So, Bob cannot derive anything from  $\sigma_n$  even though the designer knows the relation. This is because Bob is only active in run time, not in design time.

Finally, the source may also send a  $\zeta_n \in \{-1, 1\}$  to both Alice and Bob. The  $\zeta_n$  in the experiment is based on the  $\underline{\mathcal{R}}_C = \text{sample}(\mathcal{N}_N)$  and derives from a  $\zeta$  array.

The second random source,  $\underline{\mathcal{R}}_B$ , is used by B exclusively, and the third random source,  $\underline{\mathcal{R}}_C$ , is used by the source exclusively. There appears to be no physical arguments why the sketched configuration is a violation of locality or cannot be found in nature.

#### 3.3 Random Sources R. and Particles

The source sends a  $\sigma_n \in \{-1, 1\}$  and a  $\zeta_n \in \{-1, 1\}$  to both A and B. In a formal format:

$$[A(a_n)] \leftarrow (\sigma, \zeta)_n \leftarrow [S] \rightarrow (\sigma, \zeta)_n \rightarrow [B(b_n)]$$

Here, e.g., [A(a)] represents the measuring instrument A where Alice has the *a* setting. This setting "runs synchronous" with  $\sigma$  in the source because of the "shared" random source. The particle pair source is represented by [S].

The  $\sigma$  and  $\zeta$  going into the direction of A are equal to the  $\sigma$  and  $\zeta$  going to B. Each particle is, in the algorithm, a pair  $(\sigma, \zeta)_n$ .

#### 3.4 A Side Processing of the $(\sigma, \zeta)_n$

Firstly, let us for the ease of the presentation define a  $\sigma_{A,n} = \frac{1+\sigma_n}{2}$ . The  $\sigma_n$  at the n-th trial from the source *S* is a result of the sharing of  $\mathcal{R}_{AS}$ . The way the information is used remains hidden to B in order to maintain locality in the model. So, secondly, we have the setting  $a_n = \sigma_{A,n} + 1$ . Furthermore, we define two functions  $\varphi_{A,n}^- = \sigma_{A,n}$  and  $\varphi_{A,n}^+ = 1 - \sigma_{A,n}$ . The two functions, together with  $\zeta_n$ , produce, in turn, a function:

$$f_{\zeta_n}(a_n) = \zeta_n \varphi_{A,n}^+ - \varphi_{A,n}^-$$

Note that  $f_{\zeta_n} \in \{-1, 1\}$ . Hence, we can store the outcome of the computations on the A side immediately in an *N*-size array  $S_{A,n}$ , together with  $a_n$ , for trial number *n* and  $n = 1, 2, 3, \ldots, N$ .

# 3.5 B-Side Processing of the $(\sigma, \zeta)_n$

In the first place, let us determine with the B-associated random source,  $\underline{\mathcal{R}}_B$ , the setting  $b_n$ . Then, secondly and similar to the case of A, but of course completely hidden from A, the  $(\sigma, \zeta)_n$  information from the source is processed. We have  $\sigma_{B,n} = \frac{1+\sigma_n}{2}$ , then  $\varphi_{B,n}^- = \sigma_{B,n}$  and  $\varphi_{B,n}^+ = \sigma_{B,n} + (\delta_{1,b} - \delta_{2,b})(1 - \sigma_{B,n})$ . This leads to the function:

$$g_{\zeta_n}(b_n) = \zeta_n \varphi_{B,n}^+ + \frac{1 - \zeta_n}{\sqrt{2}} \varphi_{B,n}^-$$

For  $g_{\zeta_n}(b_n)$ , we may note that it projects in the real interval  $[-\sqrt{2}, \sqrt{2}]$ . If  $\sigma_{B,n} = 1$ , then  $g_{\zeta_n}(b_n) = 1$  for  $\zeta_n = 1$  and  $\sqrt{2} - 1$  for  $\zeta_n = -1$ . If  $\sigma_{B,n} = 0$ , then  $\varphi_{B,n}^- = 0$  and  $g_{\zeta_n}(b_n) = \pm 1$ .

Hence, in order to generate a response in  $\{-1, 1\}$ , a random  $\lambda_2$  from the real interval  $[-\sqrt{2}, \sqrt{2}]$  is uniformly drawn and  $S_B(b_n) = S_{B,n} = \text{sgn}(g_{\zeta_n}(b_n) - \lambda_2)$  in the *n*-th trial. We note that as long as Bob doesn't know the meaning of  $\sigma_{B,n}$ , derived from  $\sigma_n$  and related to the  $\mathcal{R}_{AS}$ , locality is warranted. Bob, like Alice, doesn't have access to the design time information.

#### 3.6 Computer Infrastructure

In computer infrastructure terms, one can imagine cables running from the source server running to the A server and running from S server to the B server. One cable,  $C_{SA}(\sigma_n)$ , carries the  $\sigma_n$  from S to A, and the other cable,  $C_{SB}(\sigma_n)$ , carries the copy

 $\sigma_n$  from S to B. Secondly, a cable,  $C_{SA}(\zeta_n)$ , carries the  $\zeta_n$  from S to A, and a cable  $C_{SB}(\zeta_n)$  carries the copy  $\zeta_n$  from S to B. In addition to these four cables, a fifth cable,  $C_{AS}(\underline{\mathcal{R}}_A)$ , is only used by A to share the (information of)  $\underline{\mathcal{R}}_A$  with S. This cable is open *only once* and carries only one "pulse" that informs S about the random source at A. The exact time when  $\underline{\mathcal{R}}_A$  is shared is in the program at an n = 0 trial or particle pair. However, the n = 0 particle pair is merely used for computational convenience and clarity.

#### 3.6.1 Predetermined

In addition, we note the following. The sharing of  $\underline{\mathcal{R}}_A$  can also be accomplished in a way that tHooft [20] would most likely call predeterministic. In this case, server A and S share a common array of randomly distributed integer numbers in an indefinite large array. Think of the large array as a design feature like a shared identical random table between computer A and computer S.

In design time, the A computer receives its N settings 1 or 2. This process starts at time  $t_{start}$  and ends at  $t_{fin} > t_{start}$ . In computer A, a subsection of the indefinite large array is identified by  $t_{start}$  and  $t_{fin}$ . This timing mechanism runs parallel in S where a copy of the large array of A resides. Note that a transformation of the numbers in the subsection can be performed to reach a similar numerical form as if we would have performed  $\underline{\mathcal{R}}_A$  =sample( $\mathcal{N}_N$ ). In this case  $\underline{\mathcal{R}}_A$  and  $\underline{\mathcal{R}}_S$  are different, and the "bridging" between A and S is done via the computation of  $\underline{\pi}$  in S. Here,  $\pi_n = 1$  when  $\underline{\sigma}_{(\underline{\mathcal{R}}_A)_n} = \underline{\sigma}_{(\underline{\mathcal{R}}_S)_n}$  and  $\pi_n = -1$  when  $\underline{\sigma}_{(\underline{\mathcal{R}}_A)_n} \neq \underline{\sigma}_{(\underline{\mathcal{R}}_S)_n}$ . In the predetermined case, the  $\sigma_n$  is computed like

$$\sigma_n = \pi_n \underline{\sigma}_{(\mathcal{R}_s)_n}$$

#### 3.6.2 Mr. X

It must also be noted that nature is neutral in the following sense. Two situations of feeding parameter settings into measuring instruments may arise. Firstly, looking at the A side, a proverbial Mr. X is sitting in front of A, and, before  $(\sigma, \zeta)_n$  enters the measurement area of A, Mr. X has selected with a coin the  $a_n$ . Secondly, we have the case where Mr. X delivers his N coin tosses *before* the experiment starts, and A runs on a batch input of Mr. X's coin tosses. In both cases, Alice only makes a record of the  $a_n$  and the resulting  $\pm 1$  output. We can imagine a Mr. Y at Bob's side and Bob only recording the outcome. The difference between on-the-spot hand-fed entrance of coin toss values for  $a_n$  and batch processing of previous series is insignificant to the problem and a mere illusion. This is so because we may assume that nature has no eyes to witness the difference between the activities of Mr. X. The reason is that the incoming particle makes contact with the instrument which has a certain setting. The incoming particle does not make contact with Mr. X who is delivering

the settings. Hence, the use of previously selected setting series, "from the days of Hammurabi", which are online, just-in-time, and hand-fed into A, can equally well and without any violation of experimental protocol be processed in a batch and translated into  $\underline{\mathcal{R}}_A$ . The  $\underline{\mathcal{R}}_A$  can subsequently be shared with S.

It must be noted also that the proverbial Mr. X may freely use one online handfed set from Hammurabi's days at the side of B. Mr. Y is then posted at Alice and makes a setting entrance batch possible. Because Mr. X has no knowledge of design time and the labels A and B can be arbitrarily interchanged, the selection of Mr. X with the single online hand-fed set from the days of Hammurabi will have a nonzero probability to violate the CHSH with the local algorithm provided in the paper. Of course, the next step is the ad hoc requirement to have two ancient handfed inputs. But before doing that, Mr. X must explain if nature at A would really note the difference. If not, then this requirement only has theatrical value. If yes, then the choice of having a Hammurabi set is allowed into the design too. Suppose Simon is running the source. Then why would the data from Hammurabi's days be accessible to Mr. X and not to Simon? The setting at Bob remains at all times random. Again, it is unlikely that nature in A will behave differently when Mr. X is holding a tablet with cuneiform markings and feeding just-in-time 1's and 2's into the selection area the lower small rectangle in the A rectangle of Fig. 1 contrasted with the situation where Mr. Y helps Mr. X with the translation and writes down the 1's and 2's from the tablet first and puts them afterward in the A area to derive a random source  $\mathcal{R}_A$ , etc. The question is how far must one allow the incorporation of theatrical requirements in the design. Depending upon the amount of omniscience a stakeholder thinks he or she has, theatrical requirements are thought necessary.

It is another matter, whether or not Mr. X is able to determine the difference between, e.g., a  $\underline{\mathcal{R}}_C$  =sample( $\mathcal{N}_n$ ) and  $\underline{\zeta} = (-1, 1, ...)$  random process and a coin toss for obtaining  $\zeta_n \in \{-1, 1\}$ , with  $\overline{n} = 1, 2, ..., N$ . Here a test resembling a Turing test can be invoked [21]. A computer generates 1's and -1's with random source and value arrays versus a human tosses a coin and generates a series of 1's and -1's. Both processes are covert. Mr. X has to decide if there is a difference. The claim is that Mr. X cannot detect the difference better than chance.

#### 4 Conclusion and Discussion

In the paper, a simple design is given that is able to violate the CHSH inequality with numerical values close to the expected quantum mechanics. The reader kindly notes that no violation of locality is employed. B doesn't know the meaning of the A-S shared information sent to B. The information from S to Alice is inaccessible to Bob. Both Alice and Bob are not allowed access to the design. Further, if the sharing of information runs along the lines of 'tHooft's predeterminism [20], then S and A do not know they share information, i.e., the random source array,  $\mathcal{R}_A$ .

The reader also notes that the computer setup is designed to explain the outcome of the A-S-B experiment such as in Weihs's [14] and should not be confused with experimental configurations unequal to  $A(a) \leftarrow S \rightarrow B(b)$ .



**Fig. 1** Explicit key concepts of computer infrastructure in predetermined format. The  $\underline{\mathcal{R}}_A$  is shared between A and S. In S, a computation of an auxiliary array  $\underline{\pi}$  is run at n = 0 to generate the  $\sigma_n$  for n > 0. The small lower rectangles in the A and B are information inflow areas. The settings a and b are handed over to data storage and to Alice and Bob. In A this handing over runs via the small rectangle on the left. In B it is the small rectangle on the right. The connection is shown by a small horizontal line. If, e.g., Bob selects a setting in the *n*-th trial (n > 0), he pushes a button and receives from B a setting either 1 or 2. He then puts the setting in the setting area of his computer (the little lower part of the small top rectangle in B). Then the ( $\sigma, \zeta$ )<sub>n</sub> enters via left side rectangle in B. The B-side algorithm starts running. After some time, a response ±1 comes out of the B computer, and Bob makes a record of it together with the setting  $b_n$ . Similar case for Alice, the generation of the sigma and zeta for Simon are of course hidden from Alice and Bob. This is indicated by the wiggely lines

In Appendix, the essential loops in the R program over n = 1, 2, 3 ... N are presented. The code is the POC of the algorithm with  $\underline{\mathcal{R}}_A = \underline{\mathcal{R}}_S = \underline{\mathcal{R}}_{AS}$ . This situation refers to "pretrial information leakage" from A to S. In the case of a predetermined format, such as in Fig. 1, we have  $\underline{\mathcal{R}}_A, \underline{\mathcal{R}}_S, \underline{\mathcal{R}}_C$ , and  $\underline{\mathcal{R}}_B$ . This is not an active information leakage but a wired-in sharing of information in design time. In the latter case,  $\underline{\pi}$  is auxiliary to the computation of the  $\sigma_n$ . The reader is referred to Fig. 1. It is noted that nobody knows if, either via A-S leakage or via wiredin predetermined sharing, the measuring instrument, A, and the particle source, S, share information yes or no. The use of encapsulating information and a distinction between design time and run time also makes sure that A and S are unaware that they share information.

In both cases, we assumed a n = 0 initial particle pair to do the necessary initial computations. Furthermore, there is a flow of particles between S and A. From S

to A, the flow is "forced" by the experimenter. In this design, flow of information from A to S can be enforced by nature on the experimenter. It is perhaps like 'tHooft claimed: ".... every no-go theorem comes with small print" [20].

To this, it must be added that the CHSH is based on Bell's formula. In turn, Bell's formula is based on the (probabilistic) distribution of hidden variables  $\lambda$ . The POC computer program is a typical "classical" algorithm. The setup of three computers is a realization of a classical system that mimics the instruments in the experiment. How would an opponent of extra local parameters interpret the numerically obtained violation, other than the rejection of the necessity of quantum probabilities to violate the CHSH?

As required by the author of [18], a computer simulation rejects the criticism raised in [18]. We may claim this because our "freezing the setting of a at particle creation" is a valid CHSH type of experiment. It would be strange to say that locality and causality cannot occur in an experiment where "in-flight" changes in both wings are allowed whereas one must admit that locality and causality occur when only B-wing "in-flight" changes of setting may occur. This is all the more so because the A and B role in the simulation can be selected randomly.

The metaphor requirements of [13] are met or are identified as solvable within the design. Note that a violation of the CHSH criterion would, most likely, not have been possible without a probability loophole in the CHSH [17]. Furthermore, the freely selected settings are created at design time. It is, moreover, hard to see how a particle pair in a distant source would behave differently when Alice and Bob or an external agent such as Mr. X employs, to them, unknown random sequences  $\underline{\mathcal{R}}_A$  and  $\underline{\mathcal{R}}_B$  for their setting selection, compared to the case where a coin to select the respective setting is employed. We note that preformed but just-in-time hand-fed ancient setting sequences by Mr. X would give a nonzero probability of CHSH violation with a local algorithm. In this sense, progress is made when looking at [17]. In the latter case, only a nonzero number of quartets of setting values  $\{(1, 1), (1, 2), (2, 1), (2, 2)\}$  violate the CHSH with local means. Finally, if the behavior of Mr. X matters at quantum level, then it must be entered into the design and can be incorporated to solve that challenge in this way. The required hardware of the computer experiment are three computers, four cables, a timing mechanism for sending pulses  $(\sigma, \zeta)_n$  from S to A and S to B, and a fifth cable from A to S that is used only once in a n = 0 preexperimental statistical trial.

Furthermore, testers must be completely unaware of the design time activities of the designer. The reason is that, obviously, design time refers to the inner workings of nature which are considered unknown in this case. Implementation of the software on the A- and B-side algorithms plus detector timers is required together with the algorithm for S. The design of the infrastructure for a predetermined format, which also can be built with the hardware given above, is provided in Fig. 1. Of course, contingency programming for n = 0 needs to be done such that no single particle pair lacks from counting. In tests on an ordinary computer, a maximum of  $N = 1 \times 10^7$  number of particle pairs was reached.

We claim that we are allowed to say that the present result corrects Peres' statement [11] that violations of the CHSH inequality "violate the canons of special

relativity." We also add here that serious doubts can be cast on the mathematical consistency of Bell's methodology [15]. To the present author, this mathematical deficit of Bell's methodology represents an additional reason to maintain the idea of local hidden variables in the sense of additional parameters to supplement the wave function. However, to quote Einstein [8] "We believe ... that such a [more complete?] theory exists." Surely, this appears quite easily said but far more difficult to be obtained.

#### Appendix

The  $\underline{\mathcal{R}}_A = \underline{\mathcal{R}}_S = \underline{\mathcal{R}}_{AS}$  algorithm is shown in the POC.

```
N<-4e5
a < - array(0, N)
aKeep<-array(0,N)
sigma<-array(0,N)</pre>
zeta<-array(0,N)</pre>
b<-array(0,N)</pre>
bKeep<-array(0,N)
RAS<-sample(seq(1,N),N,replace=FALSE,prob=NULL)
RB<-sample(seq(1,N),N,replace=FALSE,prob=NULL)</pre>
RC<-sample(seq(1,N),N,replace=FALSE,prob=NULL)</pre>
#
for(j in 1:N)
  k < -as.integer(j/2)
  m<-j/2
  if(m==k){
     a[i]<-2
     b[j]<-2
     sigma[j]<-1</pre>
     zeta[j]<-1
  }else{
     a[j]<-1
     b[j]<-1
     sigma[j]<-(-1)
     zeta[j]<-(-1)</pre>
  }
}
#
scoreA<-array(0,c(2,N))</pre>
scoreB<-array(0,c(2,N))</pre>
for (n \text{ in } 1:N)
#Source section
```

```
zetah<-zeta[RC[n]]</pre>
  sygma<-sigma[RAS[n]]</pre>
#A section
  aSet<-a[RAS[n]]
  aKeep[n] < -aSet
  phiAmin<-((syqma+1)/2)</pre>
  phiAplus<-1-((sygma+1)/2)</pre>
  f<-zetah*phiAplus-phiAmin
  scoreA[aSet,n]<-f</pre>
#B section
  phiBmin<-((sygma+1)/2)</pre>
  bSet<-b[RB[n]]
  bKeep[n] <-bSet
  if(((sygma+1)/2)==1){
    phiBplus<-1
  }else{
    if (bSet==1) {
       phiBplus<-1
     }
     if(bSet==2){
       phiBplus<-(-1)
     }
  }
  g<-zetah*phiBplus
  g<-g+((1-zetah)*phiBmin/sqrt(2))
  lambda 2<-runif(1)*sqrt(2)</pre>
  lambda 2<-sign(0.5 - runif(1))*lambda 2</pre>
  scoreB[bSet,n]<-sign(g-lambda_2)</pre>
}
E<-matrix(0,nrow=2,ncol=2)</pre>
Neq < -array(0, c(2, 2))
Nneq < -array(0, c(2, 2))
for (n in 1:N)
  aSet<-aKeep[n]
  bSet<-bKeep[n]
  if (scoreA[aSet,n]==scoreB[bSet,n]) {
    Neq[aSet,bSet] < -Neq[aSet,bSet]+1</pre>
  }else{
    Nneq[aSet,bSet] < -Nneq[aSet,bSet]+1</pre>
  }
for (aSet in 1:2) {
  for(bSet in 1:2) {
    E[aSet,bSet] <- (Neq[aSet,bSet] -Nneq[aSet,bSet]) /</pre>
     (Neq[aSet,bSet]+Nneq[aSet,bSet])
```

```
}
}
print(N)
print(E)
CHSH<-E[1,1]-E[1,2]-E[2,1]-E[2,2]
print(paste0("CHSH=",CHSH))</pre>
```

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# Efficient Energy Transfer in Network Model of Photosynthesis



Yuta Mitome, Satoshi Iriyama, Keiko Sato, and Igor V. Volivich

# 1 Introduction

Photosynthesis changes the energy from the sun into chemical energy and splits water to liberate oxygen and convert carbon dioxide into organic compounds, especially sugars. Energy from sunlight is used to convert carbon dioxide and water into organic materials to be used in cellular functions such as biosynthesis and respiration. Photosynthesis occurs in plants, algae, and many species of bacteria. Photosynthesis factory in cell consists of two complex of molecular which are antenna and the reaction center. The antenna proteins absorb light and transmit the resultant excitation energy between molecules to a reaction center. Photosynthesis starts with the absorption of a photon of sunlight by one of the light-harvesting pigments in antenna, followed by transfer of the energy to the reaction center, where the primary electron transfer reactions convert the solar energy into an electrochemical gradient. Reaction center chlorophyll-protein complexes are capable of directly absorbing light and performing charge separation events without other chlorophyll pigments, but the absorption cross section (the likelihood of absorbing a photon under a given light intensity) is small. Thus, the remaining chlorophyll in the photosystem and antenna pigment-protein complexes associated with the photosystems all cooperatively absorb and funnel light energy to the reaction center. The transfer of the excitation energy by antenna complex toward the reaction center occurs with a near-unity quantum yield. We study the efficiency of the excitation energy transfer by antenna complex in photosynthesis by using the master equation

Y. Mitome  $\cdot$  S. Iriyama ( $\boxtimes$ )  $\cdot$  K. Sato

Tokyo University of Science, Tokyo, Japan e-mail: iriyama@is.noda.ac.jp

I. V. Volivich Steklow Mathematical Institute, Moskva, Russia

© Springer International Publishing AG, part of Springer Nature 2018 A. Khrennikov, B. Toni (eds.), *Quantum Foundations, Probability and Information*, STEAM-H: Science, Technology, Engineering, Agriculture, Mathematics & Health, https://doi.org/10.1007/978-3-319-74971-6\_7 for the density matrix and discuss the influence of noise from the environment. A relation with a new paradigm of quantum computation which uses chaotic amplifier is mentioned.

#### 2 Quantum Mechanics in Photosynthesis

Recently it was discovered [1] that quantum mechanics might be involved in the process of photosynthesis in some marine algae at the room temperature. Previously the role of quantum effects in the photosynthesis at the room temperature was ruled out because of the quantum decoherence.

The evidence comes from a study of how energy travels across the lightharvesting molecules involved in photosynthesis. The work by Scholes et al. [1] demonstrated that the light-harvesting molecules involved in photosynthesis in a marine algae may exploit quantum processes at room temperature to transfer energy almost without loss.

The antenna proteins absorb light and transmit the resultant excitation energy between molecules to a reaction center. The efficiency of these electronic energy transfers was investigated in many works on antenna proteins isolated from photosynthetic organisms to uncover the basic mechanisms at play. Moreover, they have documented that light-absorbing molecules in some photosynthetic proteins capture and transfer energy according to quantum-mechanical probability laws instead of classical laws at temperatures up to 180 K.

The Fenna–Matthews–Olson (FMO) pigment–protein complex is found in low light-adapted green sulfur bacteria. Under physiological conditions, this complex is situated between the so-called baseplate protein of the large peripheral chlorosome antenna and the reaction center complex, and it is transporting sunlight energy harvested in the chlorosome to the reaction center pigments. The complex is a trimer made of identical subunits, each of which contains seven bacteriochlorophyll molecules.

In [2], the spatial and temporal dynamics of excitation energy transfer through the FMO complex at physiological temperature are investigated. The numerical results demonstrate that quantum wavelike motion persists for several 100 fs even at physiological temperature and suggest that the FMO complex may work as a rectifier for unidirectional energy flow from the peripheral light-harvesting antenna to the reaction center complex by taking advantage of quantum coherence and the energy landscape of pigments tuned by the protein scaffold.

The observation of long-lasting and robust quantum coherence prompts the speculation that quantum effects may play a significant role in achieving the remarkable efficiency of photosynthetic excitation energy transfer. In [3] it is proposed that the FMO complex performs a quantum search algorithm that is more efficient than a classical random walk suggested by the hopping mechanism. Quantum coherence enables the excitation to rapidly and reversibly sample multiple
pathways to search for bacteriochlorophyll molecules that connects to the reaction center.

This contrasts with the long-held view that long-range quantum coherence between molecules cannot be sustained in complex biological systems, even at low temperatures. In [1], two-dimensional photon echo spectroscopy measurements are presented on two evolutionarily related light-harvesting proteins isolated from marine cryptophyte algae. It reveals exceptionally longlasting excitation oscillations with distinct correlations and anti-correlations even at ambient temperature. For the experiments [1], the proteins were isolated from the algae and suspended at low concentration in aqueous buffer at ambient temperature (294 K). The femtosecond laser pulse (25-fs duration) excites a coherent superposition of the antenna protein's electronic vibrational eigenstates (absorption bands). The initial state of the system is thus prepared in a nonstationary state, where electronic excitation is localized to a greater or lesser degree compared to the eigenstates. The time-dependent solution to quantum dynamics for electronically coupled molecules with this initial condition predicts that excitation subsequently oscillates among the molecules under the influence of the system Hamiltonian until the natural eigenstates are restored owing to interactions with the environment.

#### 2.1 Quantum Network Model

Electron transport in organic molecules, such as proteins and polymers, may be described by quantum graphs [4–8]. Indeed it follows one-dimensional pathways (the bonds) changing from one path to other due to scattering centers (the vertices). Charge transport in solids is also well described by quantum graphs.

A simplified version of quantum graph is given by quantum network. Here we describe some recent works on application quantum networks to photosynthesis.

Light-harvesting complexes are typically constituted of multiple chromophores which transform photons into exciton and transport them to a reaction center. Experimental studies of the exciton dynamics in such systems reveal rich transport dynamics consisting of short-time coherent quantum dynamics which evolve, in the presence of noise into an incoherent population transport which irreversibly transfers excitations to the reaction center. In order to elucidate the basic phenomena clearly without overburdening the description with detail, we consider the relevant complexes as systems composed of several distinct sites, one of which is connected to the chromosomes while another is connected to the reaction center. This complex effective dynamics will then be modeled by a combination of simple Hamiltonian dynamics which describe the coherent exchange of excitations between sites and local Lindblad terms that take into account the dephasing and dissipation caused by the external environment.

The pigment-protein complex will be considered as a network composed of distinct sites, one of which receives a single initial excitation, while another is connected to the reaction center.

A network of *N* sites will be described by the Hamiltonian [9]

$$H = \sum_{j=1}^{N} \omega_j \sigma_j^+ \sigma_j^- + \sum_{j \neq k} v_{jk} (\sigma_j^- \sigma_j^+ + \sigma_j^+ \sigma_k^-)$$

where  $\sigma_j^+ = |j\rangle\langle 0|$  and  $\sigma_j^- = |0\rangle\langle j|$  are raising and lowering operators for site *j*, the state  $|j\rangle$  denotes one excitation in site *j*, and  $|0\rangle$  is the zero exciton state. The local site energies are  $\omega_j$ , and  $v_{jk}$  is the coherent tunneling amplitude between the sites *j* and *k*.

The dynamics of the network's density matrix  $\rho(t)$  is described by a Markovian master equation of the form

$$\frac{d}{dt}\rho(t) = -i[H,\rho(t)] + L_{\text{diss}}(\rho(t)) + L_{\text{deph}}(\rho(t))$$

where the local dissipative and pure dephasing terms are described, respectively, by the GKSL super-operators[9]

$$L_{\text{diss}}(\rho) = \sum_{j=1}^{N} \Gamma_j (-\{\sigma_j^+ \sigma_j^-, \rho\} + 2\sigma_j^- \rho \sigma_j^+),$$
$$L_{\text{deph}}(\rho) = \sum_{j=1}^{N} \gamma_j (-\{\sigma_j^+ \sigma_j^-, \rho\} + 2\sigma_j^+ \sigma_j^- \rho \sigma_j^+ \sigma_j^-)$$

The total transfer of excitation is measured by the population in the "sink," numbered N + 1, which is populated by an irreversible decay process with rate  $\Gamma_{N+1}$  from a chosen site k as described by the GKSL super-operator

$$L_{\rm sink}(\rho) = \Gamma_{N+1}(2\sigma_{N+1}^+\sigma_k^-\rho\sigma_k^+\sigma_{N+1}^- - \{\sigma_k^+\sigma_{N+1}^-\sigma_{N+1}^+\sigma_k^-,\rho\})$$

The initial state of the network at t = 0 is assumed to be a single excitation in site 1 (i.e., state  $|1\rangle$ ). The model is completed by introducing the quantity of energy transport efficiency by the population transferred to the sink  $p_{sink}(t)$ , which is given by

$$p_{\rm sink}(t) = 2\Gamma_{N+1} \int_0^t \rho_{kk}(\tau) d\tau.$$

For a fully connected uniform network, when  $v_{jk} = J$  for any  $j \neq k$  and, moreover, when  $\omega_j$ ,  $\Gamma_j$ , and  $\gamma_j$  are the same on every site, i.e.  $\omega_j = \omega$ ,  $\Gamma_j = \Gamma$ , and  $\gamma_j = \gamma$ [9, 10], the dynamics of the density matrix  $\rho$  is given by Efficient Energy Transfer in Network Model of Photosynthesis

$$\dot{\rho}_{00} = 2 \sum_{j=1}^{N} \Gamma_{j} \rho_{jj}$$
$$\dot{\rho}_{ij} = -[2\Gamma + \Gamma_{N+1}(\sigma_{iN} + \sigma_{jN}) + 2\gamma - 2\gamma \sigma_{ij}]\rho_{ij} + iJ\left(\sum_{l \neq j} \rho_{il} - \sum_{l \neq i} \rho_{li}\right)$$

In the case that  $\Gamma = 0$  (no dissipation), an exact analytical solution is found in [9], where one obtains different behaviors of the network for the cases  $\gamma = 0$  and  $\gamma \neq 0$ . If  $\gamma = 0$  then

$$\lim_{t \to \infty} p_{\rm sink}(t) = \frac{1}{N-1}.$$

If  $\gamma \neq 0$  then

$$\lim_{t \to \infty} p_{\rm sink}(t) = 1.$$

The result  $p_{sink}(\infty) = 1$  means that there is the complete excitation transfer. Therefore, it is shown that the dephasing noise leads to the enhancement of the transport of exciton in this quantum network modeling the photosynthetic complexes. It is found in [11] that the quantum and classical capacities for a family of quantum channels in the complex network dynamics can be enhanced by introducing dephasing noise.

Note that a constructive role of chaos in quantum computations was investigated in [12].

#### **3** Transfer Efficiency in a General Case

In this section, we calculate the transfer efficiency for fully connected network in a general case, i.e.,  $\Gamma \neq 0$ . The dynamics of the density matrix  $\rho$  is described in [9] by

$$\dot{\rho}_{ii} = -2\Gamma\rho_{ii} + iJ(R_i - \bar{R}_i) \quad i \neq N$$

$$\rho_{ij} = -2(\Gamma + \gamma)\rho_{ij} + iJ(R_i - \bar{R}_j) \quad i \neq N, \ j \neq N$$

$$\dot{\rho}_{iN} = -(2\Gamma + 2\gamma + \Gamma_{N+1})\rho_{iN} + iJ(R_i - \bar{R}_N)$$

$$\dot{\rho}_{NN} = -2(\Gamma_{N+1} + \Gamma)\rho_{NN} + iJ(R_i - \bar{R}_N)$$

$$\dot{\rho}_{00} = 2\Gamma \mathrm{tr}\rho$$

where

$$R_i = \sum_{j=1}^N \rho_{ij}, \Lambda = \sum_{i=1}^N R_i$$

and  $\overline{R}$  is a complex conjugate of R. The time derivatives of  $R_i$ ,  $R_N$ , and  $\Lambda$  are obtained as

$$\dot{R}_{i} = -iJ\Lambda + iJNR_{i} - 2(\Gamma + \gamma)R_{i} - \Gamma_{N+1}\rho_{iN} + 2\gamma\rho_{ii}$$
$$\dot{R}_{N} = -iJ\Lambda + iJNR_{N} - (2\Gamma + 2\gamma + \Gamma_{N+1})R_{N} + (2\gamma - \Gamma_{N+1})\rho_{NN}$$
$$\dot{\Lambda} = -2(\Gamma + \gamma)\Lambda - \Gamma_{N+1}(R_{N} + \bar{R_{N}}) + 2\gamma \mathrm{tr}\rho$$

Let us put

$$R_N = X + iY$$

we obtain the following differential equations[9]:

$$\begin{split} \dot{\Lambda} &= -2(\Gamma + \gamma)\Lambda - 2\Gamma_{N+1}X + 2\gamma(1 - \rho_{00} - p_{sink}) \\ \dot{X} &= -(2\Gamma + 2\gamma + \Gamma_{N+1})X + (2\gamma - \Gamma_{N+1})\rho_{NN} - JNY \\ \dot{Y} &= -(2\Gamma + 2\gamma + \Gamma_{N+1})Y + JNX - J\Lambda \\ \dot{\rho}_{NN} &= -2(\Gamma + \Gamma_{N+1})\rho_{NN} - 2JY \\ \dot{\rho}_{00} &= 2\Gamma(1 - \rho_{00} - p_{sink}) \\ p_{sink} &= 2\Gamma_{N+1}\rho_{NN} \end{split}$$

The initial conditions are  $\Lambda = 1$ , X = 0, Y = 0,  $\rho_{NN} = 0$ ,  $\rho_{00} = 0$ , and  $p_{sink} = 0$ . In order to calculate  $p_{sink}(t)$ , one can reduce the problem obtaining solutions of above equations into the following equations for the Laplace *s*-domain variables  $\Lambda = \mathcal{L}[\Lambda(t)]$ 

$$(s+2\Gamma+2\gamma)\tilde{\Lambda}+2\Gamma_{N+1}\tilde{X}+2\gamma\,\tilde{p}_{sink}+2\gamma\,\tilde{\rho}_{00}-2\gamma/s-1=0$$
(1)

$$(s+2\Gamma+2\gamma+\Gamma_{N+1})\tilde{X} + (\Gamma_{N+1}-2\gamma)\tilde{\rho}_{NN} + JN\tilde{Y} = 0$$
(2)

$$(s + 2\Gamma + 2\gamma + \Gamma_{N+1})\tilde{Y} + J\tilde{\Lambda} - JN\tilde{X} = 0 \qquad (3)$$

$$(s+2\Gamma+2\Gamma_{N+1})\tilde{\rho}_{NN}+2J\tilde{Y}=0 \qquad (4)$$

$$(s+2\Gamma)\tilde{\rho}_{00} + 2\Gamma\tilde{p}_{sink} - 2\Gamma/s = 0 \qquad (5)$$

$$s\tilde{p}_{sink} - 2\Gamma_{N+1}\tilde{\rho}_{NN} = 0 \qquad (6)$$

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We obtain the solution  $\tilde{p}_{sink}$  as follows:

#### Lemma 1

$$\tilde{p}_{sink} = 4J^2 \Gamma_{N+1} \frac{(s+2\Gamma+2\gamma)(s+2\Gamma+2\gamma+\Gamma_{N+1})}{s\Delta(s)}$$

where

$$\begin{split} \Delta(s) &= (s+2\Gamma)(s+2\Gamma+2\gamma)(s+2\Gamma+2\gamma+\Gamma_{N+1})^2(s+2\Gamma+2\Gamma_{N+1}) \\ &+ J^2 N^2(s+2\Gamma)(s+2\Gamma+2\gamma)(s+2\Gamma+2\Gamma_{N+1}) \\ &+ 2J^2 N(s+2\Gamma) \left\{ \Gamma_{N+1}(s+2\Gamma+2\Gamma_{N+1}) - (\Gamma_{N+1}-2\gamma)(s+2\Gamma+2\gamma) \right\} \\ &- 4J^2 (\Gamma_{N+1}^2 - 2\Gamma_{N+1}\gamma)(s+2\Gamma) + 8J^2 \Gamma_{N+1}\gamma(s+2\Gamma+2\gamma+\Gamma_{N+1}) \end{split}$$

**Proof** From (5) and (6) one has

$$\tilde{\rho}_{NN} = \frac{s\,\tilde{p}_{sink}}{2\Gamma_{N+1}}\tag{7}$$

$$\tilde{\rho}_{00} = 2\Gamma \frac{1 - s\,\tilde{p}_{sink}}{s(s+2\Gamma)} \tag{8}$$

 $\tilde{Y}$  is transformed by (4) and (6) into

$$\tilde{Y} = -\frac{(s + 2\Gamma + 2\Gamma_{N+1})\tilde{\rho}_{NN}}{2J}$$
$$= -\frac{s + 2\Gamma + 2\Gamma_{N+1}}{4J\Gamma_{N+1}}s\tilde{p}_{sink}$$
(9)

From (2), (6), and (7),  $\tilde{X}$  becomes

$$\tilde{X} = -\frac{(\Gamma_{N+1} - 2\gamma)\tilde{\rho}_{NN} + JN\tilde{Y}}{s + 2\Gamma + 2\gamma + \Gamma_{N+1}}$$

$$= -\frac{(\Gamma_{N+1} - 2\gamma)\frac{s\tilde{\rho}_{sink}}{2\Gamma_{N+1}} - JN\frac{s + 2\Gamma + 2\Gamma_{N+1}}{4J\Gamma_{N+1}}s\tilde{\rho}_{sink}}{s + 2\Gamma + 2\gamma + \Gamma_{N+1}}$$

$$= \frac{N(s + 2\Gamma + 2\Gamma_{N+1}) - 2(\Gamma_{N+1} - 2\gamma)}{4\Gamma_{N+1}(s + 2\Gamma + 2\gamma + \Gamma_{N+1})}s\tilde{\rho}_{sink}$$
(10)

One obtains from (3), (9), and (10)

$$\begin{split} \tilde{\Lambda} &= \frac{JN\tilde{X} - (s + 2\Gamma + 2\gamma + \Gamma_{N+1})\tilde{Y}}{J} \\ &= JN \frac{N(s + 2\Gamma + 2\Gamma_{N+1}) - 2(\Gamma_{N+1} - 2\gamma)}{4J\Gamma_{N+1}(s + 2\Gamma + 2\gamma + \Gamma_{N+1})} s \tilde{p}_{sink} \\ &+ (s + 2\Gamma + 2\gamma + \Gamma_{N+1}) \frac{s + 2\Gamma + 2\Gamma_{N+1}}{4J^2\Gamma_{N+1}} s \tilde{p}_{sink} \\ &= \frac{J^2 N^2 (s + 2\Gamma + 2\Gamma_{N+1}) - 2J^2 N (\Gamma_{N+1} - 2\gamma)}{4J^2\Gamma_{N+1}(s + 2\Gamma + 2\gamma + \Gamma_{N+1})} s \tilde{p}_{sink} \\ &+ \frac{(s + 2\Gamma + 2\gamma + \Gamma_{N+1})^2 (s + 2\Gamma + 2\Gamma_{N+1})}{4J^2\Gamma_{N+1}(s + 2\Gamma + 2\gamma + \Gamma_{N+1})} s \tilde{p}_{sink} \end{split}$$
(11)

Substituting (8), (10), and (11) into (1), we have

$$\begin{split} (s+2\Gamma+2\gamma) \frac{J^2 N^2 (s+2\Gamma+2\Gamma_{N+1})-2J^2 N (\Gamma_{N+1}-2\gamma)}{4J^2 \Gamma_{N+1} (s+2\Gamma+2\gamma+\Gamma_{N+1})} s \tilde{p}_{sink} + \\ (s+2\Gamma+2\gamma) \frac{(s+2\Gamma+2\gamma+\Gamma_{N+1})^2 (s+2\Gamma+2\Gamma+2\Gamma_{N+1})}{4J^2 \Gamma_{N+1} (s+2\Gamma+2\gamma+\Gamma_{N+1})} s \tilde{p}_{sink} + \\ 2\Gamma_{N+1} \frac{N (s+2\Gamma+2\Gamma_{N+1})-2 (\Gamma_{N+1}-2\gamma)}{4\Gamma_{N+1} (s+2\Gamma+2\gamma+\Gamma_{N+1})} s \tilde{p}_{sink} + \\ 2\gamma \tilde{p}_{sink} + 2\gamma \frac{2\Gamma \tilde{p}_{sink}-2\Gamma/s}{s+2\Gamma} - 2\gamma/s - 1 = 0 \end{split}$$

Therefore, one obtains

$$\begin{split} (s+2\Gamma)(s+2\Gamma+2\gamma) \frac{J^2 N^2 (s+2\Gamma+2\Gamma_{N+1})-2J^2 N (\Gamma_{N+1}-2\gamma)}{4J^2 \Gamma_{N+1} (s+2\Gamma+2\gamma+\Gamma_{N+1})} s \tilde{p}_{sink} + \\ (s+2\Gamma)(s+2\Gamma+2\gamma) \frac{(s+2\Gamma+2\gamma+\Gamma_{N+1})^2 (s+2\Gamma+2\Gamma_{N+1})}{4J^2 \Gamma_{N+1} (s+2\Gamma+2\gamma+\Gamma_{N+1})} s \tilde{p}_{sink} + \\ 2J^2 \Gamma_{N+1} (s+2\Gamma) \frac{N (s+2\Gamma+2\Gamma_{N+1})-2 (\Gamma_{N+1}-2\gamma)}{4J^2 \Gamma_{N+1} (s+2\Gamma+2\gamma+\Gamma_{N+1})} s \tilde{p}_{sink} + \\ \frac{8J^2 \gamma \Gamma_{N+1} (s+2\Gamma+2\gamma+\Gamma_{N+1})}{4J^2 \Gamma_{N+1} (s+2\Gamma+2\gamma+\Gamma_{N+1})} s \tilde{p}_{sink} - \frac{4\Gamma \gamma s - (s+2\Gamma) (s+2\gamma)}{s} = 0 \end{split}$$

From the above equation, we obtain the lemma.  $\blacksquare$ 

Because the  $\tilde{p}_{sink} = 0$  is five-dimensional equation of *s*, it is known that we generally cannot obtain its complex roots analytically. In this case, we apply the partial fraction decomposition to  $\tilde{p}_{sink}$ . Then we obtain

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$$\tilde{p}_{sink} = \frac{F}{s} + \frac{D(s)}{\Delta(s)} \tag{12}$$

where

$$F = \frac{F_1}{F_2}$$

$$\begin{split} F_{1} &= J^{2}\Gamma_{N+1}(\Gamma+\gamma)\left(2\Gamma+2\gamma+\Gamma_{N+1}\right) \\ F_{2} &= 4\Gamma^{5}+12\Gamma^{4}\gamma+8\Gamma^{4}\Gamma_{N+1}+12\Gamma^{3}\gamma^{2}+20\Gamma^{3}\gamma\Gamma_{N+1} \\ &+5\Gamma^{3}\Gamma_{N+1}^{2}+\Gamma^{3}J^{2}N^{2}+4\Gamma^{2}\gamma^{3}+16\Gamma^{2}\gamma^{2}\Gamma_{N+1}+9\Gamma^{2}\gamma\Gamma_{N+1}^{2} \\ &+\Gamma^{2}\gamma J^{2}N^{2}+2\Gamma^{2}\gamma J^{2}N+\Gamma^{2}\Gamma_{N+1}^{3}+\Gamma^{2}\Gamma_{N+1}J^{2}N^{2}+4\Gamma\gamma^{3}\Gamma_{N+1} \\ &+4\Gamma\gamma^{2}\Gamma_{N+1}^{2}+2\Gamma\gamma^{2}J^{2}N+\Gamma\gamma\Gamma_{N+1}^{3}+\Gamma\gamma\Gamma_{N+1}J^{2}N^{2}-\Gamma\gamma\Gamma_{N+1}J^{2}N \\ &+4\Gamma\gamma\Gamma_{N+1}J^{2}+\Gamma\Gamma_{N+1}^{2}J^{2}N-\Gamma\Gamma_{N+1}^{2}J^{2}+2\gamma^{2}\Gamma_{N+1}J^{2}+\gamma\Gamma_{N+1}^{2}J^{2} \end{split}$$

and D(s) is four-dimensional function of s. Using this decomposition, we obtain the following theorem.

#### Theorem 2

$$p_{sink}(t) = F + \sum_{i=1}^{5} D_i e^{ts_i}$$

where  $D_i$  are functions of  $\Gamma$ ,  $\gamma$ ,  $\Gamma_{N+1}$ , J, and N.

**Proof** In Eq. (12), the second term is decomposed into the form

$$\frac{g(s)}{\Delta(s)} = \sum_{i=1}^{5} \frac{D_i}{(s-s_i)}.$$

where  $s_i$  are five complex roots of equation  $\Delta(s) = 0$ . Applying inverse Laplace transformation to (12), we have the lemma.

Because  $p_{sink}$  is a probability function, there are no positive roots. Therefore we obtain

$$\lim_{t\to\infty}p_{sink}(t)=F.$$

Using this analysis, we can calculate when  $\Gamma > 0$  and  $\gamma > 0$ , it holds

$$\frac{1}{N-1} < \lim_{t \to \infty} p_{sink}(t) < 1.$$



When the time is large enough,  $p_{sink}$  is close to F which is given by the function of  $\Gamma$  and  $\gamma$ . Here, we introduce the following noise ratio r

$$G = \frac{\Gamma}{\gamma}.$$

For several  $\gamma$ , we plot  $p_{sink}$  at time  $t \to \infty$  with changing the ratio G. In Fig. 1, we can see that  $p_{sink}$  increases as G decreases. It means that the transfer efficiency becomes better when the dephasing noise is stronger than the dissipative noise.

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# **Clockwork Rebooted: Is the Universe a Computer?**



**Gregg Jaeger** 

#### 1 Introduction

In recent years, there has been an effort to reduce quantum mechanics and quantum field theory to computation by identifying information-theoretical principles on which physics might be based. This effort can be traced to various earlier suggestions by, among others, Konrad Zuse, John Wheeler, Norman Margolus, and Edward Fredkin [6, 8, 20, 36]. The latter two investigators influenced Richard Feynman to engage the relationship between information and matter via the *simulation* of quantum mechanical behavior using quantum computers [8, 20]. The sense of simulation used by Feynman was the traditional one, which involves calculating the *physical behavior of a mechanical system using another physical system* but stopping short of considering the physical system the behavior of which is simulated to be a mere computational process or simulation.<sup>1</sup> By contrast, the most thoroughgoing attempts to reach this goal seek to remove light and matter from the fundamental picture of the world, leaving only mathematical and informational entities.

Wheeler proposed an information-oriented world picture early on, but one in which humans are required to participate actively in the world's ongoing "creation"

G. Jaeger (⊠)

<sup>&</sup>lt;sup>1</sup>Feynman considered the question of whether quantum devices could simulate the dynamics of extended quantum systems by functioning as quantum computers [6].

Quantum Communication and Measurement Laboratory, Department of Electrical and Computer Engineering and Division of Natural Science and Mathematics, Boston University, Boston, MA, USA e-mail: jaeger@bu.edu

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at the fundamental level by carrying out measurements which give rise to bits of information. This was advocated by him under the enduring slogan "it from bit": "every it—every particle, every field of force, even the space-time continuum itself—derives its function, its meaning, its very existence entirely—even if in some contexts indirectly—from the apparatus-elicited answers to yes-or-no questions, binary choices, bits. It from bit symbolizes the idea that every item of the physical world has at bottom—a very deep bottom, in most instances—an immaterial source and explanation" [33]. This statement has had a lasting impact on informationcentered approaches to physics, although largely at the rhetorical level. Any specific such "sources" and "explanations" proposed for physical behavior, when offered, have been from outside physics; indeed, the most extreme contemporary form of this position, that of Frank Tipler, is explicitly theological [29].

The specific idea that "the universe is a cellular automaton" has been called the Fredkin–Zuse thesis: "the universe is being deterministically computed on some sort of giant but discrete computer" [23, 36].<sup>2</sup> Zuse and others, such as Stephen Wolfram [34], Mauro D'Ariano [4], and Gerard 'tHooft [27], each in a way significantly different from the other, have provided more detail than Wheeler in laying out their information-based theories but each focusing specifically on the *automaton* as the fundamental element in the mathematical reconstruction of physics. Some have argued that no computing system is needed but only the *logical possibility* of a computational *simulation* [29].

There are at least three general positions in terms of which such explorations can be considered: (i) informational ontology, (ii) digital ontology, and (iii) pancomputationalism. The information-ontological position is that all existence is reducible to information structures; it is compatible with the structural realistic philosophy and, so, allows for "informational structural realism" [7]. The digital ontological position is that the ultimate nature of reality is *discrete* in some sense, with a computable, deterministic state evolution; more precisely, it is the position that there are deterministic, discrete processes underlying all physical phenomena. Pancomputationalism is the very specific position that the universe is a computational system equivalent to a Turing machine of some sort. Positions (i)-(iii) can also be combined and have been so in various ways, cf. [7]. Recently, Seth Lloyd has taken an approach to the universe that can be identified as informationontological and explicitly incorporates both the digital ontology and a variant of pancomputationalism, in which the Turing machine in question can be thought of as a quantum cellular automaton but with the caveat that *energy* continues to play an important role in the universe over in addition to information [17, 18]; he has argued that the universe as a whole is *literally* a quantum computer, a notion which, as is shown below, encounters significant difficulties that others, including Tipler, have attempted to remedy via even more radical assumptions.

<sup>&</sup>lt;sup>2</sup>The most detailed conceptual product of this line of attack involving automata is represented by the work of G.M. D'Ariano and collaborators, cf., e.g., [4].

Here, a critical assessment is given of arguments of Lloyd and Tipler, often shared by others, in support of the thesis that the universe is a computer. Section 2 considers the notions of computer and computational capacity involved in these arguments and their dependence on the availability of genuine universal computation as introduced by Alan Turing. An assessment of the role of simulation in attempts to replace physical entities by information in the related informationreductionist and idealist ontologies is also given. Section 3 considers similarities between Llovd's approach and previous historical attempts to identify the universe with a simpler automatic device, namely, the *clock*. Section 4 considers the specific claim that the universe-cum-computer thesis offers a novel explanation for the complexity of the universe, one which is supposed to be lacking, describes how it falls short, and identifies various general difficulties with any attempt to view the physical universe as an automaton capable of universal computation in the precise sense. It is shown here that the ontological identification of the universe with a quantum computer, as is the case for its historical predecessor the "clockwork universe," is unwarranted, whatever value it might have as heuristic or analogy.

#### 2 The Universe as "Giant Quantum Computer"

Let us begin by considering what is meant here by the notion that the universe *is* an enormous information processor. Such notions have been discussed for nearly a century but, in the wake of the growth of quantum computing theory and advanced information technology [12], are now considered quite literally, with the universe being called a *computer* and even an *immaterial* one. The following comments lay out the broad vision of such an informational universe.

The new science of information processing, of which Turing was one of the primary inventors, spawned a technology of information processing and computation. . . . The rapid spread of information processing technologies, in turn, has ignited an explosion of scientific and social inquiry. The result is a paradigm shift of how we think about the world at its most fundamental level. Energy is still an important ingredient of our understanding of the universe, of course, but information has attained a conceptual and practical status equal to—and frequently surpassing—that of energy. [17]

Such declarations of revolution provoke one to review fundamental concepts; in order to properly frame the idea that the universe is fundamentally a computer or only information being processed, it is necessary first to know what such a "computer" is understood by its advocates to be, how it is to process information, and what its relation to apparent matter is supposed to be.

The sort of computer in question is now most often, in the end, said to be the *cellular automaton*, a machine composed of an array of "local," digitally operating units (cells) in a regular array that function automatically together according to predetermined, coded instructions and that can perform simulations. To be a *computer*, it is necessary for such an automaton to be capable of a range of pre-programmed responses to different input data; it is in this way that computers

differ most from non-computing mechanisms, such as clocks, that do not respond to input data while operating but function in accordance with their structures and initial states *only*. Because simulation is also in play here, one should note that something's being *simulable* differs from its *being a simulation* in that the former is *having a calculable behavior*, whereas the latter is *being a calculation of behavior*. Something's having behavior that is capable of being simulated, in itself, implies neither that the thing is merely a calculation nor that it is a computer calculating its own behavior.

Two papers of Lloyd, "Computational capacity of the universe" and "The Universe as quantum computer," are considered here because they represent two importantly different levels of strength of this thesis: the first, in which the thesis may be understood metaphorically, and the second, in which it is clearly taken literally. The first article is more modest in its goal: the computational capacity of the universe is to be estimated, that is, the question of how much computation the universe could perform *if it were* a computer carrying out programs is posed and answered, as Feynman might have had it.

If one *chooses* to regard the Universe as performing a computation, most of the elementary operations in that computation consist of [particles] moving from place to place and interacting with each other according to the basic laws of physics. *In other words, to the extent that most of the Universe is performing a computation, it is "computing" its own dynamical evolution.* 

(emphasis mine). The conclusion of the analysis, a product of essential factors, is that "... the amount of information processing that can have been performed by the Universe as a whole since the big bang... can be shown to have the capacity to perform a maximum of  $(t/t_P)^2 \approx 10^{120}$  elementary quantum logic operations on  $(t/t_P)^{3/4} \approx 10^{90}$  bits registered in quantum fields [with a potential for  $(t/t_P)^2 \approx 10^{120}$  bits if gravitational degrees of freedom are taken into account]. Here,  $t \approx 10^{10}$  years is the age of the Universe and  $t_P = \sqrt{G\hbar/c^5} = 5.391 \times 10^{-44}$  s is the Planck time..." [17], that is, a very large number of such operations might have taken place that accord with the laws of physics *were* the universe a computer, that is, a device engineered and programmed to perform "conventional digital computations."

Again, the question is taken up in the first article hypothetically and more metaphorically than literally as indicated, for example, by the use above of quotation marks around the word *computing*. Lloyd points out that the numbers of operations and bits involved here could be interpreted in several ways: (I) "As upper bounds to the amount of computation that can have been performed by all the matter in the Universe since the Universe began"; (II) "As lower bounds to the number of operations and bits required to simulate the entire universe on a quantum computer [1, 16, 35]"; (III) "If one chooses to regard the Universe as performing a computation," that is, as a computer, "these numbers give the numbers of ops and bits in that computation." Here, (1) a distinction is made between digital computation and other computation because it is said that "Only a small fraction of the Universe is performing conventional digital computations," and,

so, (2) the universe is not *just* a system "computing its own evolution." A clear accounting of the total amount of computation that could have been performed within the universe is given in the form of a specific value corresponding to its history of physical activity from an information-processing perspective.

Although the sort of "computer" under consideration is not given by reference to a specific schema, the relationship between the elements of the process of computation and physics are directly engaged via the consideration of specific operations involving logic gates, memory registers, and bits of information. The number of elementary logic operations performable by a given physical system is taken in accordance with the Margolus–Levitin theorem [21], which dictates that the minimum time required for the system to move from one quantum state to an orthogonal quantum state is given as

$$\Delta t = \pi \hbar/2E , \qquad (1)$$

where E is the average energy of the system above that of the ground state, providing an upper limit to the computation rate. It is noted that this also applies for a number of systems operating in parallel: Although with N quantum logic gates involved, each gate operates N times more *slowly* than a single logic gate operating with energy E, the maximum total number of operations per second is the same.

The number of bits capable of being held in the largest possible memory register is found by first noting the amount of information, I, that can be registered in the physical universe, which is derivable from the number of orthogonal quantum states available to it, given its physical properties.

$$I = S/k_B ln2 , \qquad (2)$$

where *S* is the maximum system entropy and  $k_B$  is the Boltzmann constant. The maximum entropy of the universe is then calculated assuming it to have volume  $V \approx c^3 t^3$ . (The gravitational degrees of freedom are included by applying the Bekenstein bound and the holographic principle.) The ultimate result of the derivation is that the maximum number of bits that could be registered by the universe using matter, energy, and gravity is found to be  $\approx c^2 t^2/l_P^2 = t^2/t_P^2$ .

Under interpretation I above, the inferred number of quantum gate operations  $(\approx 10^{120})$  that might have been performed could be helpful to future engineers in that, for example, it serves as an upper bound to attempts to harness ever large portions of the universe for the purpose of computation.<sup>3</sup> More pertinently to our more general considerations here is that physicists, in general, would consider this

<sup>&</sup>lt;sup>3</sup>This is not unlike the consideration of how much solar energy a Dyson sphere could collect. More modestly, it was long ago noticed that the solar system (or the Jupiter system) can be used for the calculation of time, when conjoined with a Stonehenge-like construction or the simple addition of a sundial on the Earth within it; see Sect. 3.

simply physical behavior, whether occurring in a computer or not.<sup>4</sup> This claim offers a version of the least problematic manner of approaching the behavior of the universe via the notion of computation: *heuristically*. Interpretation II, by contrast, effectively involves a science-fiction-like scenario in which our universe is simulated by a computer of some super-user outside of it, who could in principle provide it with input or reset it, much as physical behavior was considered in the picture of the universe as a created clockwork considered by some in the times preceding Newton, discussed in Sect. 3 below. Finally, on interpretation III, as Lloyd himself points out, "that the numbers of bits and ops calculated here represent the actual memory capacity and number of elementary quantum logic operations performed by the Universe—is more controversial. ... whether or not it makes sense to identify an elementary quantum logic operation with the local evolution of information-carrying degrees of freedom by an average angle of  $\pi/2$  is a question whose answer must await further developments in the relationship between physics and computation" [17].

The latter paper of Lloyd takes up the question of whether the universe is *literally* a quantum computer evolving in such a quantum mechanical way and so strong forms of interpretations II and III. There, the nature of computation is specified in a more precise, computer-scientific fashion by making explicit use of the theory of automata and, as a variant of the pancomputationalist thesis, taken to accord with the Zuse–Fredkin thesis. Its arguments therefore go beyond the conservative question of the universe being similar to a computer to its being *identified literally* as a computer: The universe is thought of as *not only* metaphorically "computing its own evolution" or being simulated from some basic level of physical reality but of "simulating *itself*." There are many assumptions involved in such a move, such as the validity of considering the quantum state of the entire universe in Hilbert space, that are similar to those of various attempts make sense of the Everett interpretation of quantum mechanics [13] which, although they should not be forgotten, we pass over here in the interest of considering the architecture of Lloyd's argument.

The relevant sense of computation and general sort of computer considered is that of the *Turing machine*, in its several variants, including the universal and quantum versions. Recall that Turing machine is an *abstract machine* having a reader (its "head") of symbols encoded on some medium (its linear "tape", "memory") that computes a certain fixed partial computable function from input strings over a finite set of symbols (its "alphabet"). Intuitively, a computable mathematical function is an effectively calculable function. Recall also that a function is *partially computable* if, again intuitively, it is one for which we have an algorithm enabling one to compute its value for the elements of the domain on which it operates but for elements outside of its domain it will continue to compute forever, attempting to obtain a value without ever indicating that no value will be found [5].

<sup>&</sup>lt;sup>4</sup>Indeed, for example, Lloyd's colleague Neil Gershenfeld has written a book on the subject, *The Physics of Information Technology*, that culminates in the consideration of quantum computation and communication and clearly lays out its physical practice [10].

The set of rules (instructions) specifying the stepwise operation of the Turing machine's "control unit"—such as specifying the move to be made by the tape, forward or backward one step along the sequence, upon the head's reading a given symbol—is its "action table." The action table can be fixed and also stored as a string on the tape. A Turing machine is an abstraction from aspects of physical computing devices to idealized features, most notably, those of being truly digital, of *never failing* to follow the actions prescribed for it, and of having access to *indefinitely large quantities of the resources* associated with an indefinitely large memory tape, providing unlimited storage capacity. Thus, its realization inherently goes beyond the resources of any finite universe or its contents, though a universe of a sufficiently large number of degrees of freedom might behave *approximately*, that is, imperfectly relative to this idealization.

In this later analysis, Lloyd focuses on *universal* computing, asking "How...can one claim that the universe *is* a computer? The answer lies in the definition of computation...According to Turing, a universal digital computer is *a system that can be programmed to perform any desired sequence of logical operations...*", that is, a machine that can reproduce the computations of any other machine of a similar sort. Turing first suggested the universal computing machine (universal Turing machine) in 1936. Logically, in principle

It is possible to invent a single machine which can be used to compute any computable sequence. If this machine U is supplied with a tape on the beginning of which is written the ["standard description" of an action table] of some computing machine M, then U will compute the same sequence as M. [30]

Both the action table and the input can be encoded as sequences of symbols, the input string (i.e., sequence of symbols) following this action table string on the tape. The universal Turing machine expects its tape to have just this—a string providing an action table, followed by a string for the input tape—and computes the tape that such a Turing machine so encoded would itself compute. Thus, the universal Turing machine is a Turing machine that can simulate an *arbitrary* Turing machine on *arbitrary* input; at a given step in its operation, the state of the Turing machine should include the expression on the tape at that point in operation, the internal configuration of the machine's control unit, and the symbol being "scanned." The question of whether the universe itself is such a universal digital computer is then considered by Lloyd via two questions: (1) Is the universe capable of performing universal digital computation in the sense of Turing? That is, can the universe or some part of it realize the universal Turing machine? (2) Can a universal Turing machine efficiently simulate the dynamics of the universe itself?

One could immediately object that computers (like clocks) by general definition are *artifacts*, devices designed to be prepared and actively used by agents, that is, tools created for technological application, not found things. Assumptions about superphysicists or deities do not explicitly appear in this chapter nor, presumably, would they be made by the vast majority of the scientists in the context of science itself. In the absence of assumptions of a supernatural sort, the question at hand is immediately rendered a scientific nonstarter if the universe is not assumed *not*  to be an artifact. We briefly discuss this point in the following section—for now, let us simply keep in mind that the sense of "programming" involved would have to be different from the usual one, which assumes the existence of a programmer. In this case, some looser sense of operating according to an a priori given set of algorithmic rules, without regard to how this might have come about, must instead be under consideration, so that the everyday sense of computer is *not* what must actually be involved here, despite claims or first impressions to the contrary.

The Turing machine schema is quite abstract, incorporating very little in the way of even quasi-physical characteristics beyond those of having components, involving (spatiotemporal) sequentiality and discreteness (being "digital"). As mentioned, additional structure is given by Lloyd to the notion of computation involved via a specific model of implementation of universal computation, the *cellular automaton* model, basic elements of which were first provided by John von Neumann [32]. The idea that the universe is such a cellular automaton—first mentioned in print by Martin Gardner [9], who cited Fredkin's previous advocacy of it—is part of the *strong version* of the thesis that the universe is a computer. "That is, not only does the universe compute, and only compute, but also if one looks at the guts of the universe—the structure of matter at its smallest scale—then those guts *consist of nothing more than bits undergoing local, digital operations*," that is, the ontology is both informational and digital in the senses given in our introduction.

For Lloyd, this version of the computer-universe thesis is to be phrased in the form of the following variant-pancomputationalist question, (3) "Is the universe a cellular automaton?", to which he responds, "the answer to this question is No. In particular, *basic facts about quantum mechanics prevent the local dynamics of the universe from being reproduced by a finite, local, classical, digital dynamics*" (emphasis mine). But, for him, this is only because the physics of the universe cannot be *classically* simulated: He sees the difficulty with this portrayal *not in the notion of universe as computer itself*, in accordance with the digital ontology or in the pancomputationalist thesis, *but rather in considering the universe as a computer that operates classically* instead of in a "quantum" way.

The analysis accordingly continues by considering a computer that is to exhibit computational behavior that is not "classical" but "quantum" at its fundamental level. "If we quantize our three questions," Lloyd argues, the strong computeruniverse thesis can be saved. He argues that the first question in "quantized" form "(Q1) Does the universe allow quantum computation? has the provisional answer, Yes. As before, the question of whether the universe affords a potentially unlimited supply of quantum bits remains open. Moreover, it is not clear that human beings currently possess the technical ability to build large scale quantum computers capable of code breaking. However, from the perspective of determining whether the universe supports quantum computation, it is enough that the laws of physics allow it." That quantum computation can be carried out using physical systems in specialized, non-universal form is uncontroversial, of course. However, the assumption of the presence of an "unlimited supply of quantum bits" is one of the greatest relevance to the question of *universal* computer in the fully precise sense under consideration, which demands *perfect* simulation capability, which is first given short shrift by Lloyd and subsequently dropped. In fact, there is no good reason to assume that an unlimited supply of any resource is available in the universe, particularly given that such a thing is, by its very nature, ultimately unverifiable.

Regarding the second "quantized" question, "(Q2) 'Can a quantum computer efficiently simulate the dynamics of the universe? ... The Feynman-Lloyd results show that, unlike classical computers, quantum computers can simulate efficiently any quantum system that evolves by local interactions, including for example the standard model of elementary particles. While no broadly accepted theory of quantum gravity currently exists, as long as that theory involves local interactions between quantized variables, then it can be efficiently simulated on a quantum computer. So the answer to the quantized question 2 is Yes" (emphasis mine). Although this may be significant, it does not establish the desired conclusion, namely, that this be possible for the entire universe from within, assuming a positive answer to Q1. Note that the programming involved is finally to be "accomplished by inducing interactions between the variables of the simulator that imitate the interactions between the variables of the system to be simulated," the system and the simulator being quantum systems in some sense, as "simulation is a process by which one system is made to mimic another." Moreover, the "the efficiency of a simulation depends on how hard it is to set up the simulator-system correspondence, to control the simulator to perform the simulation, and to extract its results" [16]. Of course, unless an entire sub-universe controlled by hidden structure is present, for which there is currently no evidence, one should not expect that a quantum simulator will be more efficient than the system it is simulating, given the results of the first paper establishing the limits of the universe-cum-computer; on the contrary, it would need to carry out further operations in order to perform the simulation due to differences in its physical characteristics from the system simulated, rendering it less efficient. Hence, what would be expected to be accomplished by an internal simulation is part of the universe being simulated by the complementary, greater portion of it.

Again, leaving out both supernatural factors and the trivial sense in which anything behaves as itself, any portion of the universe to be simulated would require another part to be simulating it, which means, according to the analysis of Lloyd's first paper, only part the universe could be simulated from within the universe, because the remaining portion would be involved in simulating the remaining part. The only way the entire universe could be simulating itself from within *in any nontrivial sense* would be that the universe involves some perfect mirror symmetry of behavior which is just one part simulating the other part and vice-versa, with perfect efficiency, again something for which there is no evidence. As for being simulated from without, there is no evidence of or explanatory superiority in assuming the existence of anything beyond the universe which would serve as a simulating computer.

Finally, the ultimate question, "(Q3) 'Is the universe a quantum cellular automaton?'," is engaged. Lloyd argues that "while we cannot unequivocally answer this

question in the affirmative, we note that the proofs [cited] that show that a quantum computer can simulate any local quantum system efficiently immediately imply that any homogeneous, local quantum dynamics, such as that given by the standard model and (presumably) by quantum gravity, can be directly reproduced by a quantum cellular automaton. Indeed, lattice gauge theories, in Hamiltonian form, map directly onto quantum cellular automata. Accordingly, all current physical observations are consistent with the theory that the universe is indeed a quantum cellular automaton," and so "the universe is observationally indistinguishable from a giant quantum computer" [18]. There is a clear gap in the argument here: it passes immediately over the subtle relations between observation and theory and requires an extreme reductionist assumption-that all phenomena from those of the entire range of physics to chemistry to biology to human cognition reduce to those of elementary particles and fields. Even were all observations made of the universe so far consistent with it being a giant, elaborate quantum computer/cellular automaton, they are insufficient for its identification with one solely on the basis of there being a mapping from the description of quantum systems (as described by current physical theory) to the input and output of automata. At best, one has an alternative theory of physics, similarly to the situation of Bohmian mechanics as an alternative to standard quantum mechanics, but not a reduction of the physical to pure information.

Recall that, by virtue of the limited physical resources available to it, any finite computer is only an approximation of a universal Turing machine because the universal machine contains an indefinitely extendable memory ("tape"). Lloyd considers this a minor concern. "The question of whether or not infinite memory space is available is not so serious, as one can formulate notions of universal computation with limited memory. After all, we treat our existing electronic computers as universal machines even though they have finite memory (until, of course, we run out of disc space!). The fact that we possess computers is strong empirical evidence that laws of physics support universal digital computation." This conclusion should be regarded with significant suspicion, particularly given the limited range of situations to which our computing technology has been applied, relative to the broad spectrum of available physical phenomena which we have only recently begun to probe due to very recent advances in various diverse technologies and its limited performance in more challenging situations such as long-range and extreme weather prediction. We see that a central assumption, the precise characterization of the computer as a universal Turing machine, is effectively *dropped* in the course of the argument in favor of an approximate version. Given that the level of precision required in the ability of the computer to provide simulations-that is, the requirement of "perfect simulation"-this creates a critical vulnerability.<sup>5</sup> Lloyd ultimately acknowledges this: "...it is an open question whether this simulation can be performed efficiently in the sense that a relatively small amount of computational resources are devoted to simulating what happens in

<sup>&</sup>lt;sup>5</sup>Especially for further arguments of Tipler, discussed directly below.

a small volume of space and time" [17]. After all, the universe is composable and decomposable into small, ephemeral, fundamental components [14].

Next, Lloyd looks to quantum mechanics and randomness to move from the classical universal Turing machine model of quantum computing to the quantum cellular automaton model. The nature of the computation achievable with the quantum cellular automaton presumably encounters the same difficulty of failing to achieve genuine universality, again because the existence of a finite supply of resources is better supported than an infinite supply, to say the least. Thus, one sees-after passing over the issue of the extent to which all current physical observations are supportive of the standard model, lattice gauge theories and the hypothetical quantum gravity theories (a notoriously difficult thing to construct with adequacy) mentioned here-that Lloyd's argument for the thesis that the universe is a giant quantum computer, in effect, amounts instead to an argument for the far weaker thesis that it is not manifestly inconsistent with physics or the theory of computation applied in broad strokes, leaving aside the fact that it cannot meaningfully be considered a genuinely universal computing machine. For even this weaker thesis to turn out to be correct, either (i) future observations involving future technological developments in experimental practice must continue to make no distinction between it and that of standard physics alone or, if that turns out not to be the case, that (ii) any observable distinction between the supposed simulation and physics must tell in favor of the automaton. The character of the history of physical theory as an ongoing sequence of conceptual revolutions strongly suggests that (i) will not be the case; there is currently no reason to suppose (ii). In addition to the claim that all physical activity can be simulated discretely, there is a supposition that once physical behavior is reduced to the operation of this automaton, a reduction of all phenomena involved in observing it would also be accomplished, because that is necessary for the agreement with our having obtained empirical data involving them, both directly and using technology. However, the reduction of all activity ranging in scope from fundamental physics, to the biological and cognitive functioning of physicists, to the activity of the quantum automaton would still have to be demonstrated, which is an exceedingly tall order: there are a great number of hurdles for demonstrating the reduction of cognitive, biological, and chemical phenomena to physics, to say the least.

The greatest difficulty with the argument that Q3 is to be answered in the affirmative, with the universe simulated by "pure information," is that it involves either a circularity or an infinite regress. In particular, it requires that *either* the universe computes itself into existence, something which is a priori impossible, *or* the universe is a reified simulation arising from a simulation that simulates it, which depends on the existence of another reified simulation simulating *it*, etc., reaching no ultimate ground. The mere *logical consistency* of the notion of the universal quantum Turing machine schema does not in itself make the universe identically and only such a schema. No adjustment of this world picture intended to circumvent this problem is offered by Lloyd to strengthen the argument. Frank Tipler has attempted independently to address this problem from an epistemological angle by considering a series of levels of computer code implementation, where one "is only aware of

the higher levels of implementation, which can be thought of as levels of reality. The lowest level can be termed *ultimate reality*... we cannot know if the universe in which we find ourselves is actually ultimate reality"[29], as portrayed in David Cronenberg's film *Existenz*. That is, he introduces the assumption that science faces a fundamental epistemic limitation. He also asks the question "Is it possible for the universe to be in precise one-to-one correspondence with some simulation?", answering "I think it is, if we generalize what we mean by simulation... we don't really need the physical computer; the initial sequence of integers and the general rule (instructions or map) for replacing the present sequence by the next is all that is required."

The claim is that the "actual universe is something in the collection of all mathematical objects," because "the universe has a perfect simulation, and we all agree to identify the universe with its perfect simulation, that is, with its emulation." But, there is no particular reason for one to agree with this and several reasons not to. First and foremost, there is no reason why one should view the universe as a mathematical object, because it is not actually just like one. Tipler argues that one is compelled to make this identification by the Principle of Identity of Indiscernibles (PII), according to which, in its simplest form, any (assumed) two entities not differing in their properties are to be considered *one and the same* entity. Tipler argues that this follows from the PII because a perfect computer simulation, being perfect, would be indistinguishable from the physical universe. Thus, he argues, "at the most basic ontological level, the physical universe is a concept." This argument fails because, in order for the PII to support this identification, one must accept that the universe is such an object and nothing more in order to enable the required indistinguishability at the logical level, empirical evidence aside. The PII was introduced by Leibniz as a principle of logic, but it does have relevance to mathematics and so to physics and thus could, in principle, be applied in the physical context [15]. However, the PII does not justify the identification of the universe with its own simulation unless it is a valid assumption first that the universe is a purely mathematical object so comparable to others.

Could the universe be pure mathematics? Well, for one thing, the sources of our knowledge of the two differ: the former can be experienced directly via the senses, whereas the former cannot be and, in fact, is *not* so experienced; our experience of the physical world is external experience in the straightforward sense. Any attempt to explain this would require the externality of the physical world to be an illusion. In addition, the history of such experiences in science is that the unexpected and the scientifically inexplicable—that is, inexplicable at that specific time in the development of physics—occurs.<sup>6</sup> The mathematical and the physical differ in the respect that mathematics provides the description of various aspects of the physical

<sup>&</sup>lt;sup>6</sup>Except, perhaps, outside of an idealist metaphysics in which its appearance is understood as conspiratorial in nature. Whether or not it is, in some sense, a concept in the mind of a supernatural entity is, quite simply, *not a scientific question*. Indeed, that the world "kicks back" is one of more straightforward arguments for realism in relation to the physical, cf., e.g., [24].

behavior of something *and only that*, whereas the latter *is* the behavior *as a property* of that something, a thing that acts independently. Were it otherwise, there would be and will have been no need for theoretical physics as distinct from both experimental physics and direct experience because the latter two, not differing from the first, could be discovered entirely by reasoning alone; this has never been found to be so.

The ability to provide an algorithm for reproducing the content of a mathematical description of the behavior of a physical system has no bearing on the *existence* of the system referred to by the description, but means only that one could thereby create a simulation of the behavior of something based on a means other than direct data curation. Moreover, our manner of engagement with the universe is constantly changing, and some of its objects are repeatedly found in a reproducible fashion to be doing things beyond current comprehension and expectations; the history of science is that of ongoing series of unpredictable conceptual revolutions in conjunction with our constant accumulation of ultimately consistent empirical data. One could argue that this is because the scientific community does not yet have a complete understanding of the *programming* of the hypothetical nonphysical automaton, but one is then again confronted with the question: *Of what scientific benefit* is the additional hypothesis that physics is in some sense a simulation? In the absence of novel phenomena underlying such a purported simulation, the assumption of one over lawfully characterized physical behavior is unfounded.

The argument from simulation aside, the thesis that the universe is one giant computer requires that both (a) our accepted scientific approach to the world be deeply mistaken and (b) either that there be an entirely different underlying level of existence beyond the physical, having no evident additional physical implication, or that the world exist only as a concept. When sufficient conceptual precision is required in the formulation of the strong version of the computer-universe thesis and in the explication of the relationship of a simulated universe to scientific activity, the notion is seen not only to be extremely speculative and conceptually flawed, but also to be scientifically unwarranted.<sup>7</sup>

#### **3** Clockwork Rebooted

There is a range of different sorts of automata with, at one end, the very simple mechanisms which have nothing external to their "central processor" (no tape or connection to an environment for "input" or "output") and which proceed through a succession of states, through the finite automata such as Turing machines for which a memory tape is moved along in only one direction or are otherwise restricted with regard to memory and, at the other end of the range, those without such limitations, the universal Turing machines, and those that incorporate aspects of quantum state

<sup>&</sup>lt;sup>7</sup>See Sect. 4 below for the discussion of an argument that attempts to justify this world picture by its purported ability to provide a novel scientific explanation.

transitions [2, 12]. To better understand the possibility of a relationship of physics to automata, let us consider the similar, previously considered claim that the universe is a specific type of automatic device, the *clock*. The clock itself can be thought of as an indicator of a physical parameter, time.<sup>8</sup> Like computers, clocks can be designed to function independently for large numbers of cycles of operation or long periods without intervention or repetition. The Clock of the Long Now, for example, is an extremely large clock (hundreds of feet tall), designed to run entirely independently and chime periodically in a way that, each time its chimes ring, the resulting melody is one that will not repeat until 10,000 years have passed [3].

Consider the thesis that the universe—in its original proto-Newtonian conception in which time is considered absolute—is an automaton, a very basic nonrelativistic classical clockwork. Many natural physical processes within it can serve as such clocks, that is, specialized time-indicating automata. Consider, for example, that (1) the motion of a point on the Earth's surface relative to the location of the sun in the sky gives rise to a shifting shadow about a prominence in the desert—say the Atacama, where some weather stations have never reported rain—reliably indicating the hour during the daytime, and (2) Cepheid variable stars in the heavens at night have highly regular periods of brightness alteration serving as cyclical indicators of time having periods of up to many days. The notion of the universe serving as a clock, in its essential aspects, is already present in Genesis, where the day and the year are basic periods is addressed. "And God said, Let there be lights in the expanse of the sky to separate the day from the night, and let them serve as signs to mark seasons and days and years..." [28].

The way that many parts of the universe have been thought of as constituting components of a giant clockwork is similar to the way that the universe is currently being considered by some to be a quantum computer. Indeed, the clock can even be categorized as a limited, special purpose reckoner. The common feature of the notions of clockwork universe and computer universe is functional: they are both automata in the general sense. The first version of the universe as automaton was the idea that the universe is a deterministic clockwork. This notion was explicitly used by Oresme in the fourteenth century, having grown out of the notion of the machina mundi introduced two centuries before in the work of Robert Grosseteste and of Johannes de Sacrobosco, who used it in his astronomical text Sphaera, later used by Galileo Galilei in his Paduan lectures [22]. The need for accurate determination of ship longitude in the era depended on accurate, universal timekeeping, raising the significance of this technology to European society much as the demands of accounting, communication, and space exploration have done for computing technology in our time. Galileo argued in 1612 that the positions in orbit of the four brightest moons of Jupiter, the Medicean "stars," could be used as a universal clock set in the heavens for all to see with a simple telescope [26].

<sup>&</sup>lt;sup>8</sup>A particularly interesting example of a calculating clockwork to keep in mind in this regard is the *Antikythera* mechanism [19] and clockwork-based simulators of motion of celestial objects.

Copernicus used the expression *machina mundi* and wrote in his *On the revolution of the heavenly spheres* that the universe "was created for us by the best and most systematic craftsman." *Machina mundi* refers to the notion of a "mechanical," ordered world—the Latin coming from the Greek  $\mu \alpha \chi \alpha v \dot{\alpha}$ , from  $\mu \eta \chi \alpha v \dot{\eta}$  referring primarily to compound technological devices. However, as the historian of science Stephen Snobelen has emphasized, the notion "that the universe is like a machine or clockwork mechanism" was not used by Newton himself or accepted by him. He points out that "not a single example of Newton unambiguously referring to the universe as a clockwork system has surfaced" and that

The myth of Newton's clockwork universe is one of the most persistent and pervasive myths in the history of science...Examples of the myth abound....Michio Kaku says: 'Newton believed that the universe was a clock. A gigantic clock—a machine—that God wound up at the beginning of time, and its been ticking ever since due to his laws of motion.' ...Regrettably, while the scholarly community has begun to outgrow this myth, it had a hand in perpetuating it, especially during the first half of the twentieth century. The situation changed dramatically in the second half of the twentieth century, although not all at once. [25]

Snobelen notes that for Newton, any portion of the universe is in need, not only of being created but also of being externally *sustained*; it would, at various points in its evolution, fail to "tick" properly and be in need of tinkering and so would be much more like a clock of ordinary experience than the ideal, perfectly ordered, deterministic "clockwork universe" would have it be. The notion of the universe as a perfect, deterministic, automatic device is a pre-Newtonian notion that failed not only to convince the greatest contributor to classical physics, who took its character as a created entity seriously, but also under the demands of later evidence. The ideal clockwork notion applied to the universe by others required it to be a compound system flawlessly reducible to component parts and never in need of repair or of resetting; it is one that, in practice, actual machines fail to match. Although it is valuable to be able to devise physical clocks because they can serve particular practical needs, much as with computers' providing numerical and other output, the notion has turned out not to fit the observed universe under either close philosophical scrutiny or later empirical evidence.

#### **4** The Complexity Argument

The notion of the "computer universe" shares difficulties in common with that of the "clockwork universe" and, as we have seen, has additional ones arising from the more complicated nature of the universal computer in comparison with the clock. In Sect. 2 above, it was noted that Lloyd's positive answer to his Question 3 supporting this notion was argued for by taking the universe to be entirely and only a self-sufficient "perfect simulation" of known physics. On its own, this appears to be either odd metaphysical speculation or playful science fiction. But, one can still ask whether there could be something to compel one scientifically to accept the

*literal identification* of the entire universe as an automaton, particularly a purely mathematical one that could be said to be a "computer without hardware." Is there some naturalistic explanatory value to the thesis that the universe is literally and primarily such an information processing automaton that has been overlooked above?

Perhaps recognizing the highly speculative nature of the claim that the universe is a quantum computer, Lloyd goes on rhetorically to ask "immediate question... 'So What'?" if O1–O3 all receive affirmative answers. Similarly to Tipler's making the radically reductive assumption that a perfect physical simulation of basic physics would also automatically provide a perfect simulation of the phenomenal level of human experience of the world, Lloyd first takes these affirmative answers to imply that the universe would be "observationally indistinguishable from a giant quantum computer." Then, in an attempt to show the scientific value of the notion of the universal computer as a simulation, he claims that the answer to this "so what?" is that this would offer something "new and important about its behavior," namely, why "the universe is so complex" [18]. In particular, he argues that physics as computation provides a distinct advantage over "the ordinary laws of physics," because such a large computer together with randomness (quantum fluctuations) would yield "complex, ordered structures with high probability," much like the infamous singes dactylographes (typing monkeys) of Borel, which he mentions [18], yet more efficiently.

Let us now see whether this is the case. First, to set the stage, consider the sort of argument involved in the simpler, "monkey" theorems regarding the provision of ordered states via randomness.<sup>10</sup> Suppose a symbol generator that can produce *n* symbols is taken to produce a sequence of *m* of them independently in a way described by a uniform probability distribution, that is, with no preference of one symbol over any other. Then, each symbol has an equal chance of appearing in any given position in the sequence, doing so with the probability  $\frac{1}{n}$ . The probability of producing any given such an *m*-symbol sequence in one attempt is, therefore,

$$P_n(m) = \left(\frac{1}{n}\right)^m \tag{3}$$

and the probability of not having thus produced it is

$$P_n^{(\text{not})}(m) = 1 - P_n(m) , \qquad (4)$$

<sup>&</sup>lt;sup>9</sup>It is supposed that the ordinary laws of physics together with randomness cannot provide an adequate such explanation.

<sup>&</sup>lt;sup>10</sup>Cf. [11] for a textbook example.

so that it will fail to be produced in l attempts with probability

$$P_n^{(\text{not})}(m,l) = \left(1 - P_n(m)\right)^l = \left(1 - \left(\frac{1}{n}\right)^m\right)^l.$$
 (5)

Therefore, as the number of attempts available for producing the sequence increases,  $P_n^{(\text{not})}(m, l)$  becomes increasingly small, and approaches 0 in the limit as the number of attempts *l* tends to infinity, that is, the probability of *not producing the sequence* will be found to be as small as desired for an appropriately large *l*, so that the probability of *producing* the desired sequence approaches unity, that is, becomes nearly certain.<sup>11</sup> To produce a given sequence with certainty, either an *infinite* number of generators or an *infinite* amount of time is required be *sure* to produce any desired sequence: Given a finite number of these generators working for an amount of time even on the order of the age of the universe, it will not be that with any probability as large as desired that a given complex ordered sequence, such as the text of *Hamlet*, would be produced.

We see that requirements guaranteeing that any sequence will be produced in this way are not satisfied in this situation under consideration here. However, despite his reference to Borel's *singes dactylographes*, Lloyd's argument is not that such random activity allows a giant quantum automaton to give rise *directly* to the complexity found in the universe but rather that it can produce relatively short sequences which *in turn* provide circumstances in which a complex state such as that currently obtaining for the universe as a whole could be generated: He argues that, instead of a number of 'monkeys,' that is, random symbol sequence generators producing sequences relating directly to the state of the universe, sequences can be randomly produced that themselves serve as *programs*, that is, sequences serving as logical operations to be subsequently carried out, because "many complex, ordered structures can be produced from short computer programs, albeit after lengthy calculations." Moreover, the argument goes, the sequences need not be obviously logically related to the state: "the shortest programs to produce these complex structures are necessarily random. If they were not, then there would be an even shorter program that could produce the same structure. So the monkeys, by generating random programs, are producing exactly the right conditions to generate structures of arbitrarily great complexity" [18].

This suggests that a good explanation to an important question is to be found here. Yet this is questionable, given that the proffered explanation is embedded in the context of a world picture in which physics is taken to be exactly and only a hardware-free simulation. One basic possible problem with this is that, in that context, there are no actual, physical "monkeys" to "type." There must be some entity that carries out such "programs" for anything physical at all, of whatever complexity, to result. Second, even if this potential difficulty is put aside, there

<sup>&</sup>lt;sup>11</sup>It also does not matter whether one has one symbol-producer working serially on the l attempts or several simultaneously operating sequence generators.

remains an issue having nothing to do with being able in principle to generate the complex, current state of the universe in the way suggested, namely, the significance of any added value that having an answer to this question would bring, for it is anyway to be expected that a system as large as the universe would be complex, however it came about, not least of all because its many parts are not all causally connected with each other. Indeed, if the universe were found to be exceedingly simple and orderly, that simple order would be and is what is in greater need of *explanation*, as is the case, for example, for the relative uniformity of the cosmic microwave background. The move to programming scripts for cellular automata raises the issue of the ability of such a process to affect all of the relevant portions of the universe in a uniform fashion, as it would have to do. Even more significant than this second issue is that our *particular universe* with its behaviors and its specific structures is singular, like the original Hamlet manuscript. All evidence suggests that it has evolved through one and only "run." Related to this is that, again, the universe is not programmable, in particular, it cannot be read, written upon, or have its state reset.<sup>12</sup>

For one to assent to the *identification* of the universe as an automaton, beyond internal coherence of the notion and its compatibility with observation, neither of which has been established, it should offer one a *superior* world picture to that of current physics. Aside from the several logic issues and the radical reductions required for the automaton to perfectly account for physical behavior *as observed*, this thesis appears to fail to be superior according to the standard aesthetic and ontological simplicity criteria for theory choice. This is perhaps not surprising, given that the arguments offered in support of this thesis have been ones essentially from information theory rather than physics; the explanatorily strongest argument offered, that from complexity, regards a measure of something informational rather than physical, however much it can be productively applied to aspects of physical systems. The automaton may be relatively elegant and simple as mathematical "machines" go, but it lacks explanatory force and simplicity in its application to the physical and cosmological realms.

#### 5 The Universe is Not a Computer

The arguments considered here which have been presented for the identification of the quantum universe with a computer—and, more specifically, with a universal computing machine or with a cellular automaton—fail to establish it. There are several reasons specific to the theory of computation for this. First, because the universe is bounded in time and storage capacity, it is not an instance of a genuinely

<sup>&</sup>lt;sup>12</sup>In order to be considered a true computer and not, for example, just an elaborate clock, the universe operating according to a program would need to be capable of reacting *conditionally* accordingly to something like variable external circumstances (input).

*universal* computing automaton and so is not able to perform perfect simulations of an arbitrary Turing automaton as suggested. Second, because the universe is not a system that can be read out or, most importantly, react conditionally to external input data or reset by a programmer, however much formal similarity its behavior might otherwise seem to have to a computer, it is not a *computer* in a sense distinct from more primitive automata, such as clocks, that cannot do so and cannot perform repeated trials of its total program. Third, the notion of the universe as fundamentally, rather than incidentally, operating or having portions being viewable as digital computing devices, encounters the problem that the very distinction between the analog and digital that underlies the notion of a digital universe (whether classical or quantum) may be unsound [7]; Turing himself saw the very distinction between analog and digital as ultimately artificial when applied in the physical world: "... strictly speaking there are no such machines [as discrete state machines]" [31].<sup>13</sup> It can be argued that this distinction is one only introduced by epistemic agents and one that can be made only relative to degree of abstraction, cf. [7]. Indeed, Turing's own position was only that "there are many kinds of machine, which can profitably be thought of as being discrete state machines" as a heuristic but not literally as being so [31].

The assertion that the universe is a quantum computer can be viewed as an updating of the notion of the universe as an automatic mechanism so as to accommodate the fact, unknown in previous eras, that the universe at smaller scales, in many instances, behaves according to quantum, not classical theory, and requires the presence of the mathematics of probability at the fundamental level, a mathematical tool which can be used to quantify information. However more abstract in character it might become as a result of shifting the emphasis from matter to information, updating the notion of the universe as automatic device mainly obscures the fact that the notions of the computer universe and the clockwork universe are similar in that they both seek to replace, reduce, or explain the state of the universe, its contents, and its order and complexity in terms of idealized automata. Despite the invocation of various information-theoretical concepts and the numerical calculations deployed by its advocates, the purported results of the quantum cellular automaton model discussed above are beside the point in regard to the existence of an underlying informational ontology. The notion of automatism in itself, whether "material" or "informational," at least in the absence of significant additional assumptions, adds nothing of explanatory value to physics beyond what natural laws can achieve directly. One formulates better scientific theory by avoiding any literal or metaphorical use of the notion of the automaton when providing theory applicable to the physical universe.

<sup>&</sup>lt;sup>13</sup>Moreover, it is normally in the analog, rather than the digital, that is, the continuation that one finds the infinite within bounded ranges. Note that the difference between information and the characteristic of digitality is the basis of the difference between the digital ontological and information-ontological stances.

Although there may be heuristic value in considering physical systems from the point of view of the theory of computation—much as there is some value, for example, to considering the motion of balls moving on a flat surface within a rectangular boundary also containing various holes as part of a game of billiards under certain specific circumstances, namely, those in which we have chosen to become actively involved and to use them as such—this adds nothing to the understanding of the *physical* behavior underlying it.

#### 6 Conclusion

The identification of the universe with a quantum computer, like that of its historical predecessor, the identification of the universe with a clockwork, is unwarranted: Although there is little question that, under appropriate conditions, portions of the universe could in principle be used as quantum computing devices over relatively short periods of time compared with the age of the universe and that it is logically possible that it could be simulated given *unlimited* computational resources, the universe itself as a whole is better not identified as a computer, whether of a quantum sort or otherwise. The various arguments provided for this thesis, using the notion of simulation or attempts to use it to explain the physical complexity of the universe, fail either because they lead to infinite regress or because the physical universe does not share all the characteristics of the sort of computer required, in the case of some of the arguments or, in case of the remaining argument, fail to provide a superior explanation for the ordered complexity of the universe to the one that can be provided using the standard conception of the universe and its physics. Considering physical processes as behaving similarly to computers, including quantum computers, may be beneficial as a heuristic-in particular, in the search for novel mathematical bases for physical theory, because it may provide various means for breaking away from what may ultimately be found to be unnecessary assumptions, such as that continua are necessary for the mathematical description of the behavior of the physical universe-but this remains to be shown.

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### External Observer Reflections on QBism, Its Possible Modifications, and Novel Applications



Andrei Khrennikov

#### 1 Introduction

As is well known, QM which manifests huge success in the mathematical representation of the basic problems of physics of the microworld suffers heavily of diversity of interpretations of this mathematical representation. QBism is one of the most recent attempts to provide a consistent interpretation of QM, free of all possible mysteries and paradoxes. In this short review, I present my personal reflections on QBism.<sup>1</sup> The paper starts with a historical remark on the first years of QBism. It continues with brief representation of its essentials, mainly referring to and citing its creators. Then the main postulates of QBism are critically analyzed.

We point out that the cornerstone of QBism is the interpretation of QM as a machine for update of probabilities based on a modification of *the classical formula of total probability* (FTP). In this paper we emphasize this dimension of QBism

A. Khrennikov (🖂)

International Center for Mathematical Modelling in Physics and Cognitive Sciences, Linnaeus University, Växjö, Sweden

e-mail: Andrei.Khrennikov@lnu.se

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<sup>&</sup>lt;sup>1</sup>The discussion is definitely not systematic enough to serve as an introduction to QBism. If the reader seeks a scholarly discussion, a good starting point would be the fairly recent books of Friederich [25] and Timpson [80], for example (see also their papers [24, 79]). Readers who are already conversant with QBism are unlikely to find anything new in our presentation. These notes have two closely related aims: (a) to add some details to the history of foundation and evolution of QBism and (b) to send a message to the part of physical community which still strongly rejects QBism as a totally unphysical interpretation of QM. It is important that these notes were written by one of the active representatives of this anti-QBist lobby which still strongly dominates in quantum foundations. I definitely have not been completely converted into QBism, but recently I started to find rational points in QBist views on quantum theory, and I want to present these points, but, so to say, with a spicy sauce of doubt.

which is typically shadowed by the emphasis on the subjective interpretation of probability and private agent perspective to quantum measurements. The latter emphasize often makes the impression that QBism is merely about philosophy of quantum mechanics. (At least this is my personal experience based on hundreds of conversations about QBism.) It is important to stress that QBism's version of FTP is very special, and it is derived with the aid of *symmetric* informationally complete positive operator-valued measures (SIC-POVMs).<sup>2</sup> This choice of quantum modification of FTP is critically analyzed. The main output of this analysis is that it seems that QBism would earn a lot by proceeding without the assumption of symmetry of IC-POVM or may be even without appealing to information completeness.

In this paper QBism is compared with two interpretations of QM which are very close to QBism but in two totally different aspects, cf. [24]. In Sect. 5 we compare QBism with the Växjö interpretation [45, 46, 50] of QM. The latter is a contextual realistic interpretation based on the objective interpretation of probability (with sympathy [42, 49] to von Mises' frequency probability theory [81–83]). From the first sight, there is nothing in common between these two interpretations; see [45] and [27] for the critical debate. However, they have one very important thing in common: in both interpretations, the Born rule is treated as a quantum modification of classical FTP, although the modifications of FTP are mathematically very different. In Sect. 8 QBism is compared with the information interpretation of QM elaborated by Zeilinger [86, 87] and Brukner [7–10]. From the first sight, these interpretations are very similar. However, we shall show that, in fact, they differ crucially.

The rest of the paper is devoted to interpretations of probability. Here diversity is not so huge as in QM, but the gap between two main interpretations, objective and subjective, is no smaller than the gap between two basic trends in interpretations of QM, realist (in the spirit of Einstein) and non-realist (in the spirit of Copenhagen). We present the original Kolmogorov interpretation of probability [60] (which is not so well known, even in the probability community) and compare it with the genuine frequency interpretation of von Mises [81–83] and subjective interpretation of de Finetti [20, 21].

Then, following de Finetti, we point out that consistent appealing to the subjective interpretation of probability should lead to reconsideration of the objective treatment of the scientific methodology. Finally we point that de Finetti was even more revolutionary than QBists, because his subjective treatment of scientific method was not restricted to "special quantum world." In some way QBists made one good turn but refrain from another, they revolutionary declared the private agent (user) perspective to knowledge about "quantum world," but they were not brave

<sup>&</sup>lt;sup>2</sup>From this viewpoint, i.e., QM as a probability update machine, QBism is similar to the Växjö interpretation of QM. The latter is a realist contextual statistical interpretation, so ideologically it is opposite to QBism. However, the probability update basis makes it close to QBism. At the same time, even this closeness is only formal, since the QBism version of generalized FTP differs crucially from the Växjö version.

enough to follow de Finetti completely, i.e., to declare the private agent perspective for knowledge about classical world as well. The latter is an exciting project still waiting its realization.

As was pointed out at the very beginning of the paper, it presents *critical* reflections about QBism. In particular, some doubt is expressed regarding how much the QBists' subjectivism is actually important for the overall project. I note that there may be some sort of rapprochement between subjectivism and objectivism. Of course, this may significantly underplay the role of the QBists' subjectivity in the resolution of the old puzzles about measurement and locality in quantum mechanics. At the same time, it may stimulate QBists to concentrate their efforts on development of the "probability update machinery" dimension of QBism. The same can be said about critique of another basic element of QBism—derivation of SIC-POVM-based modification of FTP.

#### 2 QBism Childhood in Växjö

In 2001 QBism was strongly represented at the second Växjö conference on quantum foundations, "Quantum Theory: Reconsideration of Foundations" (QTFT2001), June 17–21, 2001. We (organizers and participants of this conference) strongly believed that the quantum information revolution would soon lead to great foundational revolution. Unfortunately, dreams did not come true. Nevertheless, the energy of the quantum information revolution was transformed in a series of stormy debates during the series of the Växjö conferences, 2000–2015. Although these debates did not lead to a complete resolution of the basic problems of quantum mechanics, they clarified some of these problems, especially the problem of the interpretation of a quantum state. QBism was definitely one of the main foundational outputs of the quantum information revolution.<sup>3</sup>

As the organizers of QTFT-2001, I and C. Fuchs both dreamed for the creation of a consistent and clear interpretation of QM, free of mysteries and paradoxes. However, we went in two opposite directions. I followed Einstein and later, as the result of better understanding of Bohr's writings [4–6] (and especially comments of A. Plotnitsky on them), tried to unify Einstein's realist statistical interpretation with Bohr's contextual interpretation by filtering out Bohr's non-realist attitude; see [45, 46, 50] for so-called *Växjö interpretation* of QM. Both Einstein and Bohr (as well as, e.g., von Neumann) used the statistical (ensemble) interpretation of quantum probabilities. Therefore the Växjö interpretation is based

<sup>&</sup>lt;sup>3</sup>Besides QBism, we can mention the *Växjö interpretation* of QM (statistical realist and contextual) [45, 46] derivation of the QM-formalism from simple operational principles, D' Ariano [17, 18] and Chiribella et al. [15, 16] (first time this project was also announced in Växjö), and the *statistical Copenhagen interpretation* (statistical non-realist) which final formulation was presented at the Växjö-15 conference by A. Plotnitsky and based on his previous studies about the probabilistic structure of QM [67–70].

on this statistical interpretation. It also was important that as a student, I was strongly influenced by A.N. Kolmogorov and B.V. Gnedenko<sup>4</sup> who always emphasized that probability is objective and statistical. Later, after PhD, I discovered the works of von Mises [81–83]. I really enjoyed this reading! Von Mises' interpretation of probability differs from Kolmogorov's interpretation. Nevertheless, Misesian probability is also objective and statistical. In any event, nobody of them (Einstein, Bohr, von Neumann, Kolmogorov, Gnedenko) and neither I would agree with de Finetti's slogan *Probability does not exist!* and with his subjective interpretation of probability. My views on interpretation of quantum states and probabilities were

C. Fuchs went in the opposite direction; he (with support of C.M. Caves, R. Schack, and D. Mermin) openly, loudly, and proudly declared [13, 14, 26, 28, 29, 31–35] that QM is only about knowledge (and here QBists are very close to the fathers of the Copenhagen interpretation, N. Bohr and W. Heisenberg [4–6]). But this widely supported viewpoint was completed with very strained and revolutionary declaration that this quantum knowledge has to be treated as *personal knowledge*. Subjective interpretation of quantum probability matches perfectly such a private agent perspective of quantum theory. QBists emphasize the Bayesian probability update and decision-making structure of the quantum probability calculus.

From my viewpoint, the latter is one of the main contributions of QBism in clarification of quantum foundations. Independently this viewpoint was presented in the framework of the Växjö interpretation, sections [45, 46, 50].

At the beginning I and C. Fuchs did not recognize this similarity, namely, interpretation of the calculus of quantum probabilities as a machinery for update of probabilities. And it is clear why at that time I emphasized realism and objectivity and C. Fuchs privacy and subjectivity. And the probability update dimension was shadowed by these philosophic issues. This explains the appearance of Fuchs' anti-Växjö paper [27].

Nevertheless, intuitively I felt sympathy to QBism, but roots of this sympathy were not clear for me.<sup>5</sup> At the Växjö-15 conference, QBism was widely represented and celebrated its worldwide recognition. Nobel Prize Laureate T. Hänsch presented the great lecture about QBism as the only possible consistent foundational basis of quantum information theory. This lecture ignited the stormy debate, and T. Hänsch and C. Fuchs were attacked by the realist opposition (leaded by L. Vaidman and A. Elitzur).

presented in [45].

<sup>&</sup>lt;sup>4</sup>Gnedenko was the author of one of the best textbooks on probability theory [36]. The introduction of this book contains the manifesto of objective probability and sharp critique of subjective probability.

<sup>&</sup>lt;sup>5</sup>Once Christopher Fuchs asked me: "Why did you support QBism so strongly during the Växjöseries of conferences? QBism contradicts your own Växjö interpretation!" In fact, I was not able to explain this even for myself. I had a feeling that QBIsm can be useful. But how? and where?

## **3** Quantum Theory Is About Evaluation of Expectations for the Content of Personal Experience

In contrast to von Neumann, Fuchs proposed to interpret probability in the subjective way. To present essentials of some theory, sometimes it is practical simply to cite works of its creators (this is definitely not the case of Bohr, or von Neumann, or even myself). Here we cite Fuchs and Schack [34, pp. 3–4]:

The fundamental primitive of QBism is the concept of experience. According to QBism, quantum mechanics is a theory that any agent can use to evaluate her expectations for the content of her personal experience.

QBism adopts the personalist Bayesian probability theory pioneered by Ramsey [73] and de Finetti [21] and put in modern form by Savage [74] and Bernardo and Smith [3] among others. This means that QBism interprets all probabilities, in particular those that occur in quantum mechanics, as an agent's personal, subjective degrees of belief. This includes the case of certainty - even probabilities 0 or 1 are degrees of belief. ...

In QBism, a measurement is an action an agent takes to elicit an experience. The measurement outcome is the experience so elicited. The measurement outcome is thus personal to the agent who takes the measurement action. In this sense, quantum mechanics, like probability theory, is a single user theory. A measurement does not reveal a pre-existing value. Rather, the measurement outcome is created in the measurement action.

According to QBism, quantum mechanics can be applied to any physical system. QBism treats all physical systems in the same way, including atoms, beam splitters, Stern-Gerlach magnets, preparation devices, measurement apparatuses, all the way to living beings and other agents. In this, QBism differs crucially from various versions of the Copenhagen interpretation...

An agent's beliefs and experiences are necessarily local to that agent. This implies that the question of nonlocality simply does not arise in QBism.

We shall revisit the interpretational issues of QBism after the presentation of its basic probabilistic principle in the next session.

#### 4 QBism as a Probability Update Machinery

The previous section might create the impression that the subjective interpretation of quantum probabilities is the key point of QBism. It might be that even its creators have the same picture of their theory. For me, the essence of QBism is neither this very special interpretation of quantum probabilities nor the concrete agent perspective of QM. For me, the main ideological invention of C. Fuchs and R. Schack was treatment of the mathematical formalism of QM as a generalization of the classical Bayesian machinery of the probability update. This viewpoint clarifies the meaning of the basic rule of QM—the Born rule as a complex Hilbert space representation of generalization of the *classical formula of total probability* (FTP).

This dimension of QBism is identical to the probability update dimension of the Växjö interpretation [45, 46, 50]. There are a few differences.

One is the difference in the interpretations of probability. However, nowadays I do not consider it as the crucial difference (in contrast to my first debates with C. Fuchs in 2001–2003, [45] and [27]). Really, in a long series of updates, the subjective and statistical viewpoints coincide.<sup>6</sup>

For me, the main difference between QBism and the Växjö interpretation is in the mathematics, not in physics or in philosophy. Both the Växjö interpretation of QM [43, 44, 50] and QBism [29, 31–35] *the Born rule is treated as generalization of classical formula of total probability* (FTP) in the language of linear operators. However, these interpretations are based on two totally different mathematical generalizations of FTP—both matching the Born rule.

Starting with the Born rule, QBists derived their special version of generalized FTP which is based on a very special class of the quantum probability updates, based on atomic instruments with SIC-POVMs; see Appendix 1.

We now briefly present the QBism scheme for the probability update, namely, the representation of the Born rule as a generalization of FTP; here we again follow Fuchs and Schack [29, 31-34].<sup>7</sup>

Quantum states are represented by density operators  $\rho$  in a Hilbert space assumed to be finite dimensional. A measurement (an action taken by the agent) is described by a POVM  $F = (F_j)$ , where j labels the potential outcomes experienced by the agent. The agent's personalist probability<sup>8</sup>  $p(F_j)$  of experiencing outcome j is given by the Born rule:

$$p(F_i) = \operatorname{Tr} F_i \rho. \tag{1}$$

Similar to the probabilities on the left-hand side of the Born rule, QBism regards the operators  $\rho$  and  $F_j$  on the right-hand side as judgments made by the agent, representing her personalist degrees of belief.

<sup>&</sup>lt;sup>6</sup> In the mentioned debates, I also was strongly against the anti-realist attitude of QBism. However, now this attitude does not disturb me so much as 12 years ago. Either I started to understand QBists' views on the problem of realism better or QBists changed their views (or both). QBism needs not appeal to any subquantum model providing the ontic description of quantum systems and processes, in particular, to hidden variables. Nor is QBism concerned with struggle against such models. It seems that the personal position of C. Fuchs is similar to the position of N. Bohr [4–6]: for quantum model or not. For the present state of development of quantum theory, this is the most reasonable position, cf. with Zeilinger's strong anti-realist attitude. Moreover, just recently (through a series of email exchanges), I understood better the position of C. Fuchs on the problem of non-realism/realism. Surprisingly QBists (at least C. Fuchs) do not consider QBism as a non-realist interpretation of QM.

<sup>&</sup>lt;sup>7</sup>We remark that in coming considerations, the interpretation of probabilities does not play any role. They can be subjective probabilities (as originally in QBism), but they also can be statistical, e.g., Kolmogorovian or Misesian, as well.

<sup>&</sup>lt;sup>8</sup>As was remarked, probability can be interpreted in other ways. The situation is similar to the classical probability update. De Finetti would treat this probability as subjective but Kolmogorov, or Gnedenko, or von Mises as statistical.
The Born rule as written in Eq. (1) appears to connect probabilities on the left-hand side of the equation with other kinds of mathematical objects—operators—on the right-hand side.

QBists assume that the agent's reference measurement is an arbitrary *infor*mationally complete POVM,  $E = (E_i)$ , such that each  $E_i$  is of rank 1, i.e., is proportional to a one-dimensional projector. Such measurements exist for any finite Hilbert space dimension. Furthermore, we assume that, if the agent carries out the measurement  $E = (E_i)$  for an initial state  $\rho$ , upon getting outcome  $E_i$ , he would update to the post-measurement state

$$\rho_i = \frac{E_i \rho E_i}{\mathrm{Tr} E_i \rho E_i}.$$

This is the assumption of atomicity of this quantum instrument. (This is a strong constraint on the class of instruments which are used in QBism. It would be interesting to analyze the possibility to proceed with arbitrary instruments.)

Because the reference measurement is informationally complete, any state  $\rho$  corresponds to a unique vector of probabilities

$$p(E_i) = \operatorname{Tr} E_i \rho,$$

and any POVM  $F = (F_j)$  corresponds to a unique matrix of conditional probabilities

$$p(F_i|E_i) = tr(F_i\rho_i).$$

The operators  $\rho$  and  $F_j$  on the right-hand side of the Born rule are thus mathematically equivalent to sets of probabilities  $p(E_i)$  and conditional probabilities  $p(F_j|E_i)$ . (We remark that all these probabilities depend on the state  $\rho$ , i.e.,  $p(E_i) \equiv p_{\rho}(E_i), p(F_j) \equiv p_{\rho}(F_j), p(F_j|E_i) = p_{\rho}(F_j|E_i)$ .)

Then Fuchs and Schack [29, 31–34] stress that POVMs as well as quantum states represent an agent's personal degrees of belief. However, this is not essential for the formal scheme of probability update. We can as well interpret the probabilities  $p(E_i)$  and  $p(F_j|E_i)$  statistically. The main point which was rightly emphasized by them is that the Born rule can be interpreted as one special form of transformation of probabilities:

$$p(F_i) = f(p(E_i), p(F_i|E_i)).$$
 (2)

Comparing with the classical FTP which is in these notations written as

$$p(F_j) = \sum_i p(E_i) p(F_j | E_i), \qquad (3)$$

they formulate the statement which I consider as the cornerstone of QBism:

The Born rule is one of the forms of generalization of FTP.

For me, the main problem of QBists is that they started with a SIC-POVM  $E = (E_i)$ . They say [31] "The Born rule allows the agent to calculate her outcome probabilities  $p(F_j)$  in terms of her probabilities  $p(E_i)$  and  $p(F_j|E_i)$  defined with respect to a counterfactual reference measurement." This reference to counterfactuals is really redundant. Why should SIC-POVM measurement appear at all? As in the Växjö approach, one can start with an arbitrary POVM measurement, say  $G = (G_i)$ , to define probabilities  $p(G_i) = \text{Tr}\rho G_i$  providing information about the state  $\rho$ .

By taking into account such a possibility of generalization of QBist consideration<sup>9</sup> I completely agree with the following statement of QBism [31]:

In QBism, the Born rule functions as a coherence requirement. Rather than setting the probabilities  $p(F_j)$ , the Born rules relates them to those defining the state  $\rho$  and the POVM  $F = (F_j)$ . Just like the standard rules of probability theory, the Born rule is normative: the agent ought to assign probabilities that satisfy the constraints imposed by the Born rule.

The functional relationship given by (2) depends on details of the reference measurement. In the special case that the reference measurement is a symmetric informationally complete (SIC)-POVM, (2) takes the simple form:

$$p(F_j) = \text{Tr}F_j \rho_i = \sum_i \left( (d+1)p(E_i) - \frac{1}{d} \right) p(F_j|E_i).$$
(4)

This is a consequence of the complete information representation of a quantum state and the use of SIC-POVMs; see Appendix 1.

# 5 QBism and the Växjö Interpretation of Quantum Mechanics

As was pointed out, QBists have conjectured that the FTP-like form of the Born rule (4) may be used as the basic (and may be the unique) axiom in a derivation of quantum theory. The key question that remains is in identifying what minimal further principles must be added to Eq. (4) for the project to be successful.

This program is identical to attempts to justify the Växjö interpretation  $[45, 46, 50]^{10}$  by deriving the complex Hilbert space formalism from the generalized

<sup>&</sup>lt;sup>9</sup>However, for QBists the above generalization—to start the probability update scheme with an arbitrary POVM measurement  $G = (G_j)$  and not with a SIC-POVM  $E = (E_i)$ —seems to be unacceptable. They are really addicted on SIC-POVMs and on completeness of information gained at the first step, information about the state, even at the price of appearance of counterfactuals.

<sup>&</sup>lt;sup>10</sup>This is a contextual realistic interpretation of QM. Contextuality is understood in the wider sense than typically in modern discussions on Bell's inequality in which contextuality is reduced to joint

FTP with an interference term [42, 47, 49, 50]. This FTP arises as the additive perturbation of classical FTP; the perturbation term represents the interference of probabilities which is characteristic for incompatible quantum observables. We shall briefly present the derivation of such a generalized FTP later, after the coming foundational discussion.

Similarly to QBists, I tried to derive the complex Hilbert space structure of QM solely from the latter generalization of FTP, i.e., without additional axioms. This approach was successful only for dichotomous observables. Already the case of three-valued observables is very difficult mathematically. Here only a partial success was achieved by Nyman and Basieva [64, 65].

Maybe Fuchs and Schack are right that one has to find additional axioms leading to the complete derivation of the quantum formalism, as, e.g., was done by D' Ariano et al. [15–18]. However, proceeding with such additional axioms does not match completely the basic principle that the quantum formalism is just a special form of the probability update generalizing the classical Bayesian update. This principle is very attractive in both QBism and the Växjö interpretation (though they have different mathematical realizations).

Completing a generalized probability update scheme by additional operational principles diminishes the value of this scheme as the *unique fundamental principle* lying in the ground of QM. It shifts the line of research to more traditional operational approaches starting with the pioneer contribution of Heisenberg [38], then Mackey [62], and nowadays D' Ariano et al. [15–18]. In this paper we do not plan to analyze the operational axiomatics of D'Ariano et al. However, in previous derivations of QM from "natural operational principles," complex Hilbert space was always encrypted, practically explicitly, in one of the axioms; see, e.g., Mackey [62] for one of the first operational derivations of the quantum formalism.

We now derive the quantum analog of FTP, FTP with the interference term, in the simplest (but very important for foundations) case—for the two-slit interference experiment. Here we follow Feynman [23]. The author's contribution is the representation of Feynman's argument by using conditional probabilities and in this way interpreting interference of probabilities in the two-slit experiment as a violation of classical FTP and generalization to arbitrary incompatible observables [43, 48–50] and recently POVMs [54].

Consider the following pair of observables a and b. We select a as the "slit passing observable," i.e., a = 0, 1 (see Fig. 1) (we use indexes 0 and 1 to be close

measurement with another observable. In the Växjö interpretation, contextuality is understood in the spirit of Bohr [4–6]: as dependence of the outcomes of observables on the whole experimental arrangement. In particular, violation of Bell's inequality is a consequence of complementarity of experimental contexts corresponding to different pairs of orientations of polarization beam splitters. In some sense the Växjö interpretation is an attempt to unify the views of Einstein and Bohr. This interpretation matches with the statistical interpretation of probability. In works [42, 47] the frequency (von Mises [81–83]) approach to the notion of probability was explored. We remark that both Einstein and Bohr shared the statistical viewpoint on probability; see [71] for the corresponding discussion.





to qubit notation), and observable *b* as the position on the photosensitive plate (see Fig. 1). We remark that the *b*-observable has the continuous range of values, the position *x* on the photosensitive plate. We denote p(a = i) by p(i) (i = 0, 1) and p(b = x) by p(x). Physically the *a*-observable corresponds to measurement of position (coarse grained to "which slit?"), and the *b*-observable represents measurement of momentum.

The probability that a photon is detected at position x on the photosensitive plate is represented as

$$p(x) = \left| \frac{1}{\sqrt{2}} \psi_0(x) + \frac{1}{\sqrt{2}} \psi_1(x) \right|^2$$
  
=  $\frac{1}{2} |\psi_0(x)|^2 + \frac{1}{2} |\psi_1(x)|^2 + |\psi_0(x)| |\psi_1(x)| \cos \theta,$  (5)

where  $\psi_0$  and  $\psi_1$  are two wave functions, whose squared absolute values  $|\psi_i(x)|^2$  give the distributions of photons passing through the slit i = 0, 1.

Here we explored the rule of addition of complex probability amplitudes, a quantum analog of the rule of addition of probabilities. This rule is the direct consequence of the linear space structure of quantum state spaces.

The term

$$|\psi_0(x)| |\psi_1(x)| \cos \theta$$

implies the interference effect of two wave functions. Let us denote  $|\psi_i(x)|^2$  by p(x|i), then Eq. (5) is represented as

$$p(x) = p(0)p(x|0) + p(1)p(x|1) + 2\sqrt{p(0)p(x|0)p(1)p(x|1)}\cos\theta.$$
 (6)

Here the values of probabilities p(0) and p(1) are equal to 1/2 since we consider the symmetric settings. For general experimental settings, p(0) and p(1) can be taken

as the arbitrary nonnegative values satisfying p(0) + p(1) = 1. In the above form, classical FTP

$$p(x) = p(0)p(x|0) + p(1)p(x|1)$$
(7)

is violated, and the term of interference  $2\sqrt{p(x|0)p(0)p(x|1)p(1)}\cos\theta$  specifies the violation.

Modification (6) of classical FTP (7) is very natural; the classical law is additively perturbed. If the interference term is equal to zero, then quantum FTP is transferred into classical FTP, cf. with Qbism's FTP (4). Thus by the Växjö interpretation, the quantum formalism is about modification of classical FTP by additional interference terms.

We remark that classical FTP is a theorem of the commonly used the measuretheoretic model of probability [60]. To prove it one has to operate with the fixed probability measure or in more rigorous mathematical framework in the fixed probability space. Thus in purely probabilistic terms, a violation of FTP implies the impossibility to embed statistical data collected in a few experiments in a single probability space. Since in the Kolmogorov approach the probability space is fixed, we can say that the quantum probabilistic calculus which leads to a violation of FTP is an example of non-Kolmogorovian probability model.

#### 6 Agents Constrained by Born's Rule

In 2001 the private user's experience viewpoint on quantum *physics* made me really mad, and this was the main reason for my anti-QBism attitude [45].<sup>11</sup> However, recently I understood that the situation may be not so bad as one can imagine by reading the QBism manifests, such as presented in Sect. 3. Maybe this long way to understanding is not only my fault. QBists judge too highly the private user interpretation of QM comparing with the problem of concretization of the class of such private users. I remember that in 2001 in Växjö, I asked C. Fuchs: "Suppose that your user, Ivan, lives in taiga by hunting and he has never heard about QM. Would Ivan make proper predictions about simplest quantum experiments?" I do not remember the precise answer of C. Fuchs, but it seems it was a long story about his version of FTP (4), which was considered by me as totally irrelevant to my question. Then I asked C. Fuchs the same question during a few next Växjö conferences, and I did not get a satisfactory answer (at least from my viewpoint). Recently, during the Växjö-2015 conference, where QBism was heavily represented by the talks of

<sup>&</sup>lt;sup>11</sup>The strong anti-Copenhagen attitude in the first declaration about the Växjö interpretation was partially a consequence of the active advertising of QBism at Växjö-2001 conference. My reaction (as many others) was: "See, the Copenhagen interpretation finally led to such a perverse view on QM as the private agent's perspective on the quantum state."

its founders, I got a new possibility to discuss its foundations with C. Fuchs, and in the after-conference email correspondence, I finally got a clear answer to my old question. Of course, this answer could be found in the works of Fuchs and Schack, but it was dimmed by the very strong emphasis on the private agent perspective.

So, if I understood C. Fuchs correctly, the class of agents has to be *constrained!* And the basic constraint is given by the Born rule which is treated as an empirical rule reflecting some basic features of nature; see Sect. 4 for discussion. For a moment, for us the concrete natural basis of the Born rule is not important. It is important that QBism uses this rule as an information constraint to determine a class of so to say "quantum agents," i.e., those who "get tickets to the QBism performance." Thus private users of QM are those who know the main rule of the game: *the probability update for quantum systems has to be done with the aid of the Born rule (or QBist version of FTP; see (4)).* It seems reasonable that such agents would produce reasonable predictions. Thus Ivan from Taiga is excluded from QBist agents—finally!

The Born rule constraint is the basic necessary condition for entrance to the QBism club. At the same time, it is practically sufficient conditions, because other personal characteristics of an agent making predictions about quantum experiments play subsidiary roles in relation to these predictions. Thus in principle one may invent an abstract (conceptual) QBism agent who makes her probabilistic predictions about experiment results on the basis of the Born rule. In this way QBism comes closely to the recent version of the information interpretation of QM of Zeilinger-Brukner proposed by Brukner [7]. However, while QBistd would, in principle, accept an interpretation a la Brukner, i.e., referred to a conceptual agent, they definitely would not like to diminish the role of private agent perspective in QBism.

#### 7 Is QBism a Version of the Copenhagen Interpretation?

By following the talks of C. Fuchs or R. Schack, I always had the feeling that their views are very much in the spirit of Copenhagen. Bohr and Heisenberg always pointed out that the quantum formalism is not about the "quantum physical world" but it is a representation (mathematical) of measurements performed on micro-systems. Thus, from their viewpoint QM is about knowledge (especially for Heisenberg). Do Fuchs and his coauthors, Schack, Mermin, and Caves, try to say the same thing by just using the special interpretation of probability, the subjective probability? I still do not have my own definite opinion about this issue. Therefore here I present a long citation of D. Mermin who knows QBism much better than me and who claims that QBism differs crucially from all interpretations in the spirit of Copenhagen (see [63, pp. 7–8]):

A fundamental difference between QBism and any flavor of Copenhagen, is that QBism explicitly introduces each user of quantum mechanics into the story, together with the world external to that user. Since every user is different, dividing the world differently into external

and internal, every application of quantum mechanics to the world must ultimately refer, if only implicitly, to a particular user. But every version of Copenhagen takes a view of the world that makes no reference to the particular user who is trying to make sense of that world.

Fuchs and Schack prefer the term "agent" to "user." "Agent" serves to emphasize that the user takes actions on her world and experiences the consequences of her actions. I prefer the term user to emphasize Fuchs' and Schack's equally important point that science is a user's manual. Its purpose is to help each of us make sense of our private experience induced in us by the world outside of us.

It is crucial to note from the beginning that "user" does not mean a generic body of users. It means a particular individual person, who is making use of science to bring coherence to her own private perceptions. I can be a "user." You can be a "user." But we are not jointly a user, because my internal personal experience is inaccessible to you except insofar as I attempt to represent it to you verbally, and vice-versa. Science is about the interface between the experience of any particular person and the subset of the world that is external to that particular user. This is unlike anything in any version of Copenhagen. It is central to the QBist understanding of science.

Of course, the reader can find this Mermin's viewpoint on QBism as private agent (user) business does not match completely the conclusion from my discussion on the class of users belonging to the "QBism club" and constrained by the knowledge about the Born rule; see Sect. 6. This is a consequence of the private user's perspective to interpreting QBism—both David Mermin and I are good friends of the founder of QBism, Christopher Fuchs, and we both got our information about QBism directly from its founder....

## 8 QBism and the Information Interpretation of Quantum Mechanics of Zeilinger and Brukner

In the *information interpretation* of QM, information is the most fundamental, basic entity. Every quantized system is associated with a definite discrete amount of information (see Zeilinger [86] and also [87]). This information content remains constant during evolution of a closed system. Here a quantum state is defined in the spirit of Schrödinger (see [75]): *the quantum state is an expectation catalog (of probabilities for all possible outcomes)*.

Here we do not see the private agent perspective to information encoded in a quantum state. Thus, in spite of some similarity—the QM formalism is about information processing—the information interpretation differs crucially from QBism, by the absence of the private agent perspective. These interpretations also differ in their relation to the Copenhagen interpretation. In contrast to, e.g., Fuchs and Mermin who distanced from this interpretation (Sect. 7), A. Zeilinger who presented the basic principles of the information interpretation in 1999 [86] always emphasized its close connection with the Copenhagen interpretation; in particular, he often cited N. Bohr [4–6] to emphasize connection with Bohr's ideas. The same line of presentation continues in joint publications of Zeilinger and Brukner [7– 10], Kofler and Zeilinger [59] and Brukner et al. [11]. Indeed, the information interpretation of QM can be considered as a modern information-theoretic version of the orthodox Copenhagen interpretation. It has some commonality with von Neumann's version of this interpretation. In particular, Zeilinger and Brukner explore heavily the concept of *irreducible quantum randomness* which was invented by von Neumann [84].

Another key person of the information approach to QM, C. Brukner, recently published a paper on what I interpret as the universal (i.e., not private as in QBism) agent perspective on the information interpretation; we cite Brukner [7]:

The quantum state is a representation of knowledge necessary for a hypothetical observer respecting her experimental capabilities to compute probabilities of outcomes of all possible future experiments.

Here an explicit reference to the observer's experimental capabilities is crucial, cf. with my analysis of QBism in Sect. 6.

It has to be noted that in this paper, Brukner emphasized the closeness to QBism. With this I strongly disagree. From the QBism perspective, the wave function is in the head of a concrete private agent, e.g., in Fuchs' head, not in the head of a hypothetical observer.

#### 9 Classical Probability Theory

#### 9.1 Measure-Theoretic Axiomatics (Kolmogorov [60])

Modern probability theory [60] is based on the representation of events by sets, subsets of some set  $\Omega$ , the so-called sample space, or *space of elementary events*. The system of sets representing events, say  $\mathcal{F}$ , allows operations of Boolean logic;  $\mathcal{F}$  is the so-called  $\sigma$ -algebra of sets.<sup>12</sup> It is closed with respect to the (Boolean) operations of (countable) union, intersection, and complement (or in logical terms "and," "or," "no").

The set-theoretic model of probability was presented by Andrei Nikolaevich Kolmogorov in 1933 [60]; it is based on the following two natural (from the Boolean viewpoint) axioms:

- (AK1) events are represented as elements of a  $\sigma$ -algebra, and operations on events are described by Boolean logic;
- (AK2) probability is represented as a probabilistic measure.

We remind that a probabilistic measure p is a (countably) additive function on a  $\sigma$ -algebra  $\mathcal{F}$ :  $p(\bigcup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} p(A_i)$  for  $A_j \in \mathcal{F}, A_i \cap A_j = \emptyset, i \neq j$ , which

 $<sup>^{12}</sup>$  Here the symbol  $\sigma$  encodes "countable." In American terminology, such systems of subsets are called  $\sigma$ -fields.

is valued in [0, 1] and normalized by 1. We also recall the definition of a *random* variable as a measurable function,  $a : \Omega \to \mathbf{R}$ .<sup>13</sup> In classical probability theory, random variables represent observables.

#### 10 Kolmogorov's Interpretation of Probability

In applications any mathematical formalism has to be endowed with the corresponding interpretation of its entities. Here we present the original Kolmogorov interpretation of probability; see Sect. 11 for another interpretation of the same mathematical formalism.

Kolmogorov proposed [60] to interpret probability as follows: "[...] we may assume that to an event A which may or may not occur under conditions  $\Sigma$ , [there] is assigned a real number P(A) which has the following characteristics:

- (a) one can be practically certain that if the complex of conditions Σ is repeated a large number of times, N, then if n be the number of occurrences of event A, the ratio n/N will differ very slightly from P(A);
- (b) if P(A) is very small, one can be practically certain that when conditions Σ are realized only once, the event A would not occur."

The (a) part of this interpretation is nothing else than the frequency interpretation of probability, cf. with von Mises theory and his *principle of the statistical stabilization of relative frequencies* [81–83].<sup>14</sup> In the measure-theoretic approach, this viewpoint on probability is justified by the *law of large numbers*. However, for Kolmogorov, approximation of probability by frequencies was not the only characteristic feature of probability. The (b)-part (known in foundations of probability as *Cournot's principle*) also plays an important role [76]. This is the purely weight-type argument: if the weight assigned to an event is very small, then one can expect that such an event would never happen. We emphasize that Kolmogorov presented this weight-type argument in its strongest form—"never happen." One may proceed with a weaker form—"practically never happen."

<sup>&</sup>lt;sup>13</sup>Here measurability has the following meaning. The set of real numbers **R** is endowed with the *Borel*  $\sigma$ -*algebra*  $\mathcal{B}$  : the minimal  $\sigma$ -algebra containing all open and closed intervals. Then for any  $A \in \mathcal{B}$  its inverse image  $a^{-1}(A) \in \mathcal{F}$ . This gives a possibility to define on  $\mathcal{B}$  the probability distribution of a random variable,  $p_a(A) = p(a^{-1}(A))$ .

<sup>&</sup>lt;sup>14</sup>By this principle the probability of some concrete output  $\alpha$  of measurement is defined as the limit of the relative frequency of realizations of  $\alpha$  in a long (in fact, infinitely long) sequence of trials. The class of sequences of trials which can serve to determine probabilities is constrained by another fundamental principle of von Mises' theory—*the principle of randomness*. Sequences of trials satisfying the latter are called *collectives* (random sequences). The principle of randomness involves the ambiguous notion of a place selection. On one hand, the ambiguity of this notion was the main pitfall for applications of von Mises' frequency theory of probability. And nowadays it is practically forgotten. On the other hand, this ambiguity (as often happens in science) played the crucial role in establishing of modern theory of randomness and algorithms.

#### **11** Subjective Interpretation of Probability

# 11.1 Measure-Theoretic Model with Subjective Interpretation of Probability

Each scientific theory consists of two parts, a mathematical model and an interpretation of the mathematical entities. Now we make a point: in a scientific theory the same mathematical model can have a variety of interpretations. In particular, it happened with Kolmogorov's measure-theoretic model of probability. Besides the commonly used statistical interpretation, probability measures can also be interpreted in the framework of *subjective probability theory*.

This interpretation was used by T. Bayes as the basis of his theory of probability inference; see then Ramsey [73], de Finetti [21], and Savage [74], Bernardo and Smith [3]. Here the probability P(A) represents an *agent's personal, subjective degrees of belief* in non-occurrence/occurrence of the event A. In contrast to the statistically interpreted probability which is objective by its nature, the subjective probability is by definition not objective, so to say, "it does not exist in nature" independently of an agent assigning probabilities to events. This viewpoint on probability is in the direct conflict with von Mises' viewing of probability theory as a theory of natural phenomena, similar to, e.g., hydrodynamics. Kolmogorov and the majority of Soviet probability theory as a mathematical theory (so his viewpoint on probability theory did not coincide with Mises' viewpoint), he also interpreted it as representing objective feature of repeatable phenomena, statistical stability of them.

At the same time, since the measure-theoretic definition of Kolmogorov probability is heuristically based on the weighting-like procedure for events, it seems that the subjective interpretation matches well the mathematical framework of Kolmogorov probability spaces. Instead of assigning to events objective weights (as Kolmogorov proposed to do), subjectivists assign to events personal weights; each agent assigns to an event *A* his own degree of belief.

#### 11.2 De Finetti's Views on the Methodology of Science

Personalization of probability contradicts not only to the views of von Mises, Kolmogorov, and all their followers but even the basic methodology of modern science. And, for example, de Finetti understood this well and emphasized this in his exciting and provocative essay [20]. He started with a citation of the important science methodological statements of Tilgher (see [20, p. 169]) (in all following citations, the italic font was inserted by me):

Truth no longer lies in an imaginary equation of the spirit with what is outside it, and which, being outside it, could not possibly touch it and be apprehended; truth is in the very act of

the thinking thought. The absolute is not outside our knowledge, to be sought in a realm of darkness and mystery; it is in our knowledge itself. *Thought is not a mirror in which a reality external to us is faithfully reflected*; it is simply a biological function, a means of orientation in life, of preserving and enriching it, of enabling and facilitating action, of taking account of reality and dominating it.

This viewpoint, thought as just a biological function and not reflection of the objective features of external reality, was shared by de Finetti and used by him to question the conventional ideology of modern science; see Appendix 2 for the corresponding citations of de Finetti and analysis of them. For him, the main point was that *subjectivity of probability leads to subjectivity of cause*.

# 11.3 Comparison of de Finetti's Views with Copenhagen Interpretation

The rejection of objectivity of cause by de Finetti can be compared with rejection of causality by von Neumann in his interpretation of QM. (Causality is rejected in all versions of the Copenhagen interpretation of QM. However, its probabilistic nature was discussed most clearly in von Neumann book [84].) However, in contrast to de Finetti, by rejecting causality von Neumann did not reject objectivity of probability. He used the statistical interpretation of probability in its genuine von Mises' frequency version. Von Neumann "saved" objectivity of probability in the absence of causality by inventing the concept of *irreducible quantum randomness*. Bohr and Pauli also interpreted probability statistically and, for them, it was definitely objective. This objectivity was based on objectivity of outputs of classical measurement devices. In contrast to von Neumann, they did not need irreducible quantum randomness.

However, in general de Finetti's denial of objectivity of cause had to be sympathetic for Copenhagenists. Therefore it is surprising that in QM, nobody tried to proceed with the subjective probability interpretation. Only recently C. Fuchs supported by R. Schack proposed to use in QM subjective probability and personal agent's perspective (see Sect. 4). This interpretation of QM is known as Quantum Bayesianism (QBism).

# 11.4 Classical Bayesianism: Subjective Probability in Classical Physics?

For the fathers of QM, both Copenhagenists (as Bohr, Pauli, Dirac, von Neumann) and anti-Copenhagenists (as Einstein, De Broglie), probability was objective and statistical. Why? Why not subjective? One of the reasons for this was that all physicists learned probability starting with classical statistical mechanics and the

statistical interpretation was firmly incorporated in their mind. Some of them were able to give up even causality, but not statistical nature of probability. However, it seems that the main reason was that de Finetti's views on probability and more generally on scientific theory were *too revolutionary* even for "quantum folk." The latter still wanted to have solid objective ground—in classical world, the world of macroscopic measurement devices. But de Finetti tried to teach us that even in this macro-world neither probability nor cause is objective, they have to be treated subjectively, person dependent. It seems that even Copenhagenists would not accept such a position. By following de Finetti consistently, they should reconsider not only physics of microworld, as was done in the process of creation of QM, but even physics of macro-world.

What is about QBism? QBism loudly declared that quantum probabilities have to be treated as subjective entities. For this, it was admired by some people and heavily beaten by others. It seems to be reasonable if QBists by exploring the subjective interpretation of probability in QM would say:

CBism Bayesianism has to be extended to classical statistical physics and thermodynamics!

Unfortunately, we do not hear such a message from them—at least loudly. Only through the private communication with C. Fuchs it became clear for me that CBism is not foreign for QBists. In particular, in 2003 C. Fuchs pointed out (see, e.g., [30, p. 812]).

Since becoming immersed in the subject, I have found nothing more exciting than these trains of thought. For they indicate the extent to which quantum foundations research may be the tip of an iceberg—indeed, something with the potential to drastically change our worldview, even outside the realm of physical practice.

However, I stress once again that this message was totally shadowed by active advertising of the Bayesian subjective probability perspective solely for quantum physics. Thus CBism still waits similar advertising and justification as QBism. And this is the program of huge importance and complexity.

# 12 QBism as the Basis of General Theory of Decision-Making

My personal viewpoint on the subjective interpretation of probability is sufficiently complicated. As a student of the Department of Mechanics and Mathematics of Lomonosov Moscow State University, I was lucky to have a few lectures of Kolmogorov. Then he became too ill to continue, but lectures were given by his former student A.N. Shiryaev; in any event for us, "subjective probability" was the swearword. Therefore by working on quantum foundations [42, 50], I always keep the statistical interpretation of probability.

However, recently by working in applications of quantum probability to cognition, psychology, and decision-making [51] (see also recent papers [2, 52, 53]), I started to think that the subjective interpretation is adequate for modeling of decision-making process by an individual agent. The recent wave of multidisciplinary activity on applications of the mathematical formalism of quantum theory and especially its probabilistic part in cognitive science, psychology, social and political sciences, economics, and finances as well as in molecular biology and genetics and modeling of biological evolution (see, e.g., [2, 12, 19, 56–58, 72, 78] and references herein) is very supportive for QBism as very general approach to decision-making. It seems that QBism is the most natural candidate for foundational justification of applications of the quantum calculus of probabilities outside of physics.

Nowadays in theory of decision-making, agents are commonly considered as assigning subjective probabilities to possible actions; see Savage [74] (although the original theory of expected utility of von Neumann-Morgenstern [85] was based on the frequency interpretation).

As is well known, the use of classical probabilistic model in decision-making leads to numerous paradoxes, the most famous are the Ellsberg [22] and Machina paradoxes [61]. As was pointed out in [1, 12, 37], these paradoxes can be resolved by using the quantum calculus of probabilities.<sup>15</sup> However, one has to justify the applicability of the quantum probabilistic calculus for decisions made about events in the macro-world. QBism can do this easily. The private agent perspective is not rigidly coupled to events happening in the microworld. It can be extended to decisions of agents predicting outcomes of events, e.g., at the financial market. This viewpoint on QBism as the basis of general decision-making by agents processing information in accordance with the rules formalized in the quantum probabilistic formalism was presented in [55].

Once again (cf. with the last comment of the Introduction section) by extending the domain of QBism applicability to general theory of decision-making, we definitely go beyond the original ideas of QBism's fathers (Fuchs, Schack, Mermin), and it is not clear whether they would be happy to see such attempts of application of QBism, e.g., to economics or finances.

Fuchs and Schack declared [34]: "According to QBism, quantum mechanics can be applied to any physical system. QBism treats all physical systems in the same way, including atoms, beam splitters, Stern-Gerlach magnets..." If so, then why only "to any physical system"? Why not to any system, biological, cognitive, social, or political? From my viewpoint, QBism is an excellent interpretation to motivate extension of the domain of applications of the quantum formalism. We also remark that C. Fuchs actively uses works of W. James (see, e.g., [39–41]), as supporting the QBism perspective to decision-making for outcomes of measurements. W. James was one of the great psychologists of the nineteenth century. In particular, he

<sup>&</sup>lt;sup>15</sup>It is a good place to point out that these paradoxes cannot be solved simply by playing with the interpretations of probability. The essence of the problem is not an interpretation but the structure of the probability calculus. Thus by using QBism to resolve these paradoxes we use both its fundamental counterparts, interpretational—the subjective interpretation of probability, and mathematical—the Born rule.

invented the principle of complementarity (conscious and unconscious thoughts) to psychology. Later N. Bohr borrowed this principle for QM [4–6]. Thus the interest to works of James might stimulate QBists to think about interconnection between QBism and psychology, cognition.

However, it seems that, for a QBist, it is difficult (if possible at all) to accept the possibility of such wider use. The reaction of C. Fuchs to my comments in this direction cannot be characterized as excitement. Of course, this calm reaction might have social roots. By assuming that QBism is a theory about generalized probability update done not only in physics but, in fact, everywhere, QBists would depart even farther from the mainstream physics.

However, it might be that distancing from applications outside of physics has fundamental grounds. In contrast to the Växjö interpretation, in QBism, the Born rule is not just a consequence of a very general scheme of the probability update. Its appearance in quantum physics is a consequence of some fundamental feature of nature, namely, a kind of intrinsic quantum randomness. Thus by extending the domain of applications of the quantum formalism to cover, e.g., cognition, one has to assign to cognition a kind of intrinsic quantum(-like) randomness. In principle, one cannot exclude that not only quantum physical systems, but even bio-systems are intrinsically random. However, this is a very complicated problem. It seems that, for a moment, QBists (who are busy with their own problems in physics) simply do not like to be involved in the problem of justification of intrinsic bio-randomness.

However, as we know well, any idea lives its own life, and sometimes its evolution may be unexpected and surprising for its creators (or even unwanted).<sup>16</sup>

# Appendix 1: Symmetric Informationally Complete Quantum Measurements

We consider one special class of atomic instruments with quantum observables given by *symmetric informationally complete* POVMs, SIC-POVMs. Here informational completeness means that the probabilities of observing the various outcomes (given by Born's rule) entirely determine any quantum state  $\rho$  being measured. This requires  $d^2$  linearly independent operators for the state space of the dimension *d*.

The simplest definition is that a SIC-POVM is determined by a system of  $d^2$  normalized vectors ( $\phi_i$ ) (they are not orthogonal) such that

$$\langle \phi_i | \phi_j \rangle^2 = \frac{1}{d+1}, i \neq j.$$
(8)

<sup>&</sup>lt;sup>16</sup>According to Derrida, "what we get when we read a text is not an objective account of logos or even what the author really meant, but our present interpretation or understanding of the text itself. This understanding becomes so to speak, our own [text] of the text" (quoted from [66, p. 368]).

The elements of the corresponding SIC-POVM ( $E_i$ ) are subnormalized projectors  $E_i = \frac{1}{d} \Pi_i$ , where  $\Pi_i$  is the orthogonal projector on  $\phi_i$ . The elements of SIC-POVM  $E_i$  determine the corresponding quantum operations (atomic instruments).

The characteristic property of SIC-POVMs, symmetry, is that the inner product in the space of operators (or  $d \times d$  matrices) given by the trace is constant, i.e.,

$$\operatorname{Tr} E_i E_j = \operatorname{const} = \frac{1}{d^2(d+1)}, i \neq j.$$

By using this equality, it is easy to obtain the following representation of an arbitrary density operator  $\rho$ :

$$\rho = \sum_{i} \left( (d+1)p(i) - \frac{1}{d} \right) \Pi_i \tag{9}$$

where  $p(i) = \text{Tr}E_i\rho$  is the probability to obtain the result *i* for a measurement presented by the SIC-POVM ( $E_i$ ).

This SIC-POVM based representation of a density operator  $\rho$  plays the crucial role in Quantum Bayesianism (QBism), cf. with the QBist version of quantum generalization of FTP (see Sect. 4).

#### **Appendix 2: De Finetti's Views**

In this appendix the views of de Finetti to the methodology of science (see Sect. 11.2) are presented in more details. We start with a long citation of de Finetti accompanying the citation of Tilgher from Sect. 11.2. De Finetti wrote the high degree of enthusiasm and excitement [20, p. 169]:

For those who share this point of view, which is also mine, but which I could not have framed better than with these incisive sentences of Tilgher's [..], *what value can science have?* In what spirit can we approach it? Certainly, we cannot accept determinism; we cannot accept the 'existence,' in that famous alleged realm of darkness and mystery, of immutable and necessary 'laws' which rule the universe, and we cannot accept it as true simply because, in the light of our logic, it lacks all meaning. Naturally, then, science, understood as the discoverer of absolute truths, remains idle for lack of absolute truths. But *this doesn't lead to the destruction of science;* it only leads to a different conception of science. Nor does it lead to a 'devaluation of science': there is no common unit of measurement for such disparate conceptions. Once the cold marble idol has fallen in pieces, the idol of perfect, eternal and universal science that we can only keep trying to know better, we see in its place, beside us, a living creature, the science which our thought freely creates. A living creature: flesh of our flesh, fruit of our torment, companion in our struggle and guide to the conquest.

Nature will not appear to it as a monstrous and incorrigibly exact clockwork mechanism where everything that happens is what must happen because it could not but happen, and where all is foreseeable if one knows how the mechanism works. To a living science nature will not be dead, but alive; and it will be like a friend about whom one can learn in sweet

intimacy how to penetrate the soul and spirit, to know the tastes and inclinations, and to understand the character, impulses and abandonments. So *no science will permit us say: this fact will come about, it will be thus and so because it follows from a certain law, and that law is an absolute truth.* Still less will it lead us to conclude skeptically: the absolute truth does not exist, and so this fact might or might not come about, it may go like this or in a totally different way, I know nothing about it. What we can say is this: I foresee that such a fact will come about, and that it will happen in such a way, because past experience and its scientific elaboration by human thought make this forecast seem reasonable to me. Here the essential difference lies in what the 'why' applies to: I do not look for why THE FACT that I foresee will come about, but why I DO foresee that the fact will come about. It is no longer the facts that need causes; it is our thought that finds it convenient to imagine causal relations to explain, connect and foresee the facts. Only thus can science legitimate itself in the face of the obvious objection that our spirit can only think its thoughts, can only conceive its conceptions, can only reason its reasoning, and cannot encompass anything outside itself.

This statement contains such charge of energy that even one treating probability objectively cannot reject it without deep analysis. Of course, primarily de Finetti is right that in scientific prediction "I foresee that such a fact will come about, and that it will happen in such a way, because past experience and its scientific elaboration by human thought make this forecast seem reasonable to me." We have only our thought and even existence of objective reality is just one of its fruits.

For me the essential difference lies in the interpretations of "human thought": either as personalized or as collective. In the above citation from de Finetti, it seems that "human thought" has the meaning of thought of a kind of the *universal agent* doing scientific research. If we take subjective probability as the degree of belief of such a universal agent, then the dispute about objectivity or subjectivity of probability would be resolved peacefully. If de Finetti does not assumed the existence of objective reality ruled by natural laws but just assumed the use of the scientific experience of the mankind, represented as the universal thinking agent, then von Mises or at least Kolmogorov might agree that such kind of subjective probability has the right for existence. This my reflections about the universal agent perspective on the subjective probability can be compared with Gnedenko's statement [77]: "Subjective probabilities, if necessary, can be made objective."

However (and this the main point), de Finetti strongly supports the personal viewpoint on subjective probability and, hence, "human thought" and "past experience and its scientific elaboration." This *personal agent viewpoint* is unsympathetic for the majority of scientists, especially those exploring natural sciences. One of the main problems is that subjectivity of probability leads to *subjectivity of cause*.

It has to be noticed that de Finetti's radicalism shares much with American pragmatism and with logical positivism/logical empiricism, and neither kind of position has featured much as going concerns in discussions over the last 50 or so years in general philosophy or philosophy of science, perhaps for good reason. In this paper I do not plan and have no possibility to discuss these philosophic connections of de Finetti's approach to scientific methodology. This is a good topic for a special philosophic essay.

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# **Epistemic View of Quantum Communication**



Subhash Kak

### 1 Introduction

A formal theory comes with its well-defined entities and rules of analysis. In addition, certain other entities are usually implicit in the theory but are not formally defined. These implicit entities and the underlying assumptions about reality, together with the different ways abstract entities may be mapped to intuitive notions, lead to divergent interpretations of the theory. Such divergences are particularly true for quantum theory for which the interpretations include the Copenhagen, stochastic evolution, consistent histories, transactional, QBism, MWI, and so on (e.g., [1–6]). Roughly these interpretations fall into the epistemic and the ontic views, where in the epistemic view one is speaking of the knowledge obtained from the experiment without going into the ultimate nature of reality and in the ontic view one is describing reality as a particular assemblage of objects. These views are so far from each other that their synthesis is impossible.

Even though the epistemic Copenhagen Interpretation has been the dominant view among quantum theorists [6], it has been criticized for being at variance with the contemporary program of science of finding an ontic (ontological) basis of reality. This basis is sought in the structure of being (in its physical embodiment) and that of its becoming (e.g., [7].) as well as other algorithmic models of physics and intelligence. Physicists describe a physical system mathematically and logically in a manner that can speak to its evolution, and in such an ontological description, there is no place for observers. This program has grown hand in hand with the

S. Kak (🖂)

School of Electrical and Computer Engineering, Oklahoma State University, Stillwater, OK, USA e-mail: subhash.kak@okstate.edu

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deepening use of computers in society, and there are models where the unfolding of the universe itself is seen in terms of the workings of a computer program.

The ontic understanding of reality becomes problematic when one brings in information into the mix, as is done extensively in modern physics. This is because information implies the existence of a mind, which category lies outside of the realm of physics. The study of the mind is normally done using the tools and concepts of psychology and neuroscience. Standard neuroscience accepts the doctrine of an identity of the brain and mind. In this view, the mind emerges from the complexity of the interconnections, and its behavior must be completely described by the corresponding brain function leaving no room for agency of the individual [8]. No specific neural correlate of consciousness has been found [9, 10]. There are also attempts to ascribe certain counterintuitive characteristics of the mind to underlying quantum processing [11–13]. But even if quantum mechanics were shown to play a role in brain processes, it will remain a machine paradigm, and so it cannot be the complete explanation of the phenomenon of consciousness.

The perspective of epistemology presents a way to highlight the differences in the implicit assumptions. As the study of the nature of knowledge, epistemology is of relevance in examining interpretations of theory, and the case of quantum information in a communications setting makes its conceptual basis most clear for it brings in more than one agent into the equation. We agree with the philosopher Fred Dretske, who argued that [14] "A more precise account of information will yield a more creditable theory of knowledge. Maybe ... communication engineers can help philosophers with questions raised by Descartes and Kant."

Information in a communication involves two things: first, commonalities in the vocabulary of communication between the two parties; and second, the capacity to make choices. The commonality of vocabulary requires that the underlying abstract signs used by the parties be shared, which stresses the social aspects of communication. The capacity to make a choice means agency, which has no place in a world governed by closed laws unless one considers psychophysical parallelism that excludes causal interaction between the mind and body. In the view of such parallelism, mental and physical phenomena are two aspects of the same reality like two sides of a coin.

Note that psychophysical parallelism was a dominant philosophical view in Europe in the late nineteenth and early twentieth centuries but now has been relegated to the margins [15]. According to Moritz Schlick, who was the leader of the Vienna Circle of Logical Positivists in the 1930s, psychophysical parallelism is the "epistemological parallelism between a psychological conceptual system on the one hand and a physical conceptual system on the other. The "physical world" *is* just the world that is designated by means of the system of quantitative concepts of the natural sciences" [16]. The idea is in an old one having been first enunciated as *samavāya* (inherence) in the Vaiśeșika Sūtra of Kaṇāda in India [17] and later in Europe by Leibnitz.

Now consider how choices are made and how these choices are intelligible. With Heidegger, one may speak of the difference between the ontical and the ontological where the first is concerned with facts about objects and the second is concerned with the meaning of Being, with how objects are intelligible as entities. According to Heidegger [18], "Basically, all ontology, no matter how rich and firmly compacted a system of categories it has at its disposal, remains blind and perverted from its ownmost aim, if it has not first adequately clarified the meaning of Being, and conceived this clarification as its fundamental task."

There are usually several unstated assumptions regarding the process of obtaining information from an experimental situation that involve the nature of the observer. Specifically, we endow the observer with the capacity to make intelligent classifications and choices, either directly or through the agency of instruments and computing devices, which are not a part of the formal framework that describes the physical processes being investigated. It is interesting that some interpretations strive to take out the observer from the framework, without explaining how the central role of the selectivity in the observation process is to be explained.

In this essay we first review the problem of observation in epistemic and ontic interpretations of quantum theory presenting the key insight of Bohr, von Neumann, and Schrödinger in which the epistemic understanding emerges from the principle of psychophysical parallelism. Next, we examine the question of information in classical and quantum settings highlighting how its definition in the framework of ensembles requires an epistemic basis. We argue that the Copenhagen Interpretation provides the best resolution to the problems associated with information.

#### 2 The Observation Process and Complementarity

We first consider the orthodox Copenhagen Interpretation, in which the physical universe is separated into two parts: the first part is the system being observed, and the second part is the human-observing agent, together with the instruments. The agent is therefore an extended entity described in mental terms, and it includes not only his apparatus but also instructions to colleagues on how to set up the instruments and report on their observations. The Heisenberg cut (also called the von Neumann cut) is the hypothetical interface between quantum events and the observer's information, knowledge, or awareness. Below the cut everything is governed by the wave function, whereas above the cut one must use classical description.

Although the arbitrariness of the cut has come in for criticism and spurred the development of other interpretations, it is a device for aggregating the effects of the mind or minds associated with the observational regime, and it is a reasonable way to separate the inanimate from the animate especially since the brain itself may be viewed as a machine. Bohr stressed the elusive separation between subject and object:

The epistemological problem under discussion may be characterized briefly as follows: For describing our mental activity, we require, on one hand, an objectively given content to be placed in opposition to a perceiving subject, while, on the other hand, as is already implied in such an assertion, no sharp separation between object and subject can be maintained, since the perceiving subject also belongs to our mental content. [19]

von Neumann describes the principle thus: "[I]t must be possible so to describe the extra-physical process of the subjective perception as if it were in reality in the physical world—i.e., to assign to its parts equivalent physical processes in the objective environment, in ordinary space" [6]. He adds further:

The boundary between the two is arbitrary to a very large extent. In particular we saw in the four different possibilities in the example above, that the observer in this sense needs not to become identified with the body of the actual observer: In one instance in the above example, we included even the thermometer in it, while in another instance, even the eyes and optic nerve tract were not included. That this boundary can be pushed arbitrarily deeply into the interior of the body of the actual observer is the content of the principle of the psycho-physical parallelism – but this does not change the fact that in each method of description the boundary must be put somewhere, if the method is not to proceed vacuously, i.e., if a comparison with experiment is to be possible. Indeed experience only makes statements of this type: an observer has made a certain (subjective) observation; and never any like this: a physical quantity has a certain value.

Now quantum mechanics describes the events which occur in the observed portions of the world, so long as they do not interact with the observing portion, with the aid of the process 2, but as soon as such an interaction occurs, i.e., a measurement, it requires the application of process 1. The dual form is therefore justified. However, the danger lies in the fact that the principle of the psycho-physical parallelism is violated, so long as it is not shown that the boundary between the observed system and the observer can be displaced arbitrarily in the sense given above.

The above quotes make it clear that psychophysical parallelism is not equivalent to brain-mind identity of neuroscience in which the mind is an emergent property with neural structures as ground, thus admitting a causal link going from biology to the mind.

The question of interaction between mental states and the wave function was addressed in the Copenhagen Interpretation (CI) [2], by understanding the wave function epistemologically, that is, it represents the experimenter's knowledge of the system, and upon observation there is a change in this knowledge. Operationally, it is a dualist position, where there is a fundamental split between observers and objects. The placement of the cut between the subject and the object is arbitrary to the extent it depends on the nature of the interaction between the two.

In the ontic view of the wave function, as in the Many-Worlds Interpretation (MWI), there is no collapse of the wave function, and the interaction is seen through the lens of decoherence, which occurs when states interact with the environment producing entanglement [20]. By the process of decoherence, the system makes transition from a pure state to a mixture of states that observers end up measuring. The problem of collapse of the wave function is sidestepped by speaking of interaction between different subsystems. But since the entire universe is also a quantum system, the question of how this whole system splits into independent subsystems arises. It would seem that the splitting into subsystems is itself an

observational choice, rather than fundamental. This splitting serves about the same function as the Heisenberg cut of CI. Furthermore, such an ontic view has no place for minds, which can at best be taken as traces of mathematical operations, thus ruling out agency.

Finally, the principle of psychophysical parallelism is consistent with complementarity and indeed the inspiration for it [21]. Bohr argued that the consideration of the biological counterpart to the observation of the relation between the mind and body does not become part of an infinite regress. He added: "We have no possibility through physical observation of finding out what in brain processes corresponds to conscious experience. An analogy to this is the information we can obtain concerning the structure of cells and the effects this structure has on the way organic life displays itself.... What is complementary is not the idea of a mind and a body but *that* part of the contents of the mind which deals with the ideas of physics and the organisms and *that* situation where we bring in the thought about the observing subject" [22].

Schrödinger implicitly invoked the principle in describing the state function of a quantum state (psi) as representing our knowledge about the system. He said:

Reality resists imitation through a model... We have nothing but our reckoning scheme, i.e., what is a *best possible* knowledge of the object. The psi-function ... is now the means for predicting probability of measurement results. In it is embodied the momentarily-attained sum of theoretically based future expectation, somewhat as laid down in a *catalog*... [This] the catalog of expectations is initially compiled. From then on it changes with time, just as the state of the model of classical theory, in constrained and unique fashion... For each measurement one is required to ascribe to the psi-function (= the prediction-catalog) a characteristic, quite sudden change, which *depends on the measurement result obtained*, and so *cannot be foreseen*; from which alone it is already quite clear that this second kind of change of the psi-function has nothing whatever in common with its orderly development *between* two measurements... And indeed because one might never dare impute abrupt unforeseen changes to a physical thing or to a model, but because in the realism point of view observation is a natural process like any other and cannot per se bring about an interruption of the orderly flow of natural events. [23]

It is clear that Schrödinger is stressing the epistemic nature of the state function. Elsewhere, he presents the psychophysical parallel basis of this claim in a clearer form: "Consciousness cannot be accounted for in physical terms. For consciousness is absolutely fundamental. It cannot be accounted for in terms of anything else" [24].

The complementarity of aspects, such as wave and particle, is a consequence of the kind of measurement that is made which emanates from the choice made by the observer. It is not the description of an ontologically defined entity in two equivalent forms as in the representation of a number directly or in terms of its inverse sequence [25]. The experimenter is not describing reality ontologically; rather, he is obtaining knowledge about it that is related to the nature of his interaction with the system. The particle view is the one imposed on reality by the mind governed by a classical mode [26]. Nonlocality is an issue only if one takes the particle picture, together with local interaction, to be an underlying reality. Therefore, the violation of Bell's theorem by experiments does not imply a fundamental difficulty [27].

#### **3** The Communications Setting

Consider the problem of exchange of information between two parties. Figure 1 describes the communications context for the accounting of information [28]. It consists of a sender and a receiver together with an ensemble of signals (which could be letters). The statistical characteristics of the signals are known both to the sender and the receiver. There could be further relationship between the symbols and physical or abstract objects in which case one can also speak of a semantic content communicated through the transmissions.

Let the probabilities of the signals that are transmitted and then received by the sender, *S*, and the receiver, *R*, be  $p(x_i)$  and  $p(y_j)$ , respectively (the discrete index refers to the specific signal being considered out of a list that ranges from 1 onwards).

The p values are the a priori probabilities associated with the sender, the receiver, and their world. The sender now chooses a specific one out of the ensemble and sends it to the receiver and repeats this process. The information exchanged between S and R is:

$$I(x_i, y_j) = \log \frac{p(x_i | y_j)}{p(x_i)}$$
(1)

and this information is always positive, if not zero. The informational entropy I(X; Y), is, therefore:

$$I(X;Y) = \sum_{x,y} p(x,y) \log \frac{p(x,y)}{p(x)p(y)}$$
(2)

Also,

$$I(X;Y) = H(X) - H(X|Y)$$
(3)



Fig. 1 Exchange of information

where  $H(X) = -\sum_{x} p(x) \log p(x)$  and  $H(X|Y) = \sum_{x,y} p(x, y) \log \frac{p(y)}{p(x,y)}$ , which are the entropy of *S* and the conditional entropy of *S* given *R*, respectively. We ask: what is the connection between probabilistic information provided by the entropy expressions above and the knowledge obtained by the receiving party? At the most basic level, the following claims may be made regarding the communication process:

- 1. There exist associations of data, which requires separating it from other data, and abstractions (input *X* and output *Y*) which are assumed without explaining how this is achieved.
- 2. There exists training with set with correct classifications (or data typical of the ensemble) that involves different modes of behavior on the part of the two agents.
- 3. There are classification tasks (as in AI and neural networks) that come with hierarchical levels of understanding.
- 4. There exists a duality between the process of the identification of the ensemble (learning) and that of subsequent measurements.

Implicit in the identification of the ensemble is the mind, and it is also implicitly acknowledged in the problem of classical information. The sharing of the ensemble must be part of a social process.

Now consider the communications context for the quantum case. Assume the sender and the receiver both are informed of the ensemble of states { $\rho_1$ ,  $\rho_2$ , ...,  $\rho_n$ } with probability { $p_1$ ,  $p_2$ , ...,  $p_n$ }. Every density operator may be viewed as a mixture of pure states

$$\rho = \sum_{i} \lambda_{i} |\phi_{i}\rangle \langle \phi_{i}| \tag{4}$$

where  $\lambda_i$  are the eigenvalues and  $|\phi_i\rangle$  are the eigenvectors of  $\rho$ . The entropy may be written as [13]

$$S_n(\rho) = -\sum_i \lambda_i \log \lambda_i \tag{5}$$

The measurements along the reference bases may be associated with probability values  $\lambda_i$  in analogy with the classical entropy expression of  $-\sum_i p_i \log p_i$ , where

the *i*th outcome, out of a given set, has probability  $p_i$ .

Operationally, classical and quantum information work differently. Given an unknown state distributed over two systems, consider how much information needs to be sent to transfer the full state to a system. In the classical case, partial information must always be positive, but in the quantum case it can be negative. If the partial information is positive, its sender needs to communicate this number of quantum bits to the receiver; if it is negative, then sender and receiver instead gain the corresponding potential for future quantum communication [29]. The idea





of negative partial information makes sense only in the context of observers that are epistemologically connected.

Now consider the case of Fig. 2 in which the sender has access to states in an ensemble and he is sending these to the receiver. We are interested in considering the entropy of this situation. If the sender is Nature, the receiver is the experimenter who is determining both the ensemble as well as the information that is associated with it.

If the ensemble consists of a single unknown letter, the Shannon entropy associated with the ensemble is zero. The information in any single communication is also zero. Starting with the hypothesis that there are two potential states, the receiver will find in the *n*th test that the probability that it is a single letter is  $1-2^{-n}$ .

In contrast, in the quantum case, let the ensemble consist of a single pure state. We assume that the reference bases of the sending and the receiving parties are aligned without going into the question of the cost associated with that process. The von Neumann entropy associated with this case is zero. Nevertheless, the amount of information that the receiver can obtain is infinite [13]. This infinite information will be in terms of the specific phase information associated with the state which, theoretically, has infinite precision.

Parenthetically, an application of this is when two parties wish to share a random number. The sender codes the random number into the polarization angle of the many copies of the photons. The determination of the angle by the receiver will eventually transfer the random sequence to the receiver [12, 30].

The ability to obtain information from the unknown state implies access to a corresponding energy. The equivalence between energy and information is given by  $kT\ln 2$  (or about 0.69 kT) which is both the minimum amount of work needed to store one bit of binary information and the maximum that is liberated when this bit is erased, where k is Boltzmann's constant and T is the temperature of the storage medium in degrees Kelvin [31].

Assuming that the unknown state is localized (contra the central idea of nonlocality) at a physical point leads to the conclusion that energy is associated with space. This is restating the concept of zero-point energy that is normally derived

using Heisenberg's uncertainty principle. The ability to obtain information from space would depend on how the experimenter interacts with it.

The consideration of information also requires choices that go into the formation of the ensemble that is used by the communicating parties. This is only possible by the observer making choices. The manner in which these choices are made will change the value of the entropy associated with the process of information exchange [13]. The choices establish that the information is epistemic. Without consideration of this aspect of information basis, we are confronted by difficulties such as the information paradox of cosmology [32].

#### 4 Discussion

The notion of psychophysical parallelism rules out the need of hidden-variable theories. According to it, quantum mechanics is an epistemic theory and it is impossible to introduce additional variables that will convert it into an ontic theory. The lack of experimental support for hidden-variable theories is to be expected within the framework of this parallelism. It is also not surprising that extensions to quantum theory cannot give more information about the outcomes of future measurements than quantum theory itself [33].

One must also assume that the psychological part of the psychophysical parallelism notion implies that there exists no specific correlate of consciousness in the brain (as it cannot have a physical basis). The quantum Zeno effect [34] does provide a mechanism on how observation can influence dynamics, but it does not explain the ontological position of the observer.

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# **Quantum Decoherence Emulated** in a Classical Device



Brian R. La Cour, Corey I. Ostrove, Michael J. Starkey, and Granville E. Ott

## 1 Introduction

Decoherence in quantum systems arises as an inevitable consequence of interactions with the environment. Theoretically, it has been used to understand the measurement problem and provide a gateway to the classical world [1]. From a practical perspective, decoherence poses a challenge to developing large-scale quantum computers, whose efficacy degrades with the loss of coherence. Quantum error correction meets this challenge by providing a scalable means of correcting a continuum of possible errors, representable by a finite set of operators, using only a discrete number of components [2, 3]. In this paper, we will investigate whether classical analog systems can exhibit similar behavior.

We shall begin in Sect. 2 with a description of a classical emulation of a gatebased quantum computer. There, we describe how arbitrary quantum states may be represented by classical signals conforming to the mathematical tensor-product structure of a multi-qubit Hilbert space. We go on to describe how one- and twoqubit gate operations can be performed on these representative states and even how quantum measurements can be faithfully emulated. Finally, describe briefly a hardware implementation of a device capable of emulating a two-qubit quantum computer.

We go on, in Sect. 3, to describe how one may use such a device to perform quantum state tomography and, therefore, infer the equivalent mixed quantum state from an ensemble of imperfect state preparations. In Sect. 4 we extend our investigation to modeling gate operations in our classical device in terms of quantum operations. This provides the natural mathematical framework for studying classical

B. R. La Cour  $(\boxtimes) \cdot C$ . I. Ostrove  $\cdot M$ . J. Starkey  $\cdot G$ . E. Ott

Applied Research Laboratories, The University of Texas at Austin, Austin, TX, USA e-mail: blacour@arlut.utexas.edu

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performance degradation in terms of quantum decoherence. By applying a sequence of gate operations iteratively, we are able to measure the systematic falloff in performance of the device and model it as a parameterized quantum channel. Our conclusions are summarized in Sect. 5.

#### **2** Classical Emulation of a Quantum Device

In previous work, we have described the use of classical signals and analog electronics to emulate or "mimic" the behavior of a gate-based quantum computer [4]. The basic idea is quite simple. Given an abstract Hilbert space  $\mathcal{H}$  used to represent an *n*-qubit quantum state  $|\psi\rangle \in \mathcal{H}$ , we seek a classical representation of these abstract mathematical objects. Many possibilities suggest themselves. The one we shall choose is motivated by our desire to easily perform operations on it. To that end, we adopt sinusoidal analog signals as a convenient physical representation of a pure quantum state.

If we denote by  $|x\rangle$ , where  $x \in \{0, ..., 2^n - 1\}$ , a basis function in the so-called computational basis of  $\mathcal{H}$ , then its classical representation is defined as follows. Let  $[x_{n-1} \cdots x_0]$  be the little endian binary representation of x. The corresponding classical representation is then written as a complex signal  $\phi_x$  defined such that

$$\phi_{x}(t) = \exp[(-1)^{x_{n-1}} i\omega_{n-1}t] \cdots \exp[(-1)^{x_{0}} i\omega_{0}t], \qquad (1)$$

where the frequencies  $\omega_{n-1} > \cdots > \omega_0$  correspond to each of the *n* qubits. In particular, taking  $\omega_k = 2^k \omega_0$  allows for a uniform spacing among the  $2^n$  different combinations of sums and differences. Clearly, the required bandwidth for such a representation grows exponentially with the number of qubits. Linear combinations of basis signals provide a representation for an state in  $\mathcal{H}$ . Thus, if  $\langle x | \phi \rangle = \alpha_x$ , then

$$\psi(t) = \sum_{x=0}^{2^n - 1} \alpha_x \, \phi_x(t) \tag{2}$$

provides a classical representation of the quantum state  $|\psi\rangle$ . If  $T = 2\pi/\omega_0$  is the period of the signal, then an inner product may be defined as

$$\langle \phi_x | \psi \rangle = \frac{1}{T} \int_0^T \phi_x(t)^* \psi(t) \, dt \; . \tag{3}$$

Note that the set of computational basis signals forms an orthonormal basis.

Gate operations are performed using projection operations. Given a quantum state  $|\psi\rangle$  and a qubit *i* to be addressed, we can formally decompose it into projections onto the subspaces in which the qubit is either 0 or 1. Thus, we may write

Quantum Decoherence Emulated in a Classical Device

$$|\psi\rangle = \Pi_0^{(i)} |\psi\rangle + \Pi_1^{(i)} |\psi\rangle = |0\rangle_i |\psi_0^{(i)}\rangle + |1\rangle_i |\psi_1^{(i)}\rangle , \qquad (4)$$

where  $|\psi_0^{(i)}\rangle$  and  $|\psi_1^{(i)}\rangle$  will be called partial projection states. As described in [4], the corresponding signals  $\psi_0^{(i)}$  and  $\psi_1^{(i)}$  may be produced from the signal  $\psi$  using classical analog signal processing devices. In this manner, the nonseparable subspace projections may be separated and operated upon individually. Doing so allows one to perform a single-qubit gate operation U on qubit i by noting that

$$U_{i} |\psi\rangle = U |0\rangle_{i} |\psi_{0}^{(i)}\rangle + U |1\rangle_{i} |\psi_{1}^{(i)}\rangle .$$
(5)

So, simple multiplication and addition of analog signals is all that is needed to effect this transformation.

Measurements are performed in a similar manner. Given the partial projection signals  $\psi_0^{(i)}$  and  $\psi_1^{(i)}$ , we may perform a measurement on qubit *i* by first measuring the root-mean-square (RMS) voltages  $v_0 = \|\psi_0^{(i)}\|$  and  $v_1 = \|\psi_0^{(i)}\|$  of each signal and, from these, computing the probability

$$p = \frac{v_0^2}{v_0^2 + v_1^2} \,. \tag{6}$$

A random variable  $u_i \in [0, 1]$ , which serves the role of a hidden variable, is drawn such that  $u_i \leq p$  indicates an outcome of 0 and  $u_i > p$  indicates an outcome of 1. Upon measurement, the state "collapses" to form the new signal  $\psi' \propto \psi_0^{(i)}$  or  $\psi' \propto \psi_1^{(i)}$ , depending upon the measurement outcome. Additional qubits may be measured sequentially in this manner. This procedure, then, faithfully reproduces the quantum statistics dictated by the Born rule.

We have implemented a small-scale quantum emulation device in hardware using breadboards and analog electronic components interfaced to a digital desktop computer. The device can be operated in one- or two-qubit mode at frequencies of 1000 Hz and 2000 Hz, respectively. Arbitrary one-qubit gate operations can be performed as well as controlled gate operations using qubit 0 as the control and qubit 1 as the target. Typical gate fidelities are found to be over 99% [5]. Measurement gates are performed using true-RMS voltage chips and digital switching. Sequential gate operations can be performed using a software interface. For example, a simple implementation of Deutsch's algorithm can be programmed for an unknown Boolean function. In practice, we find that the device is able to correctly identify whether the function is constant or balanced about 96% of the time. Since the algorithm should, ideally, produce the correct answer every time, the nonzero error rate must be due to device imperfections. In the following sections, we will investigate whether these imperfections can be modeled as quantum decoherence.

#### **3** Application of Quantum State Tomography

Using the representation and measurement procedure described in Sect. 2, we are able to use our device to prepare and measure any quantum state and observable of up to two qubits. Of course, imperfections in the device itself can give only a limited approximation of the ideal mathematical operations. This situation is quite similar to that found in actual quantum devices or experiments, and we may use similar tools to study it.

We have heretofore discussed the representation of *pure* quantum states using our device, but the more general quantum description is that of a *mixed* state. Mixed quantum states may be thought of as an ensemble of pure states. Equivalently, in our classical representation, they may be thought of as noisy signals. For example, it can be shown that additive Gaussian white noise is equivalent to a mixture of the ideal state and a fully mixed state [6]. Noise can also be added intentionally to reproduce certain quantum measurement effects, as was done with so-called dressed states [5]. For the purposes of the present study, however, we are simply interested in estimating the equivalent quantum mixed state given a set of measurement outcomes. This may be done using the technique of quantum state tomography (QST).

A general (mixed) *n*-qubit state  $\rho$  may be decomposed into a basis of  $4^n$  separable orthonormal operators using the Hilbert-Schmidt inner product, as follows:

$$\rho = \sum_{j_{n-1}=1}^{4} \cdots \sum_{j_0=1}^{4} \operatorname{Tr}\left[\rho \; \frac{\sigma_{j_{n-1}}^{(n-1)} \otimes \cdots \otimes \sigma_{j_0}^{(0)}}{2^{n/2}}\right] \frac{\sigma_{j_{n-1}}^{(n-1)} \otimes \cdots \otimes \sigma_{j_0}^{(0)}}{2^{n/2}} , \quad (7)$$

where

$$\sigma_1^{(k)} = \mathbf{I}_k , \quad \sigma_2^{(k)} = \mathbf{X}_k , \quad \sigma_3^{(k)} = \mathbf{Y}_k , \quad \sigma_4^{(k)} = \mathbf{Z}_k$$
(8)

are the four Pauli spin operators applied to qubit k. Since the trace represents an expectation value under the Born rule [7], we may use this decomposition to empirically determine the quantum state by measuring each of the basis operators.

Let  $\bar{B}_{j_{n-1},...,j_0} \in \mathbb{R}$  denote the mean value obtained from a finite sample of measurements of the operator  $\sigma_{j_{n-1}}^{(n-1)} \otimes \cdots \otimes \sigma_{j_0}^{(0)}$ . From these results, one may estimate the quantum state to be

$$\bar{\rho} = \sum_{j_{n-1}=1}^{4} \cdots \sum_{j_0=1}^{4} \bar{B}_{j_{n-1},\dots,j_0} \frac{\sigma_{j_{n-1}}^{(n-1)} \otimes \cdots \otimes \sigma_{j_0}^{(0)}}{2^n} \,. \tag{9}$$

In practice,  $\bar{\rho}$  will not be a valid quantum state, since the numerical coefficients are not guaranteed to yield an operator that is both positive definite and of unit trace. A better procedure is to restrict one's search to valid quantum states and find the maximum likelihood estimate (MLE) of the quantum state, here denoted  $\hat{\rho}$ , that both satisfies this constraint and best fits the measured mean values. To this end, we use an MLE procedure developed by Altepeter, Jeffrey, and Kwiat under the assumption of independent Gaussian errors [8].

Once a valid estimate  $\hat{\rho}$  of the quantum state is obtained, it may be compared to the ideal quantum state  $|\psi\rangle$  by computing the fidelity *F* of the former to the latter using the expression [9]

$$F = \sqrt{\langle \psi | \hat{\rho} | \psi \rangle} . \tag{10}$$

Note that *F* is bounded between zero and one. If  $\hat{\rho} = \mathbf{I} \otimes \cdots \otimes \mathbf{I}/2^n$  (a completely mixed state), then  $F = 1/2^n$ . Thus, in practice, we expect to find intermediate values of *F* such that  $1/2^n < F < 1$ .

As an example, we considered the pure entangled state  $|\psi\rangle = \frac{1}{\sqrt{2}}[|01\rangle - |10\rangle]$ . So, in matrix form in the computational basis, the ideal quantum state is

$$\rho = |\psi\rangle \langle \psi| = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0\\ 0 + 1 & -1 & 0\\ 0 & -1 & +1 & 0\\ 0 & 0 & 0 & 0 \end{pmatrix} .$$
(11)

The estimated quantum state was found to be

$$\hat{\rho} = \begin{pmatrix} 0.0001 & -0.0011 - 0.0082i & 0.0008 + 0.0075i & -0.0006 + 0.0004i \\ -0.0011 + 0.0082i & 0.5412 & -0.4968 - 0.0082i & 0.0019 - 0.0364i \\ 0.0008 - 0.0075i & -0.4968 + 0.0082i & 0.4562 & -0.0012 + 0.0335i \\ -0.0006 + 0.0004i & 0.0019 + 0.0364i & -0.0012 - 0.0335i & 0.0025 \end{pmatrix},$$

giving a fidelity of F = 0.9978. The two states are shown graphically in Fig. 1.



Fig. 1 Cityscape plot of the ideal quantum state (a) and that inferred from quantum state tomography (b). Only the real part of the matrix elements is shown

## 4 Application of Quantum Process Tomography

In quantum mechanics, the evolution of a closed system is given by a unitary transformation generated by the system's Hamiltonian, in accordance with the Schrödinger equation. In practice, no system is ever truly isolated, and this can lead to apparent non-unitary evolution. The formalism of quantum operations gives us a framework with which to characterize the behavior of open quantum systems and, in particular, decoherence [10, 11]. A quantum operation may be viewed as a superoperator on quantum states such that, if  $\rho$  is the initial quantum state, then  $\rho' = \mathscr{E}(\rho)$  is the state that results from some, possibly non-ideal, transformation.

We will make use of an equivalent formulation of quantum operations known as the operator-sum representation [12]. Using this formalism, the quantum operation  $\mathscr{E}$  may be characterized by a discrete set of operators such that

$$\mathscr{E}(\rho) = \sum_{k} E_k \, \rho \, E_k^{\dagger} \,. \tag{12}$$

The matrices  $\{E_k\}$  are known as Kraus operators [13]. A further decomposition of the Kraus operators may be performed in terms of, say, the Pauli operators, as was done for QST.

For our present purposes, we will consider, for simplicity, only single-qubit states. In this case, each Kraus operator may be written as a linear combination of the four Pauli operators, so that

$$E_k = \sum_{i=1}^{4} e_{k,i} \frac{\sigma_i}{2} .$$
 (13)

Using this representation, the quantum operation may be written as

$$\mathscr{E}(\rho) = \sum_{k} \left( \sum_{i=1}^{4} e_{k,i} \frac{\sigma_{i}}{2} \right) \rho \left( \sum_{j=1}^{4} e_{k,j} \frac{\sigma_{j}}{2} \right)^{\dagger} = \sum_{i=1}^{4} \sum_{j=1}^{4} \chi_{i,j} \sigma_{i} \rho \sigma_{j}^{\dagger}, \quad (14)$$

where

$$\chi_{i,j} = \sum_{k} e_{k,i} \, e_{k,j}^* \tag{15}$$

are the elements of the 4  $\times$  4 chi process matrix  $\chi$  [14, 15]. Determination of the equivalent quantum operation therefore reduces to the problem of estimating the corresponding chi matrix. This, in turn, may be accomplished using the techniques of quantum process tomography (QPT) [15–17].
As an example, we performed QPT on a single-qubit identity gate using the procedure outlined in [11] but modified to use a maximum likelihood QPT technique [18–20]. We started by generating an ensemble of input states of the following form:

$$|\psi_1\rangle = |0\rangle$$
,  $|\psi_2\rangle = |1\rangle$ ,  $|\psi_3\rangle = \frac{1}{\sqrt{2}}[|0\rangle + |1\rangle]$ ,  $|\psi_4\rangle = \frac{1}{\sqrt{2}}[|0\rangle + i|1\rangle]$ . (16)

The process, in this case an identity gate, was applied to the ensemble of states, which were then measured using this same basis. The chi matrix was parameterized using a Cholesky factorization such that  $\chi = \Delta \Delta^{\dagger}$ , where  $\Delta$  is a lower triangular matrix with real, positive diagonal elements. This form guarantees that the constraints of Hermiticity, trace preservation, and complete positivity are satisfied. We then optimize over  $\Delta$  with respect to the following likelihood function:

$$L(\Delta) = \frac{1}{2} \sum_{\alpha} \sum_{\beta} \frac{\left[ N_{\alpha,\beta} - C \sum_{i} \sum_{j} \langle \psi_{\beta} | \sigma_{i} | \phi_{\alpha} \rangle \langle \phi_{\alpha} | \sigma_{j} | \psi_{\beta} \rangle (\Delta \Delta^{\dagger})_{i,j} \right]^{2}}{C \sum_{i} \sum_{j} \langle \psi_{\beta} | \sigma_{i} | \phi_{\alpha} \rangle \langle \phi_{\alpha} | \sigma_{j} | \psi_{\beta} \rangle (\Delta \Delta^{\dagger})_{i,j}},$$
(17)

where  $|\phi_{\alpha}\rangle$  and  $|\psi_{\beta}\rangle$  are the input states and measurement settings, respectively, and  $N_{\alpha,\beta}$  are the experimentally measured counts for the corresponding pair of input state and measurement settings. The factor *C* is the total number of such counts.

The resulting estimated chi matrix,  $\hat{\chi}$ , is illustrated graphically in Fig. 2. Ideally, the matrix should be such that  $\chi_{i,j} = \delta_{i,j}$ , indicating that the quantum operation takes the simple form  $\mathscr{E}(\rho) = \sigma_1 \rho \sigma_1 = \rho$ . Empirically, we do indeed find that  $\hat{\chi}_{1,1}$  is nearly 1 and is, therefore, the dominant component. A closer inspection reveals that there are other nonzero components. In particular, the  $\hat{\chi}_{1,j}$  and  $\hat{\chi}_{j,1}$  components appear to have non-negligible imaginary terms.



Fig. 2 Cityscape plot of the QPT results for a single application of the identity gate. The real part of  $\hat{\chi}$  is shown on the left, while the imaginary part of  $\hat{\chi}$  is shown on the right. Note that the two figures are shown on very different scales to illustrate the nonzero contributions to the estimate

The gate fidelity relative to an ideal unitary operator U may be determined from the estimated quantum operation  $\mathscr{E}$  according to the formula [21]

$$F = \min_{\rho} \operatorname{Tr} \sqrt{\sqrt{\mathscr{E}(\rho)} \ U\rho U^{\dagger} \sqrt{\mathscr{E}(\rho)}} \ . \tag{18}$$

For the present case, U is the identity, and  $\mathscr{E}$  is estimated by the chi matrix  $\hat{\chi}$ , for which we find that F = 0.9933 for a single identity gate operation. This is comparable to what was found earlier for the quantum state fidelity using QST, and, so, these results appear to be consistent.

Ideally, the chi matrix should give a full characterization of the quantum process (in this case, a single application of the identity gate operation). In particular, it should provide a means of forecasting the gate fidelity over multiple iterations. Indeed, if the initial quantum state is determined to be  $\rho_0$ , then the state after *n* iterations, denoted  $\rho_n$ , is given iteratively by

$$\rho_n = \mathscr{E}(\rho_{n-1}) = \mathscr{E}(\cdots \mathscr{E}(\rho_0) \cdots) .$$
<sup>(19)</sup>

Consider the depolarizing channel with parameter  $p \in [0, 1]$ , for which

$$\mathscr{E}(\rho) = (1-p)U\rho U^{\dagger} + p\mathbf{I}.$$
<sup>(20)</sup>

The fidelity of this channel is then

$$F = \sqrt{1 - \frac{2p}{3}} . \tag{21}$$

The depolarizing channel is closed under multiple iterations, with an effective parameter  $p_n$  after *n* iterations of

$$p_n = \frac{3}{4} \left[ 1 - \left( 1 - \frac{4p}{3} \right)^n \right] \,, \tag{22}$$

yielding a cumulative fidelity of

$$F_n = \sqrt{1 - \frac{1}{2} \left[ 1 - \left( 1 - \frac{4p}{3} \right)^n \right]} .$$
 (23)

In addition to the gate fidelity defined in Eq. (18), we make use of an alternative benchmark known as the quantum process fidelity defined as [21]

$$F_{\rm proc} = {\rm Tr}(\hat{\chi} u u^{\dagger}) \tag{24}$$



Fig. 3 Plot of experimentally measured process fidelity (determined via QPT) versus iteration count (red line), along with forecasted results based on direct propagation of the initially estimated chi matrix (black dashed line) and the depolarizing channel model (blue crosses)

where  $\hat{\chi}$  is the measured chi matrix and  $uu^{\dagger}$  is the rank-one chi matrix for the ideal unitary transformation *U*. The process fidelity has the benefit of being less computationally intensive to calculate as we need not perform the optimization step over input states. For the depolarizing channel, it may be interpreted as the probability that the ideal operation was performed.

Using our device, we explored the behavior of the measured process fidelity upon performing multiple iterations of the identity gate, using QPT to estimate the fidelity for each iteration. The results are summarized in Fig. 3. Surprisingly, the process fidelity after 90 iterations drops only to about 0.874. This is well above the 0.55 cumulative process fidelity that is predicted from a simple fit to a depolarizing channel based on the fidelity of a single-gate operation, which has a parameter value of p = 0.010. Using instead the actual chi matrix estimate, and iterating the corresponding quantum operation, yields a sequence of process fidelity values with a curious, oscillatory behavior, as shown in Fig. 3. Initially, it seems, the fidelity drops sharply. After the 35th iteration, however, it begins to climb up again, only to crest and fall once more after about the 70th iteration. This shows the folly of extrapolation based on a single QPT estimate.

If one instead considers the whole sequence of iterations, a much better fit can be achieved, as illustrated in Fig. 4. In this case, forecasting was done based on optimizing the channel parameterization in order to minimize the least-squares error to *all* of the measured data (i.e., over all 90 iterations). Doing so, we found that a simple depolarizing channel actually did provide a good fit to data, albeit with a model parameter value of p = 0.006. This is just slightly lower than the value estimated from a single-gate iteration, but the impact on the forecasted fidelity is quite significant. We note that the resulting depolarizing channel also agrees quite well with the forecasted chi matrix, when fitted to all 90 iterations.



Fig. 4 Plot of experimentally measured process fidelity versus iteration count along with forecasted results based on fitting both an estimated chi matrix and a depolarizing channel model to the data using least squares fitting

#### 5 Conclusions

We have considered the performance of a classical device in terms of quantum operations. Using simple electronic hardware, we are able to emulate the behavior of a two-qubit quantum computer by representing the quantum state as an analog voltage signal. An arbitrary sequence of one- and two-qubit gate operations can be performed on these signals, thereby allowing for full programmability. As with any physical device, these operations are not performed perfectly but, instead, exhibit some level of degradation. In order to understand this better, we have chosen to use to the mathematical framework of quantum operations to model this classical degradation of performance in terms of quantum decoherence. In particular, we avail ourselves of the techniques from the field of quantum state and quantum process tomography to extract an empirical estimate of the equivalent quantum channel corresponding to a given gate operation.

What we find is that the estimate of the quantum channel obtained from performing QPT on a single-gate operation provides a poor prediction of its performance upon repeated iterations. If, however, the channel is estimated over a number of iterations, then a good fit can indeed be achieved. This is particularly true when, as is the case for our device, the gate fidelity on any single iteration is quite high. In such cases, the error is quite low, and the estimation process will be very sensitive to the behavior over the first few iterations. When these considerations are taken into account, we find that we are able to achieve a good fit to the measured results by assuming a simple depolarizing channel as a model for the effective quantum operation. Given that decoherence may be viewed as a classical process that can be modeled quantum mechanically, the possibility arises for the use of quantum error correction techniques to improve performance. In particular, we have shown that errors in a classical analog device can be modeled solely in terms of discrete bit-flip and phase error quantum operations, which are sufficient for modeling all forms of decoherence. This presents the exciting new prospect of using the methods of fault-tolerant quantum computing to improve the fault tolerance of classical analog devices. Whether the inclusion of additional, albeit faulty, classical resources can improve overall performance will be a subject for future investigations.

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# Local Realism Without Hidden Variables



Ghenadie N. Mardari

# 1 Hidden Variables Exclude Superposition in Quantum Mechanics

Local hidden variables cannot violate Bell's inequality. Yet, quantum variables can. This is conclusively proven theoretically, as well as experimentally. For example, last year, three major experiments closed the loopholes of quantum observation and still revealed significant violations of Bell's inequality [1-3]. So, we know that hidden variables do not work very well in quantum mechanics. Nonetheless, we have to ask: is this a good reason to dismiss local realism? In other words, is it true that we cannot have one without the other? The main goal of this presentation is to show you that there are two kinds of local realism. The difference between them is determined by the role of quantum superposition. Single quanta often behave as if they are in many states at the same time. If we *do not* accept this appearance, we can assume that single quanta occupy only one state at a time and that superposition is a measurement artifact. This approach requires hidden variables. Yet, we can also assume that quantum superposition is a real phenomenon, in which case we can formulate a local theory without hidden variables. Such an approach would be immune to the implications of Bell's theorem.

Here is an intuitive explanation of hidden variables. Suppose that we have two coherent classical beams in superposition. The output is a projection with interference fringes. If we isolate a single dark fringe, we notice that it does not contain any energy. Yet, the textbook interpretation is that we still have two beams that go through each other unperturbed. It just so happens that the two components are out of phase and cancel out at this point. In other words, the superposed dark

G. N. Mardari (⊠)

Open Worlds Research, Sparks, MD, USA

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state is an illusion. What we really have is two unobservable components, acting against each other. Keep in mind that we are dealing with a classical state, so we expect to have many elementary entities acting at the same time. However, when we move into the quantum regime, we only get one detection at a time. It is no longer possible to say that we have many "particles," but we still get fringes. Quantum mechanics tells us that one single system is in both states at the same time and expresses the effect of interference. In contrast, hidden variable theories deny this explanation. They insist that superposition is not real. What is real is that a single quantum occupies only one of the two possible states. Of course, this creates a problem, because fringes cannot be explained anymore. And so, a hidden variable or process needs to be postulated, in order to explain why quanta conspire to behave *as if* interference is taking place.

Let us now look at this equation, which was used by John Bell to derive his famous inequality [4]:

$$\mathbf{E}(\mathbf{a}, \mathbf{b}) = \int d\lambda_{\rho}(\lambda) A(\mathbf{a}, \lambda) B(\mathbf{b}, \lambda)$$

It tells us that the joint probability of two observations is only dependent on the measurement settings **a** and **b**, as well as the all-inclusive parameter  $\lambda$ . Many people believe that  $\lambda$  is allowed to contain any classical quality or process, but this cannot possibly be true. This might be hard to grasp just by looking at the quoted equation, but it becomes less subtle when we see its implied place in the final inequality:

$$1 + E(\mathbf{b}, \mathbf{c}) \ge |E(\mathbf{a}, \mathbf{b}) - E(\mathbf{a}, \mathbf{c})|$$

Suddenly, we have three terms: E(a,b), E(a,c), and E(b,c), and each of them could—in theory—have a range between -1 and +1. This means that the inequality cannot hold, unless the three terms share a special relationship. Specifically, they must describe a common population, sharing a common reality. More importantly, individual objects have to be prohibited from changing states in between measurements. If a particle is in the state "up" for A when determining  $E(\mathbf{a},\mathbf{b})$ , it must also have the same value when determining  $E(\mathbf{a}, \mathbf{c})$ . Consequently, unstable distributions violate the criteria for deriving Bell's inequality, even if they emerge for local reasons. One might, of course, wonder: why should the population profile change for repeated identical measurements? The answer is straightforward: this is a natural side effect of linear superposition, when the net state is consequential. Contrary to the EPR criterion or reality, it is possible for classical entities to have properties with wide spectra and undefined measurement outcomes. Sometimes, these net states evolve to have sharp spectra, with well-defined states in special circumstances. Yet, these transient properties of quanta should not be mistaken for permanent sharp properties of measured entities. As a corollary, Bell's inequality only follows from the shown equation if  $\lambda$  is *not* allowed to depend on superposition effects, even if the process is classical.

To be fair, superposition is widely believed to defy classical rules at the level of single entities. The problem is that classical interference is perceived as a collective effect of multiple inputs, acting together. For a single entity to express the same behavior, it would have to be in many states at the same time. So, how can we have superposition and local realism at the same time? The trick is to keep in mind that many state vectors in superposition always add up to one net-state vector. For example, when two players kick a football at the same time, we can assign a different vector to each individual contribution. On paper, we have two state vectors. Yet, in real life, we know that the ball can only travel in the net direction. In the same way, we can say that quanta express many states at the same time on paper, but only one net state in real life. This would be particularly natural in a pilot-wave model. The thing to keep in mind is that quantum properties are not directly observable. It is purely a matter of personal preference how to describe undetected behavior. If we assume that all the component states are real at the same time, then we get nonclassical behavior with paradoxes. If we assume that the net state is real, then we get classical behavior without paradoxes [5].

The bottom line is that every wave property can be interpreted in two ways, whether we deal with polarization, momentum, or frequency spectra. We can either assume that the complex net state is real or that the simple component states are real. Yes, there are many independent components if a wave is broken down, but the question is: what happens when these components are superposed? Do they interfere with each other or not? These two approaches entail the same macroscopic predictions, because they emphasize different sides of the same equation  $(\mathbf{A} + \mathbf{B} = \mathbf{C})$ . Still, their microscopic implications are different. Keep in mind that matter does not propagate in the case of classical waves. The only real thing is that something oscillates. So, we need to decide: can a classical medium oscillate in many directions at the same time? This is the same problem that we get if we assume that single quanta express many states at the same time.

Here is a simple way to visualize the difference between the two approaches to superposition. When two narrow beams intersect, they have an interference volume with fringes, followed by another double-beam projection (Fig. 1). If we assume that interference is not real, then we describe the quanta as if they propagate along straight rays through the volume of interference. This is why we believe that quanta can reveal path knowledge. On the other hand, if we assume that interference is *real*, then we have to assume that quanta always reflect the local net state of the wave function. In the interference volume, they bunch into fringes, and afterward they redistribute again. Yet, they are no longer able to carry any information from the source to the detector. Their properties change at every step, in order to reflect the net state of the wave function, as it passes through many different profiles. As suggested above, it is this difference that can be detected with the help of Bell's theorem.

So, let us briefly summarize the main starting points of this presentation. Firstly, it is possible to develop a local realist model of quantum behavior, if we assume that the net state of linear superposition is real. Secondly, this approach is immune to Bell's inequality, because it does not make predictions on the basis of hidden

Fig. 1 Two-beam superposition. Quantum distribution in each consecutive plane corresponds to the macroscopic profile of the wave front. This appearance can be taken at face value (net-state realism) or dismissed as an artifact of measurement (component-state realism)



variables. In quantum mechanics, the concept of hidden variables is defined with a very narrow meaning. It is only intended to provide an alternative to quantum superposition. Finally, quanta can be assumed to express the net state of the wave function at every step of propagation. If so, then they can only have transient properties and no longer carry information from the source to the detector at the individual level. The main implication of this approach is that quantum mechanics cannot be improved by an alternative model with hidden variables. Instead, the goal is to reclaim quantum mechanics as a classical theory, by changing the interpretation of superposition. Let us see if this is possible.

# 2 Non-locality Is Hypothetically Implied but Not Required by Quantum Mechanics

The concept of entanglement is currently interpreted as a property of inseparable quantum systems. Though, it is important to keep in mind that it began as an argument about the nature of quantum superposition [6]. The Copenhagen interpretation insisted that single quanta can be in many states at the same time. This property was seen as unavoidable in the case of non-commuting variables, because they had to obey Heisenberg's principle. If one of these properties was sharp, the other had to have a maximally wide spectrum. Ergo, every quantum had to be in many states at the same time for at least one property. In contrast, Einstein, Podolsky, and Rosen developed an argument that seemed to contradict this expectation [7]. When two quanta separate from a joint state, they have to obey the principle of energy conservation. Therefore, it is enough to measure one, in order to determine the state of both quanta, because the sum of their states is known. This holds for all the variables that belong to the initial system, including the ones that do not commute. Suppose that we measure the position of quantum

Q1. We immediately infer the position of quantum Q2, without disturbing it in any way. Therefore, we must assume that quantum Q2 has a pre-existing value for that variable. Yet, one could just as easily measure the momentum of quantum Q1, instead of measuring its position. This means that quantum Q2 has a pre-existing momentum value as well. In short, EPR suggested that quanta do not really commute, even when quantum experiments provide evidence of noncommutativity. From their point of view, complementarity might be an artifact of the process of measurement. Therefore, they did not see it likely that single quanta were actually in many states at the same time. At the level of observables, it appeared that quanta did not commute. Yet, at some deeper level of reality, they had to commute.

Let us now jump ahead to the modern times, where we have a rich experimental record, as well as a mature quantum formalism. Among other things, we now have a very advanced understanding of the behavior of correlated physical systems [8–14]. Hence, we know that there are three kinds of coefficients of correlation: subquantum, quantum, and super-quantum. When two variables have exact detectable values in any context, they have to commute. Therefore, they obey Bell's inequality. In contrast, when they display unavoidable superposition, they violate Bell's inequality with necessity. At the same time, quantum variables cannot display arbitrarily high levels of superposition, because they have to obey Heisenberg's principle. If one of them has a wide spectrum, the other has to be sharp. As a result, quantum coefficients are also bounded, in the same way in which sub-quantum coefficients are bounded by Bell's inequality. They have to obey a limit that is known as Tsirelson's inequality [8, 12]. Accordingly, all the coefficients that exceed this line are described as super-quantum. For the purpose of our discussion, the main thing is that Bell's inequality is the hard boundary between properties that are always "in one state at a time" and the properties that can be "in many states at a time." Therefore, Bell's inequality is the ideal tool for testing the implications of the EPR argument. Einstein's group suggested that quantum superposition is not real [7], and now we have the theoretical and the experimental means to test this hypothesis.

Before we move on, I wish to address a common misconception about correlations. It is often claimed, especially in popular science presentations, that quantum correlations directly imply non-locality, because they expose relationships between remote particles. In actuality, it is the other way around. We prepare or select two systems that are known to be similar in some way, so that we can investigate incompatible properties. What we want to determine is the rule of coincidence between specific values of two variables at the level of single quanta. When we work with variables that commute, this can be done directly with single objects. Yet, when selected variables do not commute, we are forced to use multiple copies of the same system. In the case of classical objects, it works like this. Suppose that we have a large warehouse full of socks and we want to measure the correlation between two properties (e.g., color and fabric) of this population. For example, we may want to know: if a sock is white, what is the probability that it is also made of cotton? Of course, it is possible to answer this question by looking at many different socks, but let us suppose that we need to obtain a large data set very quickly. So, for reasons of efficiency, we use a machine to split all the pairs and measure each sock for a different property. Then we analyze the coincidences and calculate the coefficient of correlation. The exact coefficient will vary from population to population, but it cannot be completely arbitrary, because it has to work within the boundaries of known distribution for each property. Of course, it is not reasonable to invoke a physical connection between these coincidences, even if they obey a strict quantitative relationship. The two variables are reducible to a single object, and they obey the inequality (in combination with other tests) simply because they commute.

Next, we repeat the same experiment with pairs of quanta. As you know, it is possible to produce identical photons by means of type I SPDC. So, again, we are interested in the coincidence between the states of two variables of a single system, but we use two systems to solve the problem of incompatible measurements. We do the same thing that we did with the socks, but in this case our variables do not commute. Therefore, we cannot expect an objective correlation between the measured states, because they emerge into existence independently, in different environments. Notice, again, that we do not have a reason to suspect non-locality yet. Logically, all that we know is the mathematical relationship. The reason we end up with a violation of Bell's inequality is noncommutativity. In other words, these variables are presumed to obey Heisenberg's principle objectively and locally (at the level of single quanta). We measure two copies of the same system, because the two observables are incompatible. Yet, we still obtain information about the coincidence of two properties at the level of single entities. To sum up, the formalism of quantum mechanics, by itself, does not explicitly require non-locality even if Bell's inequality is violated. Quantum superposition is a sufficient condition for that effect. Similarly, the structure of a correlation test is also not problematic from the point of view of locality. And so, we have to ask: Where does non-locality come from in quantum mechanics? Why does it seem impossible to explain quantum correlations without it?

# **3** The Copenhagen Interpretation Is Incompatible with Quantum Mechanics

The answer is very simple: we have to blame the Copenhagen interpretation. This approach is based on the presumed reality of three basic principles [15, 16]. First of all, unmeasured quanta are always supposed to be governed by informational uncertainty. This works as if our lack of knowledge forces them to lose any physically real properties, in the classical sense. Furthermore, quantum variables are expected to collapse to "well-defined" values at the moment of detection. So, they abruptly become in one state at a time. Finally, this sudden transition is supposed to happen because of the act of observation and only because of observation. No other physical mechanism is known or required for this effect. If we take these assumptions for granted, then non-locality becomes unavoidable.

Let us go back to the basic example of Einstein, Podolsky, and Rosen [7]. If we measure the *momentum* of quantum Q1, then we immediately know that the momentum of quantum Q2 is also sharp. However, we could instead measure the *position* of quantum Q1. In this case, the position of quantum Q2 becomes sharp, and—by implication—its momentum spectrum becomes immediately wide. Hence, the real state of the quantum Q2 has to change on the spot, based on how we measure quantum Q1. How does this second photon know when to have a sharp spectrum, and when to have a wide spectrum for the same variable? Given that quanta violate Bell's inequality, and given the three cited assumptions, we have no choice but to suspect the realism. Yet, we have to ask if these assumptions are necessary. Do they remain valid in every interpretation of quantum mechanics? More importantly, are they justified by the details of quantum experiments? In other words, is this a fundamental problem of quantum mechanics, or is it just an internal problem of the Copenhagen interpretation?

Let us consider a simple example. The double-slit experiment produces distributions with fringes. If we focus on a point in the middle of a dark fringe, we can expect to detect zero photons. Why is this happening? The explanation is that we have quantum superposition. Even though we detect the photons one at a time, every one of them is under the influence of the wave function as a whole. Yet, Copenhagenstyle interpretations do not stop here. They suggest that we have uncertainty as to which path was taken by the photon, and this is why we get the final effect. But what does it mean to say that something is uncertain? It means that we have several alternative possibilities, but we do not know which one of them is actually true. Yet, here we do not have alternative arrivals of photons in different states. We get zero photons, no matter how many events are detected at other locations. If we want to explain this correctly, we have to postulate that we have multiple components acting all at the same time. Therefore, we cannot say that we have "uncertainty" as to which mode of propagation applies to the quantum in question. What we have is certainty that all the components act at the same time, in order to produce the net state. Indeed, quanta are always detected in the net state of the wave function [15]. This does not mean that we have uncertainty. It means that we are dealing with a wide spectrum.

Therefore, our first conclusion is that *quantum uncertainty is not an objective physical property*. When we have superposition, quanta cannot express individual components one at a time. Even if the wave function has a wide spectrum, they have to reflect the joint effect of all the components at the level of single events. Consequently, we can dispense with the first listed assumption of the Copenhagen interpretation.

The next step is to consider the mechanism behind the so-called quantum collapse. In a geometric approach to wave propagation, we describe the rays as if they stand for real modes of propagation. Intuitively, this means that we have wave packets that follow these rays as if they were trajectories. For instance, we could say that the path of each wave packet bends inside the lens and converges on the focal point. This is the basis for the idea that measurements resolve individual histories. We get information about one property or another, as if it came unperturbed from the source. Usually, this is not a problem in classical mechanics, because all the rays

Fig. 2 Wave dynamics: wavelets vs rays. Wave-front propagation is predicted correctly by Huygens-Fresnel wavelets. They are assumed to propagate in all directions and interfere with each other. When a stable pattern of constructive interference emerges, its structure can be captured by a group of rays



are assumed to be populated by many wave packets at the same time. In contrast, quantum mechanics operates with single quanta. We still need all the modes to predict the future state of a wave function, but the measurements are supposed to collapse the system to just one component. By the way, this problem is rooted in the classical tradition of assuming that wave components go through each other unperturbed [5]. The main reason for the notion of collapse is the assumption that detected sharp states are *input components*, as suggested by the widespread illustrations with rays.

As a matter of fact, the method of ray tracing cannot predict the details of classical wave-front evolution. The only known way to do this correctly is by using the Huygens-Fresnel method (Fig. 2). In this approach, the waves are not described by rays. Instead, the dynamics is governed by a process of wavelet interference. It works like this: every point of a wave front is assumed to be a source of wavelets. All of these wavelets interfere and produce a net state, in which wave energy is redistributed. For instance, wavelets are assumed to start in all directions, but the net effect is a light cone all the way to the focal point. This is because the energy of the wave is channeled into the volume with constructive interference, away from the areas with destructive interference. Only at this stage, when we have a welldefined net state, we can use rays to describe the structure of the final beam as a whole. Consequently, geometrical rays do not have individual significance and cannot be described as wave-packet trajectories. Therefore, it is no longer possible to interpret sharp states as "resolved" input components. Instead, we have to keep in mind that wavelet interference produces net states that sometimes have transient sharp states. In the same manner, we do not have to assume that quantum wave functions collapse to reveal one input component. Instead, we can realize that wave functions evolve to acquire transiently sharp net states. These emergent properties correspond to quantum mechanical eigenvalues.

For this reason, we do not need to treat quantum collapse as an objective property of Nature. Instead, we can acknowledge that *quantum wave functions evolve smoothly from one type of net state to another, with occasional profiles that contain sharp spectra*. In other words, measurements do not automatically transform the wave function. They can simply focus on isolated moments from its history. This conclusion contradicts the Copenhagen interpretation but not the details of quantum phenomena.

Many textbooks insist that measurements change physical reality. For example, in the double-slit experiment, we can choose to detect a fringe pattern or a split projection. It sounds as if quanta know what we are going to do and change their physical properties in response. Yet, this interpretation only works if we assume that quanta can change their properties at the same location. According to the story, quanta become different because we intend to use a different type of detector. This is not what we see in actual experiments. For example, we do not have dedicated interference detectors in this case. If we want to see fringes, we take the same screen that shows a split projection and simply move it forward. Hence, the method of detection does not change. The same device is used to track the properties of quanta, as they change from location to location. Moreover, the coordinates of each property are predictable in advance, because it reflects the net state of the wave function.

The same thing can be seen in more sophisticated quantum experiments. For example, if we want to detect sharp states of momentum for single photons, we have to place a detector in the focal plane of a lens (and only in such a plane). In contrast, if we want to detect single photons with sharp position spectra, we have to place a detector in the image plane (Fig. 3). As you can see, we do not have a momentum detector that is different from a position detector. We use the same event counter and move it from one plane of measurement to the other. It is not possible to detect photon properties in violation of the laws of optics [17]. Therefore, we do not have any empirical reason to insist that the choice of measurement hardware changes measurement outcomes. In other words, *quanta do not know how they are going to be measured. It is the people that know where to place their detectors, in order to record expected properties.* 

And so, we see that all the three quantum assumptions, which were instrumental for the conclusion of non-locality, can be avoided. We do not have quantum uncertainty. We have certainty that all the spectral components are active at the same time. We do not have quantum collapse. We have wave-function evolution. Instead

Fig. 3 Complementary wave properties. The wave front evolves to acquire a sharp momentum spectrum in the focal plane of a lens and a sharp position spectrum in the image plane. A quantum event counter can be moved from one plane to the other, in order to detect each property



of component states that are resolved by measurement, we have evolving net states that become sharp at predictable locations. Finally, we can also dismiss the notion of quantum knowledge. Measurements do not create sudden realities. They track the smooth evolution of the wave function and select discrete regions with sharp properties. Therefore, we do not have to deal with the measurement problem. As a result, we have no reason to believe in non-locality either.

# 4 No Measurement Problem: No EPR Paradox in Quantum Mechanics

By now, I suspect that many of you are wondering: what about the EPR paradox? Didn't Einstein prove that non-locality is unavoidable? In order to find the answer, I want to draw your attention to the disclaimer in the penultimate paragraph of this famous paper [7]. As you can see in that passage, Einstein, Podolsky, and Rosen had shown a simple way to solve the paradox. They clearly stated that "spooky action at a distance" only follows if we assume that the two non-commuting variables have pre-existing values *at the same time*. Yet, there is no reason to assume that today. In fact, there are good reasons to assume the opposite. In actual quantum experiments, sharp states for incompatible variables are observed by changing the context of observation. In some cases, the detector is moved to a different location [17]. In other cases, the wave-function profile is physically prepared to have a different net state. It is never the case that incompatible properties are observed or even predicted in the same exact context.

Here is a schematic illustration of this conclusion (Fig. 4). Suppose that we want to use two entangled photons, prepared to be identical. The photons start with identical properties and suffer identical perturbations at every step, because the microscopic details of their propagation are identical. Assume that the red lines express a possible trajectory that they followed. In the focal plane of the lens, both photons arrive at the same position. The fact of their presence at such a location is sufficient to determine the outcome, because they always express the net state of the wave function. So, the blue lines represent the virtual structure of the net state of the wave function at the point of detection. By the way, the photons have trajectories, but this is totally theory-independent. We cannot measure that motion, and we cannot increase our predictive power with that knowledge. As stated above, observable quantum properties are determined by the wave function, and that is why this is not a hidden variable model. As a reminder, hidden variable models are not universal in quantum mechanics. They only serve to explain the appearance of superposition. Yet, here, the process of superposition is not an appearance. Hence, when we measure quantum A for momentum, we immediately determine the momentum of quantum B but only for the shown plane of detection. We cannot say anything about the properties of photon B when it is before or after the focal plane. The reason for this is that we can only infer the state of the second photon for the plane that is used to measure the first one. In any other plane, the net state of the wave function is different, and the location of the quantum is unknown.

Fig. 4 Correlated quantum measurements. The wave-function profile changes from plane to plane. Quantum A acquires a transiently sharp momentum spectrum in the focal plane (FP), and the same is true about its twin. Similarly, both quanta acquire sharp position spectra in the image plane. When the quanta are subjected to nonidentical measurements, incompatible properties are determined at different physical locations, with corresponding probability distributions



Similarly, when we measure the photon A for position, we determine the position of the photon B as well but only for the image plane. Again, we do not have constant information carried from the source, in the case of net-state realism. The quantum *corresponds* to a macroscopic profile that is associated with a point of emission (as shown by the blue rays), but this *does not* tell us anything about the actual point of emission of the detected particle. The only thing that we can determine

is the transient property that is expressed at the point of detection. Finally, when we measure the two photons for different variables, we detect one property in one plane and the other property in a different plane. Each context of observation has its own distribution of properties. In the focal plane, both photons have sharp momentum spectra and wide position spectra. In the image plane, both photons have sharp position spectra. So, we use the photon A to determine the properties of the photon B in the focal plane, and then we also measure photon B in the image plane. We use two photons to make two measurements, but we are really determining the properties of the same photon in two different planes of observation. At no stage can we infer that our photons have sharp momentum and position at the same time. Therefore, we never have to worry about the EPR paradox.

# 5 Bell's Inequality Is a Test of Net-State Realism in Quantum Mechanics

The only problem left to explain is Bell's theorem. Suppose we accept the view that quantum properties are sharp in different contexts. It still follows that we obtain a record of two sharp states for the same quantum. So, why is Bell's inequality violated? Why should it matter that we do not detect the two properties at the same location? This is a very important question, and it is rooted in the same classical approach to ray tracing. For example, if we chose one of the optical rays and treat it as a trajectory (Fig. 3), we could say: look, the wave-packet momentum is resolved in the focal plane and hidden in the image, but it is still the same property that comes directly from the source. Conversely, the position information is hidden in the former plane and resolved in the latter, but we can easily see that the two properties apply to the same mode of propagation at the same time. Therefore, Bell's inequality should be obeyed. In response, we need to remember that the rays have no individual significance, if the net state of superposition is assumed to be real. All the rays need to be considered together, as components of a single process, in order to see that the wave function has one net state with sharp momentum spectrum in the focal plane and a *different* net state with sharp position spectrum in the image plane. Even if we could measure the same quantum in both planes, we would detect a different distribution of properties in each case. In other words, the two properties correspond to output effects of interference and belong to mutually exclusive contexts, but each state is extremely sensitive to microscopic differences in its process of evolution. For this reason, there is no stable relationship between subsequent states, and repeated observations produce contradictory outcomes for the same quantity. Any time a variable is measured more than once, in order to perform a complete Bell test, physical incompatibility translates into statistical incompatibility.

The theory behind this conclusion was recently clarified in an article about the so-called Boole inequality [18]. When two different variables are sampled independently, there is a risk of statistical error. If the two properties belong to incompatible distributions, researchers could obtain spurious correlations. To check for this sort of error, Boole developed an analytical tool, which can be used to derive a Bell-type inequality. Remarkably, this inequality can only be violated by coefficients of correlation between variables with incompatible distributions [9-11], 13]. This is exactly what we expect to see in the case of multimode beams with noncommuting properties. In a rapidly changing wave function, individual quantum properties have to fluctuate at every step. They need to conform to the profile of the net state. Accordingly, a photon must acquire a sharp momentum spectrum and a wide position spectrum in the focal plane. The same photon then acquires a sharp position spectrum and a wide momentum spectrum in the image plane. As a result, the two sharp states belong to the same quantum, but they are incompatible with each other. They can only arise in different contexts. Moreover, these two contexts belong to conjugated optical planes, which mean that the two net states are Fourier transforms of each other. This relationship is known to lead to a violation of Bell's inequality that also obeys Tsirelson's inequality [12, 13]. In other words, the two sharp properties of the same photon are incompatible in just the right way to explain quantum behavior. The two points of detection can be connected by one ray, but this is irrelevant, because the rays are not trajectories. They are meant to capture the geometrical structure of the net state.

Here is another way to look at this problem. When we determine two sharp states for a single quantum, we can ask: how are these properties connected? Do they belong to the quantum at the same time, or are they incompatible? Bell's theorem gives us the answer, by falsifying the first alternative. Therefore, we have to conclude that the net state of linear superposition is always real—not the component states. In other words, Bell's inequality is the perfect instrument for determining which type of local realism is appropriate for the description of our universe.

### 6 Conclusion

Quantum behavior is predicted by wave equations, and this can be interpreted in two alternative ways. In every case of linear superposition, we can assume that unobservable component states are real, but we can also assume that observable net states are real. Bell's theorem was able to falsify the hidden variable approach, and therefore we know that wave superposition requires a net-state ontology. The hidden variable approach and the Copenhagen interpretation share a common problem they treat virtual component states of superposition as real. For this reason, they lead to strange conclusions about measurements, reality, and locality. If we acknowledge the validity of net-state realism, then we can reinterpret the quantum wave function as a local and real pilot wave. Quantum mechanics does not violate Bell's inequality because of non-locality. It only does so because of the local effects of linear superposition.

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# **Underground Test of Quantum Mechanics: The VIP2 Experiment**



Johann Marton, S. Bartalucci, A. Bassi, M. Bazzi, S. Bertolucci, C. Berucci, M. Bragadireanu, M. Cargnelli, A. Clozza, C. Curceanu, L. De Paolis, S. Di Matteo, S. Donadi, J.-P. Egger, C. Guaraldo, M. Iliescu, M. Laubenstein, E. Milotti, A. Pichler, D. Pietreanu, K. Piscicchia, A. Scordo, H. Shi, D. Sirghi, F. Sirghi, L. Sperandio, O. Vazquez-Doce, E. Widmann, and J. Zmeskal

## 1 Introduction

The Pauli exclusion principle (PEP) is a fundamental principle in physics, valid for identical-fermion systems. It forms the basis of the periodic table of elements, electric conductivity in metals, and the degeneracy pressure which makes white dwarf stars and neutron stars stable. Furthermore it is a consequence of the spinstatistics connection [1] and is embedded into the quantum field theory [2].

J. Marton (⊠) · C. Berucci · M. Cargnelli · A. Pichler · E. Widmann · J. Zmeskal Stefan Meyer Institute, Vienna, Austria e-mail: johann.marton@oeaw.ac.at; andreas.pichler@oeaw.ac.at

A. Bassi · S. Donadi · E. Milotti Dipartimento di Fisica, Universita di Trieste and INFN Sezione di Trieste, Trieste, Italy

S. Bertolucci CERN, Meyrin, Switzerland

M. Bragadireanu Horia Hulubei National Institute of Physics and Nuclear Engineering, Bucharest, Magurele, Romania

C. Curceanu · K. Piscicchia LNF-INFN, Frascati, Italy

Museo Storico della Fisica e Centro Studi e Ricerche Enrico Fermi, Roma, Italy e-mail: catalina.curceanu@lnf.infn.it

S. Bartalucci · M. Bazzi · A. Clozza · L. De Paolis · C. Guaraldo · M. Iliescu · D. Pietreanu · A. Scordo · H. Shi · D. Sirghi · F. Sirghi · L. Sperandio LNF-INFN, Frascati, Italy

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Despite the fact that the PEP is connected to so many fundamental phenomena, an intuitive explanation is still missing [3]. Moreover, in the framework of theories beyond the Standard Model, a violation of the PEP might occur (e.g., [4]). Recent work on spin-statistics has been carried out in [5, 6]. Thus, it is important to test the PEP for each fermionic particle type. In the last two decades, many experiments have been carried out, which set upper limits for the probability of its violation [7–13]. These results were primarily obtained as by-products of experiments with a different main scientific objective (like BOREXINO [8] and DAMA [7]). As some of these experiments are investigating the validity of the PEP for composite particles like nucleons and nuclei, it is important to note that the VIP2 experiment investigates atomic transitions of electrons, which are elementary particles.

The different approaches to investigate the PEP need to be distinguished concerning their possible fulfillment of the Messiah-Greenberg (MG) superselection rule [14, 15]. This rule states that the symmetry of the wave function of a steady state is constant in time. As a consequence, the symmetry of a quantum state can only change if a particle, which is new to the system, interacts with the state. All of the aforementioned experiments are looking for changes in the symmetry of steady states that would be violating the MG superselection rule.

#### 2 Tests of the Pauli Exclusion Principle

One of the first experiments looking for a small violation of the PEP was conducted by Goldhaber and Scharff-Goldhaber in 1948 [16]. It was originally designed to check if the particles that made up beta rays were the same as the electrons in atoms, but it was later used to put an upper bound to the probability of the violation of the Pauli exclusion principle. In this experiment, beta rays were absorbed by a block of lead. The idea of the authors was that if the two kinds of particles were not identical, the beta ray particle could be captured by the atom and cascade down to the ground state without being subjected to the PEP. The X-rays emitted during this cascation process were recorded and used to set upper bounds for a violation of the PEP.

To the best of our knowledge, the best way to fulfill the MG superselection rule and test the PEP with high precision is to introduce "new" electrons in a

S. Di Matteo

J.-P. Egger

M. Laubenstein INFN, Laboratori Nazionali del Gran Sasso, Assergi, L'Aquila AQ, Italy

O. Vazquez-Doce

Excellence Cluster Universe, Technische Universität München, Garching, Germany

Institut de Physique UMR CNRS-UR1 6251, Universite de Rennes1, Rennes, France

Institut de Physique, Universite de Neuchatel, Neuchatel, Switzerland



**Fig. 1** Normal atomic 2p to 1s transition with an energy of 8.05 keV in copper (left) and the corresponding non-Paulian transition with an energy of around 7.7 keV in copper (right)

conductor via a current. The electrons form new quantum states with the atoms in the conductor. The goal is to search for new quantum states, which have a symmetric component in an otherwise antisymmetric state. These non-Paulian states can be identified by the characteristic radiation they emit during atomic transitions to the ground state.

The first to employ this scheme in a pioneering experiment in 1988 were Ramberg and Snow [17]. The experiment searched for X-rays originating from Pauli-forbidden atomic transitions, in this case from the 2p to the fully occupied 1s ground state. These transitions are depicted in Fig. 1. The "new" electrons introduced by the current can be seen as test particles, as they can be used to study interactions between a fermionic system and a fermion which has not previously interacted with the studied system. The experiment of Ramberg and Snow set an upper limit for the probability that the PEP is violated for electrons of  $\frac{\beta^2}{2} < 1.7 \times 10^{-26}$ . The parameter  $\frac{\beta^2}{2}$  is quasi standard in the literature for the probability that the PEP is violated.

A much improved version of the experiment of Ramberg and Snow was set up by the VIP collaboration [18]. It employed charge-coupled devices (CCDs) as soft Xray detectors, and through careful selection of the involved materials and shielding, a reduction of background was achieved. The VIP experiment, conducted at the underground laboratory Laboratori Nazionali del Gran Sasso (LNGS) in Italy, took data for ~3 years until 2010. The sensitivity of the experiment greatly increased due to the reduction of background induced by cosmic rays. This background is reduced by six orders of magnitude at LNGS compared to experiments above ground. The experiment set a preliminary upper limit for the probability that the PEP is violated for electrons of  $\frac{\beta^2}{2} < 4.7 \times 10^{-29}$  [19, 20]. A picture of the experiment can be seen in Fig. 2.

A similar experiment of this type conducted in recent years by colleagues in the USA, with a prototype for the MAJORANA demonstrator, is described in [15]. It covers the same topic as the VIP experiment but uses a complementary apparatus. This common interest with the VIP collaboration in testing fundamental physics shows the interest of the scientific community in foundations of quantum mechanics and theories beyond the Standard Model of particle physics. The most recent experiment in this field is VIP2, which is the subject of this article. It was



Fig. 2 The VIP experiment with passive shielding mounted taking data at LNGS

in detail described in recent publications, for example [21–24]. It is the follow-up experiment of VIP. For VIP2, several crucial components were upgraded, like the target, X-ray detectors, and shielding.

## 3 VIP 2 at LNGS Underground Laboratory

The VIP2 experiment is taking data at LNGS in Italy. Conducting the experiment at this facility is advantageous, because of its low-background environment. The Gran Sasso laboratory is the facility of this kind which is easiest to reach for the experimenters from Stefan Meyer Institute, as there is no laboratory of this kind in Austria. In 2016, we took data for 4 months at LNGS.

The core parts of the setup are the SDDs which are used as soft X-ray detectors [25] (Lechner and Soltau, unpublished). The experiment utilizes six SDD cells with an active area of  $1 \text{ cm}^2$  each. The cells are located on each side of the ultrapure copper target, where the high current runs through. The target consists of two copper strips with a gap of 6 mm between the strip and the respective SDD array. Each of these strips has a length of 91 mm and a width of 20 mm. With this configuration, the SDDs cover a solid angle of  $\sim 7\%$  of the target. The probability for detecting an X-ray originating from the target is then further reduced from this value by X-ray attenuation in the copper strip. The heating of the target due to the high current is counteracted by water cooling. The water line runs between the two strips and keeps the copper strip below room temperature, even with a current of 100 A. The SDDs are cooled by liquid argon to a temperature of 100 K. The whole experimental



Fig. 3 Silicon drift detectors with cooling and readout electronics

Table 1The gain factors forincreasing the signal strengthin the VIP2 experimentcompared to the precedingVIP experiment are given inthe table

	VIP	VIP2	Gain factor
Geometry	0.021 [26]	0.03	3/2
Detector efficiency	0.48	0.99	2
Current	40 A	100 A	5/2
Total			7–8

They are in agreement with the original proposal for VIP2 (Marton, unpublished)

setup is evacuated to approximately  $10^{-5}$  mbar, in order to enable the SDD cooling at 100 K. A picture of the SDDs with the liquid argon cooling line and readout electronics is shown in Fig. 3. The increase in signal strength (i.e., the amount of detected X-rays from non-Paulian transitions per time) gained by upgrading the VIP experiment to the setup described above is summarized in Table 1. The factor in the first line describes the probability that a Pauli-forbidden X-ray produced in the target passes through a SDD. It includes effects of target and SDD geometry as well as X-ray absorption in the target. This factor was increased by mounting the SDDs closer to the target than the CCDs of VIP, which increases the solid angle covered by the detectors. These figures are verified by GEANT4 [27] based Monte Carlo simulations (M. Cargnelli, private communication, 2016). For this purpose and all other mentioned GEANT4 simulations, the complete setup was modeled in this framework. A picture of the simulated setup is shown in Fig. 4.

The second gain factor represents the higher X-ray detection efficiency of SDDs compared to CCDs. It comes from the fact that the depth of the depletion layer of CCDs is  $30 \,\mu\text{m}$  [28], whereas the depletion layer of SDDs is  $450 \,\mu\text{m}$  thick. The difference in depths results in a difference in quantum efficiency of a factor of 2. The measurements for VIP2 can be undertaken with a higher current of 100 A due to the new copper target geometry and the implemented water cooling.



Fig. 4 The setup modeled in GEANT4, with the scintillators (green), the copper conductor (brown), and the SDDs (purple). The aluminum enclosure is also shown (gray)

Overall, these factors increase the signal by around one order of magnitude. This enhancement factor is in agreement with the VIP2 proposal (Marton, unpublished). All the mentioned parts have been tested successfully in the laboratory at the Stefan Meyer Institute in Vienna and at LNGS.

The energy and the time resolution of the SDDs are core properties of the experiment. The detector performance which was anticipated in (Marton, unpublished) has been verified experimentally. The energy resolution was determined to be around 150 eV (FWHM), tested with an Fe-55 source at 6 keV, for all six SDDs. The time resolution was measured to be around 400 ns (FWHM) relative to a scintillator trigger, which exceeds the original target (Marton, unpublished).

As an active shielding system, we use an assembly of 32 plastic scintillators read out by Silicon Photomultipliers (SiPMs). They are arranged around the copper target and the SDDs. The purpose of the active shielding system is to reject all SDD events which coincide with events in the scintillators, as these are caused by radiation originating from outside of the setup. Making this time coincidence is only possible due to the good time resolution of the SDDs. A render of the copper target with the active shielding system is shown in Fig. 5. The detection efficiency of the active shielding system was determined to be around 97% for 500 MeV electrons at the beam test facility at the DA $\Phi$ NE collider at the Laboratori Nazionali di Frascati (LNF) in Italy. Tests in the laboratory at the Stefan Meyer Institute (SMI) in Vienna showed that the detection efficiency is around 95% for the given cosmic ray background.



Fig. 5 A render of the VIP2 setup including the silicon drift detectors and the active shielding system

The cosmic ray background at LNGS is lower than at SMI by about six orders of magnitude. The main sources of background at LNGS are high-energy photons in the range of around 40–500 keV, for which the detection efficiency of the active shielding system is around 5%. This was predicted by recent Monte Carlo simulations which were based on a scintillator detection threshold of 100 keV deposited energy. This is the energy equivalent of the voltage threshold used in the experiment. Further reducing the threshold is not possible due to unavoidable noise in the detection system. The result from simulations was confirmed by data taken at LNGS in 2016. The simulations lead to a quantitative understanding of the background induced by the gamma radiation reported in [29]. A comparison between the simulated and the measured spectra is shown in Fig. 6.

# 4 VIP2 Results and Future Plans

In 2016, we were able to take a total of 40 days of data with a current of 100 A and 70 days of data without current. Using an analysis technique analogous to the one used by Ramberg and Snow [17] on this data set, we are able to set a preliminary upper limit for the probability that the PEP is violated in the electron sector of  $\frac{\beta^2}{2} \leq 3.4 \times 10^{-29}$ . This result represents the most stringent test of the PEP in a system circumventing the MG superselection rule.



**Fig. 6** Comparison between 30 days of Monte Carlo simulation data (left) and 30 days of data measured at LNGS (right). The background in the region of interest (marked in red) differs only by around 30%

# 4.1 The Planned Upgrade

We are planning to further enhance the signal and reduce the background in the energy region of the forbidden transition. Together, these effects will improve the upper limit on the violation of the PEP we will be able to set after the running time of the experiment, by more than one order of magnitude.

To reduce the background, it is important to shield the detector from high-energy photon radiation. This will be done by a passive shielding consisting of two parts: an outer part, 5 cm in thickness, made of low radioactivity lead, and an inner part which is 5 cm in thickness, made of low radioactivity copper. Both parts will completely enclose the setup. The inner copper part rests on a frame constructed from Bosch profiles. The frame and the brick layouts are already planned. The geometry of the enclosure was optimized to reach maximum background suppression. The copper and lead blocks are available at LNGS and only need to be assembled. Due to our understanding of the origin of the background, and GEANT4 simulation results, we are confident that the installation of shielding will reduce the background in the energy region of interest by at least a factor 20. To further increase the passive shielding from the outside photon radiation in the energy region of the non-Paulian X-ray transition at 8 keV, a plan to include a Teflon shielding of approximately 5 mm thickness inside of the experimental setup around the copper target and the silicon detectors has been developed.

Another fundamental part of the optimized experiment (planned in Autumn 2017) will be the implementation of new SDDs [30]. The new detectors were developed in a cooperation between SMI, Politecnico di Milano, and the Fondazione Bruno Kessler (FBK). They consist of units of nine single cells of  $8 \times 8 \text{ mm}^2$ , assembled in a  $3 \times 3$  matrix with a fraction of active area as high as 85%. A picture of the SDD unit is shown in Fig. 7. Four of the SDD units will be used, with two on each side of the target. With one cell having a surface area of 64 mm<sup>2</sup>, the total active area will be around 23 cm<sup>2</sup>, i.e., about four times the current active area of



Fig. 7 New type of SDD with ceramic board for contacting and readout and a copper block for cooling



**Fig. 8** Render of the upgraded setup: The Peltier element is attached to a copper block, which is attached to the backside of the ceramic board, with a copper strap. The Fe-55 source for energy calibration is shown. Some parts of the setup are not displayed to enhance the visibility

 $6 \text{ cm}^2$ . According to GEANT4 simulations, this leads to a higher detection rate of X-rays from non-Paulian transitions by a factor of 3. This is due to the increase in the solid angle coverage of the target. Another advantage is that this type of detector can be operated at higher temperatures of around 230 K. The currently used SDDs are operated at 100 K and require argon cooling. The higher operating temperature can be provided by Peltier cooling. Peltier cooling is better suited for long-term data taking, because of its stable and failure-free operation. The setup for Peltier cooling and signal readout of the SDDs is displayed in Figs. 7 and 8.

A ceramic board for the SDD voltage supply and the readout is mounted on the side of the SDDs opposite to the radiation entrance windows. The first stage of preamplification is provided by a new preamplifier (CUBE), which was recently developed by Politecnico di Milano. These preamplifiers allow high-performance X-ray spectroscopy with standard SDD technology. The ceramic board is connected to a readout board for further amplification and data acquisition.

Upgrade	Signal enhancement	Background reduction	Gain
New SDDs	3	~0.45	~4/3
Passive shielding	-	$\geq \sqrt{20}$	≥4.5
RRS	-	$\sqrt{3}$	$\sqrt{3}$
Total gain			≥10

 Table 2 Factors contributing to the improvement of the sensitivity of the VIP2 experiment (see text)

On the backside of the ceramic board, a copper block is mounted which is attached to the cold side of a Peltier element. This attachment will be realized in the upgraded setup by a thermally conductive copper strap (see Fig. 8). It is via this copper strap that the SDD is cooled by the Peltier element. The warm side of the Peltier element is cooled by a closed water cycle with a cooling pump. A similar water cooling system is currently in use to cool the copper target. This system can be adapted to cool the Peltier elements in addition to the copper target. This system of SDD combined with Peltier cooling has already been tested at the laboratory of the Stefan Meyer Insitute in Vienna. A typical energy resolution was found to be 200 eV (FWHM) at 6 keV.

In order to reduce the background coming from radioactive radon, the whole setup, including the passive shielding, will be enclosed in an existing plastic box where nitrogen is flushed. This radon reduction system (RRS) reduces the radon concentration in the atmosphere surrounding the experiment. Radon is an important source of background at LNGS, as it is part of the decay chains of uranium and thorium, which in turn are abundant in the rocks of the Gran Sasso mountains.

### 4.2 Gain for the VIP2 Experiment

The mentioned upgrade will improve the final achievable value for  $\frac{\beta^2}{2}$  by at least one order of magnitude compared to the final value achievable with the current setup. The upgrades are summed up in Table 2.

In the first line, the effects of the new SDDs are listed. They will enhance the signal (i.e., the number of possible detected X-rays from non-Paulian transitions per time) by a factor of at least 3, due to their larger solid angle coverage. Due to their larger area, they will also increase the background counts by a factor of  $\frac{23}{6}$ . Additionally, the anticipated energy resolution of around 200 eV (FWHM) will enlarge the background in the region of interest by around a factor of  $\frac{4}{3}$ . Since the background enters as a square root into the calculations of  $\frac{\beta^2}{2}$ , this brings the total gain for the upper limit for a PEP violation to approximately  $\frac{4}{3}$ . An additional advantage of the new detectors which cannot be put in this table is the easier handling, as mentioned earlier. The Peltier cooling replaces all the parts needed for cooling with closed cycle liquid argon cooling, e.g., a helium compressor with



**Fig. 9** The preliminary upper limit for the violation of the Pauli exclusion principle obtained by data taken with VIP2 (2) compared to the preliminary result of the former VIP experiment (1) and different scenarios (3) and (4) (see text)

cold head and condenser which are used to liquefy the argon, an electronic argon temperature controller, and the argon cooling line inside the setup. The Peltier cooling is advantageous due to its easier handling and long-term stability.

The lead and copper shielding outside of the setup, and Teflon around the detectors inside of the setup, will reduce the background by at least a factor of 20. This corresponds to a gain for  $\frac{\beta^2}{2}$  of around 4.5, which has been verified with GEANT4 simulations.

The nitrogen flushed around the setup to decrease the radon concentration (RRS) will reduce the background by a factor of around 3. As a result, the gain in sensitivity will be about  $\sqrt{3}$ . Together this adds up to an improvement of at least one order of magnitude, shown in Fig. 9. In the figure, the points represent the following from left to right: (1) the preliminary value obtained with the complete data set of the predecessor experiment VIP; (2) the preliminary value from the data taken until end of 2016 with VIP2; and (3) the expected VIP2 value after around 3 more years of data taking with the current setup. Finally (4) corresponds to the expected value which can be achieved after 3 years running time with the planned upgrades.

#### 5 Conclusion and Outlook

We will be able to install the upgrade by spring 2018 after thorough tests of the detectors at SMI. Thereby the VIP2 experiment will be able to set a new upper limit for the probability that the PEP is violated in the order of  $10^{-31}$  by the end of the running time of the experiment. Compared to the preliminary result of the VIP

experiment of  $\frac{\beta^2}{2} \le 4.7 \times 10^{-29}$ , this is an improvement by more than two orders of magnitude. The new value will also improve the current value set by VIP2 by more than one order of magnitude and will represent a test of the PEP with unprecedented sensitivity.

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# Feynman Integrals for a New Class of Time-Dependent Exponentially Growing Potentials



Hammah Mohameden and Habib Ouerdiane

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## 1 Introduction

As an alternative approach to quantum mechanics, Feynman introduced the concept of path integrals [9, 10] which developed into an extremely useful tool in many branches of theoretical physics. There have been many approaches for giving a mathematically rigorous meaning to the Feynman path integral by using, e.g., analytic continuation, see [16, 19, 20] or Fresnel integrals [1, 2, 15]. For more details we refer the reader to [1] and the references therein. Here we choose a white noise approach to Feynman integrals. White noise analysis is a mathematical framework which offers generalizations of concepts from finite-dimensional analysis, like differential operators and Fourier transform to an infinite-dimensional setting. The idea of realizing Feynman integrals within the white noise framework goes back to [14]. In [24], Lascheck et al. constructed the Feynman integrand  $\mathbb{F}_V$  for a large class of time-dependent exponentially growing potentials  $V : \Delta \times \mathbb{R} \to \mathbb{R}$ , where  $\Delta = [0, T]$  is a bounded interval of length T > 0. In order to include singular potentials, they supposed that V is not a function but a finite Borel signed measure  $\nu$  on  $\Delta \times \mathbb{R}$ . They considered the marginal measures:

$$\nu_{\text{space}}(A) \equiv \nu(\Delta \times A), \quad A \in \mathcal{B}(\mathbb{R}),$$

H. Mohameden  $\cdot$  H. Ouerdiane ( $\boxtimes$ )

Department of Mathematics, Faculty of Sciences of Tunis, University of Tunis El-Manar, Tunis, Tunisia

e-mail: habib.ouerdiane@fst.rnu.tn

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$$\nu_{\text{time}}(B) \equiv \nu(B \times \mathbb{R}), \quad B \in \mathcal{B}(\Delta).$$

They assumed that  $v_{\text{space}}$  and  $v_{\text{time}}$  satisfy:

- 1. There is some  $\beta$ , R > 0 such that  $|v_{\text{space}}|(]r, +\infty[) < e^{-\beta r^2}$  for all r > R.
- 2.  $|v_{\text{time}}|$  has a  $L^{\infty}$  density.

They constructed the white noise Feynman integrand  $\mathbb{F}_V$  and proved under conditions (1) and (2) that  $\mathbb{F}_V$  is a Hida distribution [23, 26]. Moreover, they showed that the generalized expectation  $\mathbb{I}_V := \langle \langle \mathbb{F}_V, 1 \rangle \rangle$  is a Green function for the full Schrödinger equation, i.e.,

$$i\hbar\frac{\partial \mathbb{I}_V}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \mathbb{I}_V}{\partial x^2} + V\mathbb{I}_V, \quad \text{on}\Delta \times \mathbb{R}$$
(1.1)

with the initial condition:

$$\lim_{t \to 0^+} \mathbb{I}_V(t, .) = \delta. \tag{1.2}$$

Here m > 0 is the mass,  $\hbar$  is the Planck constant, and  $\delta$  is the Dirac distribution at zero.

Our purpose in this work is to prove by inspiration of their method that the white noise Feynman integrand can be rigorously constructed for a new class of time-dependent exponentially growing potentials. More precisely, let  $\theta : \mathbb{R}_+ \to R_+$  be a Young function, i.e.,

1.  $\theta$  is a continuous, convex, increasing function.

2. 
$$\theta(0) = 0$$
 and  $\lim_{s \to +\infty} \frac{\theta(s)}{s} = +\infty$ .

In addition, we suppose that  $\theta$  satisfies the condition:

$$\limsup_{s \to +\infty} \frac{\theta(s)}{s^2} < +\infty.$$
(1.3)

Let  $[\mathcal{W}]_{\theta}$  be the corresponding space of white noise test functions and  $[\mathcal{W}]_{\theta}^*$  its dual space (for the full definition of the space  $[\mathcal{W}]_{\theta}$ , see [28] or the next section for a brief introduction). Note that if  $\theta(s) = s^2$ , then  $[\mathcal{W}]_{\theta}^*$  coincides with the space of Hida distributions (see [23, 26] or the examples in the next section).

Now let  $V : \mathbb{R}_+ \times \mathbb{R} \to \mathbb{C}$  be a given potential. In order to include singular potentials, we suppose that *V* is not a function but a family  $(v_t)_{t \in \mathbb{R}_+}$  of Borel complex measure on  $\mathbb{R}$ . Moreover, we suppose that the following conditions are fulfilled:

and

- (C1) The function  $t \to v_t([a, b])$  is measurable for any  $a, b \in \mathbb{R}$ .
- (C2) There is some  $\beta > 0$  and a function  $\rho : \mathbb{R}_+ \to \mathbb{R}_+$  such that
  - (a)  $\rho$  is bounded on every bounded interval  $I \subset \mathbb{R}_+$ .
  - (b) For for all r > 0 and almost all  $t \in \mathbb{R}_+$ , it holds that

$$\int_{\mathbb{R}} e^{r|y|} |v_t| (dy) \le |\rho(t)| e^{\theta^*(\beta r)}, \qquad (1.4)$$

where  $\theta^{\star} : \mathbb{R}_+ \to \mathbb{R}_+$  is the conjugate of  $\theta$ , i.e.,

$$\theta^{\star}(r) = \sup_{s \in \mathbb{R}_+} (sr - \theta(s)), \quad r \in \mathbb{R}_+.$$

Note that condition (1.4) implies directly that  $v_t$  is a finite Borel complex measure on  $\mathbb{R}$  for almost all  $t \in \mathbb{R}_+$  (see Remark 4.3).

The main results of this paper (see Theorems 4.2 and 4.7) are to prove that under the conditions (C1) and (C2), the white noise Feynman integrand  $\mathbb{F}_V$  exists as a generalized function in the space  $[\mathcal{W}]^*_{\theta}$ . Moreover, its generalized expectation  $\mathbb{I}_V := \langle \langle \mathbb{F}_V, 1 \rangle \rangle$  is a Green function for the full Schrödinger equation (1.1). A direct comparison between the class of admissible potentials introduced by the authors in [24] and our class of admissible potentials is given in Remark 4.8. Finally, we give several examples to illustrate the functions  $\rho$ ,  $\theta$  and  $\theta^*$ .

#### 2 White Noise Analysis

Let  $S(\mathbb{R})$  be the Schwartz space of real-valued rapidly decreasing functions. More precisely, a function  $\xi : \mathbb{R} \to \mathbb{R}$  is an element of  $S(\mathbb{R})$  if and only if  $\xi \in C^{\infty}(\mathbb{R}^n)$  and,

$$\forall n, m \in \mathbb{N}, \quad \lim_{t \to +\infty} |t^n \xi^{(m)}(t)| = 0.$$

We define a family of inner product norms on  $\mathcal{S}(\mathbb{R})$  by

$$\forall p \in \mathbb{N}, \quad \forall f \in \mathcal{S}(\mathbb{R}), \quad |f|_p = |A^p f|_0 = \left(\int_{\mathbb{R}} |A^p f(t)|^2 dt\right)^{\frac{1}{2}}, \qquad (2.1)$$

where  $|.|_0$  is the inner product norm on the Hilbert space  $L^2(\mathbb{R})$  of (equivalence classes of) the  $\mathbb{R}$ -valued square integrable functions with respect to the Lebesgue measure on  $\mathbb{R}$  and the operator A is defined densely on  $S(\mathbb{R})$  by

$$\forall t \in \mathbb{R}, \quad \forall \xi \in \mathcal{S}(\mathbb{R}), \quad A\xi(t) = -\xi''(t) + (t^2 + 1)\xi(t).$$
Thus we define

$$\forall p \in \mathbb{N}, \quad \mathcal{S}_p(\mathbb{R}) = \left\{ f \in L^2(\mathbb{R}); |f|_p < +\infty \right\}.$$

We recall the definition of a nuclear space.

#### **Definition 2.1**

Let V be a topological space with the topology given by a family  $\{\|.\|_n\}_{n\in\mathbb{N}}$  of inner product norms. Let  $V_n$  be the completion of V with respect to the norm  $\|.\|_n$ . The space V is called a nuclear space if for any n, there exists  $m \ge n$  such that the inclusion map from  $V_m$  into  $V_n$  is a Hilbert-Schmidt operator, i.e., there is an  $+\infty$ 

orthonormal basis  $\{v_k\}_{k\geq 1}$  for  $V_m$  such that  $\sum_{k=1}^{+\infty} ||v_k||_n < \infty$ .

Then  $\mathcal{S}(\mathbb{R})$  equipped with the topology given by the family  $\{|.|_p\}_{p\geq 0}$  is a nuclear space. Moreover, the operator A is invertible, and  $A^{-1}$  is a bounded operator on  $L^2(\mathbb{R})$ . For each  $p \geq 0$ , we put

$$\forall f \in L^2(\mathbb{R}), \quad |f|_{-p} = \left(\int_{\mathbb{R}} |A^{-p}f(t)|^2 dt\right)^{\frac{1}{2}}.$$

Let  $S_{-p}(\mathbb{R})$  be the completion of  $L^2(\mathbb{R})$  with respect to the norm  $|.|_{-p}$ . The dual space  $S'(\mathbb{R})$  is given by

$$\mathcal{S}'(\mathbb{R}) = \bigcup_{p \in \mathbb{N}} \mathcal{S}_{-p}(\mathbb{R}).$$

The space  $S'(\mathbb{R})$  is equipped with the corresponding inductive limit topology, and so it is naturally equipped with the corresponding Borel  $\sigma$ -algebra  $\mathcal{B}(S'(\mathbb{R}))$  (for all details on the Schwartz space and general theory of nuclear spaces, see [23] and [26]). The standard Gaussian measure on  $(S'(\mathbb{R}), \mathcal{B}(S'(\mathbb{R})))$  is defined through its characteristic function, i.e.,

$$\int_{\mathcal{S}'(\mathbb{R})} \exp\left(i\langle x,\xi\rangle\right) \mu(dx) = \exp\left(-\frac{|\xi|_0^2}{2}\right), \quad \xi \in \mathcal{S}(\mathbb{R}).$$

The existence and the uniqueness of the measure  $\mu$  are a consequence of Bochner-Minlos theorem [12, 25]. The probability space  $(S'(\mathbb{R}), \mathcal{B}(S'(\mathbb{R})), \mu)$  is called the white noise space, and we have the Gel'fand triple

$$\mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R}) \subset \mathcal{S}'(\mathbb{R}).$$

By construction of the Gaussian measure  $\mu$ , the random variable  $\langle ., \xi \rangle$  is Gaussian with mean 0 and variance  $|\xi|_0^2$  for any  $\xi \in S(\mathbb{R})$ . Then by using the fact that  $S(\mathbb{R})$ 

is dense in  $L^2(\mathbb{R})$ , we define  $\langle ., \xi \rangle$  and extend the same property for any  $\xi \in L^2(\mathbb{R})$ . Thus a version of the Brownian motion is given by

$$B(t) = \langle ., \chi_{]0,t]} \rangle, \quad t \in \mathbb{R}_+.$$

Now let  $(L^2)$  be the space of (equivalence classes of) the  $\mathbb{C}$ -valued square integrable functions with respect to the standard Gaussian measure on  $\mathcal{S}'(\mathbb{R})$ .

#### **Definition 2.2**

A nuclear subspace  $\mathcal{W} \subset (L^2)$  is called a space of white noise test functions if  $\mathcal{W}$  is dense in  $(L^2)$  and the canonical injection  $\mathcal{W} \hookrightarrow (L^2)$  is continuous. In that case, the elements in  $\mathcal{W}$  are called white noise test functions or simply test functions, and the elements in the dual space  $\mathcal{W}^*$  are called white noise generalized functions or simply generalized functions, and we have the Gel'fand triple

$$[\mathcal{W}] \subset (L^2) \subset [\mathcal{W}]^*.$$

Here we introduce a family  $[\mathcal{W}]_{\theta}$  of white noise test functions associated with a Young function  $\theta : \mathbb{R}_+ \to \mathbb{R}_+$ , i.e.,

1.  $\theta$  is a continuous, convex, increasing function.

2.  $\theta(0) = 0$  and  $\lim_{s \to +\infty} \frac{\theta(s)}{s} = +\infty$ .

In addition, we suppose that  $\theta$  satisfies the condition:

$$\limsup_{s \to +\infty} \frac{\theta(s)}{s^2} < +\infty.$$
(2.2)

So let  $\theta : \mathbb{R}_+ \to \mathbb{R}_+$  be a given Young function satisfying (2.2). Let  $H = (L^2) := L^2(\mathbb{R}) + iL^2(\mathbb{R})$  be the complexified space of  $L^2(\mathbb{R})$  and define

$$\Gamma(H) := \left\{ \phi = (f_n); f_n \in H^{\odot n}, \quad \|\phi\|_0^2 := \sum_{n=0}^{+\infty} n! \|f_n\|_0^2 < +\infty \right\},\$$

where  $H^{\odot n}$  is the *n*-symmetric tensor product of *H* (see [26]). The  $\mathbb{C}$ -canonical bilinear form is given by

$$\langle\langle\phi,\psi\rangle\rangle = \sum_{n=0}^{+\infty} n! \langle f_n,g_n\rangle, \quad \phi = (f_n), \quad \psi = (g_n).$$

First, we construct a Gel'fand triple

$$[W]_{\theta} \subset \Gamma(H) \subset [W]_{\theta}^*$$
.

For each  $p \in \mathbb{Z}$  and m > 0 let  $N_p = S_p(\mathbb{R}) + iS_p(\mathbb{R})$ ,  $N = S(\mathbb{R}) + iS(\mathbb{R})$  be the complexified space of  $S_p(\mathbb{R})$  (respectively,  $S(\mathbb{R})$ ), and put

$$F_{\theta}(N) = \bigcap_{p \in \mathbb{N}, m > 0} F_{\theta, m}(N_p),$$

where

$$F_{\theta,m}(N_p) := \left\{ \phi = (f_n); f_n \in N_p^{\odot n}, \quad \sum_{n=0}^{+\infty} \theta_n^{-2} m^{-n} |f_n|_p^2 < +\infty \right\},$$
$$\theta_n := \inf_{r>0} \frac{\theta(r)}{r^n}, \quad n \in \mathbb{N}^\star,$$

and  $N_p^{\odot n}$  is the *n*-symmetric tensor product of  $N_p$  (see [26]). Then  $F_{\theta}(N)$  equipped with the projective limit topology is a nuclear space. The dual space of  $F_{\theta}(N)$  is given by

$$G_{\theta}(N') = \bigcup_{p \in \mathbb{N}, m > 0} G_{\theta, m}(N_{-p}),$$

where

$$G_{\theta,m}(N_{-p}) := \left\{ \Phi = (F_n); F_n \in N_{-p}^{\odot n}, \quad \sum_{n=0}^{+\infty} (n!\theta_n)^2 m^n |f_n|_{-p}^2 < +\infty \right\}.$$

The canonical  $\mathbb{C}$ -bilinear form on  $G_{\theta}(N') \times F_{\theta}(N)$  is given by

$$\langle \langle \Phi, \phi \rangle \rangle := \sum_{n=0}^{+\infty} n! \langle \Phi_n, \phi_n \rangle, \quad \Phi = (F_n), \quad \phi = (f_n).$$

It is known that under the condition (2.2), we obtain a Gel'fand triple

$$[W]_{\theta} = F_{\theta}(N) \subset \Gamma(H) \subset [W]_{\theta}^* = G_{\theta}(N').$$
(2.3)

For every  $\phi = (f_n) \in \Gamma(H)$ , we define a  $L^2$ -random variable in such a way that

$$[G\phi](x) = \sum_{n=0}^{+\infty} \langle : x^{\otimes n} :, f_n \rangle, \quad \phi = (f_n), \quad x \in N',$$

where :  $x^{\otimes n}$  : is the Wick tensor power (see [23, 26]). Then the map  $\phi \to G\phi$  yields a unitary isomorphism  $\Gamma(H) \cong (L^2)$ , which is the famous Wiener-Itô-Segal

isomorphism (see [23, 26]). Let  $[W]_{\theta} := G([W]_{\theta})$ . A white noise triple (2.3) gives rise to a Gel'fand triple through the Gaussian realization:

$$[\mathcal{W}]_{\theta} \subset (L^2) \subset [\mathcal{W}]'_{\theta}$$
.

#### **Definition 2.3**

The space  $[W]_{\theta}$  is called the space of entire functions with exponential growth of order  $\theta$  and of minimal type.

The canonical  $\mathbb{C}$ -bilinear form on  $[\mathcal{W}]'_{\theta} \times [\mathcal{W}]_{\theta}$  will be denoted by  $\langle \langle ., \rangle \rangle$ .

#### Example 2.4

Let  $\beta \in [0, 1[$  and let  $\theta_{\beta} : \mathbb{R}_+ \to \mathbb{R}_+$  be the Young function defined by

$$\theta_{\beta}(r) = \frac{1+\beta}{2}r^{\frac{2}{1+\beta}}, \quad r \in \mathbb{R}_+.$$

Obviously,  $\theta_{\beta}$  satisfies the condition (2.2).

- 1. The case  $\beta = 0$ : The associated space  $[W]_{\theta}$  is called the space of Hida-Kubo-Takenaka, and it is denoted by (S). The corresponding white noise generalized functions are called Hida distributions. For more details see [23, 26, 31].
- 2. The case  $0 < \beta < 1$ : The associated spaces  $[W]_{\theta}$  are called the spaces of Kondratiev-Streit, and they are denoted by  $(S)_{\beta}$ . The corresponding white noise generalized functions are called Kondratiev-Streit distributions. For more details, see [23].

Now, we put  $S_{\mathbb{C}}(\mathbb{R}) := N = S(\mathbb{R}) + iS(\mathbb{R})$  and define

$$\forall \xi \in \mathcal{S}_{\mathbb{C}}(\mathbb{R}), \quad \phi_{\xi} := \exp\left(\langle ., \xi \rangle - \frac{\langle \xi, \xi \rangle}{2}\right) = \sum_{n=0}^{+\infty} \left\langle : .^{\otimes n} :, \frac{\xi^{\otimes n}}{n!} \right\rangle.$$

**Definition 2.5** Let  $\Phi = \sum_{n=0}^{+\infty} \langle : .^{\otimes n}, \Phi_n \rangle \in [W]^*_{\theta}$  be a generalized function. The  $\mathbb{C}$ -valued functions defined on  $\mathcal{S}_{\mathbb{C}}(\mathbb{R})$  by

$$S\Phi(\xi) = \langle\!\langle \Phi, \phi_{\xi} \rangle\!\rangle = \sum_{n=0}^{+\infty} \langle \Phi_n, \xi^{\otimes n} \rangle, \quad \xi \in \mathcal{S}_{\mathbb{C}}(\mathbb{R}),$$

and

$$T\Phi(\xi) = \langle \langle \Phi, \exp\left(i\langle ., \xi \rangle\right) \rangle \rangle = \exp\left(\frac{\langle \xi, \xi \rangle}{2}\right) S\Phi(i\xi), \quad \xi \in \mathcal{S}_{\mathbb{C}}(\mathbb{R})$$

are called the S-transform (respectively, the Fourier transform or T-transform) of  $\Phi$ .

#### Remark 2.6

- (1) Since  $\phi_{\xi} \in [W]_{\theta}$  for all  $\xi \in S(\mathbb{R})$ , the *S* and *T*-transform of a white noise generalized function are well-defined.
- (2) For  $\xi = 0$  the above expression yields  $\langle \langle \Phi, 1 \rangle \rangle$ ; therefore  $T \Phi(0) = S \Phi(0)$  is called the generalized expectation of  $\Phi \in [\mathcal{W}]^*_{\theta}$ .

Let  $\theta^* : \mathbb{R}_+ \to \mathbb{R}_+$  be the Young conjugate of  $\theta$ , i.e.,

$$\theta^{\star}(r) := \sup_{\lambda \in \mathbb{R}_{+}} (\lambda r - \theta(\lambda)), \quad r \in \mathbb{R}_{+}.$$

Then  $\theta^*$  is also a Young function,  $(\theta^*)^* = \theta$ , and the condition (2.2) is equivalent to the following:

$$\liminf_{r \to +\infty} \frac{\theta^{\star}(r)}{r^2} > 0.$$
(2.4)

For more details on Young function and their properties, see [21, 27]. The next theorem is due to Gannoun et al. [11].

#### Theorem 2.7 [11]

Let  $F : S_{\mathbb{C}}(\mathbb{R}) \to \mathbb{C}$  be a function. Then  $F = T\Phi$  for some generalized function  $\Phi \in [W]^*_{\theta}$  if and only if F satisfies the following conditions:

(1) for any fixed  $\xi, \eta \in S_{\mathbb{C}}(\mathbb{R})$ , the  $\mathbb{C}$ -valued function  $z \to F(z\xi + \eta)$  is entire with respect to the complex variable  $z \in \mathbb{C}$ .

(2) there is some  $p \in \mathbb{N}$  and m, K > 0 such that

$$|F(\xi)| \leq K \exp\left(\theta^{\star}\left(m |\xi|_{p}\right)\right), \quad \forall \xi \in \mathcal{S}_{\mathbb{C}}(\mathbb{R}).$$

The next convergence theorem was proven in [30]. For all details on the strong convergence, i.e., the convergence in the sense of the strong topology on the dual of a nuclear space, see [23].

#### **Corollary 2.8**

Let  $(\Phi_n) \subset [\mathcal{W}]^*_{\theta}$  be a sequence of generalized functions, and let  $F_n = T \Phi_n$ . Then  $\Phi_n$  converges strongly to some generalized function  $\Phi \in [\mathcal{W}]^*_{\theta}$  if and only if:

- (1) The sequence  $(F_n(\xi))_{n \in \mathbb{N}}$  is a Cauchy sequence for any  $\xi \in S_{\mathbb{C}}(\mathbb{R})$ .
- (2) There is some  $p \in \mathbb{N}$ , and m, K > 0 such that

$$|F_n(\xi)| \le K \exp\left(\theta^*(m |\xi|_p)\right), \quad \forall \xi \in \mathcal{S}_{\mathbb{C}}(\mathbb{R}).$$

The next corollary can be easily proven by the same method used in the proof of Theorem 13.4 in [23].

#### **Corollary 2.9**

Let  $(\Omega, \mathcal{F})$  be a measurable space, and let v be a complex measure on  $(\Omega, \mathcal{F})$ . Thus let  $(\Phi(u))_{u \in \Omega} \subset [W]^*_{\theta}$  be a family of generalized functions. Assume that:

- (1)  $T(\Phi(.))(\xi)$  is measurable for any  $\xi \in S_{\mathbb{C}}(\mathbb{R})$ .
- (2) There is some  $p \in \mathbb{N}$ , and m, K > 0 such that

$$\int_{\Omega} |T(\Phi(u))(\xi)| |v| (du) \le K \exp\left(\theta^{\star}(m |\xi|_p)\right), \quad \forall \xi \in \mathcal{S}_{\mathbb{C}}(\mathbb{R})$$

Then  $\int_{\Omega} \Phi(u)v(du)$  exists in the Pettis sense (see [23]) and defines a generalized function in the space  $[\mathcal{W}]^*_{\theta}$ . Its *T*-transform is given by the formula

$$T\left(\int_{\Omega} \Phi(u)\nu(du)\right)(\xi) = \int_{\Omega} T\left(\Phi(u)\right)(\xi)\nu(du), \quad \forall \xi \in \mathcal{S}_{\mathbb{C}}(\mathbb{R}).$$

The same results in Theorem 2.7 and Corollaries 2.8 and 2.9 hold for the *S*-transform.

#### Example 2.10 [Interesting Hida Distributions]

(1) Hida derivative of Brownian motion: Let  $t \in \mathbb{R}_+$  and let  $F_t : S_{\mathbb{C}}(\mathbb{R}) \to \mathbb{C}$  be defined by

$$\forall \xi \in \mathcal{S}_{\mathbb{C}}(\mathbb{R}), \quad F_t(\xi) = \xi(t).$$

Obviously,  $F_t$  satisfies the conditions of Theorem 2.7. In particular, there is a unique Hida distribution  $\dot{B}(t)$  such that

$$\forall \xi \in \mathcal{S}_{\mathbb{C}}(\mathbb{R}), \quad S\left(\dot{B}(t)\right)(\xi) = \xi(t). \tag{2.5}$$

The function  $t \to \dot{B}(t)$ ,  $t \in \mathbb{R}_+$ , is called the Hida derivative of Brownian motion or white noise. In fact, we have

$$\forall t \in \mathbb{R}_+, \quad \dot{B}(t) = \lim_{h \to 0^+} \frac{B(t+h) - B(t)}{h},$$

where the limit is taken in the sense of Corollary 2.8.

(2) **Normalized kinetic energy factor:** To define the kinetic energy factor in the path integrals, one would like to give a meaning to the formal expression

$$\exp\left(c\int_{\mathbb{R}}\dot{B}(\tau)^2d\tau\right),\,$$

where c is a complex constant. When  $c \neq \frac{1}{2}$ , the normalized exponential

$$N\exp\left(c\int_{\mathbb{R}}\dot{B}(\tau)^2d\tau\right)$$

is defined to be the unique Hida distribution with the following T-transform

$$T\left(N\exp\left(c\int_{\mathbb{R}}\dot{B}(\tau)^{2}d\tau\right)\right)(\xi) = \exp\left(\frac{1}{4c-2}\int_{\mathbb{R}}\xi^{2}(\tau)d\tau\right), \quad \xi \in \mathcal{S}_{\mathbb{C}}(\mathbb{R}).$$

For more details see [4, 22].

(3) Donsker's delta function: In order to pin Brownian motion at a point x ∈ ℝ, we want to consider the formal composition of the Dirac delta distribution with Brownian motion: δ(x − B(t)). This can be given a precise meaning as a Hida distribution. Its *T*-transform at ξ ∈ S<sub>C</sub>(ℝ) is given by

$$T\left(\delta(x-B(t))\right)(\xi) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{1}{2}\int_{\mathbb{R}}\xi^{2}(\tau)d\tau + \frac{1}{2t}\left(ix+\int_{0}^{t}\xi(\tau)d\tau\right)^{2}\right).$$

Moreover, we have the integral expression formula

$$\delta(x - B(t)) = \frac{1}{2\pi} \int_{\mathbb{R}} e^{i\lambda(x - B(t))} d\lambda.$$
(2.6)

For more details see [23].

For all details on the spaces  $[W]_{\theta}$ , we refer the reader to [5, 11, 28] and the references therein.

## **3** White Noise Formulation for Feynman Integrals

Consider a nonrelativistic particle of mass m > 0 moving in  $\mathbb{R}$  under influence of a given potential  $V : \mathbb{R}_+ \times \mathbb{R} \to \mathbb{R}$ . In quantum mechanics, the state of this particle at time *t* is described by a function  $\psi(t, x)$  satisfying the Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t}(t,x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}(t,x) + V(t,x)\psi, \quad \psi(0,x) = f(x), \quad (t,x) \in \mathbb{R}_+ \times \mathbb{R},$$
(3.1)

where *h* is the Planck constant and  $f : \mathbb{R} \to \mathbb{R}$  is such that  $\int_{\mathbb{R}} |f(x)|^2 dx = 1$ . The Feynman integrand in the white noise framework is an informal expression of the form

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$$\mathbb{F}_{V}(t,x) = N \exp\left(-\frac{i}{\hbar} \int_{0}^{t} \dot{B}(\tau)^{2} d\tau\right) \times \\ \exp\left(\frac{i}{\hbar} \int_{0}^{t} V\left(\tau, x + B(\tau) - B(t)\right) d\tau\right) \times \delta(x - B(t)), \quad x \in \mathbb{R}, \quad t > 0,$$

where  $\delta(x - B(t))$  is the Donsker's delta function and  $N \exp\left(-\frac{i}{\hbar}\int_0^t \dot{B}(\tau)^2 d\tau\right)$  is a normalized kinetic energy factor (see Example 2.10). The Feynman integral is defined by

$$\mathbb{I}_V(t,x) = \left\langle \left\langle \mathbb{F}_V(t,x), 1 \right\rangle \right\rangle, \quad x \in \mathbb{R}, \quad t > 0.$$

The idea of realizing Feynman integrals within the white noise framework goes back to [14]. For all details, we refer the reader to [3, 4, 7, 8, 13, 17, 22, 24, 33] and the reference therein.

#### Example 3.1 [The Free Feynman Integral]

The white noise Feynman integrand associated to the potential V = 0 is called the white noise free Feynman integrand, and it is denoted by  $\mathbb{F}_0$ . It has been checked in [14] that  $\mathbb{F}_0$  is a Hida distribution with the following *T*-transform

$$T\left(\mathbb{F}_{0}(t,x)\right)(\xi) = \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left(\frac{im}{2\hbar t} \left(x + \frac{\hbar}{m} \int_{0}^{t} \xi(u) du\right)^{2}\right)$$
(3.2)

$$\exp\left(-\frac{1}{2}\int_{\Delta_1(t)^c}\xi^2(u)du-\frac{i\hbar}{2m}\int_0^t\xi^2(u)du\right),\ \xi\in\mathcal{S}_{\mathbb{C}}(\mathbb{R}),\ x\in\mathbb{R},\ t>0,\ (3.3)$$

where  $\Delta_1(t)^c$  is the complement of  $\Delta_1(t) := [0, t]$ . Let  $\xi = 0$ , we get

$$\mathbb{I}_{V}(t,x) = \sqrt{\frac{m}{2\pi i \hbar t}} \exp\left(\frac{im}{2\hbar t}x^{2}\right), \quad x \in \mathbb{R}, \quad t > 0,$$

which is the exact Feynman free propagator.

# 4 Feynman Integrals for a New Class of Time-Dependent Exponentially Growing Potentials

Consider a real potential  $V : \mathbb{R}_+ \times \mathbb{R} \to \mathbb{R}$  and let  $\mathbb{F}_V$  be the corresponding Feynman integrand. By definition we have

$$\mathbb{F}_{V}(t,x) = \mathbb{F}_{0}(t,x) \cdot \exp\left(-\frac{i}{\hbar} \int_{0}^{t} V(\tau,x+B(\tau)-B(t))d\tau\right), \quad x \in \mathbb{R}, \quad t > 0,$$
(4.1)

where  $\mathbb{F}_0$  is the free Feynman integrand. Let  $x \in \mathbb{R}$  and t > 0 be fixed. We start by writing

$$V(t, x) = \int_{\mathbb{R}} V(t, y)\delta(x - y)dy, \quad x \in \mathbb{R}, \quad t > 0$$

By expanding the exponential in the expression (4.1), we find that

$$\mathbb{F}_{V}(t,x) = \sum_{n=0}^{+\infty} \frac{(-i)^{n}}{\hbar^{n}} \int_{\Delta_{n}(t) \times \mathbb{R}^{n}} \left( \prod_{j=1}^{n} V(t_{j}, y_{j}) \right) \mathbb{F}_{n}^{(t,x)}\left(\overrightarrow{t}, \overrightarrow{y}\right) d^{n} \overrightarrow{y} d^{n} \overrightarrow{t}, \quad (4.2)$$

where  $\Delta_n(t)$  is the set of all  $(t_1, \dots, t_n) \in ]0, t[^n \text{ with } t_1 < \dots < t_n \text{ and }$ 

$$\mathbb{F}_{n}^{(t,x)}\left(\overrightarrow{t},\overrightarrow{y}\right) = \mathbb{F}_{0}(t,x) \cdot \prod_{j=1}^{n} \delta\left(x - y_{j} + B(t_{j}) - B(t)\right), \tag{4.3}$$

where  $\overrightarrow{t} = (t_1, \dots, t_n) \in \Delta_n(t)$  and  $\overrightarrow{y} = (y_1, \dots, y_n) \in \mathbb{R}^n$ . Thus, the integrals in the expression (4.2) disappear for n = 0, and the corresponding term is equal to  $\mathbb{F}_0(t, x)$ .

## Lemma 4.1 [22, 24, 33]

Let  $\overrightarrow{t} = (t_1, \dots, t_n) \in \Delta_n(t)$  and  $\overrightarrow{y} = (y_1, \dots, y_n) \in \mathbb{R}^n$  be given. Then  $\mathbb{F}_n^{(t,x)}(\overrightarrow{t}, \overrightarrow{y})$  defined by the expression (4.3) is a Hida distribution. Its *T*-transform is given by the formula

$$T\left(\mathbb{F}_{n}^{(t,x)}\left(\overrightarrow{t},\overrightarrow{y}\right)\right)(\xi) = T\left(\mathbb{F}_{0}(t,x)\cdot\prod_{j=1}^{n}\delta\left(x-y_{j}+B(t_{j})-B(t)\right)\right)(\xi) = \left(\prod_{j=1}^{n+1}\sqrt{\frac{m}{2\pi i\hbar\left(t_{j}-t_{j-1}\right)}}\right)\exp\left(-\frac{1}{2}\int_{\Delta_{1}^{c}(t)}\xi^{2}(s)ds-\frac{i\hbar}{2m}\int_{\Delta_{1}(t)}\xi^{2}(s)ds\right)\times$$

$$\exp\left(\sum_{j=1}^{n+1} \frac{im}{2\hbar \left(t_j - t_{j-1}\right)} \left(y_j - y_{j-1} + \frac{\hbar}{m} \int_{t_{j-1}}^{t_j} \xi(s) ds\right)^2\right), \quad \xi \in \mathcal{S}_{\mathbb{C}}(\mathbb{R}).$$
(4.4)

Here we have used the notations  $t_0 = 0$ ,  $t_{n+1} = t$ ,  $y_0 = 0$ ,  $y_{n+1} = x$ , and  $\Delta_1^c(t)$  is the complement of  $\Delta_1(t) = ]0, t[$ .

In order to include singular potentials, we suppose from now on that V is not a function but a family  $(v_t)_{t \in \mathbb{R}_+}$  of Borel complex measure on  $\mathbb{R}$ . The expression (4.2) now is taking the form

$$\mathbb{F}_{V}(t,x) = \sum_{n=0}^{+\infty} \frac{(-i)^{n}}{\hbar^{n}} \int_{\Delta_{n}(t)} \left( \int_{\mathbb{R}^{n}} \mathbb{F}_{n}^{(t,x)}\left(\overrightarrow{t},\overrightarrow{y}\right) \prod_{j=1}^{n} \nu_{t}(dy_{j}) \right) \prod_{j=1}^{n} dt_{j}.$$
(4.5)

#### Theorem 4.2

Let  $\mathbb{F}_V$  be the Feynman integrand defined by the series (4.5), and let  $\theta : \mathbb{R}_+ \to \mathbb{R}_+$ be a Young function satisfying the condition (2.6). We suppose that the following conditions are fulfilled :

- (C1) The function  $t \to v_t$  ([a, b]) is measurable for any  $a, b \in \mathbb{R}$ .
- (C2) There is some  $\beta > 0$  and a function  $\rho : \mathbb{R}_+ \to \mathbb{R}_+$  such that
  - (a)  $\rho$  is bounded on every bounded interval  $I \subset \mathbb{R}_+$ .
  - (b) For for all r > 0 and almost all  $t \in \mathbb{R}_+$ , it holds that

$$\int_{\mathbb{R}} e^{r|y|} |v_t| (dy) \le |\rho(t)| e^{\theta^{\star}(\beta r)}, \tag{4.6}$$

where  $\theta^* : \mathbb{R}_+ \to \mathbb{R}_+$  is the conjugate of  $\theta$ .

Then  $\mathbb{F}_V$  exists as a generalized function in the space  $[\mathcal{W}]^*_{\theta}$ . The integrals exist in the Pettis sense, and the series (4.5) converges strongly in the space  $[\mathcal{W}]^*_{\theta}$ . Therefore we may express the *T*-transform of  $\mathbb{F}_V(t, x)$  by

$$T\left(\mathbb{F}_{V}(t,x)\right)(\xi) = \sum_{n=0}^{+\infty} \frac{(-i)^{n}}{\hbar^{n}} \int_{\Delta_{n}(t)} \left( \int_{\mathbb{R}^{n}} T\left(\mathbb{F}_{n}^{(t,x)}\left(\overrightarrow{t},\overrightarrow{y}\right)\right)(\xi) \prod_{j=1}^{n} \nu_{t_{j}}(dy_{j}) \right) \times \prod_{j=1}^{n} dt_{j}.$$
(4.7)

Here  $\xi \in S_{\mathbb{C}}(\mathbb{R})$  and  $T\left(\mathbb{F}_{n}^{(t,x)}\left(\overrightarrow{t},\overrightarrow{y}\right)\right)(\xi)$  is given as in Lemma 4.1 by the formula (4.4). Thus in the above expression, the integrals disappear for n = 0, and the corresponding term is equal to  $T\left(\mathbb{F}_{0}(t,x)\right)(\xi)$ .

**Proof** For simplicity, we suppose that the inequality (4.6) holds for all r > 0 and all  $\tau \in \mathbb{R}_+$ . Let  $x \in \mathbb{R}$  and t > 0 be fixed.

First setup: Let us start by proving that the integral

$$\int_{\mathbb{R}^n} \mathbb{F}_n^{(t,x)}\left(\overrightarrow{t},\overrightarrow{y}\right) \prod_{j=1}^n \nu_{t_j}(dy_j)$$

exists in the Pettis sense for any  $n \ge 1$  and any  $\vec{t} \in \Delta_n(t)$ . So let  $n \ge 1$  and  $\vec{t} = (t_1, \dots, t_n) \in \Delta_n(t)$  be fixed. We note that the  $\mathbb{C}$ -valued function

$$\overrightarrow{y} \to T\left(\mathbb{F}_n^{(t,x)}\left(\overrightarrow{t}, \overrightarrow{y}\right)\right)(\xi), \quad \overrightarrow{y} \in \mathbb{R}^n$$

is measurable for any  $\xi \in S_{\mathbb{C}}(\mathbb{R})$ . On the other hand, by using the formula (4.4), we prove easily that for any  $\xi \in S_{\mathbb{C}}(\mathbb{R})$ ,

$$\left| T\left( \mathbb{F}_{n}^{(t,x)}\left(\overrightarrow{t},\overrightarrow{y}\right) \right)(\xi) \right| \leq \left( \prod_{j=1}^{n+1} \sqrt{\frac{m}{2\pi\hbar\left(t_{j}-t_{j-1}\right)}} \right) \exp\left( \left(\frac{1}{2} + \frac{\hbar}{m}\right) |\xi|_{0}^{2} \right) \times \left| \exp\left( \sum_{j=1}^{n+1} \frac{i(y_{j} - y_{j-1})}{t_{j} - t_{j-1}} \int_{t_{j-1}}^{t_{j}} \xi(s) ds \right) \right|.$$

The last term can be rewritten as

$$\exp\left(\sum_{j=1}^{n+1} \frac{i(y_{j-1} - y_j)}{t_j - t_{j-1}} \int_{t_{j-1}}^{t_j} \xi(s) ds\right) = \exp\left(\frac{ix}{t - t_n} \int_{t_n}^t \xi(s) ds\right) \times \\ \exp\left(i\sum_{j=1}^n y_j \left(\frac{1}{t_j - t_{j-1}} \int_{t_{j-1}}^{t_j} \xi(s) ds - \frac{1}{t_{j+1} - t_j} \int_{t_j}^{t_{j+1}} \xi(s) ds\right)\right).$$

By the mean value theorem, this equals

$$\exp\left(\frac{ix}{t-t_n}\int_{t_n}^t\xi(s)ds\right)\times\exp\left(i\sum_{j=1}^ny_j\left(\xi(\tau_j)-\xi(\tau_{j+1})\right)\right),$$

where  $\tau_j \in [t_j, t_{j+1}]$ . Then it follows that

$$\left| \exp\left( \sum_{j=1}^{n+1} \frac{i(y_j - y_{j-1})}{t_j - t_{j-1}} \int_{t_{j-1}}^{t_j} \xi(s) ds \right) \right| \le \exp\left( |x| \|\xi\|_{\infty} + t \|\xi'\|_{\infty} \max_{1 \le j \le n} |y_j| \right) \le$$

 $\exp\left(|x| \|\xi\|_{\infty}\right) \max_{1 \le j \le n} \exp\left(t \|\xi'\|_{\infty} |y_j|\right) \le \exp\left(|x| \|\xi\|_{\infty}\right) \sum_{j=1}^{n} \exp\left(t \|\xi'\|_{\infty} |y_j|\right),$ 

where  $\xi'$  is the derivative of  $\xi$  and

$$\|\xi\|_{\infty} := \sup_{s \in \mathbb{R}} |\xi(s)|, \quad \xi \in \mathcal{S}_{\mathbb{C}}(\mathbb{R}).$$

This implies that

$$\int_{\mathbb{R}^n} \left| T\left( \mathbb{F}_n^{(t,x)}\left(\overrightarrow{t},\overrightarrow{y}\right) \right)(\xi) \right| d^n \overrightarrow{y} \le \left( \prod_{j=1}^{n+1} \sqrt{\frac{m}{2\pi\hbar\left(t_j - t_{j-1}\right)}} \right) \times \exp\left( \left( \left(\frac{1}{2} + \frac{\hbar}{m}\right) |\xi|_0^2 \right) \exp\left(|x| \|\xi\|_{\infty}\right) \sum_{j=1}^n \int_{\mathbb{R}^n} \exp\left(t \|\xi'\|_{\infty} |y_j|\right) \prod_{j=1}^n |v_{t_j}| (dy_j).$$

By using (4.6), we find that

$$\int_{\mathbb{R}^n} \left| T\left( \mathbb{F}_n^{(t,x)}\left(\overrightarrow{t},\overrightarrow{y}\right) \right)(\xi) \right| d^n \overrightarrow{y} \leq \left( \prod_{j=1}^{n+1} \sqrt{\frac{m}{2\pi\hbar\left(t_j - t_{j-1}\right)}} \right) \times n\left( \prod_{j=1}^n |\rho(t_j)| \right) \exp\left( \left( \frac{1}{2} + \frac{\hbar}{m} \right) |\xi|_0^2 + \|\xi\|_{\infty} |x| + \theta^\star \left( t\beta \|\xi'\|_{\infty} \right) \right).$$

Since  $\theta^*$  satisfies the condition (2.4), there is some constants a > 0 and R > 0 such that

$$\theta^{\star}(r) \ge ar^2, \quad \forall r > R.$$

Then it can be easily proven that

$$\exp\left(\left(\frac{1}{2} + \frac{\hbar}{m}\right)|\xi|_0^2 + \|\xi\|_{\infty}|x|\right) \le \alpha \exp\left(\theta^{\star}\left(\lambda\left(|\xi|_0 + \|\xi\|_{\infty}\right)\right)\right), \quad (4.8)$$

where  $\alpha = \alpha(x, a, \hbar, m, R) > 0$  and  $\lambda = \lambda(a, \hbar, m) > 0$  are constants. This implies that

$$\int_{\mathbb{R}^{n}} \left| T\left( \mathbb{F}_{n}^{(t,x)}\left(\overrightarrow{t},\overrightarrow{y}\right) \right) (\xi) \right| d^{n} \overrightarrow{y} \leq \left( \prod_{j=1}^{n+1} \sqrt{\frac{m}{2\pi\hbar \left( t_{j} - t_{j-1} \right)}} \right) \\ \times \left( n \prod_{j=1}^{n} |\rho(t_{j})| \right) \times \left( n \prod_{j=1}^{n} |\rho(t_{j})| \right) \times \left( n \left( n \prod_{j=1}^{n} |\rho(t_{j})| \right) \right) \right)$$

 $\alpha \exp\left(\theta^{\star}\left((t\beta + \lambda) \| |\xi\||\right)\right), \quad \||\xi\|| := |\xi|_{0} + \|\xi\|_{\infty} + \|\xi'\|_{\infty}.$ (4.9)

Note that the norm  $||| \cdot |||$  is continuous on  $S_{\mathbb{C}}(\mathbb{R})$  (see [32]). So, there is some  $p \in \mathbb{N}$  and K > 0 such that

$$\forall \xi \in \mathcal{S}_{\mathbb{C}}(\mathbb{R}), \quad |||\xi||| \le K |\xi|_p. \tag{4.10}$$

To conclude the proof of this item, it suffices to apply Corollary 2.9. *Second step:* Let us show that the integrals

$$\int_{\Delta_n(t)} \left( \int_{\mathbb{R}^n} \mathbb{F}_n^{(t,x)}\left(\overrightarrow{t}, \overrightarrow{y}\right) \prod_{j=1}^n \nu_{t_j}(dy_j) \right) \prod_{j=1}^n dt_j$$

exist in the Pettis sense for any  $n \ge 1$ . So let  $n \ge 1$ . First of all, we note that by the first condition, the  $\mathbb{C}$ -valued function

$$\overrightarrow{t} \to \int_{\mathbb{R}^n} T\left(\mathbb{F}_n^{(t,x)}\left(\overrightarrow{t}, \overrightarrow{y}\right)\right)(\xi) \prod_{j=1}^n v_{t_j}(dy_j), \quad \overrightarrow{t} \in \Delta_n(t)$$

is measurable for any  $\xi \in S_{\mathbb{C}}(\mathbb{R})$ . On the other hand, by (4.9) we have

$$\int_{\Delta_n(t)} \left( \int_{\mathbb{R}^n} \left| T\left( \mathbb{F}_n^{(t,x)}\left(\overrightarrow{t},\overrightarrow{y}\right) \right)(\xi) \right| \prod_{j=1}^n \left| v_{t_j} \right| (d\overrightarrow{y}_j) \right) \prod_{j=1}^n dt_j \le \alpha n \left( n! \right)^{-\frac{1}{p}} M_n(t) \left( \|\rho\|_{\infty,t} \right)^n \exp\left( \theta^\star \left( (t\beta + \lambda) \| |\xi\| |) \right),$$

where  $\|\rho\|_{\infty,t} := \sup_{s \in [0,t]} |\rho(s)|$  and (see [24])

$$M_n(t) := \int_{\Delta_n(t)} \left( \prod_{j=1}^{n+1} \sqrt{\frac{m}{2\pi\hbar (t_k - t_{k-1})}} \right) \prod_{j=1}^n dt_j$$
$$= \left( \frac{m\Gamma(\frac{1}{2})}{2\pi\hbar} \right)^{\frac{(n+1)}{2}} t^{\frac{n-1}{2}} \Gamma\left(\frac{n+1}{2}\right).$$

Here  $\Gamma$  :]0,  $+\infty[\rightarrow \mathbb{R}_+$  is the Gamma function, i.e.,

$$\Gamma(z) = \int_0^{+\infty} \lambda^{z-1} e^{-\lambda} d\lambda, \quad z > 0.$$

By Stirling's formula, we have

$$\Gamma(z) \sim z^{z-\frac{1}{2}}e^{-z}$$
, i.e.,  $\lim_{z \to +\infty} \frac{\Gamma(z)}{z^{z-\frac{1}{2}}e^{-z}} = 1.$ 

Then it follows that

$$\Gamma\left(\frac{n+1}{2}\right) \sim \left(\frac{n+1}{2\pi}\right)^{\frac{1}{4}} (n!)^{-\frac{1}{2}}.$$

So there is a constant  $C = C(m, \hbar, t) > 0$  such that

$$M_n(t) \leq C\left(\frac{mt \ \Gamma\left(\frac{1}{2}\right)}{\pi \hbar}\right)^{\frac{n}{2}} (n!)^{-\frac{1}{2}},$$

which implies that

$$\int_{\Delta_{n}(t)} \left( \int_{\mathbb{R}^{n}} \left| T\left( \mathbb{F}_{n}^{(t,x)}\left(\overrightarrow{t},\overrightarrow{y}\right) \right)(\xi) \right| \prod_{j=1}^{n} \left| \nu_{t_{j}} \right| (dy_{j}) \right) \prod_{j=1}^{n} dt_{j} \leq C\alpha \left( \frac{mt \Gamma\left(\frac{1}{2}\right)}{\pi\hbar} \right)^{\frac{n}{2}} (n!)^{-\frac{1}{2}} \left( \|\rho\|_{\infty,t} \right)^{n} \exp\left( \theta^{\star} \left( (t\beta + \lambda) \| |\xi\| |) \right).$$
(4.11)

To complete the proof of this item, it suffices to use (4.10) and apply Corollary 2.9. *Third step:* We will prove in this step that the series (4.5) converges in the strong sense. By using formula (3.2) and the inequalities (4.8) and (4.11), we show easily that

$$\sum_{n=0}^{+\infty} \hbar^{-n} \int_{\Delta_n(t)} \left( \int_{\mathbb{R}^n} \left| T\left( \mathbb{F}_n^{(t,x)}\left(\overrightarrow{t},\overrightarrow{y}\right) \right) \right| (\xi) \prod_{j=1}^n \left| v_{t_j} \right| (dy_j) \right) \prod_{j=1}^n dt_j \le \alpha \left( \sqrt{\frac{m}{2\pi\hbar t}} + C \right) \Lambda \left( \frac{\|\rho\|_{\infty,t}}{\hbar} \left( \frac{mt \Gamma\left(\frac{1}{2}\right)}{\pi\hbar} \right)^{\frac{1}{2}} \right) e^{\theta^{\star} ((t\beta+\lambda)\||\xi\||)},$$

where  $\Lambda : \mathbb{R}_+ \to \mathbb{R}_+$  is defined by

$$\Lambda(r) = \sum_{n=0}^{+\infty} (n!)^{-\frac{1}{2}} r^n, \quad r \in \mathbb{R}_+.$$
(4.12)

It is very easy to show that the series (4.12) is convergent for any  $r \in \mathbb{R}_+$ , and so  $\Lambda$  is well-defined. To conclude the proof, it suffices to use (4.10) and apply Corollary 2.8. Hence the result.

#### Remark 4.3

Note that the condition (C2) implies directly that  $v_t$  is a finite Borel complex measure on  $\mathbb{R}$  for almost all  $t \in \mathbb{R}_+$ . In fact, since

$$\int_{\mathbb{R}} \exp\left(|y|\right) |\nu_t|(dy) < +\infty,$$

then by convergence dominate theorem, we have

$$\int_{\mathbb{R}} |v_t|(dy) = \lim_{n \to +\infty} \int_{\mathbb{R}} \exp\left(\frac{1}{n}|y|\right) |v_t|(dy) \le \lim_{n \to +\infty} |\rho(t)| \exp\left(\theta^{\star}\left(\frac{\beta}{n}\right)\right) = |\rho(t)| < +\infty,$$

which holds for almost all  $t \in \mathbb{R}_+$ . Hence the result.

#### **Corollary 4.4**

Let v be a Borel complex measure on  $\mathbb{R}$  satisfying the condition:

$$\forall r > 0, \quad \int_{\mathbb{R}} \exp\left(r|y|\right) |\nu|(dy) < +\infty. \tag{4.13}$$

Then the corresponding Feynman integrand  $\mathbb{F}_{\nu}$  is a generalized function in the space  $[\mathcal{W}]^*_{\theta}$  associated to the Young function  $\theta : \mathbb{R}_+ \to \mathbb{R}_+$ , which its Young conjugate function  $\theta^* : \mathbb{R}_+ \to \mathbb{R}_+$  is given by

$$\theta^{\star}(r) = \int_{\mathbb{R}} \left( e^{r|y|} - 1 \right) |\nu|(dy), \quad r \in \mathbb{R}_+.$$

**Proof** This is an immediate consequence of Theorem 4.2. In fact, for any r > 0 we have

$$\int_{\mathbb{R}} \exp(r|y|) |\nu| (dy) \le e^{|\nu|(\mathbb{R})} \exp(\theta^{\star}(r)).$$

Hence the result.

#### **Corollary 4.5**

Let  $\mathbb{F}_V$  be the Feynman integrand defined by the series (4.5), and let  $\theta : \mathbb{R}_+ \to \mathbb{R}_+$ be a Young function satisfying the condition (2.6). We suppose that the following conditions are fulfilled:

- (1) The function  $t \to v_t$  ([a, b]) is measurable for any  $a, b \in \mathbb{R}$ .
- (2) There is some  $\beta > 0$  such that  $\int_{\mathbb{R}} e^{\theta(\beta|y|)} |v_t| (dy) < +\infty$  for all  $t \in \mathbb{R}_+$ .
- (3) The real function  $t \to \int_{\mathbb{R}} e^{\theta(\beta | y|)} |v_t| (dy), t \in \mathbb{R}_+$ , is continuous.

Then  $\mathbb{F}_V$  exists as a generalized function in the space  $[\mathcal{W}]^*_{\theta}$ . The integrals exist in the Pettis sense, and the convergence of the series (4.5) is in the strong sense. Therefore, we may express the *T*-transform of  $\mathbb{F}_V(t, x)$  by the same formula (4.7).

**Proof** This is an immediate consequence of Theorem 4.2. In fact, for any r > 0 and any  $t \in \mathbb{R}_+$ , we have

$$\int_{\mathbb{R}} \exp(r|y|) |v_t| (dy) \le e^{\theta^{\star}(\frac{r}{\beta})} \int_{\mathbb{R}} \exp(\theta(\beta|y|) |v_t| (dy).$$

Hence the result.

In order to conclude that  $\mathbb{F}_V$  defines a Feynman integrand, it remains to show that the expectation  $\mathbb{I}_V := \langle \langle \mathbb{F}_V, 1 \rangle \rangle = T \mathbb{F}_V(0)$  solves the Schrödinger equation:

$$i\hbar\frac{\partial \mathbb{I}_V}{\partial t}(t,x) = -\frac{\hbar^2}{2m}\frac{\partial^2 \mathbb{I}_V}{\partial x^2}(t,x) + V(t,x)\mathbb{I}_V(t,x), \quad x \in \mathbb{R}, \quad t > 0,$$

with the initial condition  $\lim_{t\to 0^+} I_V(t, .) = \delta$ . To prove this fact, we proceed as in [24]. So let  $\xi \in \mathcal{S}(\mathbb{R})$  be fixed and define  $\mathbb{K}^{\xi} : \mathbb{R}^2 \to \mathbb{C}$  by

$$\mathbb{K}^{\xi}(t,x) := \Theta(t)T\left(\mathbb{F}_{V}(t,x)\right)(\xi)\exp\left(\frac{1}{2}\int_{\Delta_{1}(t)^{c}}\xi^{2}(s)ds - ix\xi(t)\right), \quad t,x \in \mathbb{R},$$
(4.14)

where  $\Theta=\chi_{\mathbb{R}_+}$  is the Heaviside function. By construction we have

$$\mathbb{K}^{\xi} = \sum_{n=0}^{+\infty} \mathbb{K}_n^{\xi},$$

where  $\mathbb{K}_0^\xi:\mathbb{R}^2\to\mathbb{C}$  is defined by

$$\mathbb{K}_0^{\xi}(t,x) := \Theta(t)T\left(\mathbb{F}_0(t,x)\right)(\xi) \exp\left(\frac{1}{2}\int_{\Delta_1^c(t)}\xi^2(s)ds - ix\xi(t)\right), \quad t, x \in \mathbb{R}.$$

And for all  $n \in \mathbb{N} \setminus \{0\}$ ,

$$\mathbb{K}_{n}^{\xi}(t,x) = \frac{(-i)^{n}\Theta(t)}{\hbar^{n}} \int_{\Delta_{n}(t)} \left( \int_{\mathbb{R}^{n}} \prod_{j=1}^{n+1} \mathbb{K}_{0}^{\xi}(t_{j},y_{j}|t_{j-1},y_{j-1}) \prod_{j=1}^{n} \nu_{t_{j}}(dy_{j}) \right) \prod_{j=1}^{n} dt_{j}.$$
(4.15)

Here  $\overrightarrow{t} = (t_1, \cdots, t_n) \in \Delta_n(t)$  and  $\overrightarrow{y} = (y_1, \cdots, y_n) \in \mathbb{R}^n$  and

$$\begin{aligned} \forall j \in \{0, \cdots, n+1\}, \quad \mathbb{K}_{0}^{\xi}(t_{j}, y_{j} | t_{j-1}, y_{j-1}) &:= \Theta(t) \sqrt{\frac{m}{2\pi i \hbar \left(t_{j} - t_{j-1}\right)}} \times \\ &\exp\left(-\frac{i \hbar}{2m} \int_{\Delta_{1}(t)} \xi^{2}(s) ds + i y_{j-1} \xi(t_{j-1}) - i y_{j} \xi(t_{j})\right) \times \\ &\exp\left(\frac{i m}{2\hbar \left(t_{j} - t_{j-1}\right)} \left(y_{j} - y_{j-1} + \frac{\hbar}{m} \int_{t_{j-1}}^{t_{j}} \xi(s) ds\right)^{2}\right). \end{aligned}$$

Thus we have used the notations  $t_0 = 0$ ,  $t_{n+1} = t$ ,  $y_0 = 0$  and  $y_{n+1} = x$ . We expect  $\mathbb{K}^{\xi}$  to be the propagator corresponding to the potential  $W(t, x) = V(t, x) + \xi'(t)x$ .

## Lemma 4.6

 $\mathbb{K}^{\xi}$ , as defined in (4.14), obeys the following integral equation

$$\mathbb{K}^{\xi}(t,x) = \mathbb{K}^{\xi}_{0}(t,x) - \frac{i}{\hbar} \int_{0}^{t} \left( \int_{\mathbb{R}} \mathbb{K}^{\xi}_{0}(t,x|\tau,y) \mathbb{K}^{\xi}(\tau,y) \nu_{\tau}(dy) \right) d\tau, \quad t,x \in \mathbb{R}.$$
(4.16)

In particular, the Feynman integral  $\mathbb{I}_V \equiv \mathbb{K}$  obeys the well-known propagator equation:

$$\mathbb{K}(t,x) = \mathbb{K}_0(t,x) - \frac{i}{\hbar} \int_0^t \left( \int_{\mathbb{R}} \mathbb{K}_0(t,x|\tau,y) \mathbb{K}(\tau,y) \nu_\tau(dy) \right) d\tau, \quad t,x \in \mathbb{R}.$$
(4.17)

**Proof** Let  $x \in \mathbb{R}$  and t > 0 be fixed. Since  $\xi \in \mathcal{S}(\mathbb{R})$ , we have

$$\left|\mathbb{K}_{0}^{\xi}(t,x)\right| \leq \sqrt{\frac{m}{2\pi\hbar t}},\tag{4.18}$$

and for all  $n \in \mathbb{N} \setminus \{0\}$ ,

$$\left|\mathbb{K}_{n}^{\xi}(t,x)\right| \leq M_{n}(t) \left(\frac{2 \, \|\rho\|_{\infty,t}}{\hbar}\right)^{n}.$$

Then we can apply Fubini's theorem to change the order of integration in (4.15) to obtain the following recursion relation for  $\mathbb{K}_n^{\xi}$ 

$$\mathbb{K}_{n}^{\xi}(t,x) = -\frac{i}{\hbar} \int_{0}^{t} \left( \int_{\mathbb{R}} \mathbb{K}_{0}^{\xi}(t,x|\tau,y) \mathbb{K}_{n-1}^{\xi}(\tau,y) \nu_{\tau}(dy) \right) d\tau, \quad n \in \mathbb{N} \setminus \{0\}.$$
(4.19)

On the other hand, we have

$$\left|\mathbb{K}_{0}^{\xi}(t, x | \tau, y)\right| \leq \sqrt{\frac{m}{2\pi\hbar(t-\tau)}}, \quad y \in \mathbb{R}, \quad \tau \in ]0, t[,$$

and,

$$\sum_{n=2}^{+\infty} \left| \mathbb{K}_{n-1}^{\xi}(\tau, y) \right| \le M(t), \quad y \in \mathbb{R}, \quad \tau \in ]0, t[,$$
(4.20)

where

$$M(t) := \sum_{n=2}^{+\infty} M_n(t) \left(\frac{2 \|\rho\|_{\infty,t}}{\hbar}\right)^n < +\infty.$$

This implies that

$$\begin{split} &\int_0^t \left( \int_{\mathbb{R}} \left| \mathbb{K}_0^{\xi}(t, x | \tau, y) \right| \sum_{n=1}^{+\infty} \left| \mathbb{K}_{n-1}^{\xi}(\tau, y) \right| |\nu_{\tau}| \left( dy \right) \right) d\tau \leq \sqrt{\frac{m}{2\pi\hbar}} \times \\ & \|\rho\|_{\infty, t} \left( \int_0^t \sqrt{\frac{m}{2\pi\hbar\tau \left( t - \tau \right)}} d\tau + M(t) \int_0^t \frac{1}{\sqrt{t - \tau}} \right) < +\infty. \end{split}$$

Then we may interchange summation and integration in (4.19) to get Eq. (4.16). By taking  $\xi = 0$  in (4.16), we get Eq. (4.17). Hence the result.

Now let  $\Omega = ]0, +\infty[\times\mathbb{R}]$ , and let  $D(\Omega)$  be the space of smooth functions  $\varphi : \Omega \to \mathbb{C}$  with bounded support on  $\Omega$ . More precisely, a function  $\varphi : \Omega \to \mathbb{C}$  is an element of  $D(\Omega)$  if and only if  $\varphi \in C^{\infty}(\Omega)$  and there is some bounded interval  $I \subset \Omega$  such that

$$\forall x \notin I, \quad \varphi(x) = 0.$$

The elements in the dual space  $D'(\Omega)$  are called distributions. Since the function  $t \to \frac{1}{\sqrt{t}}$  is locally integrable on  $\Omega$ , the estimations (4.18) and (4.20) show that  $\mathbb{K}^{\xi}$  is locally integrable on  $\Omega$ , i.e.,

$$\int_{I} \left| \mathbb{K}^{\xi}(t,x) \right| dt dx < +\infty$$

for any bounded interval  $I \subset \Omega$ . Thus we can regard  $\mathbb{K}^{\xi}$  as a distribution on  $D(\Omega)$ 

$$\left\langle \mathbb{K}^{\xi}, \varphi \right\rangle = \int_{\Omega} \mathbb{K}^{\xi}(t, x)\varphi(t, x)dxdt, \quad \varphi \in D(\Omega).$$

And we can also define a distribution  $V\mathbb{K}^{\xi}$  by setting

$$\langle V \mathbb{K}^{\xi}, \varphi \rangle = \int_{\mathbb{R}_{+}} \left( \int_{\mathbb{R}} \mathbb{K}^{\xi}(t, x) \varphi(t, x) \nu_{t}(dx) \right) dt, \quad \varphi \in D(\Omega).$$

Now let  $T^{\xi}: D(\Omega) \to D(\Omega)$  be the linear operator defined by

$$T^{\xi}\varphi(t,x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi(t,x) + x\xi'(t)\varphi(t,x), \quad \varphi \in D(\Omega), \quad x \in \mathbb{R}, \quad t \in \mathbb{R}_+.$$

#### Theorem 4.7

 $\mathbb{K}^{\xi}$  is a Green function for the full Schrödinger equation, i.e.,  $\mathbb{K}^{\xi}$  solves as a distribution the following equation:

$$i\hbar\frac{\partial\mathbb{K}^{\xi}}{\partial t} = T^{\xi}\mathbb{K}^{\xi} + V\mathbb{K}^{\xi} + i\hbar\delta(0,0).$$

In particular, the Feynman integral  $\mathbb{I}_V$  solves as a distribution, the Schrödinger equation:

$$i\hbar \frac{\partial \mathbb{I}_V}{\partial t} = T\mathbb{I}_V + V\mathbb{I}_V + i\hbar\delta(0,0), \quad T := T^0.$$

**Proof** Let  $\varphi \in D(\Omega)$  be fixed. By Lemma 4.6 we have

$$i\hbar\left\langle\frac{\partial}{\partial t}\mathbb{K}^{\xi},\varphi\right\rangle = -i\hbar\left\langle\mathbb{K}^{\xi},\frac{\partial}{\partial t}\varphi\right\rangle = -i\hbar\int_{\mathbb{R}_{+}\times\mathbb{R}}\mathbb{K}^{\xi}(t,x)\frac{\partial\varphi}{\partial t}(t,x)dtdx + \frac{i}{\hbar}\int_{\mathbb{R}_{+}\times\mathbb{R}}\left(\int_{0}^{t}\left(\int_{\mathbb{R}}i\hbar\mathbb{K}_{0}^{\xi}(t,x|\tau,y)\mathbb{K}^{\xi}(\tau,y)\nu_{\tau}(dy)\right)d\tau\right)\frac{\partial\varphi}{\partial t}(t,x)dtdx.$$

As  $\mathbb{K}_0^{\xi}$  is a Green function for the free Schrödinger equation, the first term equals

$$\begin{split} i\hbar\varphi(0,0) &+ \int_{\mathbb{R}_+\times\mathbb{R}} T^{\xi} \mathbb{K}_0^{\xi}(t,x)\varphi(t,x)dtdx = \\ i\hbar\varphi(0,0) &+ \int_{\mathbb{R}_+\times\mathbb{R}} \mathbb{K}_0^{\xi}(t,x)T^{\xi}\varphi(t,x)dtdx. \end{split}$$

Thus by Fubini's theorem, the last term equals

$$\frac{i}{\hbar}\int_{\mathbb{R}_+}\left(\int_{\mathbb{R}}\left(\int_{[\tau,+\infty[\times\mathbb{R}]}i\hbar\mathbb{K}_0^{\xi}(t,x|\tau,y)\frac{\partial}{\partial t}\varphi(t,x)dtdx\right)\mathbb{K}^{\xi}(\tau,y)\nu_{\tau}(dy)\right)d\tau.$$

And by integration by parts, this equals

$$\int_{\mathbb{R}_{+}} \left( \int_{\mathbb{R}} \varphi(\tau, y) \mathbb{K}^{\xi}(\tau, y) \nu_{\tau}(dy) \right) d\tau - \frac{i}{\hbar} \int_{\mathbb{R}_{+}} \left( \int_{\mathbb{R}} \left( \int_{[\tau, +\infty[\times\mathbb{R}]} \mathbb{K}_{0}^{\xi}(t, x|\tau, y) T^{\xi} \varphi(t, x) dt dx \right) \mathbb{K}^{\xi}(\tau, y) \nu_{\tau}(dy) \right) d\tau.$$

Apply again Fubini's theorem, the last expression equals

$$\frac{i}{\hbar} \int_{\mathbb{R}_+ \times \mathbb{R}} \left( \int_0^t \left( \int_{\mathbb{R}} \mathbb{K}_0^{\xi}(t, x | \tau, y) \mathbb{K}^{\xi}(\tau, y) v_{\tau}(dy) \right) d\tau \right) T^{\xi} \varphi(t, x) dt dx.$$

Then it follows that

$$i\hbar\left(\frac{\partial}{\partial t}\mathbb{K}^{\xi},\varphi\right) = i\hbar\varphi(0,0) + \int_{\mathbb{R}_{+}} \left(\int_{\mathbb{R}}\varphi(\tau,y)\mathbb{K}^{\xi}(\tau,y)\nu_{\tau}(dy)\right)d\tau + \int_{\mathbb{R}_{+}\times\mathbb{R}} \left(\mathbb{K}_{0}^{\xi}(t,x) - \frac{i}{\hbar}\int_{0}^{t} \left(\int_{\mathbb{R}}\mathbb{K}_{0}^{\xi}(t,x|\tau,y)\mathbb{K}^{\xi}(\tau,y)\nu_{\tau}(dy)\right)d\tau\right)T^{\xi}\varphi(u,v)dudv$$

To conclude it suffices to apply Lemma 4.6 and use again integration by parts. Hence the result.

#### Remark 4.8

- (1) A direct comparison shows that
  - (a) if v<sub>t</sub> = v for all t ∈ ℝ<sub>+</sub>, where v is a finite signed Borel measure on ℝ, then our corresponding class of admissible potentials contains strictly the corresponding class of admissible potentials introduced by the authors in [24]. In fact, let E<sub>1</sub> be the corresponding class of the admissible potentials introduced by the authors in [24], and let E<sub>2</sub> be our corresponding class of admissible potentials. If v ∈ E<sub>1</sub>, then v satisfies the following condition (see [24]):

$$\exists \gamma > 0; \quad \int_{\mathbb{R}} e^{\gamma x^2} |\nu(x)| dx < +\infty, \tag{4.21}$$

which implies that

$$\forall r > 0, \quad \int_{\mathbb{R}} e^{r|x|} |v(x)| dx \le \left( \int_{\mathbb{R}} e^{\gamma x^2} |v(x)| dx \right) \exp\left(\frac{r^2}{4\gamma}\right).$$

By applying Corollary 4.4, we see that  $v \in \mathcal{E}_2$ . This implies that  $\mathcal{E}_1 \subset \mathcal{E}_2$ . To see that this inclusion is strict, let v be a Poisson measure with parameter u > 0, i.e.,

$$\nu = e^{-u} \sum_{n=0}^{+\infty} \frac{u^n}{n!} \delta_n.$$
(4.22)

*Obviously,*  $v \in \mathcal{E}_1$  *does not satisfy the condition* (4.21). So  $v \notin \mathcal{E}_2$ . *Hence the result.* 

- (b) if v<sub>t</sub> = V(t, .) for all t ∈ I, where I ⊂ ℝ<sub>+</sub> is an interval and V : I × ℝ → ℝ is an ordinary function. Then, the corresponding admissible potentials V introduced by the authors in [24] are defined only on bounded intervals I = [0, T], T > 0. However, our class of admissible potentials can be defined on bounded and unbounded intervals, e.g., I = ℝ<sub>+</sub>.
- (2) Any finite signed Borel measure v satisfying (4.13) on  $\mathbb{R}$ . This can be as singular as desired, e.g., a sum of Deltas such as  $\sum_{n \in \mathbb{N}} e^{-n^2} \delta_n$  or a devil s staircase [24].
- (3) Every finite measure with compact support is in our class. More examples in the case of time-dependent are given in the next section.
- (4) This research can be useful for quantum foundations [6, 18, 29].

# **5** Examples of Admissible Potentials

In this section, we give several examples of our admissible potentials and illustrate the functions  $\rho$  and  $\theta$  used in the conditions of Theorem 4.2 and its corollaries.

#### Example 5.1

Let  $u : \mathbb{R}_+ \to \mathbb{R}$  be a continuous function. Define a family of measure  $(v_t)_{t \in \mathbb{R}_+}$  by

$$v_t := \delta_{u(t)}, \quad t \in \mathbb{R}_+,$$

where  $\delta_a$  denotes the Dirac measure at  $a \in \mathbb{R}$ . Then for any  $t \in \mathbb{R}_+$ , we have

$$\int_{\mathbb{R}} \exp\left(y^2\right) |v_t|(dy) := \exp\left(u^2(t)\right) < +\infty$$

By applying Corollary 4.5, we see that the corresponding Feynman integrand  $\mathbb{F}_V$  is a Hida distribution.

#### Example 5.2

Let  $V : \mathbb{R}_+ \times \mathbb{R} \to \mathbb{R}$  be a given potential, and let  $\theta : \mathbb{R}_+ \to \mathbb{R}_+$  be a Young function satisfying the condition (2.6). Suppose that there is a > 0 and a continuous function  $b : \mathbb{R}_+ \to \mathbb{R}_+$  such that

$$|V(t, x)| \le b(t) \exp\left(-a\theta(|x|)\right), \quad x \in \mathbb{R}, \quad t > 0.$$

Then for any  $\beta < \inf\{a, 1\}$ , we have

$$\int_{\mathbb{R}} \exp\left(\theta \left(\beta \mid y \mid\right)\right) \left|V(t, y)\right| dy \le b(t) \int_{\mathbb{R}} \exp\left(\left(\beta - a\right)\theta \left(\mid y \mid\right)\right) dy.$$

By applying Corollary 4.5, we see that the corresponding Feynman integrand  $\mathbb{F}_V$  is a generalized function in the space  $[\mathcal{W}]^*_{\mu}$ .

#### Example 5.3

Let  $a : \mathbb{R}_+ \to \mathbb{R}_+$  and  $b : \mathbb{R}_+ \to \mathbb{R}_+$  be two continuous functions with a(t) < b(t)for all  $t \in \mathbb{R}_+$ . Define  $V : \mathbb{R}_+ \times \mathbb{R} \to \mathbb{R}$  by

$$V(t,x) = \frac{1}{b(t) - a(t)} \chi_{]a(t),b(t)[}(x), \quad x \in \mathbb{R}, \quad t \in \mathbb{R}_+.$$

For any t, r > 0, we have

$$\int_{\mathbb{R}} \exp(r|y|) |V(t,y)| \, dy = \frac{1}{b(t) - a(t)} \int_{a(t) - b(t)} \exp(r|y|) \, dy \le \exp(r(b(t) - a(t))) \le \exp\left(\frac{(b(t) - a(t))^2}{2}\right) \exp\left(\frac{r^2}{2}\right).$$

By applying Theorem 4.2, we see that the corresponding Feynman integrand  $\mathbb{F}_V$  is a Hida distribution. In that case, we have

$$\theta(s) = \theta^{\star}(s) = \frac{s^2}{2}, \quad \rho(s) = \exp\left(\frac{(b(s) - a(s))^2}{2}\right), \quad s \in \mathbb{R}_+.$$

#### Example 5.4

Let  $m : \mathbb{R}_+ \to \mathbb{R}$  and  $\sigma : \mathbb{R}_+ \to \mathbb{R} \setminus \{0\}$  be two continuous functions. Define  $V : \mathbb{R}_+ \times \mathbb{R} \to \mathbb{R}$  by

$$V(t,x) = \frac{1}{\sqrt{2\pi |\sigma(t)|}} \exp\left(-\frac{(x-m(t))^2}{2 |\sigma(t)|}\right), \quad t \in \mathbb{R}_+, \quad x \in \mathbb{R}.$$

For any r, t > 0, we have

$$\int_{\mathbb{R}} \exp\left(r \mid y \mid\right) |V(t, y)| dy \le 2 \exp\left(\frac{|\sigma(t)| r^2}{2} + r |m(t)|\right) \le 2 \exp\left(\frac{m^2(t) + (1 + |\sigma(t)|)^2}{2}\right) \exp\left(\frac{r^4}{4}\right).$$

Then V satisfies the conditions of Theorem 4.2 with

$$\theta(t) = \frac{3}{4}t^{\frac{4}{3}}, \quad \theta^{\star}(t) = \frac{t^{4}}{4}, \quad \rho(t) = 2\exp\left(\frac{m^{2}(t) + (1 + |\sigma(t)|)^{2}}{2}\right), \quad t \in \mathbb{R}_{+}.$$

In the particular case where  $\sigma$  is bounded, it is very easy to prove that the Feynman integrand  $\mathbb{F}_V$  is a well-defined Hida distribution. For all details see Remark 4.8.

### Example 5.5

Let  $u: \mathbb{R}_+ \to \mathbb{R}$  be a continuous function. Define a family of measure  $(v_t)_{t \in \mathbb{R}_+}$  by

$$\nu_t := e^{-|u(t)|} \sum_{n=0}^{+\infty} \frac{|u(t)|^n}{n!} \delta_n, \quad t \in \mathbb{R}_+.$$

In other words,  $v_t$  is the Poisson measure with parameter |u(t)|. By definition, for any r, t > 0 we have

$$\int_{\mathbb{R}} \exp(r | y|) v_t(dy) = \exp(-|u(t)|) \sum_{n=0}^{+\infty} \frac{|u(t)|^n}{n!} e^{nr} = \exp(|u(t)|(e^r - 1)) \le \exp\left(\frac{1 + |u(t)|^2}{2}\right) \exp\left(e^{2r} - 1\right),$$

which satisfies the conditions of Theorem 4.2 with

$$\theta^{\star}(t) = e^{2t} - 1, \quad \rho(t) = \exp\left(\frac{1 + |u(t)|^2}{2}\right), \quad t \in \mathbb{R}_+.$$

By direct computation, we obtain

$$\theta(t) = \begin{cases} 1 + \frac{t}{2} \left( \log(\frac{t}{2}) - 1 \right) & \text{if } t > 2\\ 0 & \text{if } 0 \le t \le 2. \end{cases}$$

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# Classical Field Theory of the Photoelectric Effect



Sergey A. Rashkovskiy

# 1 Introduction

Our current understanding of quantum mechanics is based on certain basic physical effects that, it is believed, cannot be explained within the framework of classical ideas and, therefore, require quantization.

The photoelectric effect has a special place in quantum theory because it became the first physical effect, for explanation of which the quantization of light was introduced.

By the early twentieth century, the three basic laws of the photoelectric effect were experimentally established: (1) the photoelectric current is proportional to the intensity of incident light; (2) the maximum kinetic energy of the emitted photoelectrons varies linearly with the frequency of incident electromagnetic radiation and does not depend on the flux; and (3) for each substance, there is a threshold frequency (the so-called red edge of the photoelectric effect), below which the photoelectric current is not observed.

The second and third laws of the photoelectric effect would appear to contradict classical electrodynamics, which requires dependence of the kinetic energy of the emitted photoelectrons on the intensity of the incident light. Such a conclusion necessarily follows from the analysis of the motion of charged particles—electrons in the field of a classical electromagnetic wave. Thus, the attempts to explain the photoelectric effect within the framework of classical mechanics and classical electrodynamics were unsuccessful.

Institute for Problems in Mechanics of the Russian Academy of Sciences, Moscow, Russia

S. A. Rashkovskiy (🖂)

Tomsk State University, Tomsk, Russia e-mail: rash@ipmnet.ru

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This contradiction was overcome due to the quantization of radiation, which postulates that the absorption of light occurs in the form of discrete quanta  $\hbar\omega$  (Einstein 1905). At present, in connection with this finding, it is considered to be generally accepted that the photoelectric effect provides "evidence" for the quantum nature of light.

However, in the early years of quantum mechanics, it was shown that the photoelectric effect is fully described within the framework of so-called semiclassical theory, in which light is considered to be a classical electromagnetic wave, while the atom is quantized and described by the wave equation, e.g. the Schrödinger equation or the Dirac equation [1-4].

In this case, the wave equation is solved as a typical classical field equation, whereby a continuous wave field is calculated. A "quantization" of this wave field occurs only at the stage of interpreting the solution, from which the "probability of photoelectron emission" from an atom is determined.

There were also attempts to build the semiclassical theories of other quantum phenomena, namely, Lamb shift [5, 6], spontaneous emission [5–7], semiclassical radiation theory [8], radiative effects [9], Compton effect [10–15], Hanbury Brown and Twiss effect [16, 17], semiclassical theory of laser [18, 19], etc. Because the electron in such theories is considered to be a quantum particle and light is considered to be a classical electromagnetic field, such theories are considered to be "semiclassical".

Despite the success of this approach, there are many intra-atomic and optical phenomena that did not find an explanation within the framework of semiclassical theory. Because of this, it is generally accepted that a complete description of the intra-atomic phenomena and light-atom interaction is possible only within the framework of quantum electrodynamics (QED), when both the states of an atom and the radiation itself are quantized.

However, as shown in [20–26], there is no need to introduce the quantization of electromagnetic and electron fields because this interpretation is external to the wave equation, and it does not follow from these equations. Moreover, this approach is superfluous in explaining the many physical phenomena that before were interpreted as a result of the quantization of matter.

In previous papers of this series [22-26], an attempt was made to construct a completely classical theory, which is similar to classical field theory [27], in which any quanta are absent. Here, as in [20-26], classical theory is understood as a theory in which all objects are either particles or fields, and no object can simultaneously possess both wave and corpuscular properties. In other words, in classical theory, there is no such concept as corpuscular-wave dualism. Thus, in papers [20-22], it was shown that the discrete events (e.g. clicks of a detector, emergence of the spots on a photographic plate) that are observed in some of the "quantum" experiments with light (especially in the double-slit experiments), which are considered to be direct evidence of the existence of photons, can in fact be explained within classical electrodynamics without quantization of the radiation. Similarly, if the electrons are considered to not be a particle but instead a classical continuous wave field, similar to the classical electromagnetic field, one can consistently explain the "wave-

particle duality of electrons" in the double-slit experiments [23]. In this case, the Dirac equation and its specific cases (Klein-Gordon, Pauli and Schrödinger) should be considered to be the usual field equations of a classical electron wave field, similar to Maxwell's equations for classical electromagnetic fields. As was shown in [23], considering the electron wave as a classical field, we must assign to it, besides the energy and momentum which are distributed in space, also an electric charge, an internal angular momentum and an internal magnetic moment, which are also continuously distributed in space. In this case, the internal angular momentum and internal magnetic moment of the electron wave are its intrinsic properties and cannot be reduced to any movement of charged particles. This viewpoint allows for a description in natural way, in the framework of classical field theory with respect to the many observed phenomena that involve "electrons", and it explains their properties which are considered to be paradoxical from the standpoint of classical mechanics. Thus, the Compton effect, which is considered to be "direct evidence of the existence of photons", has a natural explanation if both light and electron waves are considered to be classical continuous fields [23]. The same approach can be applied to the Born rule for light and "electrons" and to the Heisenberg's uncertainty principle, which have a simple and clear explanation within classical field theory [20–23]. Using such a point of view on the nature of the "electron", a new model of the hydrogen atom that differs from the conventional planetary model was proposed and justified in [24]. According to this model, the atom represents a classical open volume resonator in which an electrically charged continuous electron wave is held in a restricted region of space by the electrostatic field of the nucleus. As shown in [24], the electrostatic field of the nucleus plays for the electron wave, the role of a "dielectric medium", and thus, one can say that the electron wave is held in the hydrogen atom due to the total internal reflection on the inhomogeneities of this "medium". In the hydrogen atom, as in any volume resonator, there are eigenmodes that correspond to a discrete spectrum of eigenfrequencies, which are the eigenvalues of the field equation (e.g. Schrödinger, Dirac). As usual, the standing waves (in this case, the standing electron waves) correspond to the eigenmodes. If only one of the eigenmodes is excited in the atom as in the volume resonator,

then such a state of the atom is called a pure state. If simultaneously several (two or more) eigenmodes are excited in the atom, then such a state is called a mixed state [24].

Using this viewpoint, it was shown in [24] that all of the basic optical properties of the hydrogen atom have a simple and clear explanation in the framework of classical electrodynamics without any quantization. In particular, it was shown that the atom can be in a pure state indefinitely. This arrangement means that the atom has a discrete set of stationary states, which correspond to all possible pure states, but only the pure state that corresponds to the lowest eigenfrequency is stable. Precisely this state is the ground state of the atom. The remaining pure states are unstable, although they are the stationary states. Any mixed state of an atom in which several eigenmodes are excited simultaneously is nonstationary, and according to classical electrodynamics, the atom that is in that state continuously emits electromagnetic waves of the discrete spectrum, which is interpreted as a spontaneous emission. In reference [24], a fully classical description of spontaneous emission was given, and all of its basic properties that are traditionally described within the framework of quantum electrodynamics were obtained. It is shown that the "jump-like quantum transitions between the discrete energy levels of the atom" do not exist, and the spontaneous emission of an atom occurs not in the form of discrete quanta but continuously.

As is well known, the linear wave equation, e.g. the Schrödinger equation, cannot explain the spontaneous emission and the changes that occur in the atom in the process of spontaneous emission (so-called quantum transitions). To explain spontaneous transitions, quantum mechanics, it is believed, must be extended to quantum electrodynamics, which introduces such an object as a QED vacuum, the fluctuations of which are considered to be the cause of the "quantum transitions".

In reference [24], it was shown that the Schrödinger equation, which describes the electron wave as a classical field, is sufficient for a description of the spontaneous emission of a hydrogen atom. However, it should be complemented by a term that accounts for the inverse action of self-electromagnetic radiation on the electron wave. In the framework of classical electrodynamics, it was shown that the electron wave as a classical field is described in the hydrogen atom by a nonlinear Eq. [24]

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m_e}\Delta\psi - \frac{e^2}{r}\psi - \frac{2e^2}{3c^3}\psi\mathbf{r}\frac{\partial^3}{\partial t^3}\int\mathbf{r}|\psi|^2 d\mathbf{r}$$
(1)

where the last term on the right-hand side describes the inverse action of the self-electromagnetic radiation on the electron wave and is responsible for the degeneration of any mixed state of the hydrogen atom. Precisely, this term "provides" a degeneration of the mixed state of the hydrogen atom to a pure state, which corresponds to the lower excited eigenmodes of an atom. As shown in [24], this term has a fully classical meaning and fits into the concept developed in [20–26] in that the photons and electrons as particles do not exist, and there are only electromagnetic and electron waves, which are classical (continuous) fields.

The nonlinearity of the Eq. (1) plays an essential role in light-atom interaction and should be taken into account in all calculations. Thus, as shown in [25, 26], based on the nonlinear Eq. (1), the light-atom interaction can be fully described within the framework of classical field theory without the use of quantum electrodynamics. In particular, in reference [25], the optical Bloch equations with damping due to spontaneous emission and with correct damping rate has been directly derived from the nonlinear Schrödinger equation (1) without quantization of radiation [25].

In reference [26] it was shown that the thermal radiation can also be described without quantization of energy in the framework of classical field theory using the nonlinear Schrödinger equation (1) which is considered as a classical field equation. As shown in [26] the Planck's law for the spectral energy density of thermal radiation and the Einstein A-coefficient for spontaneous emission are derived without using the concept of the energy quanta.

As will be shown below, the failures of classical electrodynamics in explaining the photoelectric effect are connected with the incorrect postulate that electrons are particles. I will show that for a consistent explanation of the photoelectric effect within the framework of classical field theory, it is sufficient to abandon this postulate and consider continuous classical electron waves instead of the particleselectrons [23, 24]. The considered theory is fully classical because it does not contain not only the quantization of the radiation but also the quantization of the electron wave.

## 2 Photoelectric Effect

In reference [25], it was assumed that under the influence of an incident electromagnetic wave, the electron wave in an atom is only redistributed between its eigenmodes but not emitted outward by the atom. In this case, internal electric currents arise inside the atom that, however, cannot be detected by macroscopic devices. Such a situation occurs at a relatively low frequency of the incident electromagnetic wave. If this frequency is sufficiently large, then an emission of the electron wave by the atom occurs. Because the electron wave has an electric charge that is continuously distributed in space [23, 24], in this case, an external electric current (photoelectric current) appears that can be detected by macroscopic devices. As a result, the photoelectric effect will be observed.

From the considered point of view [20–26], the photoelectric effect represents an emission of the continuous charged electron wave by an atom that was excited by the incident classical electromagnetic wave. Formally, the photoelectric effect is no different from the stimulated emission of electromagnetic waves by an atom [24], with the only difference being that the electron wave emitted by an atom is electrically charged, while the electromagnetic wave does not carry the electric charge. Assuming that the electric charge is continuously distributed in the electron wave [23, 24], one concludes that in the process of the emission of the electron wave, the atom is positively charged continuously. However, accounting for the fact that the electron wave for an as yet inexplicable reason does not "feel" its own electrostatic field [24], this process will not affect the emission of the following "portions" of the continuous electron wave because they must overcome the same electrostatic potential of the nucleus.

Let us consider the photoelectric effect for the hydrogen atom being in the classic monochromatic electromagnetic wave.

In this section, we neglect the inverse action on the electron wave of its own nonstationary electromagnetic field. For this reason, the last term in the Schrödinger equation (1), which is associated with a spontaneous emission of the electromagnetic waves, will not be considered, and we will use the conventional linear Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m_e}\Delta\psi - \frac{e^2}{r}\psi + \psi e\mathbf{r}\mathbf{E}_0\cos\omega_0 t \tag{2}$$

where  $\omega_0$  is the frequency of the incident light. We will consider here the approximation, when the wavelength of the incident electromagnetic wave is substantially larger than the characteristic spatial size of the electron field in the hydrogen atom, which is of the order of the Bohr radius  $a_B$ .

The wave function of an electron wave can be represented as in [28]

$$\psi = \sum_{k} c_k(t) u_k(\mathbf{r}) \exp\left(-i\omega_k t\right) + \sum_{n} \int_{0}^{\infty} C_n(\omega, t) f_n(\mathbf{r}, \omega) \exp\left(-i\omega t\right) d\omega \quad (3)$$

where the first sum describes that part of the electron wave that is contained in the eigenmodes of the atom (i.e. corresponding to a "finite motion" of the electron wave), and for this term, all  $\omega_k < 0$ , while the integrals describe the electron waves that are emitted by an atom (i.e. which corresponds to the "infinite motion" of the electron wave), to which it is known that  $\omega > 0$  corresponds. The indices *n* and *k* run through the appropriate integer values. The functions  $u_k(\mathbf{r})$  and  $f_n(\mathbf{r}, \omega)$  are the eigenfunctions of the stationary Schrödinger equation, while the frequencies  $\omega_k$  are the eigenvalues that correspond to the eigenfunctions  $u_k(\mathbf{r})$ .

The eigenfunctions  $u_k(\mathbf{r})$  and  $f_n(\mathbf{r}, \omega)$  satisfy the orthogonality conditions:

$$\int u_k(\mathbf{r}) u_n^*(\mathbf{r}) \, dV = \delta_{nk} \tag{4}$$

$$\int f_k \left( \mathbf{r}, \omega' \right) f_n^* \left( \mathbf{r}, \omega'' \right) dV = \delta_{nk} \delta \left( \omega' - \omega'' \right)$$
(5)

$$\int u_k(\mathbf{r}) f_n^*(\mathbf{r}, \omega'') dV = 0$$
(6)

Substituting expression (3) into Eq. (2) and using the orthogonality conditions (4)–(6), we obtain

$$i\hbar\dot{c}_{k}(t)\exp\left(-i\omega_{k}t\right) = e\mathbf{E}_{0}\cos\omega_{0}t\sum_{n}c_{n}(t)\int\mathbf{r}u_{n}\left(\mathbf{r}\right)u_{k}^{*}dV\exp\left(-i\omega_{n}t\right)$$
$$+e\mathbf{E}_{0}\cos\omega_{0}t\sum_{n}\int_{0}^{\infty}C_{n}\left(\omega,t\right)\int\mathbf{r}u_{k}^{*}f_{n}\left(\mathbf{r},\omega\right)dV\exp\left(-i\omega t\right)d\omega$$
(7)

and

$$i\hbar\dot{C}_{n}(\omega,t)\exp\left(-i\omega t\right) = e\mathbf{E}_{0}\cos\omega_{0}t\sum_{k}c_{k}(t)\int\mathbf{r}f_{n}^{*}(\mathbf{r},\omega)u_{k}(\mathbf{r})dV\exp\left(-i\omega_{k}t\right)$$
$$+e\mathbf{E}_{0}\cos\omega_{0}t\sum_{k}\int_{0}^{\infty}C_{k}(\omega',t)\int\mathbf{r}f_{k}(\mathbf{r},\omega')f_{n}^{*}(\mathbf{r},\omega)dV\exp\left(-i\omega't\right)d\omega' \quad (8)$$

Within the framework of perturbation theory and assuming that all of the modes of the electron wave (both discrete and continuous), except for the ground mode  $u_1$ , are weakly excited, we obtain

$$i\hbar\dot{c}_{1}(t)\exp\left(-i\omega_{1}t\right) = -c_{1}(t)\left(\mathbf{E}_{0}\mathbf{d}_{11}\right)\cos\omega_{0}t\exp\left(-i\omega_{1}t\right)$$
$$+ e\mathbf{E}_{0}\cos\omega_{0}t\sum_{n}\int_{0}^{\infty}C_{n}\left(\omega,t\right)\int\mathbf{r}u_{1}^{*}f_{n}\left(\mathbf{r},\omega\right)dV\exp\left(-i\omega t\right)d\omega \qquad(9)$$

$$i\hbar\dot{C}_n(\omega,t) = e\mathbf{E}_0\cos\omega_0 tc_1(t)\exp\left[-i\left(\omega_1-\omega\right)t\right]\int\mathbf{r}f_n^*(\mathbf{r},\omega)\,u_1(\mathbf{r})\,dV + e\mathbf{E}_0$$

$$\cos \omega_0 t \exp(i\omega t) \sum_k \int_0^\infty C_k(\omega', t) \int \mathbf{r} f_k(\mathbf{r}, \omega') f_n^*(\mathbf{r}, \omega) dV \exp(-i\omega' t) d\omega'$$
(10)

where

$$\mathbf{d}_{nk} = -e \int \mathbf{r} u_n \left( \mathbf{r} \right) u_k^* dV \tag{11}$$

For a weak electromagnetic wave, which causes weak excitation of an atom,  $c_1 \approx 1$ . For this reason, we can discard terms in Eq. (10) that contain  $\mathbf{E}_0 C_k(\omega', t)$ , as small of the second order. In Eq. (9), these terms cannot be discarded because the change in  $c_1$  will have a second order in  $\mathbf{E}_0$ . Then, we obtain

$$i\hbar\dot{c}_{1}(t) = -\left(\mathbf{E}_{0}\mathbf{d}_{11}\right)\cos\omega_{0}t + \frac{1}{2}e\mathbf{E}_{0}\sum_{n}\int_{0}^{\infty}C_{n}\left(\omega, t\right)\mathbf{U}_{1n}\left(\omega\right)\exp\left[-i\left(\omega-\omega_{1}-\omega_{0}\right)t\right]$$

$$d\omega + \frac{1}{2}e\mathbf{E}_0\sum_n\int_0^\infty C_n(\omega,t)\,\mathbf{U}_{1n}(\omega)\exp\left[-i\left(\omega - \omega_1 + \omega_0\right)t\right]d\omega \tag{12}$$

$$i\hbar\dot{C}_{n}(\omega,t) = \frac{1}{2}e\mathbf{E}_{0}\cdot\mathbf{U}_{1n}^{*}(\omega)\exp\left[-i\left(\omega_{1}-\omega-\omega_{0}\right)t\right]$$
$$+\frac{1}{2}e\mathbf{E}_{0}\cdot\mathbf{U}_{1n}^{*}(\omega)\exp\left[-i\left(\omega_{1}-\omega+\omega_{0}\right)t\right]$$
(13)

where

$$\mathbf{U}_{1n}\left(\omega\right) = \int \mathbf{r}u_{1}^{*}\left(\mathbf{r}\right) f_{n}\left(\mathbf{r},\omega\right) dV$$
(14)

Neglecting the purely oscillatory term  $-(\mathbf{E}_0\mathbf{d}_{11})\cos\omega_0 t$  in Eq. (12) (which can be accomplished, for example, by averaging Eq. (12) over rapid oscillations with a frequency  $\omega_0$ ), we obtain

$$i\hbar\dot{c}_{1}(t) = \frac{1}{2}e\mathbf{E}_{0}\sum_{n}\int_{0}^{\infty}C_{n}(\omega,t)\mathbf{U}_{1n}(\omega)\exp\left[-i\left(\omega-\omega_{1}-\omega_{0}\right)t\right]d\omega$$
$$+\frac{1}{2}e\mathbf{E}_{0}\sum_{n}\int_{0}^{\infty}C_{n}(\omega,t)\mathbf{U}_{1n}(\omega)\exp\left[-i\left(\omega-\omega_{1}+\omega_{0}\right)t\right]d\omega$$
(15)

Integrating Eq. (13) with respect to the time from zero to t, we obtain

$$C_{n}(\omega, t) = \frac{e}{2\hbar} \frac{\exp\left[-i\left(\omega_{1} - \omega - \omega_{0}\right)t\right] - 1}{(\omega_{1} - \omega - \omega_{0})} \mathbf{E}_{0} \cdot \mathbf{U}_{1n}^{*}(\omega) + \frac{e}{2\hbar} \frac{\exp\left[-i\left(\omega_{1} - \omega + \omega_{0}\right)t\right] - 1}{(\omega_{1} - \omega + \omega_{0})} \mathbf{E}_{0} \cdot \mathbf{U}_{1n}^{*}(\omega)$$
(16)

Because the frequencies have  $\omega_0 > 0$ ,  $\omega > 0$  and  $\omega_1 < 0$ , the value  $\omega_1 - \omega - \omega_0$ is not equal to zero for any  $\omega$ , and thus, the first term will always be limited and will describe the oscillations that are of small amplitude. At the same time,  $\omega_1 - \omega + \omega_0 = 0$  at the resonance frequency of  $\omega_0 = |\omega_1| + \omega$ , and near the resonant frequency, the second term in (16) will increase indefinitely. Therefore, the second term in (16) makes the main contribution to the effect that is under consideration. Neglecting the first term in expression (16), we obtain

$$C_n(\omega, t) = \frac{e}{2\hbar} \frac{\exp\left[-i\left(\omega_1 - \omega + \omega_0\right)t\right] - 1}{\left(\omega_1 - \omega + \omega_0\right)} \mathbf{E}_0 \cdot \mathbf{U}_{1n}^*(\omega)$$
(17)

Let us calculate the photoelectric current that arises upon excitation of the atom by the incident electromagnetic wave.

This goal can be accomplished by calculating the electric current density according to the formula

$$\mathbf{j} = i \frac{ec^2}{2\omega_e} \left( \psi^* \nabla \psi - \psi \nabla \psi^* \right) - \frac{e^2 c}{\hbar \omega_e} \mathbf{A} \psi \psi^*$$
(18)

and integrating it over the surface of an infinite sphere whose centre is in the nucleus of the atom. However, it is more convenient to accomplish this step while using the law of conservation of charge and accounting for the fact that  $q_k = -e|c_k|^2$  is the electric charge that is contained in mode k of the electron wave [24]. Then,  $\dot{q}_k$  is the internal electric current in the atom, by which mode k is exchanged with all of the other modes of the electron wave (including continuous modes, if they exist), i.e. the amount of electric charge of the electron wave, which goes into mode k from other modes or goes out of mode k into other modes, per unit time. Because in this case, it is considered that only one (ground) eigenmode  $u_1$  of the hydrogen atom is excited, then the photoelectric current

$$I_{ph} = -\dot{q}_1 \tag{19}$$

or

$$I_{ph} = -e\frac{d|c_1|^2}{dt} \tag{20}$$

Using Eq. (15), we obtain the same approximation

$$I_{ph} = -\frac{e^2}{2i\hbar} \sum_n \int_0^\infty C_n(\omega, t) \mathbf{E}_0 \cdot \mathbf{U}_{1n}(\omega) \exp\left[-i(\omega - \omega_1 - \omega_0)t\right] d\omega$$
  
$$-\frac{e^2}{2i\hbar} \sum_n \int_0^\infty C_n(\omega, t) \mathbf{E}_0 \cdot \mathbf{U}_{1n}(\omega) \exp\left[-i(\omega - \omega_1 + \omega_0)t\right] d\omega$$
  
$$+\frac{e^2}{2i\hbar} \sum_n \int_0^\infty C_n^*(\omega, t) \mathbf{E}_0 \cdot \mathbf{U}_{1n}^*(\omega) \exp\left[i(\omega - \omega_1 - \omega_0)t\right] d\omega$$
  
$$+\frac{e^2}{2i\hbar} \sum_n \int_0^\infty C_n^*(\omega, t) \mathbf{E}_0 \cdot \mathbf{U}_{1n}^*(\omega) \exp\left[i(\omega - \omega_1 + \omega_0)t\right] d\omega$$
(21)

Substituting  $C_n(\omega, t)$  from (17) into expression (21), we obtain

$$I_{ph} = \frac{e^3}{2\hbar^3} \sum_n \int_0^\infty \frac{\sin\left[(\omega - \omega_1 - \omega_0)t\right]}{(\omega - \omega_1 - \omega_0)} \left(\mathbf{E}_0 \cdot \mathbf{U}_{1n}^*\right) \left(\mathbf{E}_0 \cdot \mathbf{U}_{1n}\right) d\omega$$
$$+ \frac{e^3}{4i\hbar^3} \exp\left(-2i\omega_0 t\right) \sum_n \int_0^\infty \frac{1 - \exp\left[-i\left(\omega - \omega_1 - \omega_0\right)t\right]}{(\omega - \omega_1 - \omega_0)} \left(\mathbf{E}_0 \cdot \mathbf{U}_{1n}^*\right) \left(\mathbf{E}_0 \cdot \mathbf{U}_{1n}\right) d\omega$$
$$- \frac{e^3}{4i\hbar^3} \exp\left(2i\omega_0 t\right) \sum_n \int_0^\infty \frac{1 - \exp\left[i\left(\omega - \omega_1 - \omega_0\right)t\right]}{(\omega - \omega_1 - \omega_0)} \left(\mathbf{E}_0 \cdot \mathbf{U}_{1n}\right) \left(\mathbf{E}_0 \cdot \mathbf{U}_{1n}^*\right) d\omega$$
(22)

The second and third terms on the right-hand side of expression (22) are rapidly oscillating at a frequency of  $\omega_0$ , and they can be discarded by averaging over the fast oscillations. Then, we obtain

$$I_{ph} = \frac{e^3}{2\hbar^2} \int_0^\infty \frac{\sin\left[(\omega - \omega_1 - \omega_0)t\right]}{(\omega - \omega_1 - \omega_0)} \sum_n \left(\mathbf{E}_0 \cdot \mathbf{U}_{1n}^*\right) \left(\mathbf{E}_0 \cdot \mathbf{U}_{1n}\right) d\omega$$
(23)

Assuming that all of the orientations of the atom in space are equally probable and therefore the vector  $U_{1n}$  is statistically isotropic, one averages the current (23) overall possible orientations of the atom.

Then,

$$\overline{\left(\mathbf{E}_{0}\mathbf{U}_{1n}\right)\left(\mathbf{E}_{0}\mathbf{U}_{1n}^{*}\right)} = E_{0i}E_{0j}\overline{U_{1n,i}U_{1n,j}^{*}}$$
(24)

where the bar denotes averaging over all possible orientations and the indices *i* and *j* are the vector indexes.

For the isotropic vector  $\mathbf{U}_{1n}$ ,

$$\overline{U_{1n,i}U_{1n,j}^*} = \frac{1}{3}|\mathbf{U}_{1n}|^2\delta_{ij}$$
(25)

Then,

$$\overline{\left(\mathbf{E}_{0}\mathbf{U}_{1n}\right)\left(\mathbf{E}_{0}\mathbf{U}_{1n}^{*}\right)} = \frac{1}{3}|\mathbf{E}_{0}|^{2}|\mathbf{U}_{1n}|^{2}$$
(26)

Accordingly, for the mean photoelectric current (23), we obtain

$$\overline{I_{ph}} = \beta |\mathbf{E}_0|^2 \tag{27}$$

where the parameter

$$\beta = \frac{e^3}{6\hbar^2} \int_0^\infty \frac{\sin\left[(\omega - \omega_1 - \omega_0)t\right]}{(\omega - \omega_1 - \omega_0)} \sum_n |\mathbf{U}_{1n}(\omega)|^2 d\omega$$
(28)

does not depend on the incident light intensity  $|\mathbf{E}_0|^2$  and instead, the parameter  $\beta$  depends on the frequency  $\omega_0$  of the incident light.

Thus, we have obtained the first law of the photoelectric effect without using the photon hypothesis within the framework of only classical field theory while considering the electromagnetic and electron waves as classical fields.

Let us consider the dependence of the parameter  $\beta$  on the frequency of the incident light  $\omega_0$ .

Let us denote

$$F(\omega) = \sum_{n} |\mathbf{U}_{1n}(\omega)|^2$$
(29)

$$x = \omega - \omega_1 - \omega_0 \tag{30}$$

Then, we obtain

$$\beta = \frac{e^3}{6\hbar^2} \int_{|\omega_1| - \omega_0}^{\infty} \frac{\sin(xt)}{x} F(x - |\omega_1| + \omega_0) \, dx \tag{31}$$

Here, we account for the fact that  $\omega_1 < 0$ .

The function  $\frac{\sin(xt)}{x}$  has a sharp peak in the vicinity of x = 0 and has a width of  $\Delta x \sim \pi/t$ , and at  $t \to \infty$ , it behaves similar to a delta-function:  $\int_{-\infty}^{\infty} \frac{\sin(xt)}{x} dx = \pi$ . The function  $F(\omega)$  in the vicinity of x = 0 is smooth and varies weakly on the interval  $\Delta x \sim \pi/t$ .

Therefore, with reasonable accuracy at  $\omega_0 < |\omega_1| - \frac{\pi}{2t}$ , we can write

$$\beta \approx \frac{e^3}{6\hbar^2} F(0) \int_{|\omega_1| - \omega_0}^{\infty} \frac{\sin(xt)}{x} dx$$
(32)

At the same time, at  $\omega_0 - |\omega_1| \gg \frac{\pi}{2t}$ , it is necessary to account for the fact that a small neighbourhood of the point x = 0 will make the main contribution to the integral in (31) (due to the delta-like behaviour of the integrand). As a result, for  $\omega_0 - |\omega_1| \gg \frac{\pi}{2t}$ , we obtain

$$\beta \approx \frac{\pi e^3}{6\hbar^2} F\left(\omega_0 - |\omega_1|\right) \tag{33}$$

In this case, the parameter  $\beta$  will vary with the frequency of the incident light  $\omega_0$ .

Figure 1 shows, in a nondimensional form, the dependence of the parameter  $\beta$  on the frequency difference  $\omega_0 - |\omega_1|$  in the vicinity of the frequency  $\omega_0 = |\omega_1|$ .

We can see that the parameter  $\beta$  is virtually zero at  $\omega_0 < |\omega_1| - \frac{\pi}{2t}$ , and it almost linearly varies from zero to  $\frac{\pi e^3}{6\hbar^2}F(0)$  when  $\omega_0$  changes in the range from  $|\omega_1| - \frac{\pi}{2t}$  to  $|\omega_1| + \frac{\pi}{2t}$ , and it virtually equals the value in (33) at  $\omega_0 > |\omega_1| + \frac{\pi}{2t}$ . The width of the frequency range in which there is a noticeable change in the parameter  $\beta$  is  $\Delta \omega_0 \sim \pi/t$ .

Assuming  $|\omega_1| \sim 10^{14}$  rad/s (which corresponds to visible light) for the observation time  $t > 10^{-9}$  s, we obtain  $\Delta \omega_0 < 3 \cdot 10^9$  rad/s, which is significantly less than  $|\omega_1|$ :


Fig. 1 The dependence of the parameter  $\beta$  on the frequency difference  $\omega_0 - |\omega_1|$  in the vicinity of the frequency  $\omega_0 = |\omega_1|$ 

$$\Delta\omega_0 \ll |\omega_1| \tag{34}$$

From this analysis, it follows that for the actual duration of the observation, the parameter  $\beta$  will have almost a threshold dependence on the frequency of the incident light  $\omega_0$ : for  $\omega_0 < |\omega_1|$ , we obtain  $\beta \approx 0$ , and the photoelectric current is almost absent, while at  $\omega_0 > |\omega_1|$ , the parameter  $\beta$  will take the value in (33), and the photoelectric current (27) will be proportional to the intensity of the incident light.

Thus, we have obtained the third law of the photoelectric effect also without using the photon hypothesis, within only the framework of classical field theory.

Let us now consider the second law of the photoelectric effect. In its conventional form, it establishes the dependence of the kinetic energy of the emitted photoelectrons on the frequency and intensity of the incident radiation. However, in the experiments on the photoelectric effect, the kinetic energy of the photoelectron is not measured directly; it is determined indirectly through the measured stopping potential. Therefore, such wording of the second law of the photoelectric effect already contains some interpretation of the experimental facts; in particular, it assumes that the electrons are indivisible particles that, at the time of escape from the atom, have a definite kinetic energy. In this case, the kinetic energy of the photoelectrons can be determined through the stopping potential at which the photoelectric current is terminated. Because in the papers of this series we doubt that electrons are particles, it does not make sense to talk about the kinetic energy of the electrons, and we will need a different formulation of the second law of the photoelectric effect.

To rule out any interpretation of the experimental data, the wording of the second law of the photoelectric effect (and in general, of any laws) should use only measured parameters. From this perspective, an *objective formulation of the second law of the photoelectric effect* will be as follows: the stopping potential varies linearly with the frequency of the incident electromagnetic radiation and does not depend on the flux.

Let us consider the function in (17). The square of its modulus  $|C_n(\omega, t)|^2$  determines the density of the photoelectric current (18). This function reaches its maximum when

$$\omega_1 - \omega + \omega_0 = 0 \tag{35}$$

and for large *t*, the largest part of the photoelectric current falls on the narrow range of the frequencies of the electron wave that have the width

$$\Delta \omega \sim \pi/t \tag{36}$$

near the frequency

$$\omega = \omega_0 - |\omega_1| \tag{37}$$

When accounting for the smallness of the frequency range (36), it can be assumed that the electron wave that is emitted by an atom is almost monochromatic and has the frequency in (37), which linearly depends on the frequency of the incident light  $\omega_0$  and does not depend on its intensity.

Let us place on the path of the electron wave a decelerating potential. In this case, we come to the problem of propagation of the electron wave in the field of the decelerating potential, which is quite accurately described by the linear Schrödinger equation. At large distances from the atom, the electron wave can be considered to be approximately flat. To simplify the analysis, instead of the decelerating potential, having a linear dependence on the coordinates along which the electron wave propagates, let us consider the potential step (barrier) of the same "height"  $U_0$  and the same width L to be the actual decelerating potential. The solution of the Schrödinger equation for the potential step is well known [28]: at  $\hbar \omega > U_0$ , the electron wave passes through a potential step and is partially reflected from it, while when  $\hbar \omega < U_0$ , the electron wave is mainly reflected from the potential step, although a small part goes through the potential step due to tunnelling. The transmission coefficient of the electron wave for the potential step (in our interpretation, this coefficient is the ratio of the electric current of the electron wave behind the potential step to the electric current of the electron wave arriving to the potential steps from an atom) in the limiting case  $\hbar \omega = U_0$  is defined by the expression [28]

$$D = \left(1 + \frac{2m_e\omega L^2}{4\hbar}\right)^{-1} \tag{38}$$

Here, instead of the energy of a non-relativistic quantum particle, we use a Schrödinger frequency  $\omega$  (which is equal to the difference between the true frequency of the electron wave that is entered into the solution of the Dirac equation and its "rest frequency"  $\omega_e = mc^2/\hbar$  [23]). With the increase in the width of the potential step *L*, the transmission coefficient (38) decreases rapidly, and for an actual decelerating potential that has macroscopic sizes that substantially exceed the de Broglie wavelength  $\lambda_{dB} = 2\pi \sqrt{\frac{\hbar}{2m_e \omega}}$ , it is almost equal to zero because, in this case, we can neglect the tunnelling.

Thus, for the macroscopic decelerating potentials that are used in the experiments, there is a threshold effect: when  $\hbar \omega > U_0$ , the electron wave passes through the decelerating potential, while when  $\hbar \omega \leq U_0$ , the electron wave is fully "reflected" by the decelerating potential and the photoelectric current is not observed behind it. This arrangement means that there is a limit to the value of the decelerating potential, which is the stopping potential

$$U_s = \hbar \omega \tag{39}$$

above which the photoelectric current is absent.

When accounting for expression (37), we obtain

$$U_s = \hbar \omega_0 - \hbar \left| \omega_1 \right| \tag{40}$$

This result completely coincides with the above given formulation of the second law of the photoelectric effect, and it was obtained within the framework of classical field theory without the use of such concepts as photons and electrons.

Note that expression (40) can be formally written in the form

$$\hbar\omega_0 = E + A \tag{41}$$

where the notations  $A = \hbar |\omega_1|$  and  $E = U_s$  were introduced. The expression in (41) can be considered to be Einstein's equation for the photoelectric effect, and one can interpret it within the framework of the photon-electron representations in which the parameter *E* is interpreted as the kinetic energy of the photoelectrons, while the parameter *A* is interpreted as a work function of the atom. However, this approach is no more than an interpretation that is based on the formal similarity of the pure wave expression (40) and the mechanical law of energy conservation.

The above analysis has shown that such a corpuscular interpretation of the photoelectric effect is superfluous.

The well-known experiments by Meyer and Gerlach on the photoelectric effect on the particles of metal dust, irradiated with ultraviolet light, are considered to be one of the pieces of "irrefutable evidence" that light energy is propagated in the form of identical indivisible quanta (photons). Assuming that the electrons are particles while light is composed of continuous classical electromagnetic waves, we can calculate the time during which the metal particle will absorb a sufficient amount of energy for the ejection of an electron. In the experiments by E. Meyer and W. Gerlach, this duration was of the order of a few seconds, which means that the photoelectron cannot leave a speck of dust earlier than in a few seconds after the start of irradiation. In contrast to this conclusion, the photoelectric current in these experiments began immediately after the beginning of the irradiation. Hence, it is usually concluded that this finding is only possible if the light is a flux of photons each of which can be absorbed by the atom only entirely and, therefore, can "knock out" the electron from the atoms at the moment of its collision with the metal particle.

However, this conclusion follows only in the case in which the electrons are considered to be indivisible particles. If instead of considering the electrons to be particles we consider a continuous electron wave [23, 24], then as was shown above, the photoelectric current appears almost without delay after the start of irradiation of an atom by the classical electromagnetic wave and occurs even at very low light intensities, when the light frequency exceeds the threshold frequency for the given atom. This finding is because to start the photoelectric current, the atom does not need to accumulate the energy that is equal to the ionization potential because the electron wave is emitted by the atom continuously and not in the form of discrete electrons from an atom under the action of light led A. Einstein to the idea of light quanta, which when absorbed, gave to the atom sufficient energy for the liberation of a whole electron.

The above analysis shows that all three laws of the photoelectric effect only approximately reflect its actual regularities. In particular, the photoelectric current appears and disappears non-abruptly when "passing" through the threshold frequency  $|\omega_1|$ , and it gradually increases or decreases in the frequency range that has the width  $\Delta \omega_0 \sim \pi/t$  near the threshold frequency  $|\omega_1|$ . However, this effect can be detected only for ultrashort observation times of  $t \sim 10^{-15}$  s, which is difficult to achieve in the experiments on the photoelectric effect. Moreover, consideration of the nonlinear effects in the interaction of the light wave with an atom shows [29] that the photoelectric current appears even in the case when the frequency of the incident light is significantly less than the threshold frequency  $|\omega_1|$ , which is predicted by the linear theory. Such effects can be observed only in a very intense laser field [30]. Strictly speaking, the theory [29], which describes the ionization of an atom in an intense laser field, is fully classical in the sense under consideration because an atom is described by the Schrödinger equation, while the light wave is considered to be a classical electromagnetic field. The true result of this finding is the photoelectric current that is created by the continuous electron wave emitted by an atom because precisely the photoelectric current is calculated in the theory [29]. However, traditionally, the results of the theory [29] are interpreted from the standpoint of photon-electron representations, which make it necessary to interpret the main result of the theory [29] as the probability of the ionization of an atom (i.e. the probability of the liberation of an "electron" from the atom) per unit time. The representations with respect to the multiphoton ionization of an atom, when the atom "absorbs simultaneously several photons", the total energy of which exceeds the ionization potential of the atom, were a consequence of such an interpretation. When there is a requirement for too many "photons" for the liberation of the "electron", talking about the simultaneous absorption of such a large number of particles becomes meaningless (because of the low probability of this process); then, the results of the theory [29] are interpreted as a tunnel ionization in which the intense laser field changes the potential field in which the "electron" is positioned, which gives it the "opportunity" to leave the atom due to tunnelling. From the point of view of the ideas that are developed in this series of papers, both "multiphoton" and "tunnel" ionization of an atom are the result of the same process—the interaction of a classical electromagnetic wave with a classical electron wave.

Finally, note that there is no difficulty in calculating the angular distribution of the photoelectric current in the framework of the theory under consideration, if we account for the fact that the continuous electric current created by the electron wave emitted by an atom under the action of light is calculated by expression (18) using the wave function in (3) and (17). Once again, note that this current is not the distribution over the directions of the particles-electrons that are emitted by an atom but the distribution over the directions of the current of a continuous charged electron wave that is emitted by the atom. All of the known expressions that are obtained earlier for the photoelectric effect (see, e.g. [4, 31]) remain valid, but they should now be interpreted from the standpoint of classical field theory.

#### **3** Concluding Remarks

Thus, we see that the light-atom interaction including the photoelectric effect is fully described within the framework of classical field theory without the use of quantum electrodynamics and, in general, without any quantization. The results of this theory utilize the simple classical sense and do not require the postulation of such paradoxical properties of matter as the wave-particle duality. The paradoxes in the theory appear when a continuous light beam or a continuous charged electron wave emitted by the atoms under the influence of incident light is attempted to be interpreted as the flux of indivisible particles—photons or electrons. In this case, the probabilistic interpretation of the results of the theory arises from a need. However, as was shown in this paper and in the previous papers of this series [23–26], the processes that are under consideration are fully deterministic, while the postulate about the probabilistic nature of all quantum phenomena is the result of misinterpretation.

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# **Classification Problem in a Quantum Framework**



**Enrica Santucci and Giuseppe Sergioli** 

## 1 Introduction

In recent years there has been an increasing interest toward the use of the quantum mechanical formalism in non-microscopic contexts. The idea is that the powerful predictive properties of quantum mechanics, used for describing the behavior of microscopic phenomena, turn out to be particularly beneficial also in non-microscopic domains. At this purpose, several nonstandard applications involving the formalism of quantum theory have been proposed in research fields, such as game theory [7, 16], economics [10], cognitive sciences [1, 2], signal processing [8], and so on. Further, particular applications, interesting for the specific topics of the present paper, concern the areas of machine learning and pattern recognition. About this, some attempts which connect quantum information to pattern recognition can be found in [18], while an exhaustive survey and bibliography of the developments concerning the use of quantum computing techniques in artificial intelligence are provided in [14, 26].

In pattern recognition area, one of the main aspects is focused on the application of quantum information processing methods to solve classification and clustering problems [4, 23].

The use of quantum states for representing patterns has a twofold motivation: firstly, it gives the possibility of exploiting quantum algorithms to boost the computational efficiency of the classification process [25]. Secondly, it is possible to use quantum-inspired models in order to reach some benefit with respect to classical problems [22].

E. Santucci (🖂) · G. Sergioli

University of Cagliari, Cagliari, Italy

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Even if the state-of-art approaches suggest possible computational advantages of this sort [3, 12, 13], the main problem to find a *more convenient* encoding from classical to quantum object is nowadays an open and interesting matter of debate [14, 18]. In this context, our contribution consists in constructing a quantum-inspired version of a classical classifier in order to reach some convenience, in terms of the error in pattern classification, with respect to the corresponding classical model. We have already proposed this kind of approach in two previous works [19, 20], where a "quantum counterpart" of a well-known minimum-distance classifier, called *Nearest Mean Classifier* (NMC), has been introduced.

In both cases, the model is based on the introduction of two main ingredients: first, an appropriate encoding of arbitrary patterns into density operators, and, second, a distance measure between density operators, representing the quantum counterpart of the Euclidean distance in the "classical" NMC. The main differences between the two previous works are as follows: (1) in the first case [20], we tested our quantum classifier on two-dimensional datasets, and we proposed a generalization to arbitrary dimension from a theoretical point of view only; (2) in the second case [19], a new encoding for arbitrary *n*-dimensional patterns into quantum states has been proposed, and it was tested on different real-world and artificial datasets. Anyway, in both cases, we have observed a significant improvement of the accuracy in the classification process. In addition, we found that, by using the encoding proposed in [19] and for two-dimensional problems only, the classification accuracy of our quantum classifier can be further improved, by performing a uniform rescaling of the original dataset.

In this work we propose a new encoding of arbitrary *n*-dimensional patterns into quantum objects, which preserves information about the norm of the original pattern. This idea has been inspired by recent debates on quantum machine learning [18], according to which it is crucial to avoid loss of information when a particular encoding of real vectors into quantum states is considered. Such an approach turns out to be very promising in terms of classification performances with respect to the classifier version of the NMC. Further, differently from the NMC, our quantum classifier is invariant under uniform rescaling. More precisely, the accuracy of the quantum classifier changes by rescaling (of an arbitrary real number) the coordinates of the dataset. Consequently, we have observed that, for several datasets, the new encoding exhibits a further advantage that can be gained by exploiting the non-invariance under rescaling, also for *n*-dimensional problems (conversely to the previous works). At this purpose, some experimental results have been presented.

The paper is organized as follows: in Sect. 2 we briefly describe the classification process and, in particular, the formal structure of the NMC. Section 3 is devoted to the definition of a new encoding of real patterns into quantum states. In Sect. 4 we introduce the quantum version of the NMC, called *Quantum Nearest Mean Classifier* (QNMC) based on the new encoding previously described. In Sect. 5 we compare the NMC and the QNMC on different datasets showing that, in general, the QNMC exhibits better performances (in terms of accuracy and other significant statistical quantities) with respect to the NMC. Further, starting from the fact that, differently from the NMC, the QNMC is not invariant under rescaling, we also show

that, for some dataset, it is possible to provide a benefit from this non-invariance property. Some conclusions and possible further developments are proposed at the end of the paper.

#### 2 On the Classification Process

Here, we address the classification problem, which is an instance of supervised learning, i.e., learning from a training set of correctly labeled objects. More precisely, each object can be characterized by its features; hence, a d-feature object can be naturally represented by a d-dimensional real vector, i.e.,  $\mathbf{x}$  =  $[x^{(1)}, \ldots, x^{(d)}] \in \mathscr{X}$ , where  $\mathscr{X} \subseteq \mathbb{R}^d$  is generally a subset of the d-dimensional real space representing the *feature space*. Hence, any arbitrary object is represented by a vector **x** associated to a given class of objects (but, in principle, we do not know which one). Let  $\mathscr{Y} = \{1, \ldots, L\}$  be the class label set. A *pattern* is represented by a pair (x, y), where x is the *feature vector* representing an object and  $y \in \mathscr{Y}$  is the *label* of the class which  $\mathbf{x}$  is associated to. The aim of the classification process is to design a function (*classifier*) that attributes (in the most accurate way) to any unlabeled object the corresponding label (where the label attached to an object represents the class which the object belongs to), by learning about the set of objects whose class is known. The *training set* is given by  $\mathscr{S}_{tr} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$ , where  $\mathbf{x}_n \in \mathscr{X}, y_n \in \mathscr{Y}$  (for n = 1, ..., N) and N is the number of patterns belonging to  $\mathscr{S}_{tr}$ . Finally, let  $N_l$  be the cardinality of the training set associated to the *l*-th class (for l = 1, 2, ..., L) such that  $\sum_{l=1}^{L} N_l = N$ .

We now introduce the well-known *Nearest Mean Classifier* (NMC) [6], which is a particular kind of minimum-distance classifier widely used in pattern recognition. The strategy consists in computing the distances between an object  $\mathbf{x}$  (to classify) and patterns chosen as prototypes of each class (called *centroids*). Finally, the classifier associates to  $\mathbf{x}$  the label of the closest centroid. So, we can resume the NMC algorithm as follows:

1. the computation of the *centroid* (i.e., the sample mean [11]) associated to each class, whose corresponding feature vector is given by

$$\boldsymbol{\mu}_{l} = \frac{1}{N_{l}} \sum_{n=1}^{N_{l}} \mathbf{x}_{n}, \quad l = 1, 2, \dots, L,$$
 (1)

where *l* is the label of the class;

2. the classification of the object  $\mathbf{x}$ , provided by

$$\operatorname{argmin}_{l=1,\dots,L} d_E(\mathbf{x}, \boldsymbol{\mu}_l), \quad \text{with} \quad d_E(\mathbf{x}, \boldsymbol{\mu}_l) = \|\mathbf{x} - \boldsymbol{\mu}_l\|$$
(2)

where  $d_E$  is the standard Euclidean distance.<sup>1</sup>

Depending on the particular distribution of the dataset patterns, it is possible that a pattern belonging to a given class is closest to the centroid of another class. In this case, if the algorithm would be applied to this pattern, it would fail. Hence, for an arbitrary object  $\mathbf{x}$ , whose class is a priori unknown, the output of the above classification process has the following four possibilities [9]: (1) true positive (TP), pattern belonging to the *l*-th class and correctly classified as *l*; (2) true negative (TN), pattern belonging to a class different than l and correctly classified as not l; (3) false positive (FP), pattern belonging to a class different than l and incorrectly classified as l; and (4) false negative (FN), pattern belonging to the l-th class and incorrectly classified as not *l*.

In order to evaluate the performance of a certain classification algorithm, the standard procedure consists in dividing the original labeled dataset  $\mathscr{S}$  of N' patterns, into a training set  $\mathscr{S}_{tr}$  of N patterns and a set  $\mathscr{S}_{ts}$  of (N' - N) patterns (i.e.,  $\mathscr{S} = \mathscr{S}_{tr} \cup \mathscr{S}_{ts}$ ). This set  $\mathscr{S}_{ts}$  of patterns is called *test set* [6], and it is defined as  $\mathscr{S}_{ts} = \{(\mathbf{x}_n, y_n)\}_{n=N+1}^{N'}$ .

Then, by applying the NMC to the test set, it is possible to evaluate the classification algorithm performance by considering the following statistical measures associated to each class *l* depending on the quantities listed above:

- True Positive Rate (TPR): TPR = TP/(TP+FN);
  True Negative Rate (TNR): TNR = TN/(TN+FP);
  False Positive Rate (FPR): FPR = FP/(FP+TN) = 1 TPN;
  False Negative Rate (FNR): FNR = FN/(FN+TP) = 1 TPR.

Further, other standard statistical coefficients [9] used to establish the reliability of a classification algorithm are:

- Classification error (E):  $E = 1 \frac{TP}{N'-N}$ ;
- Precision (P):  $P = \frac{TP}{TP+FP}$ ; Cohen's Kappa (K):  $K = \frac{Pr(a) Pr(e)}{1 Pr(e)}$ , where  $Pr(a) = \frac{TP+TN}{N'-N}$ ,  $Pr(e) = \frac{(TP+FP)(TP+FN) + (FP+TN)(TN+FN)}{(N'-N)^2}$ .

In particular, the classification error represents the percentage of misclassified patterns, the precision is a measure of the statistical variability of the considered model, and the Cohen's kappa represents the degree of reliability and accuracy of a statistical classification, and it can assume values ranging from -1 to +1(K = +1 corresponds to a perfect classification procedure, while K = -1corresponds to a completely wrong classification). Let us note that these statistical

<sup>&</sup>lt;sup>1</sup>We remind that, given a function  $f: X \to Y$ , the *argmin* (i.e., the argument of the minimum) over some subset S of X is defined as:  $\operatorname{argmin}_{x \in S \subset X} f(x) = \{x | x \in S \land \forall y \in S : f(y) \ge f(x)\}.$ In this framework, the argmin plays the role of the classifier, i.e., a function that associates to any unlabeled object the correspondent label.

coefficients have to be computed for each class. Then, the final value of each statistical coefficient related to the classification algorithm is the weighted sum of the statistical coefficients of each class.

#### **3** Correspondence Between Pattern and Density Operator

In order to introduce a quantum version of the NMC, the first step is to find an appropriate quantum encoding for a real pattern.

Generally, given a *d*-dimensional feature vector, there exist different ways to encode it into a density operator [18]. In [20], the proposed encoding was based on the use of the stereographic projection [5]. In particular, it allows to unequivocally map any point  $r = (r_1, r_2, r_3)$  on the surface of a radius-one sphere  $\mathbb{S}^2$  (except for the north pole) onto an arbitrary point  $\mathbf{x} = [x^{(1)}, x^{(2)}]$  in  $\mathbb{R}^2$ , i.e.,

$$SP: (r_1, r_2, r_3) \mapsto \left(\frac{r_1}{1 - r_3}, \frac{r_2}{1 - r_3}\right).$$
 (3)

The inverse of the stereographic projection is given by

$$SP^{-1}: [x^{(1)}, x^{(2)}] \mapsto \left[\frac{2x^{(1)}}{||\mathbf{x}||^2 + 1}, \frac{2x^{(2)}}{||\mathbf{x}||^2 + 1}, \frac{||\mathbf{x}||^2 - 1}{||\mathbf{x}||^2 + 1}\right],\tag{4}$$

where  $||\mathbf{x}||^2 = [x^{(1)}]^2 + [x^{(2)}]^2$ . Then, by imposing that  $r_1 = \frac{2x^{(1)}}{||\mathbf{x}||^2+1}$ ,  $r_2 = \frac{2x^{(2)}}{||\mathbf{x}||^2+1}$ ,  $r_3 = \frac{||\mathbf{x}||^2-1}{||\mathbf{x}||^2+1}$ , if we consider  $r_1, r_2, r_3$  as Pauli components<sup>2</sup> of a density operator  $\rho_{\mathbf{x}} \in \mathbb{C}^2$ , the density operator associated to the pattern  $\mathbf{x} = [x^{(1)}, x^{(2)}]$  can be written as

$$\frac{1}{2} \begin{pmatrix} 1+r_3 & r_1 - ir_2 \\ r_1 + ir_2 & 1 - r_3 \end{pmatrix} = \frac{1}{||\mathbf{x}||^2 + 1} \begin{pmatrix} ||\mathbf{x}||^2 & x^{(1)} - ix^{(2)} \\ x^{(1)} + ix^{(2)} & 1 \end{pmatrix}.$$
 (5)

The advantage in using this encoding consists in the fact that it provides an easy visualization of an arbitrary two-feature vector on the Bloch sphere [20]. However, the main problem concerns the generalization of this encoding to *d*-feature vectors with d > 2. Although in [20] a generalization to the *d*-feature case was introduced, it exhibits some difficulties to be implemented for general cases.

 $<sup>^{2}</sup>$ We consider the representation of an arbitrary density operator as linear combination of Pauli matrices.

An alternative encoding of a *d*-feature vector  $\mathbf{x} = [x^{(1)}, \dots, x^{(d)}]$  into a density operator was proposed in [19]. It is obtained (1) by mapping  $\mathbf{x} \in \mathbb{R}^d$  into a (d + 1)-dimensional vector  $\mathbf{x}' \in \mathbb{R}^{d+1}$  according to the generalized version of Eq. (4), i.e.,

$$\mathbf{x}' = SP^{-1}(\mathbf{x}) = \frac{1}{||\mathbf{x}||^2 + 1} \left[ 2x^{(1)}, \dots, 2x^{(d)}, ||\mathbf{x}||^2 - 1 \right]$$
(6)

where  $||\mathbf{x}||^2 = \sum_{i=1}^{d} [x^{(i)}]^2$  and then (2) by considering the projector  $\rho_{\mathbf{x}} = \mathbf{x}' \cdot (\mathbf{x}')^T$ .

In this work we propose a different version of the QNMC based on a new encoding again, and we show that this exhibits interesting improvements mostly by exploiting the non-invariance under rescaling of the features.

Accordingly with [12, 17, 18], when a real vector is encoded into a quantum state, in order to avoid a loss of information, it is important that the quantum state keeps some information about the norm of the original real vector. In light of this fact, we introduce the following alternative encoding.

Let  $\mathbf{x} = [x^{(1)}, \dots, x^{(d)}] \in \mathbb{R}^d$  be an arbitrary *d*-feature vector.

1. We map the vector  $\mathbf{x} \in \mathbb{R}^d$  into a vector  $\mathbf{x}' \in \mathbb{R}^{d+1}$ , whose first *d* features are the components of the vector  $\mathbf{x}$  and the (d+1)-th feature is the norm of  $\mathbf{x}$ . Formally:

$$\mathbf{x} = [x^{(1)}, \dots, x^{(d)}] \mapsto \mathbf{x}' = [x^{(1)}, \dots, x^{(d)}, ||\mathbf{x}||].$$
(7)

2. Finally, we obtain the vector **x**' by dividing the first *d* components of the vector **x**' for ||**x**||:

$$\mathbf{x}' \mapsto \mathbf{x}'' = \left[\frac{x^{(1)}}{||\mathbf{x}||}, \dots, \frac{x^{(d)}}{||\mathbf{x}||}, ||\mathbf{x}||\right].$$
 (8)

3. We consider the norm of the vector  $\mathbf{x}''$ , i.e.,  $||\mathbf{x}''|| = \sqrt{||\mathbf{x}||^2 + 1}$  and we map the vector  $\mathbf{x}''$  into the normalized vector  $\mathbf{x}'''$  as follows:

$$\mathbf{x}'' \mapsto \mathbf{x}''' = \frac{\mathbf{x}''}{||\mathbf{x}''||} = \left[\frac{x^{(1)}}{||\mathbf{x}||\sqrt{||\mathbf{x}||^2 + 1}}, \dots, \frac{x^{(d)}}{||\mathbf{x}||\sqrt{||\mathbf{x}||^2 + 1}}, \frac{||\mathbf{x}||}{\sqrt{||\mathbf{x}||^2 + 1}}\right].$$
(9)

Now, we provide the following definition.

#### **Definition 1 (Density Pattern)**

Let  $\mathbf{x} = [x^{(1)}, \dots, x^{(d)}]$  be an arbitrary *d*-feature vector and  $(\mathbf{x}, y)$  the corresponding pattern. Then, the *density pattern* associated to  $(\mathbf{x}, y)$  is represented by the pair  $(\rho_{\mathbf{x}}, y)$ , where the matrix  $\rho_{\mathbf{x}}$ , corresponding to the feature vector  $\mathbf{x}$ , is defined as

$$\rho_{\mathbf{x}} \doteq \mathbf{x}^{\prime\prime\prime} \cdot (\mathbf{x}^{\prime\prime\prime})^{\dagger}, \tag{10}$$

where the vector  $\mathbf{x}'''$  is defined according to Eq. (9) and y is the label of the original pattern.

Hence, this encoding maps real *d*-dimensional vectors **x** into (d + 1)-dimensional pure states  $\rho_{\mathbf{x}}$ . In this way, we obtain an encoding that takes into account the information about the initial real vector norm and, at the same time, allows to easily encode also arbitrary real *d*-dimensional vectors.

#### 4 Quantum Classification

In this section we introduce a quantum-inspired version of the NMC, named *Quantum Nearest Mean Classifier* (QNMC). It can be seen as a particular kind of minimum-distance classifier between quantum objects (i.e., density patterns). The use of this new formalism could lead not only to achieve the well-known advantages related to the quantum computation with respect to the classical one (mostly related to the speedup of the computational process) but also to make a full comparison between NMC and QNMC performance by using a classical computer only.

In order to provide a quantum counterpart of the NMC, we need (1) an encoding from real patterns to quantum objects (already defined in the previous section), (2) a quantum counterpart of the classical centroid (i.e., a sort of class quantum prototype) that will be named *quantum centroid*, and (3) a suitable definition of *quantum distance* between density patterns that plays the same role as the Euclidean distance for the NMC. In this quantum framework, the quantum version  $\mathscr{S}^q$  of the dataset  $\mathscr{S}$  is given by

$$\mathscr{S}^q = \mathscr{S}^q_{\mathrm{tr}} \cup \mathscr{S}^q_{\mathrm{ts}}, \quad \mathscr{S}^q_{\mathrm{tr}} = \{(\rho_{\mathbf{x}_n}, y_n)\}_{n=1}^N, \quad \mathscr{S}^q_{\mathrm{ts}} = \{(\rho_{\mathbf{x}_n}, y_n)\}_{n=N+1}^{N'},$$

where  $(\rho_{\mathbf{x}_n}, y_n)$  is the density pattern associated to the pattern  $(\mathbf{x}_n, y_n)$ . Consequently,  $\mathscr{S}_{tr}^q$  and  $\mathscr{S}_{ts}^q$  represent the quantum versions of training and test set, respectively, i.e., the sets of all the density patterns obtained by encoding all the elements of  $\mathscr{S}_{tr}$  and  $\mathscr{S}_{ts}$ . Now, we naturally introduce the quantum version of the classical centroid  $\boldsymbol{\mu}_l$ , given in Eq. (1), as follows.

**Definition 2 (Quantum Centroid)** Let  $\mathscr{S}^q$  be a labeled dataset of N' density patterns such that  $\mathscr{S}^q_{tr} \subseteq \mathscr{S}^q$  is a training set composed of N density patterns. Further, let  $\mathscr{Y} = \{1, 2, ..., L\}$  be the class label set. The *quantum centroid* of the *l*-th class is given by

$$\rho_l = \frac{1}{N_l} \sum_{n=1}^{N_l} \rho_{\mathbf{x}_n}, \quad l = 1, \dots, L$$
(11)

where  $N_l$  is the number of density patterns of the *l*-th class belonging to  $\mathscr{S}_{tr}^q$ , such that  $\sum_{l=1}^{L} N_l = N$ .

Notice that the quantum centroids are generally mixed states, and they are not obtained by encoding the classical centroids  $\mu_l$ , i.e.,

$$\rho_l \neq \rho_{\boldsymbol{\mu}_l}, \ \forall l \in \{1, \dots, L\}.$$

Accordingly, the definition of the quantum centroid leads to a new object that is no longer a pure state and does not have any classical counterpart. This is the main reason that establishes, even in a fundamental level, the difference between NMC and QNMC. In particular, it is easy to verify [20] that, unlike the classical case, the expression of the quantum centroid is sensitive to the dataset dispersion.

In order to consider a suitable definition of distance between density patterns, we recall the well-known definition of trace distance between quantum states (see, *e.g.*, [15]).

**Definition 3 (Trace Distance)** Let  $\rho$  and  $\rho'$  be two quantum density operators belonging to the same dimensional Hilbert space. The *trace distance* between them is given by

$$d_T(\rho, \rho') = \frac{1}{2} \operatorname{Tr} |\rho - \rho'|,$$
 (13)

where  $|A| = \sqrt{A^{\dagger}A}$ .

Notice that the trace distance is a true metric for density operators, that is, it satisfies (1)  $d_T(\rho, \rho') \ge 0$  with equality iff  $\rho = \rho'$  (*positivity*), (2)  $d_T(\rho, \rho') = d_T(\rho', \rho)$  (*symmetry*), and (3)  $d_T(\rho, \rho') + d_T(\rho', \rho'') \ge d_T(\rho, \rho'')$  (*triangle inequality*).

We have introduced all the ingredients we need to describe the QNMC process that, similarly to the classical case, consists in the following steps:

- constructing the quantum training and test sets  $\mathscr{S}_{tr}^q$ ,  $\mathscr{S}_{ts}^q$  by applying the encoding introduced in Definition 1 to each pattern of the classical training and test sets  $\mathscr{S}_{tr}$ ,  $\mathscr{S}_{ts}$ ;
- calculating the quantum centroids  $\rho_l \ (\forall l \in \{1, ..., L\})$ , by using the quantum training set  $\mathscr{S}_{tt}^q$ , according to Definition 2;
- classifying an arbitrary density pattern  $\rho_{\mathbf{x}} \in S_{ts}^q$  accordingly with the following minimization problem

$$\underset{l=1,\dots,L}{\operatorname{argmin}} d_T(\rho_{\mathbf{x}}, \rho_l), \tag{14}$$

where  $d_T$  is the Trace distance introduced in Definition 3.

#### **5** Experimental Results

This section is devoted to show a comparison between the NMC and the QNMC performances in terms of the statistical coefficients introduced in Sect. 2. We use both classifiers to analyze 14 datasets. In particular, two different kinds of datasets have been studied: five of them (*Gaussian (I), Gaussian (II), Gaussian (III), Moon,* 

*Banana*) are artificial datasets, while the others (*Balance, Bands, Breast Cancer (I), Breast Cancer (II), Ilpd, Ionosphere, Liver, Pima, Tic Tac*) are real-world datasets, extracted from the UCI repository,<sup>3</sup> which follow unknown distributions. Let us note that, in real situations, we usually deal with data whose distribution is unknown, then the most interesting case is the one in which we use real-world datasets. However, the use of artificial datasets following known distribution, and in particular Gaussian distributions with specific parameters, can help to catch precious information, as we will see in the next section.

#### 5.1 Comparison Between QNMC and NMC

In Table 1 we summarize the characteristics of the datasets involved in our experiments. In particular, for each dataset, we list the total number of patterns, the number of patterns belonging to each class, and the number of features. Let us note that, although we mostly confine our investigation to two-class datasets, our model can be easily extended to multiclass problems (as we show for the three-class datasets *Balance* and *Gaussian (III)*).

In order to make our results statistically significant, we apply the standard procedure which consists in randomly splitting each dataset into two parts, the training set (representing the 80% of the original dataset) and the test set (representing the 20% of the original dataset). Finally, we perform ten experiments for each dataset, where the splitting is every time randomly taken.

In Table 2, we report QNMC and NMC performance for each dataset, evaluated in terms of mean value and standard deviation (computed on ten runs) of the statistical coefficients, discussed in the previous section. For the sake of simplicity, we omit the values of FPR and FNR because they can be easily obtained by TPR and TNR values (i.e., FPR = 1 - TNR, FNR = 1 - TPR).

We observe, by comparing QNMC and NMC performances (see Table 2), that the first provides a significant improvement with respect to the standard NMC in terms of all the statistical parameters we have considered. Further, the new encoding, for two-feature datasets, provides better performance than the one considered in [20] (where the QNMC error with related standard deviation was  $0.174\pm0.047$  for *Moon* and  $0.419\pm0.015$  for *Banana*), and it generally exhibits quite similar performance with respect to the one in [19] for multidimensional datasets, except in the case of *Breast Cancer (II)* and *Gaussian (I)* datasets, for which the new encoding provides a classification improvement of about 3% and 5%, respectively.

The artificial Gaussian datasets may deserve a brief comment. Let us discuss the way in which the three Gaussian datasets have been created. *Gaussian* (I) [21] is a perfectly balanced dataset (i.e., both classes have the same number of patterns); patterns have the same dispersion in both classes, and only some features

<sup>&</sup>lt;sup>3</sup>http://archive.ics.uci.edu/ml.

Data set	Instances	Features (d)
Balance	625 (49+288+288)	4
Banana	5300 (2376 + 2924)	2
Bands	365 (135 + 230)	19
Breast Cancer (I)	683 (444 + 239)	10
Breast Cancer (II)	699 (458 + 241)	9
Ilpd	583 (416+167)	9
Ionosphere	351 (225 + 126)	34
Liver	578 (413 + 165)	10
Moon	200 (100 + 100)	2
Pima	768 (500 + 268)	8
TicTac	958 (626 + 332)	9
Gaussian (I)	400 (200 + 200)	30
Gaussian (II)	1000 (100 + 900)	8
Gaussian (III)	2050 (50 + 500 + 1500)	8

Table 1Characteristics ofthe datasets used in ourexperiments

The number of instances in each class is shown between brackets

are correlated [24]. *Gaussian (II)* is an unbalanced dataset (i.e., classes have a very different number of patterns), patterns do not exhibit the same dispersion in both classes, and features are not correlated. *Gaussian (III)* is composed of three classes, and it is an unbalanced dataset with different pattern dispersion in all the classes, where all the features are correlated.

For these Gaussian datasets, the NMC is not the best classifier [6] because of the particular characteristics of the class dispersion. Indeed, the NMC does not take into account data dispersion. Conversely, by looking at Table 2, the improvements of the QNMC seem to exhibit some kind of sensitivity of the classifier with respect to the data dispersion. A detailed description of this problem will be addressed in a future work.

As a remark, it is important to remind that, even if it is possible to establish whether a classifier is "good" or "bad" for a given dataset by the evaluation of some a priori data characteristics, generally it is not possible to establish an absolute superiority of a given classifier for any dataset, according to the well-known *No Free Lunch Theorem* [6]. Anyway, the QNMC seems to be particularly convenient when the data distribution is difficult to treat with the standard NMC.

#### 5.2 Non-invariance Under Rescaling

The final experimental results that we present in this paper regard a significant difference between NMC and QNMC. Let us suppose that all the components of the feature vectors  $\mathbf{x}_n$  ( $\forall n = 1, ..., N'$ ) belonging to the original dataset  $\mathscr{S}$  are multiplied by the same parameter  $t \in \mathbb{R}$ , i.e.,  $\mathbf{x}_n \mapsto t\mathbf{x}_n$ . Then, the whole dataset

Dataset	E	TPR	TNR	Р	Κ
QNMC					
Balance	$0.148 \pm 0.018$	$0.852\pm0.018$	$0.915\pm0.014$	$0.862\pm0.022$	$0.767 \pm 0.029$
Banana	$0.316\pm0.017$	$0.684 \pm 0.017$	$0.660\pm0.017$	$0.684 \pm 0.018$	$0.350\pm0.034$
Bands	$0.394 \pm 0.053$	$0.606\pm0.053$	$0.528 \pm 0.071$	$0.606 \pm 0.058$	$0.133 \pm 0.112$
Breast Cancer (I)	$0.386 \pm 0.038$	$0.614 \pm 0.038$	$0.444 \pm 0.045$	$0.583 \pm 0.044$	$0.062\pm0.069$
Breast Cancer (II)	$0.040\pm0.015$	$0.946 \pm 0.023$	$0.986 \pm 0.016$	$0.993\pm0.009$	$0.912\pm0.033$
Ilpd	$0.351 \pm 0.037$	$0.649 \pm 0.037$	$0.705\pm0.056$	$0.734 \pm 0.041$	$0.292\pm0.073$
Ionosphere	$0.165\pm0.049$	$0.835\pm0.049$	$0.764 \pm 0.059$	$0.842\pm0.051$	$0.624\pm0.105$
Liver	$0.342\pm0.037$	$0.607\pm0.057$	$0.783 \pm 0.059$	$0.870\pm0.039$	$0.318 \pm 0.061$
Moon	$0.156 \pm 0.042$	$0.857\pm0.063$	$0.831 \pm 0.066$	$0.841 \pm 0.066$	$0.683\pm0.085$
Pima	$0.304 \pm 0.030$	$0.696 \pm 0.030$	$0.690 \pm 0.044$	$0.720\pm0.030$	$0.365\pm0.066$
Tic Tac	$0.410\pm0.032$	$0.590 \pm 0.032$	$0.597 \pm 0.039$	$0.629 \pm 0.036$	$0.172\pm0.061$
Gaussian (I)	$0.274 \pm 0.051$	$0.726 \pm 0.051$	$0.728 \pm 0.049$	$0.745\pm0.048$	$0.452\pm0.099$
Gaussian (II)	$0.210\pm0.025$	$0.790 \pm 0.025$	$0.744 \pm 0.061$	$0.900\pm0.019$	$0.308 \pm 0.058$
Gaussian (III)	$0.401\pm0.036$	$0.599 \pm 0.036$	$0.558 \pm 0.026$	$0.654 \pm 0.041$	$0152\pm0.043$
NMC					
Balance	$0.267\pm0.038$	$0.733 \pm 0.038$	$0.969 \pm 0.014$	$0.925\pm0.025$	$0.686\pm0.034$
Banana	$0.453\pm0.019$	$0.548 \pm 0.019$	$0.552\pm0.020$	$0.556 \pm 0.020$	$0.098 \pm 0.038$
Bands	$0.435\pm0.048$	$0.565\pm0.048$	$0.582\pm0.055$	$0.605\pm0.054$	$0.135\pm0.092$
Breast Cancer (I)	$0.442\pm0.037$	$0.558 \pm 0.037$	$0.464\pm0.046$	$0.551\pm0.039$	$0.022\pm0.076$
Breast Cancer (II)	$0.042\pm0.015$	$0.973\pm0.015$	$0.931\pm0.032$	$0.963\pm0.017$	$0.908\pm0.033$
Ilpd	$0.470\pm0.037$	$0.530 \pm 0.037$	$0.757\pm0.041$	$0.761 \pm 0.037$	$0.193\pm0.051$
Ionosphere	$0.323 \pm 0.051$	$0.677 \pm 0.051$	$0.676 \pm 0.051$	$0.680\pm0.051$	$0.351 \pm 0.102$
Liver	$0.472\pm0.048$	$0.388 \pm 0.057$	$0.891 \pm 0.055$	$0.905\pm0.045$	$0.193\pm0.060$
Moon	$0.234 \pm 0.065$	$0.772 \pm 0.089$	$0.762\pm0.085$	$0.771 \pm 0.091$	$0.528 \pm 0.130$
Pima	$0.375\pm0.033$	$0.625\pm0.033$	$0.546 \pm 0.045$	$0.622\pm0.037$	$0.173 \pm 0.075$
Tic Tac	$0.439 \pm 0.031$	$0.561 \pm 0.031$	$0.571 \pm 0.042$	$0.606\pm0.036$	$0.119\pm0.063$
Gaussian (I)	$0.322\pm0.042$	$0.679 \pm 0.042$	$0.680\pm0.043$	$0.685\pm0.042$	$0.355\pm0.085$
Gaussian (II)	$0.320\pm0.032$	$0.680\pm0.032$	$0.588 \pm 0.102$	$0.860\pm0.032$	$0.129\pm0.055$
Gaussian (III)	$0.530 \pm 0.029$	$0.470 \pm 0.029$	$0.625\pm0.030$	$0.620\pm0.036$	$0.066 \pm 0.044$

Table 2 Comparison between QNMC and NMC performance

is subjected to an increasing dispersion (for |t| > 1) or a decreasing dispersion (for |t| < 1), and the classical centroids change according to  $\mu_l \mapsto t \mu_l$  ( $\forall l = 1, ..., L$ ). Consequently, the classification problem for each pattern of the rescaled test set can be written as

$$\underset{l=1,\ldots,L}{\operatorname{argmin}} d_E(t\mathbf{x}_n, t\boldsymbol{\mu}_l) = t \operatorname{argmin}_{l=1,\ldots,L} d_E(\mathbf{x}_n, \boldsymbol{\mu}_l), \ \forall n = N+1, \ldots, N'.$$

For any value of the parameter t it can be proved [19] that, while the NMC is invariant under rescaling, for the QNMC this invariance fails. Interestingly enough, it is possible to consider the failure of the invariance under rescaling as a resource



**Fig. 1** Comparison between NMC and QNMC performance in terms of the classification error for the datasets (**a**) *Ionosphere* and (**b**) *Bands*. In both cases, the simple dashed line represents the QNMC classification error without rescaling, the dashed line with points represents the NMC classification error (which does not depend on the rescaling parameter), and points with related error bars (red in (**a**) and blue in (**b**)) represent the QNMC classification error for increasing values of the parameter *t*. In (a)  $t \in [0.1, 1.9]$  and it increases with step  $10^{-1}$ . In (b),  $t \in [0.001, 0.019]$  and it increases with step  $10^{-3}$ 

for the classification problem. In other words, a suitable choice of the rescaling factor is possible, in principle, to get a decreasing of the classification error. At this purpose, we have studied the variation of the QNMC performance (in particular of the classification error) in terms of the *free* parameter t, and in Fig. 1 the results for the datasets *Ionosphere* and *Bands* are shown. In the figure, each point represents the mean value (with corresponding standard deviation represented by the vertical bar) over ten runs of the experiments. We can observe that, for the considered datasets, the QNMC performance for most of t values is better than the NMC, but for some particular value of t the error gets a further significant reduction (with respect the unrescaled case).

Let us note that the range of the rescaling parameter t, for which the QNMC performance improves, is generally not unique and depends on the dataset. For instance, in Fig. 1, we observe that the classification error provided by the QNMC decreases for t ranging from 0.1 to 1.9 in the *Ionosphere* case and from 0.001 to 0.019 in the *Bands* case. As a consequence, we do not generally get an improvement in the classification process for any t ranges. On the contrary, there exist some intervals of the parameter t where the QNMC classification performance is worse than the case without rescaling. Then, each dataset has specific and unique characteristics (in accord to the No Free Lunch Theorem), and the incidence of the non-invariance under rescaling in the decreasing of the error, in general, should be determined by empirical evidences.

#### 6 Conclusions and Future Work

In this work a quantum counterpart of the well-known Nearest Mean Classifier was proposed. We introduced a quantum minimum-distance classifier, called Quantum Nearest Mean Classifier, obtained by defining a suitable encoding of real patterns, i.e., *density patterns*, and by recovering the trace distance between density operators.

We proposed a new encoding of a real pattern into a quantum object that was suggested by recent debates on quantum machine learning according to which, in order to avoid a loss of information caused by encoding a real vector into a quantum state, we need to normalize the real vector maintaining some information about its norm. Secondly, we defined the *quantum centroid*, i.e., the pattern chosen as the prototype of each class, which is not invariant under uniform rescaling of the original dataset (unlike the NMC) and seems to exhibit a kind of sensitivity to the data dispersion.

The experiments were organized as follows: both classifiers were compared in terms of significant statistical coefficients. In particular, we considered 14 different datasets having different nature (real-world and artificial). Further, the non-invariance under rescaling of the QNMC suggested to study the variation of the classification error in terms of a free parameter t, whose variation produces a modification of the data dispersion and, consequently, of the classifier performance. In particular we showed as, in the most of cases, the QNMC exhibits a significant decreasing of the classification error (and of the other statistical coefficients) with respect to the NMC and, for some case, the non-invariance under rescaling can provide a significant positive incidence in the classification process.

Let us remark that, even if there is not an absolute superiority of QNMC with respect to the NMC, the method we introduced allows to get some relevant improvements of the classification when we have an a priori knowledge about the distribution of the dataset we have to deal with.

In light of such considerations, further developments of the present work will be focused on (1) finding out the encoding (from real vectors to density operators) that guarantees the *optimal* improvement (at least for a finite class of datasets) in terms of the classification process accuracy, (2) obtaining a general method to find the suitable rescaling parameter range to apply to a given dataset in order to get further improvement of the accuracy, and (3) understanding for which kind of distribution the QNMC performs better than the NMC. At this purpose, it will be useful to compare the *optimal* QNMC also with other standard classifiers.

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# On Complexity for Open System Dynamics



Noboru Watanabe

## 1 Introduction

The quantum entropy for a density operator was defined by von Neumann [51] in 1932. The quantum entropy for C\*-system, which is called a C\*-mixing entropy, was introduced in [33], and its property was studied in [23, 29]. The quantum relative entropy for density operators was introduced by Umegaki [48], and it was extended for general state space by Araki [8, 9] in von Neumann algebra and by Uhlmann [47] in \*-algebra. The study of the channel for the quantum processes based on the transition expectation introduced by Accardi [3], in which quantum Markov process [1] was studied, is discussed in [4], and the beam splitting was rigorously studied by Fichtner et al. [18]. By using the quantum communication processes, the noisy optical channel was introduced in [40].

In the quantum information theory, one of the important subjects is to study how much information correctly transmitted through a quantum channel, so that it is necessary to extend the mutual entropy of the classical system to the quantum system. The classical mutual entropy was defined by the joint probability distribution between input and output systems. However, the joint probability does not exist generally (see [49]) in quantum systems. The semiclassical mutual entropy was introduced by Holevo, Levitin, and Ingarden [19, 22, 27] for classical input and quantum output passing through a semiclassical channel. By introducing a compound state, Ohya defined the quantum mutual entropy (information) in complete quantum systems in 1983 [31]. By using this mutual entropy, one can study the efficiency of the information transmission in quantum communication

N. Watanabe (⊠)

Tokyo University of Science, Noda City, Chiba 278–8510, Japan e-mail: watanabe@is.noda.tus.ac.jp

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processes, which allows the detailed analysis of optical communication [40-42, 53]. The channel capacities are studied in [20, 36, 38, 43, 44]. The mutual entropy in C\*-system was defined by Ohya [35]. These quantum entropies are expounded in [37]. Recently these methods started to be explored in applications to biology and cognition [10, 11, 24].

Kolmogorov–Sinai entropy S(T) [25] for a measure preserving transformation T was defined on a message space through finite partitions of the measurable space. Based on the mean dynamical entropy and the mean dynamical mutual entropy, the classical coding theorems of Shannon are formulated to analyze the capacity for communication processes. The quantum dynamical entropy (QDE) was first studied by Connes-Størmer [14] and Emch [17] such as a complexity (entropy of automorphism) of quantum dynamical processes. In 1985, Ohya introduced the Smixing entropy [33-35, 37, 39] in general quantum systems, which contains the von Neumann entropy [51] as a special case. By using the S-mixing entropy, Ohya defined a mean entropy and a mean mutual entropy in [29, 33] for the quantum dynamical systems, and several discussions of the mean entropies are done in [28, 53]. The mean dynamical entropy denotes the amount of information per one letter of a signal sequence transmitted from the input source, and the mean dynamical mutual entropy expresses the amount of information per one letter of the signal obtained in the output system. In 1987, Conne-Narnhoffer-Thirring introduced a dynamical entropy [15] (CNT entropy), and several researchers discussed the CNT entropy [12, 13, 21, 28, 45]. Alicki–Fannes [7] defined a dynamical entropy (AF entropy) with respect to a finite operational partitions of unity. In 1995, Voiculescu [50] proposed a dynamical entropy (dynamical approximation entropy) for C\* and W\* algebras. In 1997, Accardi–Ohya and I [6] defined a dynamical entropy (AOW entropy) through the quantum Markov process, and the relation between these dynamical entropies is discussed in [5, 28]. In 1999, Kossakowski-Ohya and I [26] introduced a dynamical entropy (KOW entropy) with respect to completely positive maps based on transition expectations and liftings in the sense of Accardi and Ohya [2].

In this chapter, we will discuss about complexity of open system dynamics to calculate (1) the mean mutual entropy with respect to the input states and the quantum channel for the open system dynamics [54] and (2) the generalized AOW entropy through the quantum channel for the open system dynamics [55].

#### 2 Quantum Channels

Let  $(\mathscr{A}_1, \mathfrak{S}(\mathscr{A}_1))$  and  $(\mathscr{A}_2, \mathfrak{S}(\mathscr{A}_2))$  be the input and output quantum systems, respectively, where  $\mathscr{A}_1$  (resp. $\mathscr{A}_2$ ) is a C\*-algebra or the set of all bounded operators  $\mathbf{B}(\mathscr{H}_1)$  (resp.  $\mathbf{B}(\mathscr{H}_1)$ ) on a separable complex Hilbert space  $\mathscr{H}_1$  (resp. $\mathscr{H}_2$ ) and  $\mathfrak{S}(\mathscr{A}_1)$  (resp. $\mathfrak{S}(\mathscr{A}_2)$ ) is the set of all states on  $\mathscr{A}_1$  (resp. $\mathscr{A}_2$ ) or the set of all density operators on  $\mathscr{H}_1$  (resp. $\mathscr{H}_2$ ). A quantum channel is defined by a mapping  $\Lambda^*$  from the input quantum state space  $\mathfrak{S}(\mathscr{A}_1)$  to the output quantum state space  $\mathfrak{S}(\mathscr{A}_2)$ . A quantum channel  $\Lambda^*$  satisfying an affine property such as

$$\Lambda^*(\sum_k \lambda_k \varphi_k) = \sum_k \lambda_k \Lambda^*(\varphi_k)$$

for any  $\varphi_k \in \mathfrak{S}(\mathscr{A}_1)$  and any  $\sum_k \lambda_k = 1$  with  $\lambda_k \ge 0$  ( $\forall k$ ) is said to be a linear.  $\Lambda^*$  is a completely positive (CP) channel [23, 30, 37, 39, 42] if its dual map  $\Lambda$  from  $\mathscr{A}_2$  to  $\mathscr{A}_1$  satisfies

$$\sum_{i,j=1}^n A_i^* \Lambda(B_i^* B_j) A_j \ge 0$$

for any  $n \in \mathbb{N}$ , any  $B_j \in \overline{\mathscr{A}}$ , and any  $A_j \in \mathscr{A}$ , where the dual map  $\Lambda$  of  $\Lambda^*$  is given by  $\Lambda^*(\varphi)(B) = \varphi(\Lambda(B))$  for any  $\varphi \in \mathfrak{S}(\mathscr{A}_1)$  and any  $B \in \mathscr{A}_2$ . We briefly review some examples of quantum channels.

#### 2.1 Quantum Communication Processes

Take  $\mathscr{A}_1 = \mathbf{B}(\mathscr{H}_1)$  (resp.  $\mathscr{A}_2 = \mathbf{B}(\mathscr{H}_2)$ ) and  $\mathfrak{S}(\mathscr{A}_1) = \mathfrak{S}(\mathscr{H}_1)$  (resp.  $\mathfrak{S}(\mathscr{A}_2) = \mathfrak{S}(\mathscr{H}_2)$ ), where  $\mathfrak{S}(\mathscr{H}_1)$  is the set of all density operators on a separable complex Hilbert space  $\mathscr{H}_1$  (resp.  $\mathscr{H}_2$ ). Let  $\mathscr{H}_1$  and  $\mathscr{H}_2$  be two Hilbert spaces describing noise and loss systems, respectively. Put  $\mathscr{B}_2 = \mathbf{B}(\mathscr{H}_1)$  (resp.  $\mathscr{B}_2 = \mathbf{B}(\mathscr{H}_2)$ ) and  $\mathfrak{S}(\mathscr{B}_1) = \mathfrak{S}(\mathscr{H}_1)$  (resp.  $\mathfrak{S}(\mathscr{B}_2) = \mathfrak{S}(\mathscr{H}_2)$ ), where  $\mathfrak{S}(\mathscr{H}_1)$  is the set of all density operators on a separable complex Hilbert space  $\mathscr{H}_1$  (resp.  $\mathscr{H}_2$ ). A mathematical scheme of quantum communication process including the influence of noise and loss is discussed in [31] as follows: Let  $\varphi$  and  $\psi$  be input and noise states in  $\mathfrak{S}(\mathscr{A}_1)$  and  $\mathfrak{S}(\mathscr{B}_1)$ .

$$\begin{array}{c} \mathfrak{S}(\mathscr{A}_1) & \xrightarrow{\Lambda^*} \mathfrak{S}(\mathscr{A}_2) \\ \gamma^* \downarrow & \xrightarrow{} \\ \mathfrak{S}(\mathscr{A}_1 \otimes \mathscr{B}_1) & \overrightarrow{\pi^*} & \mathfrak{S}(\mathscr{A}_2 \otimes \mathscr{B}_2) \end{array}$$

 $\gamma^*$ ,  $a^*$  are CP channels defined by

$$\gamma^* (\varphi) = \varphi \otimes \psi, \quad \varphi \in \mathfrak{S} (\mathscr{A}_1),$$
$$a^* (\Psi) (A) = \Psi (A \otimes I_2), \quad \Psi \in \mathfrak{S} (\mathscr{A}_2 \otimes \mathscr{B}_2) \quad (A \in \mathscr{A}_2),$$

where  $I_2$  is the identity operator in  $\mathscr{B}_1$ . The map  $\pi^*$  is a CP channel from  $\mathfrak{S}(\mathscr{A}_1 \otimes \mathscr{B}_1)$  to  $\mathfrak{S}(\mathscr{A}_2 \otimes \mathscr{B}_2)$  determined by the physical property of the communication device. The quantum channel for the communication process is given by

$$\Lambda^{*}(\varphi) (A) \equiv \pi^{*} (\varphi \otimes \psi) (A \otimes I_{2})$$
$$= (a^{*} \circ \pi^{*} \circ \gamma^{*}) (\varphi) (A) \quad (A \in \mathscr{A}_{2})$$

for any  $\varphi \in \mathfrak{S}(\mathscr{A}_1)$ . Some examples of the quantum communication channels are the noisy optical channel, the attenuation channel, and the connected channel that are constructed as follows:

#### 2.2 Noisy Optical Channel

Noisy optical channel  $\Lambda^*$  with a normal noise state  $\psi$  was introduced in [40] such as

$$\begin{aligned} \Lambda^*(\varphi) \left( A \right) &\equiv \pi^*(\varphi \otimes \psi) \left( A \otimes I_2 \right) \\ &= \left( \varphi \otimes \psi \right) \circ \pi \left( A \otimes I_2 \right) \\ &= tr V \left( \widetilde{\varphi} \otimes \widetilde{\psi} \right) V^* \left( A \otimes I_2 \right), \quad (A \in \mathscr{A}_2) \end{aligned}$$

where  $\psi(B) = tr \tilde{\psi}B = \langle m_1, Bm_1 \rangle$   $(B \in \mathcal{B}_1), \tilde{\psi} = |m_1\rangle \langle m_1|$  is the  $m_1$  photon number state in  $\mathfrak{S}(\mathcal{H}_1)$  and V is a linear mapping from  $\mathcal{H}_1 \otimes \mathcal{H}_1$  to  $\mathcal{H}_2 \otimes \mathcal{H}_2$ defined by

$$V(|n_1\rangle \otimes |m_1\rangle) = \sum_{j=0}^{n_1+m_1} C_j^{n_1,m_1} |j\rangle \otimes |n_1+m_1-j\rangle,$$

$$C_{j}^{n_{1},m_{1}} = \sum_{r=L}^{K} (-1)^{n_{1}+j-r} \frac{\sqrt{n_{1}!m_{1}!j!(n_{1}+m_{1}-j)!}}{r!(n_{1}-j)!(j-r)!(m_{1}-j+r)!} \times \alpha^{m_{1}-j+2r} \left(-\bar{\beta}\right)^{n_{1}+j-2r},$$

and  $|n_1\rangle$  is the  $n_1$  photon number state vector in  $\mathcal{H}_1$ , and  $\alpha$ ,  $\beta$  are complex numbers holding  $|\alpha|^2 + |\beta|^2 = 1$ ,  $K = \min\{n_1, j\}$  and  $L = \max\{m_1 - j, 0\}$ . The following theorem is proved.

**Theorem 1** The noisy optical channel  $\Lambda^*$  with noise state

$$\psi(B) = tr[|m\rangle \langle m|B] \quad (B \in \mathscr{B})$$

is described by

$$\Lambda^*(\varphi)(A) = tr\left[\sum_{i=0}^{\infty} O_i V Q^{(m)} \widetilde{\varphi} Q^{(m)*} V^* O_i^* A\right], \left(A \in \overline{\mathscr{A}}\right)$$
(1)

where  $Q^{(m)} \equiv \sum_{l=0}^{\infty} (|y_l\rangle \otimes |m\rangle) \langle y_l|$ ,  $O_i \equiv \sum_{k=0}^{\infty} |z_k\rangle (\langle z_k| \otimes \langle i|), \{|y_l\rangle\}$  is a CONS in  $\mathcal{H}_1, \{|z_k\rangle\}$  is a CONS in  $\mathcal{H}_2$ , and  $\{|i\rangle\}$  is the set of number states in  $\mathcal{H}_2$ .

For the coherent input state,

$$\Phi_{\xi\otimes\kappa}\left(\widetilde{A}\right) = tr\left[\left(\left|\xi\right\rangle\left\langle\xi\right|\otimes\left|\kappa\right\rangle\left\langle\kappa\right|\right)\widetilde{A}\right], \quad \left(\left|\xi\right\rangle\left\langle\xi\right|\otimes\left|\kappa\right\rangle\left\langle\kappa\right|\in\mathfrak{S}\left(\mathscr{H}_{1}\otimes\mathscr{H}_{1}\right)\right)\right]$$

the output state of  $\pi^*$  is given by

$$\pi^{*} \left( \Phi_{\xi \otimes \kappa} \right) \left( \widetilde{A} \right)$$

$$= \Phi_{\alpha \xi + \beta \kappa \otimes -\bar{\beta} \xi + \bar{\alpha} \kappa} \left( \widetilde{A} \right)$$

$$= tr \left[ |\alpha \xi + \beta \kappa \rangle \langle \alpha \xi + \beta \kappa | \otimes | -\bar{\beta} \xi + \bar{\alpha} \kappa \rangle \langle -\bar{\beta} \xi + \bar{\alpha} \kappa | \widetilde{A} \right]$$

$$\left( |\alpha \xi + \beta \kappa \rangle \langle \alpha \xi + \beta \kappa | \otimes | -\bar{\beta} \xi + \bar{\alpha} \kappa \rangle \langle -\bar{\beta} \xi + \bar{\alpha} \kappa | \in \mathfrak{S} \left( \mathscr{H}_{2} \otimes \mathscr{H}_{2} \right) \right)$$

for  $\widetilde{A} \in \mathscr{A}_1 \otimes \mathscr{A}_2$ .  $\pi^*$  defined in [40] is called a generalized beam splitting. The noisy optical channel with a vacuum noise is called an attenuation channel defined in [31].

#### 2.3 Attenuation Channel

The noisy optical channel  $\Lambda^*$  with a vacuum noise state  $\psi_0$  is called the attenuation channel defined in [31] by

$$\begin{split} \Lambda_0^*(\varphi) \left( A \right) &\equiv \pi_0^*(\varphi \otimes \psi_0) \left( A \otimes I_2 \right) \\ &= \left( \varphi \otimes \psi_0 \right) \circ \pi_0 \left( A \otimes I_2 \right) \\ &= tr V_0 \left( \widetilde{\varphi} \otimes \widetilde{\psi}_0 \right) V_0^* \left( A \otimes I_2 \right), \quad \left( A \in \mathscr{A}_2 \right) \end{split}$$

where  $\psi_0(B) = tr \widetilde{\psi}_0 B = \langle 0, B0 \rangle$   $(B \in \mathcal{B}_1), \widetilde{\psi}_0 = |0\rangle \langle 0|$  is the vacuum noise state in  $\mathfrak{S}(\mathcal{K}_1)$  and V is a linear mapping from  $\mathcal{H}_1 \otimes \mathcal{H}_1$  to  $\mathcal{H}_2 \otimes \mathcal{K}_2$  defined by

$$V_0(|n_1\rangle \otimes |0\rangle) = \sum_{j}^{n_1} C_j^{n_1} |j\rangle \otimes |n_1 - j\rangle,$$
$$C_j^{n_1} = \sqrt{\frac{n_1!}{j!(n_1 - j)!}} \alpha^j (-\bar{\beta})^{n_1 - j}$$

and  $|n_1\rangle$  is the  $n_1$  photon number state vector in  $\mathcal{H}_1$ , and  $\alpha$ ,  $\beta$  are complex numbers satisfying  $|\alpha|^2 + |\beta|^2 = 1$ . On generalized Fock spaces, the mathematical representation of beam splitting [18] is given by

$$\mathscr{E}_{0}^{*}\left(|\xi\rangle\langle\xi|\right) = |\alpha\xi\rangle\langle\alpha\xi| \otimes |\beta\xi\rangle\langle\beta\xi|$$

where  $\mathscr{E}_0^*$  is a lifting from  $\mathfrak{S}(\mathscr{H})$  to  $\mathfrak{S}(\mathscr{H}\otimes\mathscr{H})$  in the sense of Accardi and Ohya [2].

#### 2.4 Connected Channel

Here we explain a connected channel. For  $n \in \mathbf{N}$ , a *n*-connected channel  $\Lambda_{(n)}^*$  with a fixed noise state  $\zeta$  was defined by

$$\Lambda^*_{(n)}(\rho) \equiv tr_{\mathscr{K}_2} \Pi^{*n}(\rho \otimes \zeta) = tr_{\mathscr{K}_2} V^n \left(\rho \otimes \zeta\right) V^{*n},$$

for any  $\rho \in \mathfrak{S}(\mathscr{H}_1)$ , where  $\Pi^{*n}$  is *n*-folds composition of the CP channels  $\Pi^*$ and  $V^n$  and  $V^{*n}$  are also *n*-folds compositions of *V* and  $V^*$ , respectively. Then *n*-connected channel  $\Lambda^*_{(n)}$  can be denoted as the following representation [53].

**Theorem 2** The *n*-connected channel  $\Lambda^*_{(n)}$  with noise state  $|m\rangle \langle m|$  is denoted by

$$A_{(n)}^{*}(\rho) = \sum_{i=0}^{\infty} O_{i} V^{n} Q^{(m)} \rho Q^{(m)*} V^{*n} O_{i}^{*},$$

where  $Q^{(m)} \equiv \sum_{l=0}^{\infty} (|y_l\rangle \otimes |m\rangle) \langle y_l|$ ,  $O_i \equiv \sum_{k=0}^{\infty} |z_k\rangle (\langle z_k| \otimes \langle i|)$ ,  $\{|y_l\rangle\}$  and  $\{|z_k\rangle\}$  are CONS in  $\mathcal{H}_1$  and  $\mathcal{H}_2$ , respectively.  $\{|i\rangle\}$  is the set of number states in  $\mathcal{H}_2$ .

For a *n*-connected channel  $\Lambda_{(n)}^*$  with a fixed noise state  $\zeta$ , we have

**Theorem 3** For the n-connected channel  $\Lambda_{(n)}^*$  with  $\alpha = \frac{\sqrt{3}}{2}$ , if n is given by  $12\ell \quad (\ell \in \mathbf{N})$ , then  $\Pi^{*n}$  is the identity channel id, that is,

$$\Lambda_{(n)}^*\left(\rho\right) = \rho.$$

We obtain the following theorem in [53].

**Theorem 4** For the n-connected channel  $\Lambda_{(n)}^*$  with  $\alpha = \frac{1}{2}$ , if n is given by  $6\ell + \frac{3}{2}$  ( $\ell \in \mathbf{N}$ ), then  $\Pi^{*n}$  is the exchanged channel, that is,

$$\Lambda_{(n)}^*\left(\rho\right) = \zeta$$

is held for any  $\rho \in \mathfrak{S}(\mathscr{H}_1)$ . If *n* is given by  $6\ell + \frac{3}{4}$  ( $\ell \in \mathbb{N}$ ), one can obtain the output and loss states of *n*-folds composition of the CP channels  $\Pi^*$  such as the maximal entangled state

$$\Pi^{*n}\left(\rho\otimes\zeta\right) = \frac{1}{2}\left(|1\rangle\otimes|0\rangle + |0\rangle\otimes|1\rangle\right)\left(\langle 1|\otimes\langle 0| + \langle 0|\otimes\langle 1|\right)\right)$$

for the input state  $\rho = |1\rangle \langle 1|$  and the noise state  $\zeta = |0\rangle \langle 0|$ . It means that  $\Pi^{*n} \left(n = 6\ell + \frac{3}{4} \quad (\ell \in \mathbf{N})\right)$  generates the maximal entangled state.

#### 2.5 Open System Dynamics

Let  $S_1$  be a system described by a Hilbert space  $\mathscr{H}$  and  $S_2$  be an external system described by another Hilbert space  $\mathscr{H}$ , interacting with  $S_1$ . Let H be the total Hamiltonian of  $S_1$  and  $S_2$ . We denote the initial states of  $S_1$  and  $S_2$  by  $\rho$  and  $\sigma$ , respectively. The time evolution of the interacted state  $\rho \otimes \sigma$  at time t according to the unitary operator  $U_t = \exp(-itH)$  is given by the combined state  $\theta_t$ 

$$\theta_t \equiv U_t(\rho \otimes \sigma) U_t^*.$$

A CP channel of the open system dynamics [23, 37, 39] is obtained by taking the partial trace of  $\theta_t$  with respect to  $\mathcal{K}$  such as

$$\Lambda_t^*(\rho) \equiv tr_{\mathscr{K}}\theta_t,$$

where  $tr_{\mathscr{K}}\theta_t$  is defined by

$$\langle x, tr_{\mathscr{H}}\theta_t x' \rangle = \sum_n \langle x \otimes y_n, \sigma x' \otimes y_n \rangle \quad (\forall x, x' \in \mathscr{H})$$

with a complete orthogonal system  $\{y_n\} \subset \mathcal{K}$ .

#### 2.6 Quantum Channel for Open System Dynamics

Based on [4], let  $H_1$  be the Hamiltonian of a system  $S_1$  described by a Hilbert space  $\mathscr{H}_1$ . If a system  $S_1$  interacts with an external system (heat bath)  $S_2$  with the Hamiltonian  $H_2$  described by another Hilbert space  $\mathscr{H}_2$  and the initial states of  $S_1$ and  $S_2$  are  $\rho$  and  $\xi$ , respectively, then the compound state  $\sigma_t$  of  $S_1$  and  $S_2$  at time t after the interaction between two systems is given by

$$\sigma_t \equiv U_t(\rho \otimes \xi) U_t^*,$$

where  $U_t = \exp(-itH)$  with the total Hamiltonian H of  $S_1$  and  $S_2$ . A channel is obtained by taking the partial trace w.r.t.  $\mathscr{H}_2$  such as

$$\rho \to \Lambda^* \rho \equiv \operatorname{tr}_{\mathscr{H}} \sigma_t.$$

The total Hamiltonian H is described by

$$H = H_1 \otimes I + I \otimes H_2 + H_{in},$$
  
$$H_1 = a^*a,$$

$$H_{2} = \sum_{j} b_{j}^{*} b_{j},$$
$$H_{in} = \sum_{j} \left( \varepsilon_{j} b_{j} a^{*} + \overline{\varepsilon_{j}} b_{j}^{*} a \right)$$

To simplify, we assume that the system  $\Sigma_2$  is given by a single mode

$$H_2 = b^*b,$$
  
$$H_{in} = \varepsilon (ba^* + b^*a)$$

For a given state  $\xi \in \mathfrak{S}(\mathscr{H}_2)$ , the quantum channel  $\Lambda_t^*$  at time *t* for the open system is denoted by Stinespring–Sudarshan–Kraus representation such as

$$\Lambda_{t}^{*}(\rho) = \sum_{i=0}^{\infty} O_{i}(t) \left(\rho \otimes \xi\right) O_{i}^{*}(t), \quad (\forall \rho \in \mathfrak{S}(\mathscr{H}_{1}))$$

where  $O_i$  is a partial isometric operator given by

$$O_{i}(t) = \sum_{k=i}^{\infty} |k - i\rangle \left\langle \Phi_{k-i}^{(k)}(t) \right|,$$
  
$$\left| \Phi_{k-i}^{(k)}(t) \right\rangle = \sum_{j=0}^{k} \tau_{k-i,j}^{(k)}(t) |j\rangle \otimes |k - j\rangle \in [\mathscr{H}_{1} \otimes \mathscr{H}_{2}]^{(k)} \subset \mathscr{H}_{1} \otimes \mathscr{H}_{2},$$
  
$$\tau_{k-i,j}^{(k)}(t) = \sum_{\ell=0}^{k} \exp\left(-it\varepsilon\lambda_{\ell}^{(k)}\right) C_{k-i}^{k,\ell} \overline{C_{j}^{k,\ell}},$$

where  $\lambda_{\ell}^{(k)}$  is given in (2) and

$$\begin{split} C_{k-i}^{k,\ell} &= \sum_{r=L}^{k-i} (-1)^{2k-i-r} \frac{\sqrt{k!\ell! \, (k-i)!(\ell+i)!}}{r!i!(k-i-r)!(\ell+i-k+r)!} \\ &\times \alpha^{\ell-(k-i)+2r} \left(-\bar{\beta}\right)^{2k-i-2r}, \left(|\alpha|^2+|\beta|^2=1\right), \\ L &\equiv \max\left\{\ell+i-k, 0\right\}. \end{split}$$

For any k,  $[\mathscr{H}_1 \otimes \mathscr{H}_2]^{(k)}$  is a subspace spanned by a subset  $\{|j\rangle \otimes |k-j\rangle; j = 0, 1, 2, \cdots, k\}$ . Then

$$H_{in}\left[\mathscr{H}_1\otimes\mathscr{H}_2\right]^{(k)}\subseteq\left[\mathscr{H}_1\otimes\mathscr{H}_2\right]^{(k)}$$

is hold. Let  $H_{in}^{(k)}$  be a restriction of  $H_{in}$  into  $[\mathscr{H}_1 \otimes \mathscr{H}_2]^{(k)}$ .  $H_{in}^{(k)}$  is a finitedimensional self-adjoint operator on  $\mathbb{C}^{k+1}$  satisfying

$$H_{in}^{(k)} \Psi_{\ell}^{(k)} = \lambda_{\ell}^{(k)} \Psi_{\ell}^{(k)}, \quad (\ell = 0, 1, 2, \cdots, k),$$

$$\Psi_{\ell}^{(k)} = \sum_{m=0}^{k} C_{m}^{k,\ell} |m\rangle \otimes |k-m\rangle \in [\mathscr{H}_{1} \otimes \mathscr{H}_{2}]^{(k)}.$$
(2)

#### **3** Entropy and Mutual Entropy for Quantum Systems

For a density operator  $\rho \in \mathfrak{S}(\mathscr{H}_1)$ , von Neumann [51] defined the quantum entropy by

$$S(\rho) = -tr\rho \log \rho.$$

The properties of entropy are explained in [37, 39, 42].

The mutual entropy for purely quantum systems denoted by  $I(\rho; \Lambda^*)$  depends on an input quantum state  $\rho$ , and a quantum channel  $\Lambda^*$  should hold the following three conditions:

- 1. The quantum mutual entropy with the identity channel  $\Lambda^* = id$  is equal to the von Neumann entropy:  $I(\rho; id) = S(\rho)$ .
- 2. The quantum mutual entropy w.r.t. the classical systems reduces to classical one.
- 3. Shannon's type fundamental inequalities  $0 \le I(\rho; \Lambda^*) \le S(\rho)$  are satisfied.

Instead of the joint state in classical systems, Ohya defined the compound state  $\sigma_E$  of the input state  $\rho$  and the output state  $\Lambda^* \rho$  by

$$\sigma_E = \sum_k \mu_k E_k \otimes \Lambda^* E_k,$$

where *E* represents a one-dimensional orthogonal base {*E<sub>k</sub>*} of the Schatten decomposition [46]  $\rho = \sum_k \mu_k E_k$  of  $\rho$ , which is not always unique unless every eigenvalue of  $\rho$  is not degenerated. The compound state depends on how we distinguish the state  $\rho$  into basic states. By using two compound states  $\sigma_E$  and  $\sigma_0 = \rho \otimes \Lambda^* \rho$ , Ohya introduced [31, 32] the quantum mutual entropy (information) as

$$I(\rho; \Lambda^*) = \sup \{S(\sigma_E, \sigma_0); E = \{E_k\}\},\$$

where the supremum is taken over all Schatten decompositions of  $\rho$ , and  $S(\sigma_E, \sigma_0)$  is the Umegaki's relative entropy [48] defined by

$$S(\sigma_E, \sigma_0) = \begin{cases} tr\sigma_E \left(\log \sigma_E - \log \sigma_0\right) \left(s \left(\sigma_E\right) \ll s \left(\sigma_0\right)\right), \\ \infty \qquad (\text{else}), \end{cases}$$

 $s(\sigma_E) \ll s(\sigma_0)$  means the support projection  $s(\sigma_0)$  of  $\sigma_0$  is greater than the support projection  $s(\sigma_E)$  of  $\sigma_E$ . The above conditions (1)  $\sim$  (2) are held for the quantum mutual entropy. Moreover the condition (3) follows from the monotonicity of relative entropy [31]:

#### Theorem 5

$$0 \le I(\rho; \Lambda^*) \le \min\{S(\rho), S(\Lambda^* \rho)\}.$$

For a linear channel, one has the following form [31]:

**Theorem 6** The quantum mutual entropy is denoted as

$$I(\rho; \Lambda^*) = \sup\left\{\sum_k \mu_k S(\Lambda^* E_k, \Lambda^* \rho); E = \{E_k\}\right\}.$$

When the input system is classical, an input state  $\rho$  is given by a probability distribution or a probability measure. In either case, the Schatten decomposition of  $\rho$  is unique, namely, for the case of probability distribution ;  $\rho = \{\mu_k\}$ ,

$$\rho = \sum_{k} \mu_k \delta_k,$$

where  $\delta_k$  is the delta measure, that is,

$$\delta_k(j) = \delta_{k,j} = \begin{cases} 1(k=j) \\ 0(k \neq j) \end{cases}, \forall j.$$

Therefore for any channel  $\Lambda^*$ , the mutual entropy becomes

$$I(\rho; \Lambda^*) = \sum_k \mu_k S(\Lambda^* \delta_k, \Lambda^* \rho),$$

which equals to the following usual expression when one of the two terms is finite for an infinite-dimensional Hilbert space:

$$I(\rho; \Lambda^*) = S(\Lambda^* \rho) - \sum_k \mu_k S(\Lambda^* \delta_k).$$

The above equality has been taken by Levitin [27] and Holevo [19] associated with classical-quantum channels. The quantum mutual entropy by Ohya contains their semiclassical mutual entropies as a special one.

# 4 Entropy and Mutual Entropy for General Quantum Systems

In this section, I briefly explain entropies of general quantum systems [32, 34, 35, 37, 39].

Let  $\mathscr{A}$  be a C\* algebra,  $\mathfrak{S}(\mathscr{A})$  be the set of all normal states on  $\mathscr{A}$ , and  $\mathscr{S}$  be a weak\* compact and convex subset of  $\mathfrak{S}(\mathscr{A})$ . Every state  $\varphi \in \mathscr{S}$  has a maximal measure  $\mu$  pseudosupported on  $ex\mathscr{S}$  such that

$$\varphi = \int_{\mathscr{S}} \omega d\mu, \tag{3}$$

where  $ex\mathscr{S}$  is the set of all extreme points of  $\mathscr{S}$ . The measure  $\mu$  satisfying the above decomposition is not unique unless  $\mathscr{S}$  is a Choquet simplex. We describe the set of all such measures by  $M_{\varphi}(\mathscr{S})$ . We define a subset of  $M_{\varphi}(\mathscr{S})$  by  $D_{\varphi}(\mathscr{S})$  such as

$$D_{\varphi}(\mathscr{S}) = \left\{ M_{\varphi}(\mathscr{S}); \quad \exists \mu_k \subset \mathbb{R}^+ \text{ and } \{\varphi_k\} \subset exS \\ s.t. \quad \sum_k \mu_k = 1, \quad \mu = \sum_k \mu_k \delta\left(\varphi_k\right) \right\}, \tag{4}$$

where  $\delta(\varphi)$  is the Dirac measure concentrated on an initial state  $\varphi$ . We put a functional *H* by

$$H(\mu) = -\sum_{k} \mu_k \log \mu_k \tag{5}$$

for a measure  $\mu \in D_{\varphi}(\mathscr{S})$ . The  $\mathscr{S}$ -mixing entropy of a state  $\varphi \in \mathscr{S}$  with respect to  $\mathscr{S}$  is defined by

$$S^{\mathscr{S}}(\varphi) = \begin{cases} \inf \left\{ H(\mu); \quad \mu \in D_{\varphi}(\mathscr{S}) \right\} \\ +\infty \qquad \text{if } D_{\varphi}(\mathscr{S}) = \varnothing. \end{cases}$$
(6)

It describes the amount of information of the state  $\varphi$  measured from the subsystem  $\mathscr{S}$ . For example,  $\mathscr{S}$  is given by  $\mathfrak{S}(\mathscr{A})$  which is the set of all states on  $\mathscr{A}$ ,  $I(\alpha)$  which is the set of all invariant states for  $\alpha$ , and  $K(\alpha)$  which is the set of all KMS states. If  $\mathscr{S}$  is given by  $\mathfrak{S}(\mathscr{A})$ , we denote  $S^{\mathfrak{S}(\mathscr{A})}(\varphi)$  by  $S(\varphi)$ . It is an extension of von Neumann's entropy [51]

$$S(\rho) = -tr\rho \log \rho, \quad \forall \rho \in \mathfrak{S}(\mathscr{H}).$$
(7)

For an initial state  $\varphi \in \mathscr{S}$  and a quantum channel  $\Lambda^* : \mathfrak{S}(\mathscr{A}) \to \mathfrak{S}(\mathscr{B})$ , two compound states are defined by Ohya such as

$$\Phi_0 = \varphi \otimes \Lambda^* \varphi$$
 (trivial compound state)  
$$\Phi_{\mu}^{\mathscr{S}} = \int_{\mathscr{S}} \omega \otimes \Lambda^* \omega \, d\mu$$
 (Ohya compound state)

The compound state  $\Phi_{\mu}^{\mathscr{S}}$  expresses the correlation between the input state  $\varphi$  and the output state  $\Lambda^* \varphi$ . They are separable compound states.  $\Phi_0$  does not depend on any correlation between two marginal systems.  $\Phi_{\mu}^{\mathscr{S}}$  represents a certain correlation between two compound systems.

In [35], the mutual entropy with respect to  $\mathscr{S}$  and  $\mu$  is given by

$$I_{\mu}^{\mathscr{S}}\left(\varphi;\Lambda^{*}\right) = S\left(\Phi_{\mu}^{\mathscr{S}},\Phi_{0}\right),\tag{8}$$

where  $S\left(\Phi_{\mu}^{\mathscr{S}}, \Phi_{0}\right)$  is the quantum relative entropy by Araki [8] and Uhlmann [47]. The quantum relative entropy of two states was introduced by Umegaki in [48] and Lindblad for  $\sigma$ -finite and semifinite von Neumann algebras. For two density operators  $\rho$  and  $\sigma$ , it is defined by

$$S(\rho, \sigma) = tr\rho \left(\log \rho - \log \sigma\right).$$
(9)

It was extended to more general quantum systems [37] by Araki [8, 9], Uhlmann [47] and Donald [16]. Based on the relative entropy, the mutual entropy was introduced by Ohya [35] for fully general quantum systems. The mutual entropy with respect to  $\mathscr{S}$  for general quantum systems is defined by Ohya as

$$I^{\mathscr{S}}(\varphi;\Lambda^*) = \sup\left\{I^{\mathscr{S}}_{\mu}(\varphi;\Lambda^*); \ \mu \in M_{\varphi}(\mathscr{S})\right\}.$$
 (10)

When  $\mathscr{S} = \mathfrak{S}(\mathscr{A})$  and a state  $\varphi$  is given by a fixed form  $\varphi = \sum_k \lambda_k \omega_k$ , the mutual entropy (relative entropy) is described by

$$I^{\mathscr{S}}\left(\varphi;\Lambda^{*}\right) = S\left(\Phi_{\mu}^{\mathscr{S}},\Phi_{0}\right) = \sum_{k} \lambda_{k} S(\Lambda^{*}\omega_{k},\Lambda^{*}\varphi) \leq S\left(\varphi\right).$$
(11)

The fundamental inequalities among the  $\mathscr{S}$ -mixing entropy and the mutual entropy for general quantum systems are satisfied as follows [35]:

$$0 \le I^{\mathscr{S}}(\varphi; \Lambda^*) \le \min\left\{S^{\mathscr{S}}(\varphi), S^{\mathscr{S}}(\Lambda^*\varphi)\right\}.$$

#### 5 Mean Entropy and Mean Mutual Entropy

We briefly explain the quantum mean entropy and quantum mean mutual entropy defined by Ohya [28, 35].

Let  $\mathscr{A}$  be a unital  $C^*$ -algebra,  $\mathfrak{S}(\mathscr{A})$  be the set of all states over  $\mathscr{A}$ , and  $\theta_{\mathscr{A}}$  be an automorphism of  $\mathscr{A}$ . A  $C^*$ -triple  $(\mathscr{A}, \mathfrak{S}(\mathscr{A}), \theta_{\mathscr{A}})$  with a stationary state  $\varphi \in \mathfrak{S}(\mathscr{A})$  with respect to  $\theta_{\mathscr{A}}$ , that is,  $\varphi \circ \theta_{\mathscr{A}} = \varphi$  is held, represents a stationary information source in quantum information theory.

We denote an output  $C^*$ -dynamical system by the  $C^*$ -triple  $(\mathscr{B}, \mathfrak{S}(\mathscr{B}), \theta_{\mathscr{B}})$ . Let  $\Lambda^* : \mathfrak{S}(\mathscr{A}) \to \mathfrak{S}(\mathscr{B})$  be a covariant channel, that is, it's predual map  $\Lambda : \mathscr{B} \to \mathscr{A}$  is a completely positive unital map satisfying  $\Lambda \circ \theta_{\mathscr{B}} = \theta_{\mathscr{A}} \circ \Lambda$ . Let  $\mathscr{A}_m$  and  $\mathscr{B}_n$   $(m = 1, \dots, M, n = 1, \dots, N)$  be finite-dimensional unital  $C^*$ -algebras and  $\alpha_m : \mathscr{A}_m \to \mathscr{A}$  and  $\beta_n : \mathscr{B}_n \to \mathscr{B}$  be completely positive unital maps. We express a pair of finite sequences of  $\{\alpha_m\}, \{\beta_n\}$  by  $\alpha^M = (\alpha_1, \alpha_2, \dots, \alpha_M), \beta^N = (\beta_1, \beta_2, \dots, \beta_N)$ .

We briefly explain functionals  $S^{\mathscr{S}}_{\mu}(\varphi; \alpha^M)$ ,  $S^{\mathscr{S}}(\varphi; \alpha^M)$ ,  $I^{\mathscr{S}}_{\mu}(\varphi; \alpha^M, \beta^N)$ , and  $I^{\mathscr{S}}(\varphi; \alpha^M, \beta^N)$  introduced in [28, 35].

For a given  $\alpha_m : \mathscr{A}_m \to \mathscr{A}$  and a given extremal decomposition measure  $\mu \in M_{\varphi}(\mathscr{S})$  of  $\varphi$ , the compound state of  $\alpha_1^*\varphi, \alpha_2^*\varphi, \cdots, \alpha_M^*\varphi$  on the tensor product algebra  $\frac{M}{m=1}\mathscr{A}_m$  is defined by [28, 35]

$$\Phi_{\mu}^{\mathscr{S}}(\alpha^{M}) = \int_{\mathcal{S}(\mathscr{A})} {}^{M}_{m=1} \alpha_{m}^{*} \omega d\mu(\omega),$$

and  $\Phi_{\mu}^{\mathscr{S}}(\alpha^{M} \cup \beta^{N})$  is a compound state of  $\Phi_{\mu}^{\mathscr{S}}(\alpha^{M})$  and  $\Phi_{\mu}^{\mathscr{S}}(\beta^{N})$  with respect to  $\alpha^{M} \cup \beta^{N} \equiv (\alpha_{1}, \alpha_{2}, \cdots, \alpha_{M}, \beta_{1}, \beta_{2}, \cdots, \beta_{N})$  given by

$$\Phi_{\mu}^{\mathscr{S}}\left(\alpha^{M}\cup\beta^{N}\right)=\int_{S(A)}\binom{M}{m=1}\alpha_{m}^{*}\omega\right)\otimes\binom{N}{m=1}\beta_{n}^{*}\omega\right)d\mu$$

For a given pair of  $\alpha^M = (\alpha_1, \dots, \alpha_M)$ ,  $\beta^N = (\beta_1, \dots, \beta_N)$ , the functionals  $S^{\mathscr{S}}(\varphi; \alpha^M)$  and  $I^{\mathscr{S}}(\varphi; \alpha^M, \beta^N)$  are defined in [28, 35] by taking the supremum for all possible extremal decomposition measure  $\mu$  of  $\varphi$  in  $M_{\varphi}(\mathscr{S})$  such as

$$S^{\mathscr{S}}(\varphi; \alpha^{M}) = \sup \left\{ S^{\mathscr{S}}_{\mu}(\varphi; \alpha^{M}); \quad \mu \in M_{\varphi}(\mathscr{S}) \right\},$$
$$I^{\mathscr{S}}(\varphi; \alpha^{M}, \beta^{N}) = \sup \left\{ I^{\mathscr{S}}_{\mu}(\varphi; \alpha^{M}, \beta^{N}); \quad \mu \in M_{\varphi}(\mathscr{S}) \right\},$$

where  $S^{\mathscr{S}}_{\mu}(\varphi; \alpha^M)$  and  $I^{\mathscr{S}}_{\mu}(\varphi; \alpha^M, \beta^N)$  are given by

$$S_{\mu}^{\mathscr{S}}(\varphi;\alpha^{M}) = \int_{S(A)} S\left( {}_{m=1}^{M} \alpha_{m}^{*} \omega, \Phi_{\mu}^{\mathscr{S}}(\alpha^{M}) \right) d\mu (\omega) ,$$
$$I_{\mu}^{\mathscr{S}}(\varphi;\alpha^{M},\beta^{N}) = S\left( \Phi_{\mu}^{S}\left( \alpha^{M} \cup \beta^{N} \right), \Phi_{\mu}^{\mathscr{S}}(\alpha^{M}) \otimes \Phi_{\mu}^{\mathscr{S}}(\beta^{N}) \right)$$

for any pair  $(\alpha^M, \beta^N)$  of finite sequences  $\alpha^M = (\alpha_1, \dots, \alpha_M)$  and  $\beta^N = (\beta_1, \dots, \beta_N)$  of completely positive unital maps  $\alpha_m, \beta_n$  and any extremal decomposition measure  $\mu$  of  $\varphi$ , and  $S(\cdot, \cdot)$  is the relative entropy.

Let  $\mathscr{A}$  (resp.  $\mathscr{B}$ ) be a unital  $C^*$ -algebra with a fixed automorphism  $\theta_{\mathscr{A}}$  (resp.  $\theta_{\mathscr{B}}$ ),  $\alpha$  (resp.  $\beta$ ) be completely positive unital maps from a finite-dimensional unital  $C^*$ -algebra  $\mathscr{A}_0$  (resp.  $\mathscr{B}_0$ ) to  $\mathscr{A}$  (resp.  $\mathscr{B}$ ),  $\Lambda$  be a covariant completely positive unital map from  $\mathscr{B}$  to  $\mathscr{A}$ , and  $\varphi$  be an invariant state over  $\mathscr{A}$ , i.e.,  $\varphi \circ \theta_{\mathscr{A}} = \varphi$ . Let  $\alpha^N$  and  $\beta^N_\Lambda$  be finite sequences of  $\{\theta^n_{\mathscr{A}} \alpha\}, \{\Lambda \circ \theta^{n-1}_{\mathscr{B}} \circ \beta\}$  given by

$$\begin{split} \boldsymbol{\alpha}^{N} &\equiv \left(\boldsymbol{\alpha}, \, \boldsymbol{\theta}_{\mathscr{A}} \circ \boldsymbol{\alpha}, \cdots, \, \boldsymbol{\theta}_{\mathscr{A}}^{N-1} \circ \boldsymbol{\alpha}\right), \\ \boldsymbol{\beta}_{\Lambda}^{N} &\equiv \left(\boldsymbol{\Lambda} \circ \boldsymbol{\beta}, \, \boldsymbol{\Lambda} \circ \boldsymbol{\theta}_{\mathscr{B}} \circ \boldsymbol{\beta}, \, \cdots, \, \boldsymbol{\Lambda} \circ \boldsymbol{\theta}_{\mathscr{B}}^{N-1} \circ \boldsymbol{\beta}\right). \end{split}$$

For each completely positive unital map  $\alpha$  and  $\beta$ , the functionals  $\tilde{S}^{\mathscr{S}}(\varphi; \theta_{\mathscr{A}})$ ,  $\tilde{S}^{\mathscr{S}}(\Lambda^*\varphi; \theta_{\mathscr{B}})$ , and  $\tilde{I}^{\mathscr{S}}(\varphi; \Lambda^*, \theta_{\mathscr{A}}, \theta_{\mathscr{B}})$  are defined by taking the supremum for all possible  $\mathscr{A}_0$ 's,  $\alpha$ 's,  $\mathscr{B}_0$ 's, and  $\beta$ 's:

$$\begin{split} \tilde{S}^{\mathscr{S}}(\varphi;\theta_{\mathscr{A}}) &= \sup_{\alpha} \tilde{S}^{\mathscr{S}}(\varphi;\theta_{\mathscr{A}},\alpha), \\ \tilde{S}^{\mathscr{S}}(\Lambda^{*}\varphi;\theta_{\mathscr{B}}) &= \sup_{\beta} \tilde{S}^{\mathscr{S}}(\Lambda^{*}\varphi;\theta_{\mathscr{B}},\beta), \\ \tilde{I}^{\mathscr{S}}(\varphi;\Lambda^{*},\theta_{\mathscr{A}},\theta_{\mathscr{B}}) &= \sup_{\alpha,\beta} \tilde{I}^{\mathscr{S}}(\varphi;\Lambda^{*},\theta_{\mathscr{A}},\theta_{\mathscr{B}},\alpha,\beta), \end{split}$$

where  $\tilde{S}^{\mathscr{S}}(\varphi; \theta_{\mathscr{A}}, \alpha), \tilde{S}^{\mathscr{S}}(\Lambda^*\varphi; \theta_{\mathscr{B}}, \beta)$ , and  $\tilde{I}^{\mathscr{S}}(\varphi; \Lambda^*, \theta_{\mathscr{A}}, \theta_{\mathscr{B}}, \alpha, \beta)$  are given in [28, 35] by

$$\begin{split} \tilde{S}^{\mathscr{S}}(\varphi;\theta_{\mathscr{A}},\alpha) &= \lim \inf_{N \to \infty} \frac{1}{N} S^{\mathscr{S}}(\varphi;\alpha^{N}), \\ \tilde{S}^{\mathscr{S}}(\Lambda^{*}\varphi;\theta_{\mathscr{B}},\beta) &= \lim \inf_{N \to \infty} \frac{1}{N} S^{\mathscr{S}}(\Lambda^{*}\varphi;\beta_{\Lambda}^{N}), \\ \tilde{I}^{\mathscr{S}}(\varphi;\Lambda^{*},\theta_{\mathscr{A}},\theta_{\mathscr{B}},\alpha,\beta) &= \lim \inf_{N \to \infty} \frac{1}{N} I^{\mathscr{S}}(\varphi;\alpha^{N},\beta^{N}). \end{split}$$

The fundamental inequalities with respect to  $\tilde{S}^{\mathscr{S}}(\varphi; \theta_{\mathscr{A}}), \ \tilde{S}^{\mathscr{S}}(\Lambda^*\varphi; \theta_{\mathscr{B}})$ , and  $\tilde{I}^{\mathscr{S}}(\varphi; \Lambda^*, \theta_{\mathscr{A}}, \theta_{\mathscr{B}})$  are held in [35].

#### **Proposition 1**

$$0 \leq \tilde{I}^{\mathscr{S}}(\varphi; \Lambda^*, \theta_{\mathscr{A}}, \theta_{\mathscr{B}}) \leq \min\{\tilde{S}^{\mathscr{S}}(\varphi; \theta_{\mathscr{A}}), \tilde{S}^{\mathscr{S}}(\Lambda^*\varphi; \theta_{\mathscr{B}})\}$$

Since these functionals are given by using a channel transformation, they contain the dynamical entropy (e.g., usual K-S entropies) as a special case [28, 35].

**Proposition 2** If  $\mathcal{A}_k$ ,  $\mathcal{A}$  are abelian  $C^*$ -algebras and each  $\alpha_k$  is an embedding, then our functionals coincide with classical K-S entropies:

$$S_{\mu}^{\mathfrak{S}(\mathscr{A})}(\varphi; \ \alpha^{M}) = S_{\mu}^{\text{classical}} \begin{pmatrix} M \\ m=1 \\ \tilde{A}_{m} \end{pmatrix},$$
$$I_{\mu}^{\mathfrak{S}(\mathscr{A})}(\varphi; \ \alpha^{M}, \beta_{id}^{N}) = I_{\mu}^{\text{classical}} \begin{pmatrix} M \\ m=1 \\ \tilde{A}_{m}, n=1 \\ \tilde{B}_{n} \end{pmatrix}$$

for any finite partitions  $\tilde{A}_m$ ,  $\tilde{B}_n$  of a probability space  $(\Omega, \mathfrak{F}, \varphi)$ .

In general quantum systems, the following theorems are proved in [28, 35].

**Theorem 7** Let  $\alpha_m$  be a sequence of completely positive maps  $\alpha_m : \mathcal{A}_m \to \mathcal{A}$  such that there exist completely positive maps  $\alpha'_m : \mathcal{A} \to \mathcal{A}_m$  satisfying  $\alpha_m \circ \alpha'_m \to id_{\mathcal{A}}$  in the pointwise topology. Then

$$\tilde{S}^{\mathscr{S}}(\varphi; \ \theta_{\mathscr{A}}) = \lim_{m \to \infty} \tilde{S}^{\mathscr{S}}(\varphi; \ \theta_{\mathscr{A}}, \alpha_m).$$

**Theorem 8** Let  $\alpha_m$  and  $\beta_m$  be sequences of completely positive maps  $\alpha_m : \mathscr{A}_m \to \mathscr{A}$  and  $\beta_m : \mathscr{B}_m \to \mathscr{B}$  such that there exist completely positive maps  $\alpha'_m : \mathscr{A} \to \mathscr{A}_m$  and  $\beta'_m : \mathscr{B} \to \mathscr{B}_m$  satisfying  $\alpha_m \circ \alpha'_m \to id_{\mathscr{A}}$  and  $\beta_m \circ \beta'_m \to id_{\mathscr{B}}$  in the pointwise topology. Then one has

$$\tilde{I}^{\mathscr{S}}(\varphi;\Lambda^*,\theta_{\mathscr{A}},\theta_{\mathscr{B}}) = \lim_{m \to \infty} \tilde{I}^{\mathscr{S}}(\varphi;\Lambda^*,\theta_{\mathscr{A}},\theta_{\mathscr{B}},\alpha_m,\beta_m).$$

The above theorems show Kolmogorov–Sinai-type convergence theorems for the entropy and the mutual entropy [28, 29, 34, 35]. Based on these settings, one can study Shannon's coding theorems in quantum compound systems by using the quantum capacity [36–39, 41–44].

# 6 Computation of Mean Entropy and Mean Mutual Entropy for Open System Dynamics

We here calculate the mean entropy and the mean mutual entropy for open system dynamics based on [54].

For a stationary initial states  $\rho = \sum_{m} \eta_{m} \bigotimes_{i=-\infty}^{\infty} \rho_{i}^{(m)} \in \mathfrak{S}\left(\bigotimes_{i=-\infty}^{\infty} \mathscr{H}_{1}\right)$  and  $\xi = \sum_{m'} \omega_{m'} \bigotimes_{j=-\infty}^{\infty} \xi_{j}^{(m')} \in \mathfrak{S}\left(\bigotimes_{j=-\infty}^{\infty} \mathscr{H}_{2}\right)$ , let  $\rho_{i}^{(m)} = \sum_{n_{i}=1}^{M} \lambda_{n_{i}}^{(m)} E_{n_{i}} \in \mathfrak{S}(\mathscr{H}_{1})$  and  $\xi_{j}^{(m')} = \sum_{n_{i}=1}^{M} \mu_{n_{i}}^{(m')} F_{n_{i}} \in \mathfrak{S}(\mathscr{H}_{2})$ . Then we have two compound states
$$\Phi_E(\alpha^N) = \sum_{n_0=1}^M \cdots \sum_{n_{N-1}=1}^M \left( \sum_m \eta_m \prod_{k=0}^{N-1} \lambda_{n_k}^{(m)} \right) \left( \bigotimes_{i=0}^{N-1} E_{n_i} \right),$$
  
$$\Phi_E(\beta_{\Lambda_t}^N) = \sum_{n_0=1}^M \cdots \sum_{n_{N-1}=1}^M \left( \sum_m \eta_m \prod_{k=0}^{N-1} \lambda_{n_k}^{(m)} \right) \left( \bigotimes_{i=0}^{N-1} \Lambda_t^* E_{n_i} \right).$$

When  $\Lambda_t^*$  is the quantum channel given by the above open system dynamics in Sect. 2.6, we get

$$\Lambda_t^* E_{n_i} = \sum_{j_i=0}^{n_i} \sum_{\ell_i=L_i}^{j_i} \mu_{\ell_i-n_i+j_i}^{(m)} |\tau_{j_i,n_i}^{(\ell_i+j_i)}(t)|^2 F_{j_i},$$

where  $F_{j_i} = |j_i| > \langle j_i|$  is the  $j_i$ -photon number state in  $\mathfrak{S}(\mathscr{H}_2)$ . Two compound states through the channel  $\Lambda_t^*$  of open system dynamics are obtained by

$$\Phi_{E}(\alpha^{N} \cup \beta_{\Lambda_{t}}^{N}) = \sum_{n_{0}=1}^{M} \cdots \sum_{n_{N-1}=1}^{M} \left( \sum_{m} \eta_{m} \prod_{k=0}^{N-1} \lambda_{n_{k}}^{(m)} \right) \\
\times \sum_{j_{0}=0}^{n_{0}} \cdots \sum_{j_{N-1}=0}^{n_{N-1}} \left( \prod_{k'=0}^{N-1} \left( \sum_{\ell_{k'}=L_{k'}}^{j_{k'}} \mu_{\ell_{k'}-n_{k'}+j_{k'}}^{(m)} |\tau_{j_{k'},n_{k'}}^{(\ell_{k'}+j_{k'})}(t)|^{2} \right) \right) \\
\times \left( \bigotimes_{i=0}^{N-1} E_{n_{i}} \right) \left( \bigotimes_{i'=0}^{N-1} F_{j_{i'}} \right)$$
(12)

$$\Phi_{E}(\alpha^{N}) \otimes \Phi_{E}(\beta^{N}_{\Lambda_{t}}) 
= \sum_{n_{0}=1}^{M} \cdots \sum_{n_{N-1}=1}^{M} \left( \sum_{m} \eta_{m} \prod_{k=0}^{N-1} \lambda^{(m)}_{n_{k}} \right) 
\times \sum_{n'_{0}=1}^{M} \cdots \sum_{n'_{N-1}=1}^{M} \left( \sum_{m'} \eta_{m'} \prod_{k'=0}^{N-1} \lambda^{(m')}_{n'_{k'}} \right) 
\times \sum_{j'_{0}=0}^{n'_{0}} \cdots \sum_{j'_{N-1}=0}^{M} \left( \prod_{k''=0}^{N-1} \left( \sum_{\ell_{k''}=L_{k''}}^{j'_{k''}} \mu^{(m')}_{\ell_{k''}-n'_{k''}+j'_{k''}} |\tau^{(\ell_{k''}+j'_{k''})}_{j'_{k''},n'_{k''}}(t)|^{2} \right) \right) 
\times \left( \bigotimes_{i=0}^{N-1} E_{n_{i}} \right) \left( \bigotimes_{i'=0}^{N-1} F_{j'_{i'}} \right)$$
(13)

On Complexity for Open System Dynamics

**Lemma 1** For a stationary initial state  $\rho = \sum_m \eta_m \bigotimes_{i=-\infty}^{\infty} \rho_i^{(m)} \in \mathfrak{S}\left(\bigotimes_{i=-\infty}^{\infty} \mathscr{H}_1\right)$ , we have

$$\begin{split} I_{E}(\rho; \Lambda_{t}^{*}, \alpha^{N}, \beta^{N}) &= \sum_{j_{0}=0}^{M} \cdots \sum_{j_{N-1}=0}^{M} \sum_{n_{0}=J_{0}}^{M} \cdots \sum_{n_{N-1}=J_{N-1}}^{M} \left( \sum_{m} \eta_{m} \prod_{k=0}^{N-1} \lambda_{n_{k}} \right) \\ &\times \left( \prod_{k'=0}^{N-1} \left( \sum_{\ell_{k'}=L_{k'}}^{j_{k'}} \mu_{\ell_{k'}-n_{k'}+j_{k'}}^{(m)} |\tau_{j_{k'},n_{k'}}^{(\ell_{k'}+j_{k'})}(t)|^{2} \right) \right) \right) \\ &\times \log \left( \frac{\left( \prod_{k'=0}^{N-1} \left( \sum_{\ell_{k'}=L_{k'}}^{j_{k'}} \mu_{\ell_{k'}-n_{k'}+j_{k'}}^{(m)} |\tau_{j_{k'},n_{k'}}^{(\ell_{k'}+j_{k'})}(t)|^{2} \right) \right)}{\sum_{n'_{0}=J_{0}}^{M} \cdots \sum_{n'_{N-1}=J_{N-1}}^{M} \left( \sum_{m'} \eta_{m'} \prod_{k'=0}^{N-1} \lambda_{n'_{k'}}^{(m')} \right) \\ &\frac{1}{\left( \prod_{k'=0}^{N-1} \left( \sum_{\ell_{k''}=L_{k''}}^{j_{k''}} \mu_{\ell_{k''}-n_{k''}+j_{k''}}^{(m')} |\tau_{j_{k'},n_{k''}}^{(\ell_{k''}+j_{k''})}(t)|^{2} \right) \right)} \right). \end{split}$$

By using the above lemma, we have the following theorem.

#### **Theorem 9**

(1) For a stationary initial state  $\rho = \sum_{m} \eta_{m} \bigotimes_{i=-\infty}^{\infty} \rho_{i}^{(m)} \in \mathfrak{S}\left(\bigotimes_{i=-\infty}^{\infty} \mathscr{H}_{1}\right)$ , we have the lower bound of  $\tilde{S}(\rho; \theta_{\mathscr{A}}, \alpha^{N})$  such as

$$\tilde{S}(\rho; \theta_{\mathscr{A}}, \alpha^N) \ge \sum_m \eta_m S\left(\rho_0^{(m)}\right).$$

(2) If  $\eta_0 = 1$ ,  $\eta_k = 0$  ( $\forall k \ge 1$ ), and  $\lambda_{n_i}^{(0)} = \lambda_{n_i}$  of  $\rho = \sum_m \eta_m \bigotimes_{i=-\infty}^{\infty} \rho_i^{(m)}$ , then

$$\tilde{S}(\rho; \theta_{\mathscr{A}}, \alpha^{N}) = \lim_{N \to \infty} \frac{1}{N} S(\rho; \alpha^{N}) = -\sum_{n=1}^{M} \lambda_{n} \log \lambda_{n}$$

and

$$\tilde{I}(\rho; \Lambda_{t}^{*}, \theta_{\mathscr{A}}, \theta_{\mathscr{B}}, \alpha^{N}, \beta^{N}) = \sum_{j=1}^{M} \sum_{n=J}^{M} \lambda_{n} \left( \sum_{\ell=L}^{j} \mu_{\ell-n+j}^{(0)} |\tau_{j,n}^{(\ell+j)}(t)|^{2} \right) \\ \times \log \frac{\left( \sum_{\ell=L}^{j} \mu_{\ell-n+j}^{(0)} |\tau_{j,n}^{(\ell+j)}(t)|^{2} \right)}{\sum_{n'=J}^{M} \lambda_{n'} \left( \sum_{\ell'=L}^{j} \mu_{\ell'-n'+j}^{(0)} |\tau_{j,n'}^{(\ell'+j)}(t)|^{2} \right)}.$$

## 7 Quantum Dynamical Entropy for CP Maps

According to [26, 52], we explain the formulation of the KOW entropy.

Let  $\mathscr{A}$  and  $\mathscr{B}$  be the full algebras  $\mathbf{B}(\mathscr{H})$  and  $\mathbf{B}(\mathscr{H})$ , respectively. Let  $\omega$  be a normal state on  $\mathscr{B}$  and  $\Gamma$  be a normal, unital CP linear map from  $\mathscr{B} \otimes \mathscr{A}$  to  $\mathscr{B} \otimes \mathscr{A}$ . For any normal states  $\varphi$  on  $\mathscr{A}$ , a transition expectation  $E^{\Gamma,\omega}$  from  $\mathscr{B} \otimes \mathscr{A}$  to  $\mathscr{A}$  is defined by

$$\varphi\left(E^{\Gamma,\omega}\left(\widetilde{A}\right)\right) \equiv \left(\omega \otimes \varphi\right)\left(\Gamma\left(\widetilde{A}\right)\right) = \operatorname{tr}_{\mathscr{K} \otimes \mathscr{H}}\left[\left(\widetilde{\omega} \otimes \widetilde{\varphi}\right)\Gamma\left(\widetilde{A}\right)\right]$$

for any  $\widetilde{A} \in \mathscr{B} \otimes \mathscr{A}$  in the sense of [2, 26], where  $\widetilde{\omega} \in \mathfrak{S}(\mathscr{K})$  and  $\widetilde{\varphi} \in \mathfrak{S}(\mathscr{H})$  are density operators associated with  $\omega$  and  $\varphi$ . The dual map  $E^{*\Gamma,\omega}$  of  $E^{\Gamma,\omega}$ 

$$E^{*\Gamma,\omega}\left(\varphi\right)\left(\widetilde{A}\right)=\varphi\left(E^{\Gamma,\omega}\left(\widetilde{A}\right)\right),\quad\widetilde{A}\in\mathscr{B}\otimes\mathscr{A}$$

is a lifting from  $\mathfrak{S}(\mathscr{A})$  to  $\mathfrak{S}(\mathscr{B}\otimes\mathscr{A})$  in the sense of Accardi and Ohya [2]. Then it represents

$$E^{*\Gamma,\omega}\left(\widetilde{\varphi}\right) = \Gamma^*\left(\widetilde{\omega}\otimes\widetilde{\varphi}\right), \quad \widetilde{\varphi}\in\mathfrak{S}\left(\mathscr{H}\right)$$

Let  $\Lambda$  be a normal, unital CP map from  $\mathscr{A}$  to  $\mathscr{A}$  and id be the identity map on  $\mathscr{B}$ .  $\varphi\left(E_{\Lambda}^{\Gamma,\omega}\left(\widetilde{A}\right)\right)$  is described by

$$\varphi\left(E_{\Lambda}^{\Gamma,\omega}\left(\widetilde{A}\right)\right) = (\omega \otimes \varphi)\left((id \otimes \Lambda) \Gamma\left(\widetilde{A}\right)\right)$$
$$= \operatorname{tr}_{\mathscr{K} \otimes \mathscr{K}}\left[\left(\widetilde{\omega} \otimes \Lambda^{*}\left(\widetilde{\varphi}\right)\right) \Gamma\left(\widetilde{A}\right)\right]$$

for any normal states  $\varphi$  and any  $\widetilde{A} \in \mathcal{B} \otimes \mathcal{A}$ , where  $id \otimes \Lambda$  is a normal, unital CP map from  $\mathcal{B} \otimes \mathcal{A}$  to  $\mathcal{B} \otimes \mathcal{A}$  and  $\Lambda^*$  is a quantum channel [2, 23, 30, 37, 39, 42] from  $\mathfrak{S}(\mathcal{H})$  to  $\mathfrak{S}(\mathcal{H})$  with respect to an input signal state  $\tilde{\varphi}$  and a noise state  $\tilde{\omega}$ . The dual map  $E_{\Lambda}^{*\Gamma,\omega}$  of  $E_{\Lambda}^{\Gamma,\omega}$  is a lifting from  $\mathfrak{S}(\mathcal{A})$  to  $\mathfrak{S}(\mathcal{B} \otimes \mathcal{A})$  given by

$$E_{\Lambda}^{*\Gamma,\omega}(\varphi)\left(\widetilde{A}\right) = \varphi\left(E_{\Lambda}^{\Gamma,\omega}\left(\widetilde{A}\right)\right), \quad \widetilde{A} \in \mathscr{B} \otimes \mathscr{A}.$$

Then it represents

$$E_{\Lambda}^{*\Gamma,\omega}\left(\widetilde{\varphi}\right) = \Gamma^{*}\left(\widetilde{\omega} \otimes \Lambda^{*}\left(\widetilde{\varphi}\right)\right), \quad \widetilde{\varphi} \in \mathfrak{S}\left(\mathscr{H}\right)$$

Based on the following relation

$$\varphi\left(E_{\Lambda}^{\Gamma,\omega}\left(A_{1}\otimes E_{\Lambda}^{\Gamma,\omega}\left(A_{2}\otimes\cdots\otimes E_{\Lambda}^{\Gamma,\omega}\left(A_{n-1}\otimes E_{\Lambda}^{\Gamma,\omega}\left(A_{n}\otimes B\right)\right)\cdots\right)\right)\right)$$
$$=\varPhi_{\Lambda,n}^{*\Gamma,\omega}(\varphi)\left(A_{1}\otimes\cdots\otimes A_{n}\otimes B\right)$$
$$=\operatorname{tr}_{\left(\otimes_{1}^{n}\mathscr{K}\right)\otimes\mathscr{K}}\widetilde{\varPhi}_{\Lambda,n}^{*\Gamma,\omega}(\widetilde{\varphi})\left(A_{1}\otimes\cdots\otimes A_{n}\otimes B\right)$$

for all  $A_1, A_2, \dots, A_n \in \mathcal{B}, B \in \mathcal{A}$ , and any  $\varphi \in \mathfrak{S}(\mathcal{A})$ , a lifting  $\Phi_{A,n}^{*\Gamma,\omega}$  from  $\mathfrak{S}(\mathcal{A})$  to  $\mathfrak{S}((\bigotimes_{n=1}^{n} \mathcal{B}) \otimes \mathcal{A})$  and marginal states are given by

$$\psi_{\Lambda,n}^{\Gamma,\omega} (A_1 \otimes \cdots \otimes A_n) = \Phi_{\Lambda,n}^{*\Gamma,\omega} (\varphi) (A_1 \otimes \cdots \otimes A_n \otimes I) (A_1, \cdots, A_n \in \mathscr{B})$$
  
$$\varphi_{\Lambda,n}^{\Gamma,\omega} (B) = \Phi_{\Lambda,n}^{*\Gamma,\omega} (\varphi) (I \otimes \cdots \otimes I \otimes B) \qquad (B \in \mathscr{A})$$

For any  $\widetilde{\varphi} \in \mathfrak{S}(\mathscr{H})$ , a lifting  $\widetilde{\Phi}_{\Lambda,n}^{*\Gamma,\omega}$  from  $\mathfrak{S}(\mathscr{H})$  to  $\mathfrak{S}((\otimes_1^n \mathscr{H}) \otimes \mathscr{H})$  and marginal states

$$\sigma_{\Lambda,n}^{\Gamma,\omega} = \operatorname{tr}_{\mathscr{H}} \widetilde{\Phi}_{\Lambda,n}^{*\Gamma,\omega}(\widetilde{\varphi}) \in \mathfrak{S}\left(\otimes_{1}^{n} \mathscr{K}\right) \text{ and } \rho_{\Lambda,n}^{\Gamma,\omega} = \operatorname{tr}_{\otimes_{1}^{n} \mathscr{K}} \Phi_{\Lambda,n}^{*\Gamma,\omega}(\widetilde{\varphi}) \in \mathfrak{S}\left(\mathscr{H}\right)$$

are obtained, where  $\Phi_{\Lambda,n}^{*\Gamma,\omega}(\varphi)$  (resp.  $\Phi_{\Lambda,n}^{*\Gamma,\omega}(\widetilde{\varphi})$ ) is a compound state with respect to  $\psi_{\Lambda,n}^{\Gamma,\omega}$  (resp.  $\sigma_{\Lambda,n}^{\Gamma,\omega}$ ) and  $\varphi_{\Lambda,n}^{\Gamma,\omega}$  (resp.  $\rho_{\Lambda,n}^{\Gamma,\omega}$ ) in the sense of [26, 52].

**Definition 1** The quantum dynamical entropy with respect to  $\Lambda$ ,  $\varphi$ ,  $\Gamma$ , and  $\omega$  is defined by

$$\tilde{S}(\Lambda;\varphi,\Gamma,\omega) \equiv \limsup_{n\to\infty} \frac{1}{n} S\left(\varphi_{\Lambda,n}^{\Gamma,\omega}\right),$$

where  $S\left(\varphi_{\Lambda,n}^{\Gamma,\omega}\right)$  is the  $\mathscr{S}$ -mixing entropy of  $\varphi_{\Lambda,n}^{\Gamma,\omega} \in \mathfrak{S}\left(\otimes_{1}^{n}\mathscr{B}\right)$  given by  $S\left(\varphi_{\Lambda,n}^{\Gamma,\omega}\right) = -tr\widetilde{\varphi}_{\Lambda,n}^{\Gamma,\omega}\log\widetilde{\varphi}_{\Lambda,n}^{\Gamma,\omega}$ . The dynamical entropy with respect to  $\Lambda$  and  $\varphi$  is defined as

$$\tilde{S}(\Lambda;\varphi) \equiv \sup \{S(\Lambda;\varphi,\Gamma,\omega);\Gamma,\omega\}.$$

## 7.1 Generalized AF and Generalized AOW Dynamical Entropies

Here we briefly review the formulation of the generalized AF entropy and the generalized AOW entropy given by the KOW entropy [26]. Transition expectations  $E_{\Lambda}^{\gamma}$  from  $M_d \otimes \mathscr{A}$  to  $\mathscr{A}$  and  $E_{\Lambda}^{\gamma(0)}$  from  $M_d^0 \otimes \mathscr{A}$  to  $\mathscr{A}$  are defined by

$$E_{\Lambda}^{\gamma}\left(\sum_{i,j=1}^{d} E_{ij} \otimes A_{ij}\right) = \sum_{i,j=1}^{d} \Lambda\left(\gamma_{i}^{*}A_{ij}\gamma_{j}\right),$$
$$E_{\Lambda}^{\gamma(0)}\left(\sum_{i,j=1}^{d} E_{ij} \otimes A_{ij}\right) = \sum_{i=1}^{d} \Lambda\left(\gamma_{i}^{*}A_{ii}\gamma_{i}\right)$$

for a finite operational partition of unity  $\gamma_1, \dots, \gamma_d \in \mathscr{A}(=\mathbf{B}(\mathscr{H}))$ , i.e.,  $\sum_{i=1}^d \gamma_i^* \gamma_i = I$ , and a normal unital CP map  $\Lambda$  from  $\mathscr{A}$  to  $\mathscr{A}$ , where  $E_{ij} = |e_i\rangle \langle e_j|$ with normalized vectors  $e_i \in \mathscr{H}$ ,  $i = 1, 2, \dots, d \leq \dim \mathscr{H}$ ,  $M_d$  in  $\mathscr{A}$  is the  $d \times d$  matrix algebra and  $M_d^0$  is a subalgebra of  $M_d$  consisting of diagonal elements of  $M_d$ . The liftings  $E_{\Lambda}^{\gamma*}$  from  $\mathfrak{S}(A)$  to  $\mathfrak{S}(M_d \otimes \mathscr{A})$  and  $E_{\Lambda}^{\gamma(0)*}$  from  $\mathfrak{S}(A)$  to  $\mathfrak{S}(M_d^0 \otimes \mathscr{A})$  are described by

$$E_{\Lambda}^{\gamma*}(\widetilde{\varphi}) = \sum_{i,j=1}^{d} E_{i,j} \otimes \gamma_{i} \Lambda^{*}(\widetilde{\varphi}) \gamma_{j}^{*},$$
$$E_{\Lambda}^{\gamma(0)*}(\widetilde{\varphi}) = \sum_{i=1}^{d} E_{ii} \otimes \gamma_{i} \Lambda^{*}(\widetilde{\varphi}) \gamma_{i}^{*}.$$

Then the quantum Markov states  $\widetilde{\varphi}_{A,n}^{\gamma}$  and  $\widetilde{\varphi}_{A,n}^{\gamma(0)}$  are obtained by

$$\widetilde{\varphi}_{\Lambda,n}^{\gamma} = \sum_{i_1,\cdots,i_n=1}^d \sum_{j_1,\cdots,j_n=1}^d \operatorname{tr}_{\mathscr{H}} \widetilde{\varphi} \Lambda \left( W_{j_1 i_1} \left( \Lambda \left( W_{j_2 i_2} \left( \cdots \Lambda \left( W_{j_n i_n} \left( I_{\mathscr{H}} \right) \right) \right) \right) \right) \right) \\ \times E_{i_1 j_1} \otimes \cdots \otimes E_{i_n j_n}$$

and

$$\widetilde{\varphi}_{\Lambda,n}^{\gamma(0)} = \sum_{i_1,\cdots,i_n=1}^d \operatorname{tr}_{\mathscr{H}} \widetilde{\varphi} \Lambda \left( W_{i_1i_1} \left( \Lambda \left( W_{i_2i_2} \left( \cdots \Lambda \left( W_{i_ni_n} \left( I_{\mathscr{H}} \right) \right) \right) \right) \right) \right) \\ \times E_{i_1i_1} \otimes \cdots \otimes E_{i_ni_n} \\ = \sum_{i_1,\cdots,i_n=1}^d p_{i_1,\cdots,i_n} E_{i_1i_1} \otimes \cdots \otimes E_{i_ni_n},$$

where

$$\begin{split} W_{ij}\left(A\right) &= \gamma_{i}^{*}A\gamma_{j}, \quad A \in \mathbf{B}\left(\mathscr{H}\right), \\ W_{ij}^{*}\left(\widetilde{\varphi}\right) &= \gamma_{j}\widetilde{\varphi}\gamma_{i}^{*}, \quad \widetilde{\varphi} \in \mathfrak{S}\left(\mathscr{H}\right), \\ p_{i_{1},\cdots,i_{n}} &= \operatorname{tr}_{\mathscr{H}}\widetilde{\varphi}\Lambda\left(W_{i_{1}i_{1}}\left(\Lambda\left(W_{i_{2}i_{2}}\left(\cdots \Lambda\left(W_{i_{n}i_{n}}\left(I_{\mathscr{H}}\right)\right)\right)\right)\right)) \\ &= \operatorname{tr}_{\mathscr{H}}W_{i_{n}i_{n}}^{*}\left(\Lambda^{*}\cdots\Lambda^{*}\left(W_{i_{2}i_{2}}^{*}\left(\Lambda^{*}\left(W_{i_{1}i_{1}}^{*}\left(\Lambda^{*}\left(\widetilde{\varphi}\right)\right)\right)\right)\right)). \end{split}$$

Based on [26], there exist CP maps  $\Xi_n^* : \widetilde{\varphi}_{\Lambda,n}^{\gamma} \to \widetilde{\varphi}_{\Lambda,n}^{\gamma(0)}$  and  $\Theta_n^* : \widetilde{\varphi}_{\Lambda,n}^{\gamma(0)} \to \widetilde{\varphi}_{\Lambda,n}^{\gamma}$ . Therefore the generalized AF entropy  $\widetilde{S}_{\mathscr{B}}(\Lambda; \varphi)$  and the generalized AOW entropy  $\widetilde{S}_{\mathscr{B}}^{(0)}(\Lambda; \varphi)$  of  $\Lambda$  and  $\varphi$  with respect to a finite-dimensional subalgebra  $\mathscr{B} \subset \mathbf{B}(\mathscr{H})$  are defined by

$$\tilde{S}_{\mathscr{B}}(\Lambda;\varphi) = \sup_{\{\gamma_i\}\subset\mathscr{B}} \tilde{S}(\Lambda;\varphi,\{\gamma_i\}),$$
$$\tilde{S}_{\mathscr{B}}^{(0)}(\Lambda;\varphi) = \sup_{\{\gamma_i\}\subset\mathscr{B}} \tilde{S}^{(0)}(\Lambda;\varphi,\{\gamma_i\}),$$

where the dynamical entropies  $\tilde{S}(\Lambda; \varphi, \{\gamma_i\})$  and  $\tilde{S}^{(0)}(\Lambda; \varphi, \{\gamma_i\})$  are obtained by

$$\tilde{S}(\Lambda;\varphi,\{\gamma_i\}) = \limsup_{n \to \infty} \frac{1}{n} S\left(\varphi_{\Lambda,n}^{\gamma}\right),$$
$$\tilde{S}^{(0)}(\Lambda;\varphi,\{\gamma_i\}) = \limsup_{n \to \infty} \frac{1}{n} S\left(\varphi_{\Lambda,n}^{\gamma(0)}\right).$$

Then the following theorem [26] is held:

#### Theorem 10

$$\tilde{S}_{\mathscr{B}}(\Lambda;\varphi) \leq \tilde{S}_{\mathscr{B}}^{(0)}(\Lambda;\varphi)$$
.

 $\tilde{S}_{\mathscr{B}}^{(0)}(\Lambda;\varphi)$  is equal to the AOW entropy if  $\{\gamma_i\}$  is PVM (projection-valued measure) and  $\Lambda$  is given by an automorphism  $\theta$ .  $\tilde{S}_{\mathscr{B}}(\Lambda;\varphi)$  is equal to the AF entropy if  $\{\gamma_i^*\gamma_i\}$  is POV (positive-operator-valued measure) and  $\Lambda$  is given by an automorphism  $\theta$ .

## 8 Calculation of Generalized AOW Dynamical Entropy for Open System Dynamics

We here compute the generalized AOW entropy for open system dynamics according to [55].

Let  $\rho$  and  $\xi$  be

$$\rho = \widetilde{\varphi} = \sum_{n=1}^{M} \lambda_n E_n \in \mathfrak{S}(\mathscr{H}_1) \quad \text{and} \quad \xi = \widetilde{\omega} = \sum_{k=1}^{M} \mu_k F_k \in \mathfrak{S}(\mathscr{H}_2).$$

For  $\gamma_j = |x_j\rangle \langle x_j|$  ({ $|x_j\rangle$ } is a CONS in  $\mathcal{H}_2$ ), the output state of  $\Lambda_t^*$  is obtained by

$$\Lambda_{t}^{*}(\widetilde{\varphi}) = \sum_{n=1}^{M} \lambda_{n} \Lambda_{t}^{*} E_{n} = \sum_{n=1}^{M} \lambda_{n} \sum_{m=0}^{n} \sum_{\ell=L}^{m} \mu_{\ell-n+m} |\tau_{m,n}^{(\ell+m)}(t)|^{2} F_{m},$$
$$= \sum_{m=0}^{M} \left( \sum_{n=m}^{M} \lambda_{n} \sum_{\ell=L}^{m} \mu_{\ell-n+m} |\tau_{m,n}^{(\ell+m)}(t)|^{2} \right) F_{m}$$

$$W_{jj}^{*}\left(\Lambda_{t}^{*}\left(\widetilde{\varphi}\right)\right) = \gamma_{j}^{*}\Lambda_{t}^{*}\left(\widetilde{\varphi}\right)\gamma_{j}$$
$$= \sum_{k=0}^{M} \left(\sum_{n=m}^{M} \lambda_{n} \sum_{\ell=L}^{m} \mu_{\ell-n+m} |\tau_{m,n}^{(\ell+m)}\left(t\right)|^{2}\right) \left|\left\langle m, x_{j}\right\rangle\right|^{2} |x_{j}\rangle \langle x_{j}|.$$

$$\begin{split} &\Lambda_{t}^{*}\left(W_{j_{1}j_{1}}^{*}\left(\Lambda_{t}^{*}\left(\widetilde{\varphi}\right)\right)\right) \\ &= \sum_{m_{1}=0}^{M}\left[\sum_{n_{1}=k_{1}}^{M}\lambda_{n_{1}}\sum_{\ell_{1}=L_{1}}^{m_{1}}\mu_{\ell_{1}-n_{1}+m_{1}}|\tau_{m_{1},n_{1}}^{(\ell_{1}+m_{1})}\left(t\right)|^{2}\right]\left|\left\langle m_{1},x_{j_{1}}\right\rangle\right|^{2} \\ &\times\left[\sum_{m_{2}=0}^{j_{1}}\sum_{\ell_{2}=L_{2}}^{m_{2}}\mu_{\ell_{2}-j_{1}+m_{2}}|\tau_{m_{2},j_{1}}^{(\ell_{2}+m_{2})}\left(t\right)|^{2}\right]F_{m_{2}}, \end{split}$$

$$W_{j_{2}j_{2}}^{*}\left(\Lambda_{t}^{*}\left(W_{j_{1}j_{1}}^{*}\left(\Lambda_{t}^{*}\left(\widetilde{\varphi}\right)\right)\right)\right)$$

$$=\gamma_{j_{2}}^{*}\Lambda_{t}^{*}\left(W_{j_{1}j_{1}}^{*}\left(\Lambda_{t}^{*}\left(\widetilde{\varphi}\right)\right)\right)\gamma_{j_{2}}$$

$$=\sum_{n_{1}=1}^{M}\lambda_{n_{1}}\left[\sum_{m_{1}=0}^{n_{1}}\sum_{\ell_{1}=L_{1}}^{m_{1}}\mu_{\ell_{1}-n_{1}+m_{1}}|\tau_{m_{1},n_{1}}^{(\ell_{1}+m_{1})}\left(t\right)|^{2}\left|\left\langle m_{1},x_{j_{1}}\right\rangle\right|^{2}\right]$$

$$\times\left[\sum_{j_{2}=0}^{j_{1}}\sum_{\ell_{2}=L_{2}}^{j_{2}}\mu_{\ell_{2}-j_{1}+m_{2}}|\tau_{m_{2},j_{1}}^{(\ell_{2}+m_{2})}\left(t\right)|^{2}\left|\left\langle m_{2},x_{j_{2}}\right\rangle\right|^{2}\right]|x_{j_{2}}\rangle\langle x_{j_{2}}|$$

are satisfied for  $n \ge 3$ . Then the above compound state  $\widetilde{\varphi}^{\gamma(0)}_{A_t,n}$  is written by

$$\widetilde{\varphi}_{A_t,n}^{\gamma(0)} = \sum_{j_1,\cdots,j_n=1}^M q_{j_1,\cdots,j_n}(t) \bigotimes_{k=1}^n |x_{j_k}\rangle \langle x_{j_k}|,$$

where

$$q_{j_1,\dots,j_n}(t) = tr_{\mathscr{H}} W_{j_n j_n}^* \left( \Lambda_t^* \left( \cdots \Lambda_t^* \left( W_{j_2 j_2}^* \left( \Lambda_t^* \left( W_{j_1 j_1}^* \left( \Lambda_t^* \left( \widetilde{\varphi} \right) \right) \right) \right) \cdots \right) \right) \right).$$

Based on [26, 52], one can obtain

$$\Lambda_{t}^{*}(|x_{j}\rangle\langle x_{j}|) = \sum_{m=0}^{j} \sum_{\ell=L}^{m} \mu_{\ell-j+m} |\tau_{k,j}^{(\ell+m)}(t)|^{2} F_{k},$$

On Complexity for Open System Dynamics

$$\begin{aligned} q_{j_1,\dots,j_n}(t) &= \prod_{k=2}^n \left( \sum_{m_k=0}^{j_{k-1}} \sum_{\ell_k=L_k}^{m_k} \mu_{\ell_k - j_{k-1} + m_k} |\tau_{m_k,j_{k-1}}^{(\ell_k + m_k)}(t)|^2 \left| \langle m_k, x_{j_k} \rangle \right|^2 \right) \\ &\times \left( \sum_{n_1=1}^M \lambda_{n_1} \sum_{m_1=0}^{n_1} \sum_{\ell_1=L_1}^{m_1} \mu_{\ell_1 - n_1 + m_1} |\tau_{m_1,n_1}^{(\ell_1 + m_1)}(t)|^2 \left| \langle m_1, x_{j_1} \rangle \right|^2 \right) \\ &= \prod_{k=2}^n q_{j_k,j_{k-1}}(t) q_{j_1}(t) . \end{aligned}$$

Thus we have the following theorem.

**Theorem 11** When  $\varphi$  and  $\omega$  are normal states given by

$$\varphi(A) = tr\left[\widetilde{\varphi}A\right] = tr\left[\left(\sum_{n=1}^{M} \lambda_n E_n\right)A\right] \quad (\forall A \in \mathscr{A}),$$
$$\omega(B) = tr\left[\widetilde{\omega}B\right] = tr\left[\left(\sum_{m=1}^{M} \mu_m F_m\right)B\right] \quad (\forall B \in \mathscr{B})$$

and  $\Lambda_t^*$  is the quantum channel of open system dynamics satisfying the condition  $\sum_j q_{k,j}(t) q_j(t) = q_k(t)$ , the quantum dynamical entropy with respect to  $\Lambda_t$ ,  $\varphi$ , and  $\{\gamma_i\}$  is obtained by

$$\tilde{S}^{(0)}\left(\Lambda_t;\varphi,\left\{\gamma_j\right\}\right) = -\sum_{j,k} q_{k,j}(t)q_j(t)\log q_{k,j}(t),$$

where

$$q_j(t) = \sum_{n_1=1}^M \lambda_{n_1} \sum_{m_1=0}^{n_1} \sum_{\ell_1=L_1}^{m_1} \mu_{\ell_1-n_1+m_1} |\tau_{k_1,n_1}^{(\ell_1+m_1)}(t)|^2 |\langle m_1, x_j \rangle|^2$$

and

$$q_{k,j}(t) = \sum_{m_k=0}^{j} \sum_{\ell_k=L_k}^{m_k} \mu_{\ell_k-j+m_k} |\tau_{m_k,j}^{(\ell_k+m_k)}(t)|^2 |\langle m_k, x_k \rangle|^2.$$

## 9 Conclusion

We explained the quantum channels associated with the open system dynamics and the quantum communication processes. Some examples of quantum communication channels are discussed. The quantum mutual entropy by Ohya is treated for purely quantum systems, and semiclassical mutual entropy is a special case of the quantum mutual entropy. We briefly reviewed the mean entropy and the mean mutual entropy for general quantum systems. The lower bound of the mean entropy for the open system dynamics is obtained. For a given assumption, the mean entropy and the mean mutual entropy for the open system dynamics are calculated. We briefly review the definition of the KOW dynamical entropy and the formulation of the generalized AF and AOW entropies, and we calculate the generalized AOW dynamical entropy for a simple model of open system dynamics.

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# **Bell Correlations and the Common Future**



Ämin Baumeler, Julien Degorre, and Stefan Wolf

## 1 Introduction

Reichenbach's principle [46] states that, in a fixed causal structure, correlations either stem from a *common cause* or from one part *directly influencing* the other. The principle looks natural since it imagines a *mechanism* that leads to the correlations. Bell's theorems [9, 10] limit the explanatory power of a *common cause* in the form of *classical* information, while quantum theory predicts correlations beyond that so-called Bell non-local correlations (see also [14]). But then, strangely enough, not all correlations compatible with no-signaling are attainable in nature: An example of an idealization beyond what quantum physics predicts are PR correlations [43], i.e., binary inputs *X*, *Y* and outputs *A*, *B* satisfying  $A \oplus B = XY$ .

The absence of a *mechanism* behind Bell non-local correlations is disturbing, and several patches have been proposed: One can loosen Reichenbach's principle and simply regard the quantum state as a common cause (then, no further mechanism is to be expected) [2, 16]; one can resort to one measurement event influencing another (that would have to be an *instantaneous fine-tuned* influence in a preferred frame [4, 5, 15, 19, 48, 52]); one can assume signals to travel to the past [20, 44] or suppose the existence of multiple realities [13]—but even at that price, no striking story has been told yet.

If the data in question are never brought together, no correlation can be *seen* (Fitzi, M., 2008, personal communication). At the occasion of that necessary *rendezvous* in the future, the (physically represented) pieces of information locally

Faculty of Informatics, Università della Svizzera italiana, Lugano, Switzerland

Ä. Baumeler · J. Degorre · S. Wolf ( $\boxtimes$ )

Facoltà indipendente di Gandria, Lunga scala, Gandria, Switzerland e-mail: baumea@usi.ch; degorj@usi.ch; wolfs@usi.ch

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interact—and this *detection procedure* of the correlation may be considered its *origin*: Such violations of causality can become possible, e.g., through closed time-like curves (CTCs). CTCs are world-lines *closed* in time: A system traveling along it can meet its "younger self." CTCs are *consistent* with general relativity [32, 38]. We consider the case where all information is *classical* and all interactions *local*: The established correlations are sent to the past via a CTC as described by Deutsch [25], ending up in a classical story behind Bell non-local correlations.

This text is organized as follows. Sections 2 and 3 review specific modifications of causality, namely, Hermann's relative causality and Costa de Beauregard's retro-causality. Section 3.2 presents a new formulation of this "zigzag" model through relaxing measurement independence. Section 4 describes a simple classical mechanism simulating Bell non-local correlations. Section 5 discusses relations to previous stories (parallel lives, retro-causality, and *Viennese* "process matrices").

## 2 Relative Causality

The works of *Grete Hermann*, physicist and philosopher, have been strangely overlooked. Not only did she spot a mistake (later called "silly" by Bell) in von Neumann's [50] "proof" that quantum theory cannot be extended to yield deterministic predictions, she also provided her own arguments against such an extension—besides contributing to a better understanding of *causality*. In this context, she described the measurement process in the spirit of the *relative-state interpretation* [29, 30] of quantum theory—10 years before *Hugh Everett III* did.

Hermann's 1948 article [34] looks into the process of measuring an electron's position as described quantum-physically: If that electron interacts with a photon (described quantum-physically as well), the result is

a new wave-function which is uniquely determined by the given wave-functions: It does, therefore, not contain the uncertainty that we would have to attribute to that mystic process.<sup>1</sup>

At this stage, one would have to *measure* this new wave-function to determine the position of the electron.

Without any such new observations, the quantum-mechanical formalism leads to a progressing not visualizable braiding of the fundamental particles.<sup>2</sup>

According to Hermann, this means that

the electron, after colliding with the photon, is described by a wave-function with a sharp position only relatively to the new measurement,<sup>3</sup>

<sup>&</sup>lt;sup>1</sup>"eine neue Wellenfunktion, die eindeutig durch die beiden gegebenen Wellenfunktionen [...] bestimmt ist. [...] [S]ie enthält also nicht die Unbestimmtheit, die wir jenem mystischen [...] [P]rozess zuschreiben müßten."

<sup>&</sup>lt;sup>2</sup>"Ohne solche neuen Beobachtungen führt der quantenmechanische Formalismus zu einer immer weitergehenden, aber ganz unanschaulichen Verflechtung der Elementarteilchen."

<sup>&</sup>lt;sup>3</sup>"Erst relativ zu der neuen Messung wird der Zustand des Elektrons nach seinem Zusammenstoß mit dem Lichtquant durch eine Wellenfunktion mit scharfer Ortsangabe [...] beschrieben [,]"

and in that perspective (the key of the argument)

it, therefore, constitutes an autonomous physical system characterized by its own wavefunction immediately after the collision with the photon.<sup>4</sup>

In other words, after the interaction, the measured system's wave-function *relates* to the measurement outcome—which is in what she sees the *cause* for the electron to be at that position. Such a cause, however, cannot be brought in to give better predictions as it is only accessible to the experimenter *after* the measurement. In [35], she writes:

These causes could not have been used for predictions; they determine the system in a relative way, relatively to the observation which was obtained only at the moment of the measurement. They, therefore, could be accessed after this observation only and do, hence, not allow to predict the outcome.<sup>5</sup>

Through these thoughts, Hermann anticipates Everett's formalism [29, 30] and, at the same time, *disentangles causality and predictability*. More specifically, Hermann [36] describes an ontology in which a measurement entangles the observed object to the apparatus, and only *relative statements* are possible. Everett goes beyond Hermann's view by invoking the *wave-function of the whole universe*. His formalism has often been called "many worlds": Whenever a system gets entangled with the apparatus, all possible results are realized in *parallel* universes—a view brought forward, for example, by DeWitt and Deutsch [26, 28]. This is a leftover of *classical* concepts: "The coëxisting branches [...] can only be related to 'worlds' described by classical physics. [...] [T]he [...] meaning of Everett's ideas is not the coëxistence of many [classical] worlds, but on the contrary, the existence of a *single quantum one*" [39].

A variation of the Hermann/Everett theme are "*parallel lives*" [13]: Instead of *globally*, the individual experimenters split *locally* into "bubbles" that are later only visible to each other if the quantum predictions result—the model is local *and* realistic.

If one incorporates time into the description, then a *timeless* wave-function of the universe as a whole can be imagined [41, 53]: The state of *one* part of the universe is determined relatively to *another*, called "clock." By that, all dynamics (the Schrödinger equation) can be cast in *static form: Relatively* to the clock, the systems undergo the quantum *dynamics*.

<sup>&</sup>lt;sup>4</sup>"bildet es also unmittelbar nach dem Zusammenstoß mit dem Lichtquant durchaus ein für sich bestehendes, durch seine eigene Wellenfunktion charakterisiertes physikalisches System."

<sup>&</sup>lt;sup>5</sup>"Zu einer Voraussage [...] wären jene Gründe [...] nicht zu gebrauchen; denn auch sie bestimmen [...] das System nur relativ, und zwar relativ zu der Beobachtung, die bei der Messung selber erst gemacht wurde. Sie konnten also dem Physiker erst nach dieser Beobachtung zur Verfügung stehen und ihm somit keine Vorausberechnung von deren Ergebnis gestatten."

## 3 From Measurement-Dependence to Retro-Causality

One way of relaxing the causal structure is by a *retro-causal effect*: The "Parisian zigzag" was introduced by Costa de Beauregard 70 years ago [20] and recently revived by Price [44]; we relate it to measurement-dependence.

## 3.1 "Parisian Zigzag"

In 1947,<sup>6</sup> Olivier Costa de Beauregard questioned the no-signaling assumption (*no instantaneous causality*) made by Einstein, Podolsky, and Rosen ("*EPR*" for short) in 1935 and considered actions to and from the common past: "[A]ll the weight of Einstein's argument is moved from instantaneous causality to retroactive causality"<sup>7</sup>[20]. This represents a reply to *EPR*—circumventing the claim to augment quantum theory by hidden variables—that can even be seen as a reply to *Bell's later reply to EPR*.

The "Parisian zigzag" [21, 22, 44] gives a description of Bell non-local correlations via *retro-causation*, i.e., causation from the future to the past.<sup>8</sup> Assume an experiment in which Alice and Bob each get a photon to be measured. In that model, the photons "do not possess polarizations of their own," but rather "borrow one later" [22]: When Alice performs the measurement on her photon, it gets a random polarization that is then sent to the photon's source in the past, from where the "borrowed" polarization travels on to Bob in the future (this is why the speculation is called "*zigzag*"). In that model, "Einstein's prohibition to 'telegraph to the past' does not hold at the level" of the photons but at the one of macroscopic (in other words, classical) objects only [22]. A crucial point is that no photon travels *directly* from one party to the other (a path that is "physically empty"). Instead, it goes "along the Feynman-style zigzag [...] made of two time-like vectors (which is physically occupied)." The view is related to models [31] with measurement-dependence through a retro-causal effect, perfectly simulating a singlet. Section 3.2 links retro-causal approaches to measurement-dependence.

<sup>&</sup>lt;sup>6</sup>In 1947, Olivier Costa de Beauregard shared this idea with Louis de Broglie who disapproved. It was published in 1953 [23].

<sup>&</sup>lt;sup>7</sup>"[T]out le poids de l'argument d'Einstein est ainsi transporté du paradoxe de la causalité immédiate à la causalité rétroactive".

<sup>&</sup>lt;sup>8</sup>In quantum information, Schumacher [11] suggested such a "zigzag" for interpreting superdense coding: "[O]ne of the two bits is sent forward in time through the treated particle, while the other bit is sent backward in time to the *EPR* source, then forward in time through the untreated particle, until finally it is combined with the bit in the treated particle to reconstitute the two-bit message. Because the bit 'sent backward in time' cannot be used to transmit a meaningful message without the help of the other particle, no opportunity for time travel or superluminal communication is created, just as none is created in the classic *EPR* experiment in which simultaneous measurements are used to establish non-message-bearing correlations over a spacelike interval."



**Fig. 1** Bell's locality: Time flows from top to bottom. Alice (Bob) inputs X (Y) and obtains A (B). Alice and Bob share an infinite amount of randomness  $\Lambda$  distributed independently of Alice's and Bob's inputs

## 3.2 Retro-Causal Models

The retro-causality of the "Parisian zigzag" is related to the relaxation of measurement independence in the *Bell model*: We denote by X(Y) Alice's (Bob's) input, the outputs being A and B. The behavior of interest is a conditional distribution  $P_{AB|XY}$ . Bell-locality allows Alice and Bob to share an infinite amount of randomness  $\Lambda$  (see Fig. 1): A distribution  $P_{AB|XY}$  is called *Bell-local* if it can be written as

$$P_{AB|XY} = \sum_{\lambda} P_{\Lambda}(\lambda) P_{A|X,\Lambda=\lambda} P_{B|Y,\Lambda=\lambda} \,.$$

It is remarkable that quantum theory is consistent with correlations which are *not* Bell-local [9]. The definition of *Bell-locality* decomposes into three conditions.

- 1. No-signaling: Alice's output is independent of Bob's input, and vice versa.
- 2. *Locality*: The correlations between Alice and Bob stem from a shared random variable  $\Lambda$ .
- 3. *Measurement independence*: The shared randomness is independent of Alice's and Bob's inputs.

The third assumption is usually implicit as  $\Lambda$  is understood to root in the *common past* of Alice and Bob. If we allow the shared randomness to depend on Alice's and Bob's inputs, it is possible to reproduce the joint distribution of a Bell non-local quantum state [12]. Relaxing this assumption can mean, e.g., that the shared randomness influences the measurement settings of Alice and Bob. This does not change the causal structure: The common cause is in the past, and there is no retro-



Fig. 2 A Bell-like model with measurement-dependence and retro-causal influence: The distribution of the shared random variables depends on Alice's and Bob's inputs

causal effect (this is a flavor of determinism or the fully causal hidden variable approach of Brans [12, 33]). Alternatively, it can mean that the inputs influence the shared randomness. This points to the distributed-sampling problem [24] and retro-causal models as discussed above.

Here, we are interested in a model with relaxed causal structure and focus on the second option: A Bell-local model with measurement-dependence through a retro-causal influence (Fig. 2). This model can reproduce no-signaling correlations: A first idea is to send Alice's input retroactively to the common past and to share it with Bob. Alternatively, Alice's input can be retro-causally used to bias the uniform distribution of the shared randomness ( $\Lambda \sim P_{uniform}$ ). This is the retro-causal model of Feldman [31], solving a *distributed-sampling problem*, and it has been shown to allow Alice and Bob for simulating a singlet [24]: The Toner-Bacon protocol with one bit of communication translates to a "zigzag" with a retro-causal bit (from Alice to the common past). Note that in these models, the mutual information between the shared randomness  $\Lambda$  and Alice's input is nonzero.<sup>9</sup> It means that there is a *hidden* influence going from Alice to Bob via a fine-tuned "zigzag" [52]. Alternatively, we can build a mechanism without signaling between Alice and Bob. We use the fact [24] that the protocol reproducing a maximally entangled state with the help of one PR-box [17] leads to a "zigzag-style protocol" with two "retro-causal bits:" One bit each travels from Alice and Bob, respectively, to their common past, the PR correlation is established there, and the singlet can be simulated.

<sup>&</sup>lt;sup>9</sup>There are numerous results on calculating and minimizing its amount [6, 33, 37, 47, 49].

## 4 From Relative and Retro-Causality to Closed Time-Like Curves

Both models of Sect. 3.2 have in common that the future affects the past. In "parallel lives," this manifests itself in the parties *meeting up* for the correlation to be established/detected. In the "zigzag" models, the inputs of Alice and Bob are sent to the common past, and the correlation is established there. A combination of these pictures sees the respective data meet in the *future*, and the local computation necessary for the *verification* of the correlation is at the same time *its origin*—if the data can travel back in time via a *closed time-like curve* (*CTC*).<sup>10</sup>

#### 4.1 Closed Time-Like Curves with Classical Information

The idea of Deutsch's model for CTC dynamics is that two systems undergo a joint evolution after which one of them travels back to the past and reenters. Whereas Deutsch described his model for *quantum* states, we use *classical* information [1]. The *causality-respecting* system is denoted by *R*, the *causality-violating* one by *V*, and the joint evolution is  $\varepsilon = P_{R'V'|RV}$ . For an initial state  $P_R^{\text{init}}$  of *R* and given  $\varepsilon$ , Deutsch's consistency condition is

$$P_{V}^{\text{cons}} = \sum_{r',r,v} P_{R'=r',V'|R=r,V=v} P_{R=r}^{\text{init}} P_{V=v}^{\text{cons}},$$
(1)

i.e., the states of *V* before and after the evolution are identical (see Fig. 3). Generally, several consistent states can exist: In that case, Deutsch suggests to choose the one maximizing the entropy, avoiding the *information antinomy*. The final state  $P_R^{\text{fin}}$  of the causality-respecting system is then

$$P_{R}^{\text{fin}} = \sum_{v',r,v'} P_{R',V'=v'|R=r,V=v} P_{R=r}^{\text{init}} P_{V=v}^{\text{cons}}.$$
(2)

Fig. 3 A causality-respecting system jointly evolves with a causality-violating one: The latter system's state is the fixed point with maximal entropy



<sup>&</sup>lt;sup>10</sup>The latter have already been widely discussed in quantum information [1, 3, 25, 54].



**Fig. 5** A PR box is simulated locally in the common future of Alice and Bob. The outputs of the PR box travel back in time through a Deutsch closed time-like curve. The dashed lines represent the light cones. Time flows bottom-up

## 4.2 No-Signaling Correlations from Closed Time-Like Curves

We present the setup with Deutsch CTCs based on random variables to reproduce any no-signaling correlation. We show the representative example of the *Popescu/Rohrlich (PR) box* [43] defined as (see Fig. 4):

$$P_{AB|XY}^{\text{PR}}(a,b,x,z) = \frac{\delta_{xy,a\oplus b}}{2}.$$
(3)

If Alice and Bob want to simulate the PR box with *shared classical randomness*, they can reach a success probability of 3/4. When, instead, Alice and Bob share a quantum state, then (at most [18]) roughly 85% is possible. If, on the other hand, Alice and Bob have access to a classical CTC, they can *perfectly* simulate a PR box by *local* interactions. The idea is that Alice and Bob send their inputs *X*, *Y* to the common future to have them interact *locally*, resulting in outputs according to the PR condition, and let them travel back along the CTC (see Fig. 5).

The setup uses an "open" time-like curve [42, 54]: The systems traveling to the past do *not* self-interact. When the local operations are swaps, then a *single* fixed

point of the evolution exists (the PR box); this avoids the *information antinomy*. Note that the setup does not become signaling even if Alice or Bob choose to apply a *different* operation locally. First, the joint distribution  $P_{AB|XY}^{PR}(a, b, x, z)$  of the PR box is *no-signaling*, and second, the state of all systems *just before* the parties apply their local operations is  $P_X P_Y \rho$ , where Alice's part of  $\rho$  contains no information on *Y*, and vice versa: Deutsch CTCs are *no-signaling preserving*. (They are, however, still an "overkill" because they allow for reproducing *any* no-signaling distribution. A question worth exploring is to find a consistent mechanism, weaker than classical Deutsch CTCs, restricting the resulting correlations—ideally to exactly the *quantum* correlations.)

#### **5** Relation to the Other Models

We discuss the relation of our speculation to previously considered "stories" behind the emergence of Bell correlations.

## 5.1 Hermann/Everett and "Parallel Lives"

The parallel-lives model [13] (see also [27]) assumes that every party, when performing a measurement, splits into "bubbles" in different realities, labeled by the measurement outcome. When Alice and Bob meet in the common future to compare their results, only those "bubbles" are visible to each other for which the labels reproduce the desired correlation. CTCs are an alternative to such a matching rule.

#### 5.2 Retro-Causality and Distributed Sampling

In the retro-causal "Parisian zigzag" [20–22, 44, 45], the input of Alice is sent to the past where it influences the shared random variable of Bob. According to Sect. 3.2, this model is *fine-tuned* [52] and harmonizes with our own speculation in the sense that a CTC can be seen as a mechanism for achieving retro-causality operationally and in a consistent way, i.e., without time-travel antinomies.

## 5.3 The "Process-Matrix" Framework

In [40], no causal structure is assumed a priori, but only local assumptions are made: The parties receive a system from the environment, interact with it, and

output it back to the environment. The latter is noncausal: The inputs to the parties can depend on their outputs. The framework allows for correlations incompatible with definite orders of the parties. Since such correlations can be obtained even for the classical case [8], one might wonder whether also Bell-like correlations can. This is, however, not so. More specifically, the question is whether Bell non-local correlations can be seen as arising from some classical (as opposed to quantum) mechanism which is noncausal. The answer to this question is: "If yes, then only at the expense of signaling." Thus, the classical variant of the process-matrix framework does not allow for a *non-signaling* explanation of Bell non-local correlations are causal (they can be simulated in a causal way); and the contrapositive thereof is that noncausal correlations are signaling. In other words, any classical process matrix that allows for noncausal correlations—this is the surplus of the process-matrix framework—allow for signaling as well.

### 6 A Look Back and a Look Forward

In Sects. 2 and 3, we revisit two routes—proposed more than 20 years *before* Bell's argument—to relaxing the causal structure for reconciling Reichenbach's principle and quantum correlations: Hermann's relative causality and Costa de Beauregard's retro-causality. In Sect. 3.2, we show a new formulation of the "zigzag" model rooted in measurement-dependence and shedding light on the hidden signaling involved. In Sect. 4, we realize the retro-causal effect with *closed time-like curves*, hereby speculating about a *classical* mechanism establishing *Bell non-local correlations*.

When the parts of a system in an entangled quantum state are measured, then shared classical information can be insufficient for explaining the observed correlations: John Stewart Bell's "exploit" in 1964 questioned fundamentally the validity of an attack to quantum theory by Einstein, Podolsky, and Rosen in 1935—but the puzzle is, after Bell, as unsolved as ever: What could be a classical mechanism leading to correlations of classical information? Reichenbach's principle states that in a given causal structure, this can root either in a common cause in the common past or in a *direct influence* from one of the correlated events to the other. Various results question its applicability in the light of Bell correlations not only but in particular in the *multipartite* scenario [4, 5, 19, 48, 52]. There are at least three escapes from the dilemma: First, Reichenbach's principle is declared wrong, Bell correlations being a counterexample. It could then, second, be replaced by a modified—quantum—principle accepting as a reason for correlations of classical pieces of information also an *entangled state*. Third, we can drop the assumption of a fundamental causal structure (Reichenbach's principle's basis). With the first two "emergency exits," the story ends here; we consider the third option: Drop fundamental causality.<sup>11</sup> This text is concerned with how *loopholes* of rigid causality, such as closed time-like curves, can be used to obtain Bell violations. Let us finish with a wilder speculation: *What if, in the spirit of Wheeler's* "*It from Bit*" [51], space-time causality emerges from "laws of large numbers" at the macroscopic level of the thermodynamic limit hand in hand with—and not prior to—the classical<sup>12</sup> information so strangely correlated? (Can we come up with a coherent combinatorial canvas comprehending the creation of classicality, correlations, and causality—combined?)

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<sup>&</sup>lt;sup>11</sup>Are we throwing out the baby with the bath water? Maybe—at least, this has some tradition: "The law of causality [...] is a relic of a bygone age, surviving, like the monarchy, only because it is erroneously supposed to do no harm" (Bertrand Russell, 1913)

<sup>&</sup>lt;sup>12</sup>Classicality is an idealized notion existing in the thermodynamic limit and related to *macroscopicity and redundancy* (i.e., work value [7]). Violations of Bell's inequalities indicate the emergence, in a space-like separated way, of identical classical bits. *This* is the strangeness about the missing classical story: The *same* decision seems to be taken *twice*!

The measurement is the transition from quantum to *classical* information, so one may look for the key to the quantum measurement problem—and now also, the emergence of space-time causality when seen as a feature of the classical realm—within *thermodynamics* (*combinatorics*), well aware of the fact that none of the present *interpretations of quantum theory* harmonizes with Bell non-locality. (Surely, the correlations are sometimes used by camp X to question camp Y's interpretation and vice versa—but this often pairs with blindness for the weakness of one's own favorite metaphysics in the face of the *Bell curse*; or as *Nicolas Gisin* put it: "*Bell, c'est difficile pour tout le monde.*")

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## **Temporal Vibrations in a Quantized Field**



#### Hou Yau

## **1** Introduction

Nature, in general, prefers symmetries [1, 2]. Our experiences tell us that by restoring symmetry among equations in a scientific theory, dramatic discoveries can sometimes be revealed. One of these achievements is the Maxwell equations. In developing his formulation for the electrodynamic theory, Maxwell saw the need to add an extra term to bring symmetry in his equations. The extra term ("displacement current") was added to his fourth equation to describe how the electric and magnetic fields vary in time relating to the distributions of electric charges and currents. It is Maxwell's insight that ultimately led to the full unification of electrodynamics and optics. The extra term in Maxwell's fourth equation generalizes the laws of electrodynamics that include radiation solutions for all known optical phenomena [3].

Despite nature's preference for symmetries, the treatment of time and space in quantum theory is not symmetrical. As in Newtonian mechanics, time is assumed the same for all reference frames in quantum theory [4, 5]. It is postulated as a parameter and not treated as an operator. However, this is in contrast with how relativity is formulated which requires space and time to be treated on the same footing. This contradiction, as a result, has created constellation of problems when we try to unify the two fundamental theories [6, 7]. In order to make quantum theory more symmetrical, can time have a more dynamical role in its formulation?

The reason not to consider time as an operator can be traced back to Pauli's era. According to Pauli's reasonings [8] and subsequent work by Srinivas and Vijayalakshmi [9], a time operator t should satisfy a commutation relation with the Hamiltonian operator H, i.e., [H, t] = -i. Letting t as the universal time operator

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H. Yau (🖂)

FDNL Research, Daly City, CA, USA e-mail: hyau@fdnresearch.us

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valid for all systems, its spectrum should span continuously over the entire real line. This would also imply the same for the eigenvalues of H. However, as we know, the Hamiltonian H of a physical system should be bounded from below.<sup>1</sup> Some systems also have discrete energy eigenvalues. Therefore, the assumption of a continuous unbounded energy spectrum will contradict the properties of a real physical system. A self-adjoint time operator cannot exist that is canonically conjugate to a semibounded or discrete Hamiltonian. This is widely known as Pauli's theorem.

Although Pauli's theorem is generally accepted, there are many cases that suggest time can have a more dynamical role in quantum theory, for example, tunneling time [11, 12], decay time of an unstable particle [13], arrival time of a particle [14, 15], time as a fundamentally discrete dynamical variable suggested by T. D. Lee [16], and more as shown in [17–20, 22–25], [21, and references therein]. In many of these examples, the "intrinsic time" [26] of the investigated systems can be taken as an operator. Their results show that time and space can have a more equal status in a quantum field. The treatment of time in quantum theory remains one of the challenging open questions in the foundations of physics.

In quantum theory and Newtonian mechanics, matter can have vibration in the spatial directions but not in the temporal direction. In fact, if time and space are to be treated on the same footing, it is possible to allow matter to vibrate in time [27, 28]. These temporal vibrations are additional degrees of freedom that can be introduced in a matter field. As discussed earlier, Maxwell introduced an extra term in his formulation for electrodynamic theory. Here, we will introduce extra temporal vibrations to restore symmetry between time and space in the formulation of a matter field.

This paper is organized in the following manner. In Sect. 2, we construct a plane wave with 4-vector amplitude  $(T, \mathbf{X})$  that has vibrations of matter in space and time. By studying the Hamiltonian density equation of this plane wave in Sect. 3, we find that a particle observed in this system has oscillation in proper time. This temporal oscillation can only have one unique amplitude. In Sects. 4 and 5, we investigate the quantum properties of the system (e.g., Schrödinger equation, Klein-Gordon equation, bosonic field, probability density, etc.). The system with vibrations of matter in space and time has the familiar structures of a real quantum field. In Sect. 6, we consider the "internal time" of the system as a self-adjoint operator. The spectrum of this operator spans the entire real line even though the Hamiltonian of the system is bounded from below. In our formulation, the "external time" (taking the role of a universal time for measuring the temporal vibrations) is a parameter. It is not an operator as called for by Pauli's theorem.

<sup>&</sup>lt;sup>1</sup>There are possible exception in special systems such as an electrically charged particle in an infinite uniform electric field where the continuous energy spectrum is not bounded [10].

#### 2 Temporal Vibrations

Consider the background coordinates  $(t, \mathbf{x})$  for the flat spacetime as observed in an inertial frame. Time in this background is the "external time" as measured by clocks stationary at spatial infinity that are not coupled to the system under investigation [26, 29, 30]. Taking time as a dynamical variable, we will construct a plane wave with matter that has vibrations in both the temporal and spatial directions. The external time *t* is used as reference for measuring the temporal vibrations of matter inside the wave.

Let us first study a plane wave in an inertial frame O' with matter that has vibrations in time only. We will define the wave's temporal vibration amplitude,  $T_0$  (analogous to the amplitude of vibration in space, **X**, of a classical plane wave), as the maximum difference between the time of matter inside the wave,  $t'_f$ , and the external time t'. Therefore, if matter inside the plane wave has an internal clock, its time  $t'_f$  will be different from time t' measured at spatial infinity. Time measured by the matter's internal clock is running at a varying rate relative to the inertial observer's clock. In addition, matter in the plane wave has vibrations in the temporal direction but with no vibration in the spatial direction. The "internal time"  $t'_f$  is an intrinsic property of matter. We may then write,

$$t'_{f} = t' - T_{0}\sin(\omega_{0}t') = t' + t'_{d} = t' + \operatorname{Re}(\zeta'_{t}),$$
(1)

$$\mathbf{x}_{f}^{\prime} = \mathbf{x}^{\prime},\tag{2}$$

where

$$t'_d = \operatorname{Re}(\zeta'_t) = -T_0 \sin(\omega_0 t'), \qquad (3)$$

$$\zeta_t' = -iT_0 e^{-i\omega_0 t'}.\tag{4}$$

The internal time of matter in the plane wave, therefore, passes at the rate,

$$\frac{\partial t'_f}{\partial t'} = 1 - \omega_0 T_0 \cos(\omega_0 t'), \tag{5}$$

with respect to the external time and has an average value of 1. Matter will appear to travel along a timelike geodesic when averaged over many cycles.

By an appropriate Lorentz transformation, the background coordinates  $(t', \mathbf{x}')$  of inertial frame O' can be related to the background coordinates  $(t, \mathbf{x})$  for the flat spacetime observed in another frame of reference O. We assume that frame O' travels with velocity  $\mathbf{v}$  relative to frame O. Similarly, the temporal and spatial vibrations of matter  $(t'_f, \mathbf{x}'_f)$  can be Lorentz transformed to the temporal and spatial

vibrations of matter  $(t_f, \mathbf{x}_f)$  as observed in frame *O*. We can thus relate the matter vibrations  $(t_f, \mathbf{x}_f)$  to the background coordinates  $(t, \mathbf{x})$ :

$$t_f = t + T\sin(\mathbf{k} \cdot \mathbf{x} - \omega t) = t + t_d = t + \operatorname{Re}(\zeta_t),$$
(6)

$$\mathbf{x}_f = \mathbf{x} + \mathbf{X}\sin(\mathbf{k} \cdot \mathbf{x} - \omega t) = \mathbf{x} + \mathbf{x}_d = \mathbf{x} + \operatorname{Re}(\boldsymbol{\zeta}_x), \tag{7}$$

where

$$t_d = \operatorname{Re}(\zeta_t) = T \sin(\mathbf{k} \cdot \mathbf{x} - \omega t), \tag{8}$$

$$\mathbf{x}_d = \operatorname{Re}(\boldsymbol{\zeta}_x) = \mathbf{X}\sin(\mathbf{k}\cdot\mathbf{x} - \omega t), \tag{9}$$

$$\zeta_t = -iT e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)},\tag{10}$$

$$\boldsymbol{\zeta}_{x} = -i\mathbf{X}e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)},\tag{11}$$

$$T = (\omega/\omega_0)T_0, \tag{12}$$

$$\mathbf{X} = (\mathbf{k}/\omega_0)T_0. \tag{13}$$

Amplitude **X** is the maximum displacement of matter from its equilibrium coordinate **x**, and amplitude *T* is its maximum displacement from the external time *t*. The proper time displacement  $T_0$  can be seen as a Lorentz transformation of a 4-displacement vector:  $(T_0, 0, 0, 0) \rightarrow (T, \mathbf{X})$  where  $T^2 = T_0^2 + |\mathbf{X}|^2$ . The amplitude of the plane wave is a 4-vector.

Inside the plane wave in frame O, matter has vibrations in both the temporal and spatial directions. We can further summarize these vibrations with a single function:

$$\zeta = \frac{T_0}{\omega_0} e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}.$$
(14)

The vibrations  $\zeta_t$  and  $\zeta_x$  from Eqs. (10) and (11) can be written as

$$\zeta_t = \partial_0 \zeta, \tag{15}$$

$$\boldsymbol{\zeta}_{\mathbf{X}} = -\nabla \boldsymbol{\zeta}. \tag{16}$$

## 3 Mass-Energy of a Proper Time Oscillator

Consider the function  $\zeta$  and its complex conjugate  $\zeta^*$ . The functions satisfy the wave equations:

$$\partial_u \partial^u \zeta + \omega_0^2 \zeta = 0, \tag{17}$$

$$\partial_u \partial^u \zeta^* + \omega_0^2 \zeta^* = 0. \tag{18}$$

Equations (17) and (18) are similar to the Klein-Gordon equation, except we still have to understand how  $\zeta$  can be related to the zero spin bosonic field in quantum theory. The corresponding Lagrangian density for the equations of motion is

$$\mathscr{L} = K[(\partial^{u}\zeta^{*})(\partial_{u}\zeta) - \omega_{0}^{2}\zeta^{*}\zeta], \qquad (19)$$

and the Hamiltonian density is

$$\mathscr{H} = K[(\partial_0 \zeta^*)(\partial_0 \zeta) + (\nabla \zeta^*) \cdot (\nabla \zeta) + \omega_0^2 \zeta^* \zeta],$$
(20)

where K is a constant of the system under investigation. For a system that can have multiple number of particles with mass m in a cube with volume V, we make the ansatz:

$$K = \frac{m\omega_0^2}{2V}.$$
(21)

Periodic boundary conditions are to be imposed at the box walls, and the natural units ( $c = \hbar = 1$ ) are adopted.

Let us examine the Hamiltonian density of a plane wave. Substitute  $\zeta$  from Eq. (14) into Eq. (20), the Hamiltonian density is

$$\mathscr{H} = \mathscr{H}_1 + \mathscr{H}_2 + \mathscr{H}_3, \tag{22}$$

where

$$\mathscr{H}_1 = \left(\frac{m\omega_0^2}{2V}\right)T^*T,\tag{23}$$

$$\mathscr{H}_2 = \left(\frac{m\omega_0^2}{2V}\right) \mathbf{X}^* \cdot \mathbf{X},\tag{24}$$

$$\mathscr{H}_{3} = (\frac{m\omega_{0}^{2}}{2V})T_{0}^{*}T_{0},$$
(25)

such that  $T_0$ , **X**, and *T* are taken as complex amplitudes. The first term,  $\mathcal{H}_1$ , on the right-hand side of Eq. (22) is a Hamiltonian density with oscillations in time. The second term,  $\mathcal{H}_2$ , is related to oscillations of matter in the spatial directions. In the nonrelativistic limit, our choice of *K* is not arbitrary. The term  $\mathcal{H}_2$  gives us the Hamiltonian density of a classical harmonic system with oscillations in the spatial direction. The third term,  $\mathcal{H}_3$ , is related to the oscillations in proper time. After combining  $\mathcal{H}_1$ ,  $\mathcal{H}_2$ , and  $\mathcal{H}_3$ , we have

$$\mathscr{H} = \left(\frac{m\omega_0^2}{V}\right)T^*T.$$
(26)

For a system with vibrations in proper time only, matter is stationary in space. In this case,  $\omega = \omega_0$ ,  $|\mathbf{k}| = 0$ ,  $T = T_0$ , and  $|\mathbf{X}| = 0$ . From Eq. (26), the Hamiltonian density of a plane wave with vibrations in proper time only is

$$\mathscr{H}_0 = (\frac{m\omega_0^2}{V})T_0^*T_0.$$
(27)

This result is similar to the Hamiltonian density of a harmonic oscillating system in classical mechanics, except the vibrations are in time and not in space. Since there is no vibration in the spatial directions, the Hamiltonian density  $\mathcal{H}_0$  shall correspond to certain internal energy of matter at rest. In addition, the vibrations in proper time do not involve any force field. Therefore,  $\mathcal{H}_0$  does not necessarily have energy from charges. On the other hand, we have only consider matter with mass *m* in this simple harmonic oscillating system. No other energy is present in this system except the energy of mass *m*. Here, we will consider  $\mathcal{H}_0$  as an internal mass-energy density which arises from the proper time vibrations of matter.

Let us assume there is only one particle in the system. From Eq. (27), the energy inside volume V is  $E = m\omega_0^2 T_0^* T_0$  of a harmonic oscillator in proper time with mass m. If the energy of this harmonic oscillator is the internal mass-energy of matter, it can only be observed as the energy of mass m which is on shell, i.e.,

$$E = m = m\omega_0^2 T_0^* T_0,$$
 (28)

or

$$\omega_0^2 T_0^* T_0 = 1. (29)$$

Therefore, a particle with mass *m* has oscillation in proper time with amplitude  $|\mathring{T}_0| = 1/\omega_0$ . However, we shall note that the amplitude of this oscillation is unique. A proper time oscillator with mass *m* has no other observable amplitude. Only an oscillator with the unique amplitude can be observed under the constraint that mass is on shell. In addition to the classical concepts of mass [31, 32], we suggest a possibility that matter can also have vibration in time with an unique amplitude.

Next, we will consider the temporal oscillation of the particle as observed in a reference frame O'. The internal time  $\mathring{t'}_f$  with amplitude  $\mathring{T}_0 = 1/\omega_0$  of the particle is

$$\mathring{t'}_{f}(t') = t' - \frac{\sin(\omega_0 t')}{\omega_0}.$$
(30)

We will assume the particle observed is located at the origin of coordinate  $\mathbf{x}'_0$ ,

$$\mathbf{\tilde{x}'}_f(t') = \mathbf{x}'_0. \tag{31}$$

This particle is stationary in space with an internal clock that has a frequency as conjectured by de Broglie [33]. However, instead of traveling along a smooth timelike geodesic, the particle has a temporal vibration relative to the external time. The internal time rate relative to the external time for the oscillator is

$$\frac{\partial t'_f}{\partial t'} = 1 - \cos(\omega_0 t'). \tag{32}$$

The average of this time rate is 1. Its value is bounded between 0 and 2 which is positive. Therefore, the internal time of the oscillator moves only forward. It cannot go backward to its past. In addition, as the frequency of the oscillation increases, the amplitude decreases, i.e.,  $|\mathring{T}_0| \rightarrow 0$  when  $\omega_0 \rightarrow \infty$ . As the accuracy of the measuring clock is restricted by the energy-time uncertainty relation [34, 35], a particle will appear to travel along a timelike geodesic if our measurement is not sensitive enough to detect the oscillation. On the other hand, if the measurement is sensitive enough, different decay rate will be observed for an unstable particle at different phase of the oscillation.

In another frame of reference *O* with background coordinates  $(t, \mathbf{x})$ , the particle will have oscillations in time and space. Here, we will assume frame *O'* is traveling with velocity  $\mathbf{v} = \mathbf{k}/\omega$  relative to frame *O*, and the particle begins at origin of the  $\mathbf{x}$  coordinates at t = 0. By Lorentz transforming Eqs. (30) and (31) from frame *O'* to frame *O*, the oscillations are

$$\mathring{t}_f(t) = t - \mathring{T}_p \sin(\omega_p t), \tag{33}$$

$$\mathring{\mathbf{x}}_{f}(t) = \mathbf{v}t - \mathring{\mathbf{X}}_{p}\sin(\omega_{p}t), \tag{34}$$

where

$$\mathring{T}_p = \frac{\omega}{\omega_0^2},\tag{35}$$

$$\overset{\,\,{}_{\circ}}{\mathbf{X}}_{p} = \frac{\mathbf{k}}{\omega_{0}^{2}},\tag{36}$$

$$\omega_p = \frac{\omega_0^2}{\omega}.$$
(37)

The magnitude of the amplitudes  $|\mathring{T}_p|$  and  $|\mathring{X}_p|$  are unique for the particle traveling at a velocity **v**. We shall note that as  $|\mathbf{v}| \rightarrow 1$ , the magnitude of the spatial and temporal amplitudes approaches infinity,  $|\mathring{X}_p| \rightarrow \infty$  and  $|\mathring{T}_p| \rightarrow \infty$ . On the other hand,  $\omega_p$  is the angular frequency of a moving particle. It is not the angular frequency  $\omega$  of the plane wave. As  $|\mathbf{v}| \rightarrow 1$ , the angular frequency  $\omega_p$  slows down and approaches zero,  $\omega_p \rightarrow 0$ .

#### 4 Probability Density and Wave Function

Let us consider a plane wave  $\bar{\xi}_0$  that has vibrations in proper time and an amplitude  $|T_0| = 1/\omega_0$ . From Eq. (27), its Hamiltonian density is  $\tilde{\mathcal{H}}_0 = m/V$ . This system contains the energy E = m of one particle in a cube with volume V. When we probe the system as a whole, one particle can be observed. On the other hand, the situation is different when we probe only part of the system. Since the Hamiltonian density of the plane wave is uniform throughout, the energy observable in a volume  $V_1$  (< V) is  $E_1 = mV_1/V$ . It is only a fraction of a particle's mass-energy. However, as we shall recall, a particle's energy is supposed to be on shell, and a fraction of its energy cannot be observed. If this is the case, can we still observe any mass-energy as call out by the Hamiltonian density when we probe only a part of the system?

The presence of a Hamiltonian density can be explained if we consider the plane wave as a probability wave. The situation is the same as in quantum theory. A probability density  $\bar{\rho}$  can be assigned for the observation of a particle at a particular location. Since a particle carries an energy E = m, we can average the results from many measurements and obtain a Hamiltonian density from the probability density, i.e.,  $\bar{\mathcal{H}}_0 = \bar{\rho}m$ . In other words, the probability density of finding a particle in the plane wave  $\bar{\zeta}_0$  can be written in terms of its Hamiltonian density, i.e.,  $\bar{\rho} = \bar{\mathcal{H}}_0/m$ . This approach can be extended to a generalized system with superposition of plane waves.

A plane wave  $\zeta$  from Eq. (14) has vibrations of matter in space and time. In this section, we will only consider the case when its amplitude is in the range  $0 \le |T_0| \le$ 1. Taking  $\partial_0 \zeta = -i\omega\zeta$  and  $\nabla \zeta = i\mathbf{k}\zeta$ , the Hamiltonian density of the plane wave  $\zeta$  from Eq. (20) becomes

$$\mathscr{H} = \frac{\omega_0^3 \omega^2}{V} \zeta^* \zeta. \tag{38}$$

Here, the point mass is taken as a particle with de Broglie's mass-energy ( $m = \omega_0$ ). Since a particle in plane wave  $\zeta$  has a velocity  $|\mathbf{v}|$ , its energy is  $E_{\mathbf{k}} = \gamma \omega_0 =$   $\omega$ , where  $\gamma = (1 - |\mathbf{v}|^2)^{-1/2}$ . Based on our earlier discussions, we can define a probability density of observing a particle in plane wave  $\zeta$ , i.e.,

$$\rho = \frac{\mathscr{H}}{\omega} = \frac{\omega_0^3 \omega}{V} \zeta^* \zeta. \tag{39}$$

Taking the approximation  $\gamma = \omega/\omega_0 \approx 1$  in the nonrelativistic limit, the probability density can be approximated as

$$\rho \approx \frac{\omega_0^4}{V} \zeta^* \zeta. \tag{40}$$

We can relate the plane wave  $\zeta$  and the quantum wave function  $\psi$  for a system in a cube with volume *V*:

$$\psi = \frac{a}{\sqrt{V}} e^{i(\mathbf{k}\cdot\mathbf{x}-\tilde{\omega}t+\chi)} \approx \left[\frac{\omega_0^2}{\sqrt{V}} e^{i(\omega_0t+\chi)}\right] \zeta,\tag{41}$$

where

$$a = \omega_0 T_0, \tag{42}$$

$$\tilde{\omega} = \mathbf{k} \cdot \mathbf{k} / (2\omega_0) \approx \omega - \omega_0. \tag{43}$$

As we shall note,  $e^{i\chi}$  is an arbitrary factor introduced to show that wave function  $\psi$  and plane wave  $\zeta$  can have an arbitrary phase difference. Amplitude *a* is a probability amplitude which can be expressed in terms of the proper time vibration amplitude. Equation (40) can then be written as

$$\rho \approx \psi^* \psi, \tag{44}$$

which is the probability density we find in quantum mechanics.

Applying the superposition principle, we can write

$$\psi(\mathbf{x},t) = e^{i\chi} \sum_{\mathbf{k}} \frac{\omega_0 T_{0\mathbf{k}}}{\sqrt{V}} e^{i(\mathbf{k}\cdot\mathbf{x}-\tilde{\omega}t)},\tag{45}$$

where periodic boundary conditions for a cube are imposed on the wave vector **k**. For a normalized system, one particle with the unique proper time vibration amplitude can be observed. The probability density can again be obtained from Eq. (44). Furthermore, if we examine  $\psi(\mathbf{x}, t)$ , it is a solution of the linear and homogeneous Schrödinger equation for a free particle, i.e.,  $i\dot{\psi}(\mathbf{x}, t) = -(2m)^{-1}\nabla^2\psi(\mathbf{x}, t)$ . The system with vibrations of matter in space and time therefore has basic properties of a quantum wave. Although the formulations presented here is straightforward, we

shall recall that these results are obtained from the temporal vibrations introduced which is not part of the quantum theory.

It is commonly believed that a matter wave can only have a probabilistic interpretation because the overall phase for the wave function  $\psi$  is unobservable [36]. However, as we shall note, the phase factor  $e^{i\chi}$  in Eqs. (41) and (45) does not change the probability density. In fact, as demonstrated in quantum mechanics, the theory developed with wave functions  $\psi$  is invariant under global phase transformation, but the relative phase factors are physical. Here, the wave function  $\psi$  serves as a mathematical tool for describing an underlying wave with vibrations of matter in time and space. A system with wave function  $\psi$  from the superposed plane waves can have a global phase shift  $\chi$  without changing the results in quantum mechanics. The overall phase of  $\psi$  is unobservable. However, function  $\psi$  is not required to have the same phase as  $\zeta$  that describes the physical vibrations in space and time.

#### 5 Bosonic Field

The above analysis is based on a single particle system in the nonrelativistic limit where approximations are taken to obtain the probability density. As it is well known in quantum theory, when the Klein-Gordon equation is treated as a single particle equation in a relativistic theory, one will encounter the difficulties of negative energy solutions. Since  $\zeta$  satisfies an equation similar to the Klein-Gordon equation, we expect the system with vibrations in space and time can have the same properties of a zero spin matter field in quantum theory.

For a plane wave  $\zeta_0$  that has vibrations in proper time, multiple number of particles with mass *m* can be observed if the system has the energy allowed. The internal mass-energy observable in this plane wave  $\zeta_0$  is quantized. Each particle shall have oscillation with the same proper time amplitude. The plane wave  $\zeta_0$  is a quantized system.

For a many-particle system, it can have n integer number of oscillators. We can generalize condition (29) as

$$\omega_0^2 T_0^* T_0 = n, (46)$$

which is a Lorentz invariant. The number of particles observed in the system shall remain the same under Lorentz transformations. The Hamiltonian density from Eq. (27) for a plane wave  $\zeta_0$  can be written as

$$\mathscr{H}_0 = \frac{n\omega_0}{V}.\tag{47}$$

The energy in this plane wave with vibrations in proper time only is quantized with n = 0, 1, 2, ...

Under a Lorentz transformation, plane wave  $\zeta_0$  transforms to another plane wave  $\zeta$  that has vibrations in space and time. Instead, let us consider a plane wave  $\zeta_n$  which is normalized in volume V when n = 1:

$$\zeta_n = \gamma^{-1/2} \zeta. \tag{48}$$

Replace  $\zeta$  with  $\zeta_n$  in Eq. (20), the Hamiltonian density for plane wave  $\zeta_n$  is

$$\mathscr{H}_n = \gamma \,\mathscr{H}_0 = \frac{n\omega}{V}.\tag{49}$$

The energy in this plane wave  $\zeta_n$  is quantized with *n* particles of angular frequency  $\omega$  in a volume *V*.

The vibrations in space and time are real physical quantities. In Eqs. (6) and (7), only the real component of  $\zeta$  is relevant for obtaining these physical quantities. We retained the complex component of  $\zeta$  in the previous analysis to simplify the derivation of the complex wave function. Here,  $\zeta$  (or  $\zeta_n$ ) can be combined with its complex conjugate. Instead of using  $\zeta$ , we can obtain a real scalar field by superposition of plane waves  $\zeta_n$ , i.e.,

$$\zeta(\vec{x}) = \frac{1}{\sqrt{2}} \sum_{\mathbf{k}} [\zeta_{n\mathbf{k}}(\vec{x}) + \zeta_{n\mathbf{k}}^{*}(\vec{x})] = \sum_{\mathbf{k}} (2\omega\omega_{0})^{-1/2} [T_{0\mathbf{k}}e^{-i\vec{k}\cdot\vec{x}} + T_{0\mathbf{k}}^{*}e^{i\vec{k}\cdot\vec{x}}],$$
(50)

which satisfies the Klein-Gordon equation. Again, periodic boundary conditions for a cube are imposed on the wave vector  $\mathbf{k}$ .

To adopt the same convention in quantum field theory, we will switch to the use of field  $\varphi$  for describing the vibrations, i.e.,

$$\varphi(\vec{x}) = \zeta(\vec{x}) \sqrt{\frac{\omega_0^3}{V}} = \sum_{\mathbf{k}} (2\omega V)^{-1/2} [\omega_0 T_{0\mathbf{k}} e^{-i\vec{k}\cdot\vec{x}} + \omega_0 T_{0\mathbf{k}}^* e^{i\vec{k}\cdot\vec{x}}].$$
(51)

From Eq. (20), the Hamiltonian density equation for  $\varphi(\vec{x})$  is

$$\mathscr{H} = \frac{1}{2} [(\partial_0 \varphi)^2 + (\nabla \varphi)^2 + \omega_0^2 \varphi^2].$$
(52)

As shown in quantum field theory, the transition of a classical field to a quantum field can be done via canonical quantization. Similarly, we can treat  $\varphi(\vec{x})$  and  $\mathcal{H}$  as operators. Since the quantization of a real scalar field is a familiar process, we will only highlight the key results involving the temporal vibrations that are not included in the quantum theory. For example, condition (46) can be extended to the quantized field with

$$N_{\mathbf{k}} = \omega_0^2 T_{0\mathbf{k}}^{\dagger} T_{0\mathbf{k}},\tag{53}$$
as the particle number operator. Normal ordering shall be taken into account between  $T_{0\mathbf{k}}$  and  $T_{0\mathbf{k}}^{\dagger}$ . Furthermore, an annihilation operator  $a_{\mathbf{k}}$  and a creation operator  $a_{\mathbf{k}}^{\dagger}$  can be defined,

$$a_{\mathbf{k}} = \omega_0 T_{0\mathbf{k}},\tag{54}$$

$$a_{\mathbf{k}}^{\dagger} = \omega_0 T_{0\mathbf{k}}^{\dagger},\tag{55}$$

such that  $N_{\mathbf{k}} = a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}$ . The operators  $a_{\mathbf{k}}$ ,  $a_{\mathbf{k}}^{\dagger}$ ,  $T_{0\mathbf{k}}$ , and  $T_{0\mathbf{k}}^{\dagger}$  satisfy the commutation relations,

$$[a_{\mathbf{k}}, a_{\mathbf{k}'}^{\dagger}] = \delta_{\mathbf{k}\mathbf{k}'},\tag{56}$$

$$[a_{\mathbf{k}}, a_{\mathbf{k}'}] = [a_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}'}^{\dagger}] = 0,$$
(57)

$$[T_{0\mathbf{k}}, T_{0\mathbf{k}'}^{\dagger}] = \frac{\delta_{\mathbf{k}\mathbf{k}'}}{\omega_0^2},\tag{58}$$

$$[T_{0\mathbf{k}}, T_{0\mathbf{k}'}] = [T_{0\mathbf{k}}^{\dagger}, T_{0\mathbf{k}'}^{\dagger}] = 0.$$
<sup>(59)</sup>

Based on the creation and annihilation operators, we can write down some other operators in the quantum theory and express them in terms of the proper time vibration operator  $T_0$ . One of them is the Hamiltonian H of the system. From Eq. (52),

$$H = \sum_{\mathbf{k}} \omega (a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \frac{1}{2}) = \sum_{\mathbf{k}} \omega (\omega_0^2 T_{0\mathbf{k}}^{\dagger} T_{0\mathbf{k}} + \frac{1}{2}),$$
(60)

after integration over the whole volume V. As we can see, these results have the familiar properties of a bosonic field except temporal vibrations are introduced in the system. The real scalar field with vibrations in space and time has the physical structures of a zero-spin bosonic field.

## 6 Temporal Vibration and Internal Time Operators

From Eqs. (12), (54), and (55), the temporal vibration amplitude  $T_{\mathbf{k}}$  and its Hermitian conjugate  $T_{\mathbf{k}}^{\dagger}$  for oscillators with  $\omega = \sqrt{\omega_0^2 + |\mathbf{k}|^2}$  are

$$T_{\mathbf{k}} = \frac{\omega}{\omega_0} T_{0\mathbf{k}} = \frac{\omega}{\omega_0^2} a_{\mathbf{k}},\tag{61}$$

$$T_{\mathbf{k}}^{\dagger} = \frac{\omega}{\omega_0} T_{0\mathbf{k}}^{\dagger} = \frac{\omega}{\omega_0^2} a_{\mathbf{k}}^{\dagger}, \tag{62}$$

satisfying commutation relations,

$$[T_{\mathbf{k}}, T_{\mathbf{k}'}^{\dagger}] = \frac{\omega^2}{\omega_0^4} \delta_{\mathbf{k}\mathbf{k}'},\tag{63}$$

$$[T_{\mathbf{k}}, T_{\mathbf{k}'}] = [T_{\mathbf{k}}^{\dagger}, T_{\mathbf{k}'}^{\dagger}] = 0.$$
(64)

In the Heisenberg picture,  $T_{\mathbf{k}}(t)$  and  $T_{\mathbf{k}}^{\dagger}(t)$  evolve over time as

$$\frac{d}{dt}T_{\mathbf{k}}(t) = i[H_{\mathbf{k}}(t), T_{\mathbf{k}}(t)] = i[\omega(a_{\mathbf{k}}^{\dagger}(t)a_{\mathbf{k}}(t) + \frac{1}{2}), T_{\mathbf{k}}(t)]$$
$$= -i\omega T_{\mathbf{k}}(t) \rightarrow T_{\mathbf{k}}(t) = T_{\mathbf{k}}(0)e^{-i\omega t}, \qquad (65)$$

$$\frac{d}{dt}T_{\mathbf{k}}^{\dagger}(t) = i[H_{\mathbf{k}}(t), T_{\mathbf{k}}^{\dagger}(t)] = i[\omega(a_{\mathbf{k}}^{\dagger}(t)a_{\mathbf{k}}(t) + \frac{1}{2}), T_{\mathbf{k}}^{\dagger}(t)]$$
$$= i\omega T_{\mathbf{k}}^{\dagger}(t) \rightarrow T_{\mathbf{k}}^{\dagger}(t) = T_{\mathbf{k}}^{\dagger}(0)e^{i\omega t}, \qquad (66)$$

where Hamiltonian  $H_{\mathbf{k}}(t) = H_{\mathbf{k}} = \omega(a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}} + \frac{1}{2})$  is obtained from Eq. (60). In addition,  $T_{\mathbf{k}}(0) = T_{\mathbf{k}}$  and  $T_{\mathbf{k}}^{\dagger}(0) = T_{\mathbf{k}}^{\dagger}$  are the operators in Schrödinger picture. By combining  $T_{\mathbf{k}}(t)$  and  $T_{\mathbf{k}}^{\dagger}(t)$ , we can obtain a temporal vibration operator:

$$t_{d\mathbf{k}}(t) = \frac{-i}{\sqrt{2}} (T_{\mathbf{k}} e^{-i\omega t} - T_{\mathbf{k}}^{\dagger} e^{i\omega t}) = \frac{-i\omega}{\sqrt{2}\omega_0^2} (a_{\mathbf{k}} e^{-i\omega t} - a_{\mathbf{k}}^{\dagger} e^{i\omega t}).$$
(67)

Analogous to a quantum harmonic oscillator that has vibration in the spatial direction, the temporal vibration operator  $t_{d\mathbf{k}}(t)$  can also be expressed in terms of the creation and annihilation operators.

We can further construct a field with temporal vibrations by superposition, i.e.,  $\sum t_{d\mathbf{k}}(\vec{x})$ . In fact, this is partly done in Sect. 5. As discussed,  $\zeta(\vec{x})$  from Eq. (50) is a real scalar field that can be applied to obtain the temporal and spatial vibrations of matter in a bosonic field. It can be rewritten in terms of  $T_{\mathbf{k}}$  and  $T_{\mathbf{k}}^{\dagger}$  as

$$\zeta(\vec{x}) = \sum_{\mathbf{k}} \sqrt{\frac{\omega_0}{2\omega^3}} [T_{\mathbf{k}} e^{-i\vec{k}\cdot\vec{x}} + T_{\mathbf{k}}^{\dagger} e^{i\vec{k}\cdot\vec{x}}].$$
(68)

The temporal vibration field operator is the time derivative of  $\zeta(\vec{x})$  by applying Eq. (15),

$$t_d(\overrightarrow{x}) = \zeta_t(\overrightarrow{x}) = \partial_0 \zeta(\overrightarrow{x}) = \sum_{\mathbf{k}} -i\sqrt{\frac{\omega_0}{2\omega}} [T_{\mathbf{k}}e^{-i\overrightarrow{k}\cdot\overrightarrow{x}} - T_{\mathbf{k}}^{\dagger}e^{i\overrightarrow{k}\cdot\overrightarrow{x}}], \quad (69)$$

where  $\sqrt{\omega_0 \omega^{-1}}$  is a normalization factor introduced.  $\zeta_t(\vec{x})$  is a temporal vibration real scalar field.

Next, let us consider the conjugate momenta of  $\zeta(\vec{x})$ . Based on Eq. (19), the Lagrangian density for the real scalar field is

$$\mathscr{L} = \frac{\bar{\rho}_m \omega_0^2}{2} [(\partial_0 \zeta)^2 - (\nabla \zeta)^2 - \omega_0^2 \zeta^2],$$
(70)

where

$$\bar{\rho}_m = \frac{\omega_0}{V},\tag{71}$$

is a mass density constant of the system. Hence, the conjugate momenta of  $\zeta(\vec{x})$  is

$$\eta(\vec{x}) = \frac{\partial \mathscr{L}}{\partial [\partial_0 \zeta(\vec{x})]} = -i\bar{\rho}_m \omega_0^2 \sum_{\mathbf{k}} \sqrt{\frac{\omega_0}{2\omega}} [T_{\mathbf{k}} e^{-i\vec{k}\cdot\vec{x}} - T_{\mathbf{k}}^{\dagger} e^{i\vec{k}\cdot\vec{x}}] = \bar{\rho}_m \omega_0^2 \zeta_t(\vec{x}).$$
(72)

The conjugate pair  $\zeta(\vec{x})$  and  $\eta(\vec{x})$  satisfy the equal-time commutation relations:

$$[\boldsymbol{\zeta}(t, \mathbf{x}), \boldsymbol{\eta}(t, \mathbf{x}')] = i\delta(\mathbf{x} - \mathbf{x}'), \tag{73}$$

$$[\zeta(t, \mathbf{x}), \zeta(t, \mathbf{x}')] = [\eta(t, \mathbf{x}), \eta(t, \mathbf{x}')] = 0.$$
(74)

Similarly,

$$[\zeta(t, \mathbf{x}), \zeta_t(t, \mathbf{x}')] = (\bar{\rho}_m \omega_0^2)^{-1} \delta(\mathbf{x} - \mathbf{x}'), \tag{75}$$

$$[\zeta_t(t, \mathbf{x}), \zeta_t(t, \mathbf{x}')] = 0.$$
(76)

The real scalar field  $\eta(\vec{x})$ , being the conjugate momenta of  $\zeta(\vec{x})$ , describes the temporal vibrations in a bosonic field as it is related to  $\zeta_t(\vec{x})$  as shown in Eq. (72).

A classical oscillator with spatial vibration can have displacement either in the positive or negative direction relative to its spatial equilibrium coordinate. Similarly, a temporal oscillator has displacement in either the positive or negative temporal direction relative to the external time *t*. From Eq. (6), internal time  $t_f(\vec{x})$  is the sum of the temporal vibration  $\zeta_t(\vec{x})$  and the external time *t*, i.e.,  $t_f(\vec{x}) = t + \zeta_t(\vec{x})$ . Since the temporal vibration  $\zeta_t(\vec{x})$  can be treated as an operator and the external time *t* is just a parameter, the internal time  $t_f(\vec{x})$  can also be treated as an operator.  $t_f(\vec{x})$  and  $\zeta(\vec{x})$  satisfy the equal-time commutation relations:

$$[\boldsymbol{\zeta}(t,\mathbf{x}), t_f(t,\mathbf{x}')] = (\bar{\rho}_m \omega_0^2)^{-1} \delta(\mathbf{x} - \mathbf{x}'), \tag{77}$$

$$[t_f(t, \mathbf{x}), t_f(t, \mathbf{x}')] = 0.$$
(78)

If we recall Pauli's theorem discussed in Sect. 1, the semi-bounded Hamiltonian forbids the introduction of an universal time operator. As discussed above, the external time (taking the role of a universal time) is not an operator as called for by Pauli's theorem. On the other hand, the spectra of  $t_f(\vec{x})$ ,  $\zeta(\vec{x})$ ,  $\zeta_t(\vec{x})$ , and  $\eta(\vec{x})$  span the whole real line. They are self-adjoint operators. From Eq. (77), the internal time  $t_f(\vec{x})$  does not form a conjugate pair with the Hamiltonian. It is this unique feature that allows us to write the internal time as a self-adjoint operator. There is no commutation relation with the semi-bounded Hamiltonian that restricts the spectrum of the internal time operator to be bounded. The internal time acquires its dynamical nature from the temporal vibration which is also a self-adjoint operator and does not form a conjugate pair with the Hamiltonian.

## 7 Conclusions and Discussions

In this paper, we demonstrate a possibility that time can have a more dynamical role in quantum theory. By restoring the symmetry between time and space in a matter field, we obtain the results that resemble a zero-spin bosonic field. The temporal vibrations are additional degrees of freedom introduced. A particle has an internal clock with a frequency as conjugated by de Broglie. The internal time registered by this clock is oscillating relative to the external time. The energy that arises from the oscillation is the internal mass-energy of the particle which must be on shell. As a result, the particle's proper time vibration amplitude has only one unique value. The energy in the field with space and time vibrations can only correspond to those for integer numbers of particles. Each particle has the same proper time vibration amplitude. The condition that mass is on shell forces the system to be quantized. This situation is very different from the classical theory where the amplitude of an oscillator can take any real positive number. There is no analogy like the mass on shell that quantizes a classical system with oscillation in the spatial directions.

In [37, 38], Busch clarifies the different role of "external time" and "intrinsic time" to prevent confusions when they are used to discuss time in quantum physics. The external time is a parameter used for references as adopted in our formulation. There is nothing dynamical about the external time. On the other hand, as defined by Busch, the intrinsic time shall be a dynamical variable of the studied system that functions to measure the time (e.g., position of a clock's dial or position of a classical free particle [26]). Here, we extend the concept of intrinsic time and use the term "internal time" to define the dynamical time registered by the internal clock of a particle that has physical vibration in time. In our proposed system, the internal time is the sum of external time and temporal vibration. This internal time is only a parameter. The mass energy of a particle is generated from the oscillation in proper time as shown in Eq. (28). Without the temporal vibration, the particle will have no energy, and there will be nothing dynamical about the particle's internal time.

The spatial vibration of a particle may remind us of zitterbewegung. As we shall recall, Schrödinger shows that in addition to the uniform rectilinear motion consistent with the classical electrodynamics, an extra oscillatory term (zitterbewegung) also appears in the Dirac equation [39]. This oscillation can be interpreted as fluctuation in the position of the electron with radius  $\lambda = (2m)^{-1}$  and a circular frequency  $\omega = 2m$ . Its effect is believed to have originated from the interference between positive and negative energy waves. However, there are also suggestions that zitterbewegung can have possible link with spin [40, 41]. Interference between positive and negative frequencies may not be the only reason that can give rise to zitterbewegung. Although zitterbewegung bears some semblance to the spatial vibration discussed in this paper, there are fundamental differences.

The spatial vibration of a particle with proper time vibration has nothing to do with spin. As shown in Sect. 3, even a moving zero-spin particle can have spatial vibration. The spatial vibration discussed in this paper originates from the proper time oscillation of a particle and not from spin. In addition, a plane wave with only one particle from Eq. (14) can have vibration in space. There is no interference between positive and negative energy waves. Lastly, from Eq. (34), the spatial vibration is along the particle's trajectory with an amplitude  $\mathbf{X}_p = \mathbf{k}\omega_0^{-2}$ . It is not the fluctuation as calculated for zitterbewegung. As we can see, zitterbewegung and the spatial vibration discussed in this paper have fundamental differences. Since the scope of this paper is limited to a bosonic field, we will defer any detail discussions about spin particles and zitterbewegung to a later time.

The mass-energy of a particle is generated from its vibration in proper time as shown in Eq. (28). It is reasonable to believe that all massive particles shall have this vibration in proper time, with or without spin. Under a Lorentz transformation, this proper time vibration translates to vibrations in both the temporal and spatial directions. Neglecting the effects of spin and zitterbewegung, we can estimate the spatial and temporal oscillation amplitudes of a moving electron from its proper time oscillation (i.e.,  $\omega_0 = 7.6 \times 10^{20} \text{ s}^{-1}$  and  $|\tilde{T}_0| = 1.32 \times 10^{-21} \text{ s}$ ). We are interested in the electrons because they are the most common massive particles investigated in the laboratories. From Eqs. (33) and (34), the oscillation amplitudes of an electron traveling with velocity  $|\mathbf{v}|$  are

$$|\mathbf{v}| = 0.001 \quad \Rightarrow \quad |\mathring{T}_p| = 1.3 \times 10^{-21} \,\mathrm{s}, \qquad |\mathring{\mathbf{X}}_p| = 3.9 \times 10^{-14} \,\mathrm{cm},$$
  
 $\omega_p = 7.6 \times 10^{20} \,\mathrm{s}^{-1}, \qquad (79)$ 

$$|\mathbf{v}| = 0.99999 \quad \Rightarrow \quad |\mathring{T}_p| = 2.9 \times 10^{-19} \,\mathrm{s}, \quad |\mathring{\mathbf{X}}_p| = 8.8 \times 10^{-9} \,\mathrm{cm},$$
  
 $\omega_p = 3.4 \times 10^{18} \,\mathrm{s}^{-1}.$  (80)

In the nonrelativistic example, the amplitude of the spatial vibration is approximately equal to the diameter of a nucleus. However, this vibration is very rapid. If the measurement is not sensitive enough to detect the small vibration, the particle will appear to travel along a smooth trajectory. On the other hand, the amplitudes of the oscillation are increasing, but the frequency is decreasing when the velocity of the particle increases. If the particle is traveling fast enough with lower frequency and larger amplitude, it may make the oscillation easier for detection. However, we shall bear in mind that the effects of spin and zitterbewegung are not included in this discussion.

The frequency of de Broglie's internal clock is very rapid, and the amplitude of the temporal proper time oscillation is very small. In order to detect this oscillation, a clock sensitive enough to detect the rapid oscillation is required. We can achieve this by using the internal clock of a heavy particle. As we can see, as  $\omega_0 \rightarrow \infty$ , the amplitude  $|T_0| \rightarrow 0$ . A heavy particle will appear to travel along a near timelike geodesic which is sensitive enough to detect the varying internal time rate of another particle with lower frequency. However, to obtain infinite accuracy in measuring a clock's time will mean infinite uncertainty in the clock's mass, and thus the clock's mass needs to reach infinity ( $m = \omega_0 \rightarrow \infty$ ) [42].

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