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Kragujevac Journal of Science 47 (2025) 3
Special Issue

C O N T E N T S

EDITORIAL

Foundations, History and Philosophy of Quantum Science

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Quantum Fields, Particles and Cosmology

Future of Quantum Science and Technology

EDITORIAL

This Special Issue of the *Kragujevac Journal of Science* is devoted to the *International Year of Quantum Science and Technology*. The year 2025 marks the 100th anniversary of Werner Heisenberg's groundbreaking introduction of matrix mechanics - a pivotal moment in the development of quantum mechanics. Heisenberg's formulation offered a radically new way for describing the behavior of matter at atomic and subatomic levels. Departing from the principles of classical physics, matrix mechanics laid the foundation for the quantum revolution, including the development of the famous Schrödinger equation just one year later. In recognition of this scientific milestone, the United Nations has declared 2025 the International Year of Quantum Science and Technology, aiming to inspire a year-long, worldwide celebration that raises public awareness of the importance and impact of quantum science and its applications. Considering this historical occasion, Professor Dugic initiated the preparation of this special issue. This initiative was warmly supported by the editorial board of the *Kragujevac Journal of Science*.

The contributions to this issue are due to invitation only. We hope the readers will benefit from the articles presenting quantum science and technology starting from a historical and foundational perspective up to the open issues of modern quantum cosmology. As a special part of the Issue, we want to emphasize a collection of the answers of the authors who responded to our query on the future of Quantum Science and Technology. We want to express gratitude to all the authors for their time and effort to set this special issue. We would also like to thank the Editorial Board of the Journal for disseminating awareness of the scientific importance and global relevance of Quantum Science and Technology.

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100 YEARS OF QUANTUM MECHANICS: THE MONTHS THAT CHANGED PHYSICS

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ABSTRACT. A hundred years ago, physics underwent one of its most dramatic transformations – a paradigm shift that fundamentally changed our understanding of nature. Over the course of several revolutionary months in 1925 and early 1926, quantum mechanics emerged as a new, foundational theory of the microscopic world. With the publication of key papers by Werner Heisenberg and Erwin Schrödinger, the theoretical framework was established that radically redefined our perception of physical reality. These works demonstrated that atoms and subatomic particles do not obey the laws of classical mechanics, but instead follow entirely new, quantum laws. Born in those intense months, quantum mechanics became one of the cornerstones of modern physics and a lasting source of inspiration in both theoretical and applied sciences. This paradigmatic shift opened new avenues of research and laid the groundwork for scientific discoveries that continue to shape our understanding of nature today. This paper is dedicated to those pivotal historical moments – the months in which science made one of its deepest leaps and most consequential strides in comprehending the world.

Keywords: Quantum mechanics, scientific revolution, Werner Heisenberg, Erwin Schrödinger, old quantum theory, matrix mechanics, wave mechanics.

INTRODUCTION

There are certain periods in human history marked by a sudden and intense flourishing of thought, ideas, and discoveries – epochs in which science advances by leaps rather than steps. One such period was the 1920s, and in particular the months of 1925 and early 1926, which can rightfully be called the "The Beautiful Era" of theoretical physics. It was precisely at that time that one of the greatest turning points in the history of science occurred – the birth of quantum mechanics, a new theoretical paradigm that fundamentally transformed our understanding of the microworld (WEINBERG, 2013; PANTIĆ, 2024; DUGIĆ and JEKNIĆ-DUGIĆ, 2025).

This discipline, which initially emerged as an attempt to explain anomalies within classical physics, soon evolved into one of the pillars of modern science. With the publication

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of key papers by Werner Heisenberg (1925) and Erwin Schrödinger (1926), physics entered a new era in which atoms and subatomic particles were no longer subject to the laws of classical mechanics, but required an entirely new, quantum description. During those intense months, new discoveries began to unveil deeper layers of reality, previously hidden behind the limitations of classical intuition.

The development of quantum mechanics involved the greatest minds of the time: Niels Bohr and his collaborators from Copenhagen, Max Born, Pascual Jordan, Werner Heisenberg, Erwin Schrödinger, Wolfgang Pauli, Paul Dirac, and others. Even Albert Einstein, though later skeptical of some implications of quantum theory, played a significant role in its early stages. Quantum mechanics did not emerge all at once, but rather as a response to theoretical challenges and experimental puzzles, such as the inadequacy of the classical model of electron orbits in atoms.

The United Nations has declared 2025 the International Year of Quantum Science and Technology, precisely in honor of that astonishing scientific leap that occurred a century ago. The aim of this paper is to shed light on those key and turbulent months during which science took a profound turn toward a new understanding of nature, and to show how the ideas born in that short but fruitful period forever changed the course of physics and laid the foundations of modern science and technology.

THE INTENSE MONTHS OF 1925 AND 1926: HISTORICAL MOMENTS IN THE BIRTH OF QUANTUM MECHANICS

A hundred years ago, in July 1925, twenty-three-year-old German physicist Werner Heisenberg submitted a paper to the journal *Zeitschrift für Physik* (HEISENBERG, 1925), which would mark the beginning of modern quantum mechanics and ignite a revolution in our understanding of the fundamental laws of physics – a revolution whose impact is still deeply felt today. This pioneering work not only represented a turning point, but also stimulated intense research in the months that followed, both through Heisenberg's collaboration with Max Born and Pascual Jordan, and through the work of Erwin Schrödinger, who developed a completely different, yet mathematically equivalent, approach.

Heisenberg's paper represented a bold and innovative effort to overcome the limitations of existing models in explaining atomic spectra – the frequencies and intensities of light that atoms emit and absorb. At the heart of the problem was the Bohr-Sommerfeld model of the atom, developed during the 1910s. This model formed the basis of the old quantum theory, which had emerged as an attempt to interpret certain quantum effects within the framework of classical mechanics. However, it became clear that classical physics was insufficient to provide a consistent explanation of phenomena in the microscopic world, opening the door for the emergence of an entirely new theory.

However, the gap in understanding atomic structure could only be bridged by introducing the ad hoc assumption that energy does not flow continuously, but arrives in discrete packets – quanta. The Bohr-Sommerfeld model, as an extension of Bohr's earlier atomic model, assumed that electrons move in elliptical orbits around the nucleus, with their motion governed by specific quantum conditions. This model successfully explained the spectrum of the hydrogen atom, as well as the splitting of spectral lines in the presence of external electric fields (the Stark effect) and magnetic fields (the Zeeman effect). Nevertheless, despite these successes, the model encountered serious difficulties in explaining more complex systems, such as the hydrogen molecule and atoms with multiple electrons.

Heisenberg recognized this problem in 1923, when, as a young scientist, he joined the Institute for Theoretical Physics at the University of Göttingen, where he worked as an

assistant to Max Born. Together, they carried out a series of detailed calculations of the helium atom's spectrum, using all the orbits predicted by the Bohr-Sommerfeld model. However, their results did not align with experimental data. At first, they suspected inaccuracies in the computational methods, but it soon became clear that the issue was a much deeper conceptual one. “It is becoming increasingly likely,” wrote Born (BORN, 1926), “that it will not be enough to simply introduce new assumptions in the form of physical hypotheses, but that the entire system of physical concepts will have to be rebuilt from the ground up.” In a letter to his former teacher Arnold Sommerfeld from December 1923, Heisenberg wrote: “Classical representations of orbits cannot accurately describe the energies and frequencies that appear in real atoms.”

Heisenberg and Wolfgang Pauli both questioned the viability of the orbital model. As early as 1924, Pauli wrote to Sommerfeld expressing that the language used to describe the quantum world was inadequate. Nevertheless, up until April 1925, it remained unclear how to proceed with the development of the theory without relying on classical orbital models.

Sometime later, seeking relief from hay fever on the island of Helgoland, Heisenberg laid the foundation for a more radical approach. Instead of relying on models with clearly defined orbits, he developed the concept of “quantum mechanics”, where electrons were no longer viewed as particles moving along continuous paths. In early July 1925, he wrote to Pauli that all his efforts were directed at completely eliminating the concept of orbits, which, as he pointed out, could not even be directly observed. This marked a crucial break with classical mechanics (MLAĐENOVIĆ, 2008).

In his paper (HEISENBERG, 1925), Heisenberg aimed to establish a theoretical foundation for quantum mechanics that relied exclusively on relations between quantities that are, in principle, measurable. He proposed a new approach based on the use of matrices, moving away from the classical notion of particles and waves. Instead of considering traditional concepts such as electron orbits, Heisenberg focused on describing kinematic and mechanical quantities, such as position and momentum, which were represented using matrices in this approach. His equation involved complex matrix sequences that described observable quantities, such as energies and transition amplitudes, which represent the probability of atoms transitioning from one quantum state to another. This work was not only a theoretical step forward but also laid the foundation for the development of matrix mechanics, one of the core formulations of quantum mechanics.

However, it was difficult to understand how the elimination of unobservable quantities could guide the further development of the theory. It was also unclear which quantities should be considered unobservable. As Born later reflected, although the idea of eliminating unobservable quantities seemed reasonable in 1925, in practice such a “general and vague formulation was completely useless, even wrong”. This challenge highlighted the pragmatic approach of Heisenberg’s physics, which often relied on testing various ideas until the one that actually worked in practice was found.

The development of quantum mechanics through the work of Werner Heisenberg marks a break with the classical concept of orbits and introduces a new approach based on matrices. Heisenberg considered unobservable quantities and their role in the quantum description of nature, but it became clear that a more precise approach was needed. The development of matrix mechanics, although initially uncertain in direction, continued to form through experimental and theoretical efforts, laying the foundation for quantum mechanics as a theoretical framework. In the following, Heisenberg’s matrix quantum mechanics, which represented a key step in defining modern quantum theory, will be discussed in more detail.

HEISENBERG'S MATRIX MECHANICS

The physical ideas that led to the emergence of quantum mechanics were first systematically formulated by Werner Heisenberg. Born in 1901 in Würzburg (Bavaria), Heisenberg studied in Munich under the guidance of the renowned professor Arnold Sommerfeld and defended his doctoral dissertation on hydrodynamics in 1923. However, a decisive moment in his scientific development was his encounter with Niels Bohr, the creator of the old (classical) quantum theory, in 1922. Bohr had been invited to give a seminar in Göttingen, which Heisenberg attended. The sharp and insightful remarks of the young student impressed Bohr, who invited Heisenberg to visit the Institute in Copenhagen the following spring, in 1923. This meeting laid the foundation for a long and fruitful collaboration that greatly shaped the development of quantum mechanics (DUGIĆ and JEKNIĆ-DUGIĆ, 2025; MLAĐENOVIĆ, 2008).

The warm, friendly atmosphere at the Institute and in the Bohr household, as well as Niels Bohr's own character, left a deep impression on Heisenberg. Bohr's intuitive approach to studying physical phenomena was an ideal complement to Heisenberg's more abstract method of reasoning. Bohr's method, which did not begin with mathematical formalization but with a deep understanding of the phenomena themselves, had a profound influence on Heisenberg's ability to reconsider and transform his earlier concepts. As Heisenberg himself wrote in an article dedicated to Bohr: "For Bohr, understanding the relationships between physical quantities did not arise from mathematical analysis of theoretical assumptions, but from an intense study of the phenomena themselves, which allowed him to grasp these relationships intuitively, rather than derive them formally."

This collaboration in Copenhagen not only enriched Heisenberg's understanding of quantum mechanics, but also significantly influenced the very structure of quantum theory itself. Heisenberg's work, combined with Bohr's intuition, was crucial for the development of matrix mechanics, which would later become one of the two main pillars of quantum mechanics, alongside wave mechanics developed by Erwin Schrödinger.

Upon being appointed as an assistant at the University of Göttingen, Heisenberg joined ongoing research in the field of quantum theory in collaboration with Max Born and Pascual Jordan. From 1924 to 1927, Heisenberg frequently stayed in Copenhagen, where he continued a fruitful and intense collaboration with Niels Bohr, one of the pioneers of the old quantum theory. At that time, classical quantum theory was at its peak.

Quantum theory originates from Planck's hypothesis, formulated in 1900 by Max Planck to explain the blackbody radiation law. According to this hypothesis, the exchange of energy between matter and radiation does not occur continuously, but rather in discrete, indivisible units – quanta of energy. In 1913, Niels Bohr introduced the concept of quantum jumps between discrete energy levels in his atomic model, providing a mechanism for explaining Planck's hypothesis. According to Bohr's model, when an electron transitions from a higher energy level E_m to a lower one E_n, a quantum of light – a photon – is emitted or absorbed with energy $h\nu = E_m - E_n$, where $h = 6{,}626 \cdot 10^{-34}$Js is Planck's constant, representing the elementary quantum of action.

Although quantum jumps and Planck's hypothesis successfully explained a range of experimental data, Bohr himself believed that the concept of the quantum of light served only a supplementary mathematical role and did not accept the physical reality of the photon. His position was that Einstein's corpuscular theory of light – proposed in 1905 to explain the photoelectric effect – could not be reconciled with Maxwell's classical theory of electromagnetism. However, this skepticism was shaken in 1922 when Arthur Compton discovered the scattering of X-rays by electrons – a phenomenon that could only be explained

by attributing a particle-like nature to radiation. This led to the acceptance of the idea that radiation simultaneously possesses both wave and particle properties – a phenomenon that would later become known as the wave-particle duality of light. This profound conceptual dilemma remained beyond the reach of classical quantum theory.

Faced with this challenge, Bohr spent years trying to find a way to unify the wave and particle nature of light into a single coherent theory. However, by 1924 it had become clear that the classical quantum model was insufficient to explain more complex atomic systems. While Bohr's theory successfully described the hydrogen atom – the simplest atomic model – it could not account for the fine structure of the spectrum or other experimental results. Theoretical physics found itself in a crisis that demanded a radically new approach. It was at this historical moment that Heisenberg emerged with his new perspective based on matrix mechanics – a revolutionary method that would mark the beginning of modern quantum mechanics.

In the spring of 1925, Werner Heisenberg attempted to calculate the intensities of lines in the hydrogen spectrum using the existing quantum theory. However, he was unsuccessful in this endeavor. He concluded that the difficulties were of a fundamental nature and had to be resolved before any further progress could be made. The idea for how to overcome this problem came from a thought expressed by A. Einstein in his special theory of relativity: that any physical theory must rely solely on observable quantities. Heisenberg realized that the main shortcoming of Bohr's quantum theory was its reliance on quantities inaccessible to experimental observation – such as electron orbits or trajectories within the atom.

Starting from this idea, Heisenberg focused exclusively on experimentally accessible (observable) quantities, such as the frequencies and intensities of spectral lines in atomic spectra. He constructed frequency schemes corresponding to transitions between two stationary states: $\nu_{nm} = (E_m - E_n)/h$ where $\nu_{nm} \neq 0$. Similar schemes could also be constructed for the intensities of spectral lines, as well as for other quantities associated with transitions between stationary states. To each physical quantity, Heisenberg assigned such a scheme.

On the other hand, Heisenberg introduced the assumption that the elements a_{nm} of the scheme for any physical quantity A, associated with the atom, vary harmonically with time in accordance with the corresponding frequency: $a_{nk}(t) \sim e^{2\pi i\, \nu_{nk} t}$. From this law of time dependence follows the multiplication rule for the schemes:

$$a_{nk} a_{km} = e^{2\pi i\, (\nu_{nk} + \nu_{km}) t} = e^{2\pi i\, \nu_{nm} t} = a_{nm}.$$

This law of time variation, as well as the multiplication rule for the schemes, was derived by Heisenberg based on experimental facts. It was known that if two frequencies appear in a spectrum, then their sum and difference also appear in the same spectrum. This empirical rule, known as the Ritz combination principle, receives a clear explanation in the light of quantum jumps – each transition between energy levels generates a specific frequency, and combinations of these transitions result in new spectral lines.

He believed that "a more intensive mathematical investigation" would show whether his method from July was "satisfactory." In Göttingen, this line of research was continued by Max Born and Pascual Jordan, who recognized that the quantities in Heisenberg's equations could be represented as matrices – a new, revolutionary mathematical approach. Together, they reconstructed the theory in terms of matrix mechanics and presented their results in an extensive paper BORN, *et al*. (1926), known as the *Dreimännerarbeit* ("three-man paper"), which they submitted in November 1925. With this work, which preceded paper BORN and JORDAN, (1925), the mathematical foundation of the new theory – **matrix quantum mechanics** – was established.

In the further development and general mathematical elaboration of the formalism of quantum mechanics, significant contributions were made by Paul Dirac and John von Neumann. However, even Heisenberg's initial formulation reveals a fundamental difference between classical physics and quantum mechanics. While classical physics associates physical quantities with ordinary numbers, quantum mechanics assigns matrices to these quantities, whose rules of calculation may differ. For instance, for two matrices A and B, the product AB is not always equal to the product BA. In such cases, the matrices are said to be non-commutative.

What is particularly important is that the coordinate matrix (denoted as X) and the momentum matrix (denoted as P) do not commute, which is mathematically expressed as $XP \neq PX$. This non-commutativity is not merely a mathematical peculiarity but has a profound physical significance – it lies at the heart of Heisenberg's uncertainty principle. This principle establishes fundamental limits on the simultaneous knowledge of a particle's position and momentum in the same quantum state.

Heisenberg attributed great importance to these seemingly purely mathematical aspects of the theory. He believed that the physical meaning of the theory was embedded in its fundamental postulates and that the consistent application of the mathematical framework could yield correct interpretations of physical phenomena – without the need for visual representations or classical intuition. This approach not only eliminated the classical notion of particles as objects moving along well-defined trajectories, but also led to the development of quantum mechanics as a theory based on probabilities rather than deterministic predictions. This radical departure from classical mechanics laid the foundations of modern quantum physics, where the mathematical framework – rather than physically realistic models – plays a central role in understanding the microscopic world.

However, Heisenberg's model came at a cost. As the authors explained, the new theory was not suitable for a geometric interpretation, as the motion of electrons could not be described in terms of familiar concepts of space and time[2]. While Born and Jordan enjoyed the abstraction, Heisenberg, in a letter to Pauli in June 1925, expressed doubt, questioning what the equations of motion[3] he used in his work actually meant. Pauli's successful calculations of the hydrogen atom's spectrum (PAULI, 1926) in December of that year were considered confirmation of the validity of the approach. However, most physicists found it difficult to accept this complex mathematics, so it was a relief when, just a few months later, in 1926, a completely different approach emerged. This approach, which would become known as wave mechanics, represented a new way of considering quantum phenomena and opened the path for further development of quantum theory. We now turn to the discussion of this important breakthrough that would lead to a deeper understanding of quantum systems, where the concept of waves and wave functions would play a central role.

SCHRÖDINGER'S WAVE MECHANICS

Less than a year after the development of matrix mechanics, another version of quantum theory emerged – **wave mechanics**. This new approach was formulated by Erwin Schrödinger, then a professor at the University of Zurich, in a series of revolutionary papers published in the journal *Annalen der Physik* (SCHRODINGER, 1926; SCHRODINGER, 1928). Unlike Heisenberg, who dismissed visual representations in favor of abstract algebraic

[2]This in classical mechanics implies defined positions (coordinates) and trajectories of particles.

[3]In the context of quantum mechanics, the equation of motion refers to the mathematical relation that describes how a quantum system changes or evolves over time.

structures, Schrödinger started from the idea that the fundamental equation of quantum theory should describe the propagation of matter waves.

By 1923, there was sufficient evidence that light possessed a dual nature – both wave-like and particle-like. However, there was no experimental proof that particles on the atomic scale exhibited a similar dualistic character. The first to seriously suggest this possibility was Louis de Broglie. He hypothesized that if Planck's constant relates energy and momentum to frequency and wavelength for photons, then the same relationship should also apply to material particles. De Broglie concluded that the wavelength of a particle is given by the expression $h = \lambda/p$, and the frequency by $\nu = E/h$, where h is Planck's constant, p is the momentum, and E is the energy of the particle. With this bold hypothesis, de Broglie introduced the idea of wave-particle duality not only for light but for matter as a whole.

At the time when de Broglie presented his ideas, the main weakness – aside from the lack of experimental confirmation – was that his formulation did not constitute a complete theory. Classical mechanics could no longer explain all experimental findings, and the quantum conditions that were being introduced *ad hoc* were becoming increasingly numerous and disconnected. The need for a new, unified theoretical framework was becoming more and more apparent.

While Heisenberg, as previously described, was the first to offer a successful solution by formulating matrix mechanics in 1925, only a few months later, Schrödinger developed his own approach based on ideas closely related to de Broglie's hypothesis. In this way, quantum mechanics was born a second time – this time in the form of wave mechanics.

Schrödinger believed that the rejection of visual and spatial representations of atomic processes – as done by matrix mechanics – was a step backward and a loss of hope in understanding the atomic world. In contrast, he was convinced that it was possible to formulate a theory that would describe the dynamics of atomic systems using waves. He formulated a wave equation that successfully described the energy states of the hydrogen atom, thereby confirming the validity of his approach.

Within this framework, the quantum state of a system is described by a complex function of real variables – the wave function, which is a solution to Schrödinger's equation. Although this function itself has no direct physical interpretation, it allows for the calculation of all physically relevant quantities. In this way, the wave function becomes the carrier of information about the state of a quantum system and a central concept in Schrödinger's formulation of quantum mechanics.

Heisenberg, however, did not accept Schrödinger's theory uncritically. After attending a colloquium in Munich where Schrödinger presented his version of quantum mechanics, Heisenberg expressed numerous criticisms in a letter to Wolfgang Pauli. He believed that the wave theory could not explain key quantum phenomena such as the photoelectric effect and the Stern-Gerlach experiment. He also pointed out the difficulties in describing multi-particle systems, which would require the use of a wave function in an abstract, high-dimensional space. Although he acknowledged the usefulness of Schrödinger's formulation as a computational tool, Heisenberg remained skeptical about the physical meaning of the wave function. In a letter from 1926, he wrote: "Even if a consistent wave theory in three-dimensional space were to be developed, it would hardly be capable of providing an exhaustive description of atomic processes within the framework of our known concepts of space and time" (HEISENBERG, 1926; MLAĐENOVIĆ, 2008).

During the following year, Schrödinger persistently tried to find a satisfactory physical interpretation of his theory, but without full success. Although wave mechanics quickly became an extremely useful mathematical framework for solving concrete quantum problems, it did not provide an intuitive description of individual processes within the atom in terms of

traditional concepts of space and time. Schrödinger was deeply disappointed by the fact that the new physical paradigms no longer allowed for the visualization of atomic processes in a manner similar to classical mechanics. This marked a deeper epistemological shift: the atomic world is no less real, but it requires abandoning intuitive images in favor of abstract mathematical symbols. While this allows the physicist to understand and predict phenomena, it significantly complicates the popularization of quantum theory outside professional circles.

Although it did not provide an intuitive explanation of quantum phenomena in the classical sense, wave mechanics nonetheless played a crucial role in the construction of the new theory. In combination with matrix mechanics, it laid the foundation of modern quantum physics and enabled the formulation of a unified theory – quantum mechanics. Concepts such as the wave function and its probabilistic interpretation became central elements of the theory, allowing for a deeper understanding of atomic and subatomic processes. The shift toward this new, more abstract and mathematically grounded view of quantum phenomena marked a turning point in the development of modern physics.

Nevertheless, we should not conclude without addressing some of the problems inherent in quantum mechanics itself. Despite its remarkable successes, the theory also has its weaknesses. One of them is the lack of integration with the general theory of relativity – the universal theory of gravitation. Another challenge lies in the fact that quantum mechanics is still not entirely self-sufficient: for its formulation and experimental verification, it continues to rely on classical mechanics.

The greatest challenge of modern physics may lie precisely in the ability to reexamine – and, if necessary, abandon – fundamental principles when they are shown to no longer hold in new contexts. The history of physics demonstrates that progress has often depended on the willingness to move beyond old paradigms. Although it currently seems unlikely that the ideas of quantum mechanics will be entirely abandoned in the near future, the possibility remains open that future theories will provide even deeper and more comprehensive descriptions of physical reality.

EQUIVALENCE OF MATRIX AND WAVE MECHANICS

As we mentioned earlier, immediately after presenting their theories, misunderstandings arose between Heisenberg and Schrödinger due to differing starting positions and interpretations. From today's perspective, the speed with which quantum mechanics was shaped is remarkable. However, very quickly, at the initiative of Niels Bohr, there was a reconciliation of opinions. In the end, it turned out that matrix and wave mechanics are equivalent theories, representing two different, but mathematically comparable formulations of quantum mechanics.

The equivalence of matrix and wave mechanics was established in the spring of 1926 (SCHRODINGER, 1928), which was a crucial step in the further development of quantum theory. June 1926 was also significant due to the first paper submitted by Max Born, which related to collision phenomena. In this paper, he interpreted the square of the amplitude of the wave function from Schrödinger's theory as the probability that a particle would scatter in a certain direction after colliding with an atom. Soon after, works by Pascual Jordan and Paul Dirac followed, in which they developed the "transformation theory", describing quantum states (and not just transitions between them) in terms of probability amplitudes. This concept laid the foundation for probability as one of the fundamental ideas in quantum mechanics.

A significant turning point in the development of the theory occurred in 1927, when Heisenberg, in one of his papers HEISENBERG (1927), introduced the concept of uncertainty

relations. According to this concept, the more precisely the position of an electron is determined, the less precisely its momentum can be determined (and vice versa). This paper not only completed the development of quantum mechanics but also pointed out the existence of fundamental limitations in the knowledge of two physical quantities, such as position and momentum, which quantum nature imposes, independently of the measurement process.

From mid-1926, physicists began applying quantum theory to more and more practical problems. The development of the theory was so rapid that it was difficult to keep up with all the new methods and techniques. After some physicists mastered the new method, they often found that someone else had already published the same solution earlier. This accelerated pace of development led to frequent complaints about "intellectual overload". The consideration of the deeper meanings and philosophical consequences of the new theories was a privilege of only a small number of researchers who were able to devote themselves to such detailed deliberations.

By the time of the Solvay Conference in 1927, most physicists believed that quantum mechanics had reached its final form. Heisenberg and Born, in their report, declared quantum mechanics a "complete theory", whose basic assumptions no longer needed to be changed. However, not everyone was so convinced. Scientists such as Einstein, Schrödinger, and de Broglie considered the theory deeply problematic.

"Perhaps quantum mechanics is the correct theory of statistical laws", Einstein wrote, "but it does not sufficiently explain individual elementary processes". Einstein remained a critic of quantum mechanics throughout his life, believing that there was a deeper level of reality yet to be discovered. He argued that while quantum theory was successful in mathematically describing phenomena, it did not provide a satisfactory explanation of the fundamental laws of nature and, as such, could not be considered complete. His criticism was particularly directed at the "Copenhagen interpretation", which suggested that we cannot have a complete picture of reality at the subatomic level.

Although some of the most prominent scientists were skeptical about accepting quantum mechanics as the final theory, most physicists nevertheless accepted its accuracy and used it as a foundation for explaining various phenomena. After 1925, quantum mechanics became the basis for significant advancements in physics and chemistry. For example, it explained chemical bonds between atoms, investigated the mechanism of radioactive alpha decay, and clarified the process of electrical conductivity in metals. These results were crucial for the development of new areas of science and technology, particularly in materials science and molecular biology. Theories and discoveries derived from quantum mechanics laid the foundation for numerous innovations, including the development of lasers, semiconductors, and modern computing technologies (DUGIĆ, 2009).

Although quantum theory is still the subject of deep philosophical debates and is not without controversy, it provides an extraordinarily accurate description of all experiments conducted to date. Quantum mechanics perfectly explains phenomena in the subatomic world and serves as the foundation upon which new discoveries and theories are built. Its success in explaining complex natural phenomena, as well as its unparalleled advantage in practical applications, make it one of the most successful and productive theories in the history of science.

Although there are still some open questions, such as the deeper nature of quantum mechanics and the possibility of its integration with the theory of gravity, quantum mechanics remains a key pillar of our understanding of the physical world. Its ability to accurately describe phenomena in the subatomic world, without precedent, remains one of the most significant contributions to science. Deeper questions regarding the physical interpretation of quantum theory continue to spark debates among philosophers and theoretical physicists, but

regardless of the philosophical puzzles the theory presents, which will likely continue to be raised, it has provided extraordinary insight into the nature of our reality. Quantum mechanics, although still surrounded by open questions, remains one of the most successful and fruitful theories in the history of science, opening new horizons for future discoveries and understanding of the universe.

CONCLUSION

The emergence of quantum mechanics a hundred years ago represents one of the deepest and most significant revolutions in the history of physics, fundamentally altering our understanding of nature and the way we interpret physical reality. From the early works in quantum theory to the present day, quantum mechanics has not only provided exceptionally precise mathematical models for describing the world at the subatomic level but has also laid the foundation for the development of technologies that have become indispensable in modern society.

From lasers and semiconductors to supercomputers and nanotechnology, the application of quantum mechanics has shaped the technological and scientific progress of the 20th and 21st centuries. Its significance is recognized by the international community: on June 7, 2024, the United Nations declared 2025 the **International Year of Quantum Science and Technology**, symbolically highlighting the global impact of this theory. This decision reflects a deep awareness of the importance of quantum science and its applications for the future of humanity. Through this global initiative, supported by leading scientific and academic societies around the world, awareness will be raised about the importance of quantum technologies in everyday life and future technological development.

The International Year of Quantum Science and Technology aims to bring together researchers, industry experts, students, and the general public on a global scale. This initiative will promote the advancement of quantum research and its applications in various fields such as quantum computing, quantum cryptography, quantum sensors and security, as well as quantum medicine and new types of communication. It also aims to inspire younger generations to engage in this exciting and important scientific endeavor that will shape the future.

The year 2025 was chosen not only because of the current progress in quantum science but also to mark the 100th anniversary of the emergence of quantum mechanics, one of the most revolutionary scientific theories in history. The International Year of Quantum Science and Technology represents an ideal opportunity to promote quantum mechanics and quantum physics, especially among young people, and to encourage future generations to engage in this exciting scientific field.

Research in the field of quantum mechanics has laid the foundation for the development of numerous new disciplines and technologies that shape modern science, industry, and all aspects of our daily lives. Some of the most significant applications include quantum information science, quantum computing, quantum metrology, quantum thermodynamics, the theory of decoherence, and quantum theory of open systems. These disciplines are deeply interdisciplinary, reflecting a trend in modern sciences and technologies, where collaboration among different fields leads to significant advancements.

In addition to its scientific significance, quantum science and technology hold exceptional potential for future technological development, with applications in areas such as communications, computing, security, and medical technologies. It is expected that the 21st century will be marked by rapid advancements in quantum technologies, and quantum

engineers and experts in quantum technologies will play a key role in shaping the future. In scientific circles, it is already predicted that this century will be defined as the era of quantum engineers and innovations in the field of quantum technologies (MILBURN, 1997).

Revolutionary concepts such as quantum superposition, the uncertainty principle, wave-particle duality, and the phenomenon of quantum tunneling are just some of the key discoveries that have transformed not only physics but also the way we understand reality. Although quantum mechanics continues to raise many philosophical and theoretical questions – particularly in the context of its integration with general relativity – it remains indisputable in its ability to describe, predict, and explain phenomena in the micro-world.

Today, quantum mechanics is not just a scientific theory confined to laboratory experiments – it is the cornerstone of future discoveries and technologies. By opening new paths in understanding the deepest principles of the universe, this theory continues to play a crucial role in our quest to comprehend the structure of reality, life, and the cosmos itself.

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RESOLUTION OF THE PROBLEM OF DEFINITE OUTCOMES

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Abstract: This paper resolves the problem of definite outcomes, also known as "Schrodinger's cat" and the "problem of wavefunction collapse." It's the problem of understanding how nature goes from a coherent superposition of possible outcomes to a single definite outcome. This "measurement problem" has not to my knowledge been solved. The analysis stems from an insight into entanglement demonstrated in two nonlocality experiments involving pairs of momentum-entangled photons. These show that an entangled state of two subsystems is not a superposition of products of paired *states*, but instead a superposition of *correlations between paired states.* The "premeasurement state" is just such a superposition with the proviso that one subsystem is the detector of the other subsystem. This state is not a paradoxical superposition of macroscopic detector states; it is instead a superposition of *correlations between detector states and microscopic quantum states*. Thus, Schrodinger's cat isn't "smeared" between dead and alive but instead represents a nonlocal superposition of *correlations between* states of the cat and states of the nucleus: This is what we want. We also critique one previously claimed resolution of the measurement problem and seven previously claimed proofs that the measurement problem is unsolvable.

Keywords: quantum measurement problem, problem of outcomes, entanglement, nonlocality, Schrodinger's cat, wave function collapse.

INTRODUCTION

This analysis demonstrates that the problem of definite outcomes arises from a technical misunderstanding of entanglement and nonlocality. A proper understanding resolves the problem.

Since entangled states play a central role in most formulations of the measurement problem, and since entanglement is generally associated with non-local action (HOBSON, 2024), this paper investigates connections between nonlocality and measurement. We review two 1991 experimental investigations of entangled photons that are remarkable for being the only nonlocality tests (tests of Bell's inequality) based on mechanical variables (namely photon

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momenta) rather than quantum variables such as spin (RARITY and TAPSTER, 1990; OU *et al*., 1990). We show that a proper understanding of entanglement and nonlocality resolves the problem of definite outcomes.

Section 2 reviews one of the most common formulations of the measurement problem, namely the "problem of outcomes" or "Schrodinger's cat." Briefly, the problem is that the premeasurement entangled state seems to describe a macroscopic measurement device that simultaneously exhibits all possible measurement outcomes, even if those outcomes are "dead cat" and "alive cat." Such a macroscopic superposition is absurd (SCHRODINGER, 1935).

Section 3 reviews another common formulation of the measurement problem, first described by Einstein at the 1927 Solvay Conference (GILDER, 2008; KUMAR, 2008; BACCIAGALUPPI *et al*., 2009). This is the "collapse of the wave function" that occurs when a single quantum object such as an electron is described by a dynamically evolving spatially extended wave function that interacts with a detection device such as a viewing screen, causing the wave function to instantaneously collapse into a far more compact region. As Einstein noted, this appears to violate special relativity.

Section 4 presents the experimental background for properly understanding the measurement problem. We examine two quantum optics experiments that demonstrate nonlocal action between two momentum-entangled photons (RARITY and TAPSTER, 1990; OU *et al*., 1990).

Section 5 utilizes this understanding of nonlocal action to resolve the problem of outcomes.

Similarly, Section 6 resolves the puzzle of wave function collapse.

Section 7 shows that a well-known presumed resolution of the measurement problem (GOTTFRIED, 1966, 1991; GOTTFRIED *et al*., 1991) has a fatal flaw.

Section 8 disproves seven presumed proofs (WIGNER, 1963; D'ESPAGNAT, 1966; FINE, 1970; SHIMONY, 1974; BROWN, 1986; BUSCH and SHIMONY, 1996; BACCIAGALUPPI, 2013) of the insolvability of the measurement problem.

Section 9 summarizes this paper's conclusions.

The Problem of Outcomes ("Schrodinger's Cat")

First posed by E. Schrodinger and known as "Schrodinger's Cat" (SCHRODINGER, 1935) this formulation of the measurement problem is also known as the "problem of outcomes" (SCHLOSSHAUER, 2007). Consider a quantum system A having (for simplicity) a two-dimensional Hilbert space spanned by orthonormal states |A1> and |A2> and let O be the observable whose eigenstates are |A1> and |A2>. A "detector" D of O must contain a quantum component having the following three quantum states: |Dready,> represents a state in which D is poised to detect whether A is in state |A1> or |A2>, and |Di> (i=1 or 2) represents macroscopic registration that A was detected in the state |Ai>. D must also have a component that amplifies the microscopically detected outcome to irreversibly register that outcome, perhaps by creating a visible mark or an audible click. Thus, D is a macroscopic object with a quantum component.

For example, A might be a single electron passing through a double-slit setup containing a viewing screen, with "which-slit detectors" D1 and D2 present at both slits. The states |Di> (i=1 or 2) then represent the "clicked" state of the first or second detector. Suppose that, before measurement, A is prepared in an eigenstate |Ai> (i=1 or 2). A minimally disturbing measurement is then represented by

$$|Ai\rangle\,|D\ ready\rangle \Longrightarrow |Ai\rangle\,|Di\rangle \qquad (i = 1, 2) \tag{1}$$

where $|Ai\rangle$ represents the premeasurement eigenstate, the arrow represents the measurement process, and the right-hand side represents the post-measurement state. Note that

the same state $|Ai\rangle$ appears on both sides of (1), i.e. we assume that, when A is prepared in an eigenstate of $\boldsymbol{O}$, measurement of $\boldsymbol{O}$ does not disturb that eigenstate. This is an idealization.

Now suppose A is prepared in a 50-50 superposition of its eigenstates:

$$|Y_A\rangle = \frac{(|A1\rangle + |A2\rangle.}{\sqrt{2}} \qquad (2)$$

It follows from the linearity of the time evolution that a "which state" measurement of A is then represented by

$$\frac{(|A1\rangle + |A2\rangle)}{\sqrt{2}} |D\ ready\rangle \Longrightarrow |Y_{AD}\rangle \qquad (3)$$

where $|Y_{AD}\rangle$ is defined as

$$|Y_{AD}\rangle = \frac{|A1\rangle\,|D1\rangle + |A2\rangle\,|D2\rangle}{\sqrt{2}} \quad . \qquad (4)$$

A similar enigmatic entangled state crops up in nearly every analysis of the measurement problem. Following Schlosshauer (SCHRODINGER, 1935), we will call it the "premeasurement state."

The observed result of such a "measurement" ("detection" would be a more accurate word) is known from experiment to be

outcome $|Di\rangle$ is found with 50% probability ($i=1$ or 2). (5)

Equation (4) does not appear to be equivalent to (5). This is known as the “problem of outcomes." As one expert aptly put it, "The problem of what to make of this" (namely the state (4)) "is called ‘the measurement problem’" (MYRVOLD, 2022).

Equation (4) seems to represent a superposition of two detector states. In the case of an electron passing through a double slit experiment with detectors at both slits, (4) appears to describe one electron that passes through both slits, causing both detectors to click. This is not allowed because of Max Planck’s quantization postulate: Energy is always "found" in discrete finite lumps, with each lump having energy $E = hf$. This is of course the fundamental quantum postulate.

The symmetry of the above example implies that, classically, the energy passes in equal amounts through both slits, hence energy $(hf/2)$ passes through each slit. Equation (5), which is an experimental fact, then leads naturally assumption that each term should be treated in a probabilistic sense, implying that $\langle Y_{AD}|Y_{AD}\rangle$, evaluated at the ith detector, represents the probability that the photon will register at the i^{th} detector (i= 1, 2) – the Born rule.

In 1935, Schrodinger wrote a long philosophical paper published in three issues of *Die Naturwissenschafter (The Natural Sciences)* laying out his views on quantum foundations (GILDER, 2008). His infamous cat is mentioned in only two brief paragraphs within a Section titled "are the variables in fact smeared out?" (i.e.are the subsystems A and D described by a phase-dependent superposition?).

Schrodinger gets to the heart of the matter in his example of a "very burlesque case" of "smearing." He imagines a cat locked up in a closed room together with a radioactive sample placed in a radiation detector in such a manner as to create a 50-50 chance of a radioactive decay triggering the detector within one hour. Such triggering would activate a macroscopic device that would kill the cat. Schrodinger states, "in terms of the y function of the entire system, this will be expressed as a mixture [today we would call it a "superposition"] of a living

and dead cat." He notes that "a microscopic uncertainty has been transformed into a coarse grained (macroscopic) uncertainty." Such a macroscopic quantum superposition of a state in which the cat is dead (and the radiation detector has clicked) and a state in which the cat is alive (and the detector has not clicked) would be absurd.

Let's return to (4), which represents a superposition of two states of the compound system *AD*. Those two states are represented by the two dyads $|Ai\rangle\,|Di\rangle$ *(i = 1, 2)*. For example, in the electron 2-slit experiment with detectors at both slits, the conventional interpretation of (4) would be "In a single trial, the electron was detected at the first slit AND the electron was detected at the second slit." This describes an absurd superposition of two macroscopic outcomes. What's wrong?

Prior to answering this question (Section 5), we present a second version of the problem of definite outcomes (Section 3). Section 4 will then present two experiments that provide insight into these problems.

The Problem of Wave Function Collapse

Einstein, at the 1927 Solvay Conference on Electrons and Photons, was the first to point out the conundrum now known as "collapse of the wave packet." In an impromptu remark late in the conference, he asked the audience to consider a thought experiment in which an electron passes through a tiny hole in an opaque screen and then impacts a large hemispherical detection screen centered at the hole (see Fig. 1) (GILDER, 2008; KUMAR, 2008; BACCIAGALUPPI *et al*., 2009).

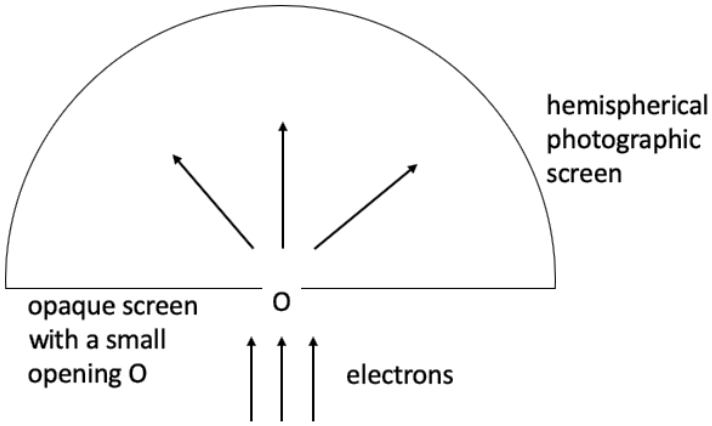

Figure 1: Einstein's thought experiment.

On each trial, a single electron diffracts widely, and then simultaneously arrives at every point on the hemispherical screen. Yet only one point registers an impact! How do the other points *instantaneously* remain dark? This appears to violate special relativity.

According to Schrodinger's equation, each electron diffracts widely after passing through the opening. A short time later, the entire electron (i.e. the entire wave function) interacts symmetrically with the *entire screen*. Because of the screen's hemispherical shape, this occurs *at a single instant*. Yet each electron registers at only a single point! How do the other points remain dark? Why don't they also register an impact? After all, the same wave function arrives simultaneously at every point on the screen.

As Einstein writes in his notes, "this entirely peculiar mechanism of action at a distance, which prevents the wave continuously distributed on the screen from producing an effect in *two* places on the screen" presents a problem. How do the points that do *not* show an impact *instantly*

"know" that they should remain dark? Einstein thought an instantaneous signal must "inform" these points that the impact occurred elsewhere. Such a signal would violate special relativity.

Experiments with momentum-entangled photons

Two quantum optics experiments (RARITY and TAPSTER, 1990; OU *et al*., 1990) published nearly simultaneously in 1991 demonstrate that the conventional interpretation of the premeasurement state (4) is incorrect, and that (4) is in fact precisely what we want and expect during a measurement. We shall call these experiments the "RTO experiments", honoring the two authors of the first report and the lead author of the second report.

RTO investigated entangled momentum states of two photons. Labeling the first photon "*A*" and the second photon "*B",* this entangled state was

$$|Y_{AB}> = \frac{|A1>|B1> + |A2>|B2>}{\sqrt{2}} \qquad (6)$$

where *I|Ai>* (*i=1, 2)* represents two orthonormal momentum eigenstates of the first photon and I|*Bi> (i = 1, 2)* represents two orthonormal momentum eigenstates of the second photon. Equation (6) is isomorphic to (4) with the important distinction that, in (6), both subsystems are microscopic. As we shall soon see, the entangled state (6) has non-local properties.

2022 Physics Nobel laureate Alain Aspect has remarked (PHILLIPS and DALIBARD, 2023) that the RTO experiments were unique because they were and are the only investigation of entangled *mechanical* degrees of freedom, namely linear photon momenta. All other entanglement experiments, including Aspect's prize-winning experiment, investigated photon polarization states.

Fig. 2 shows the layout for the RTO experiments. Two photons *A* and *B* were entangled by down-conversion of a single high-frequency photon. In Fig. 2, this entanglement is presumed to occur within the "source", so the photons were in the entangled state (6) as they emerged from the source. Photon *A* emerged moving along two paths A1 and A2, while *B* emerged moving along two other paths B1 and B2. Variable phase shifters f_A and f_B were inserted into one of *A*'s two paths and one of *B*'s two paths, respectively. We label these phase shifts f_A and f_B.

Remarkably, *neither photon Interfered with itself as a function of its own phase* f_A or f_B. That is, *individual photons were incoherent rather than phase-dependent or "smeared*:" Regardless of the phase settings f_A and f_B,

$$P(A1) = P(A2) = P(B1) = P(B2) = 0.5 \qquad (7)$$

This incoherence must be attributed to the entanglement.

However, coherence had not vanished. RTO found that the expected coherence of each photon had instead shifted: A and B now interfered with each other (rather than with themselves) as a function of the difference fA-fB of the two phase angles: When the experimenters shifted this "nonlocal phase difference" to various angles between 0 and 180 degrees, the correlation between the two photons varied as shown in Fig. 3.

Fig. 3 represents a remarkable new natural principle: When a composite system AB with microscopic sub-systems A and B becomes entangled, the pre-entanglement coherence of the subsystems is transferred to the new composite system. That is, the subsystems lose their coherence while the correlation between A and B becomes coherent or "smeared" (phase-dependent).

Indeed, Rarity and Tapster's outcomes at the four detectors violate Bell's inequality, verifying the nonlocality. Ou et al. were unable to demonstrate a violation of Bell's inequality. They state that "although experiments to demonstrate violations of Bell's inequality would require higher visibility of the interference, we have nevertheless confirmed the principle of two-photon interference under conditions of very great path difference."

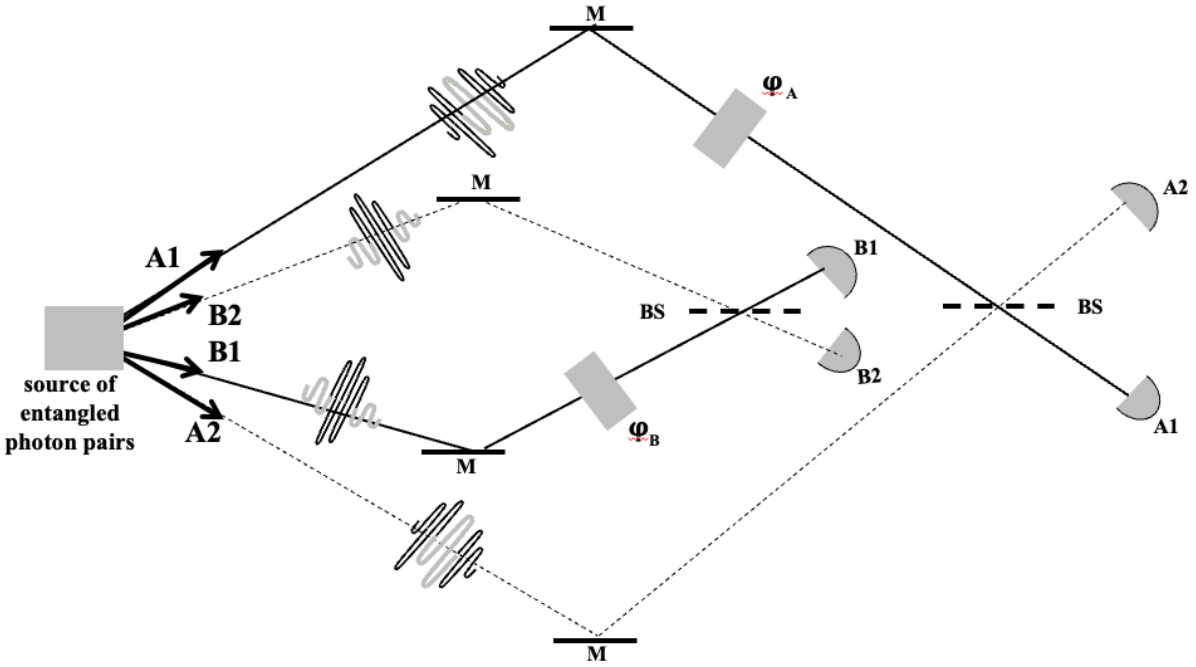

Figure 2. Layout of the RTO experiments. One photon emerges from the source along paths A1 and A2 while the other photon emerges along paths B1 and B2. The two photons form a single entangled "biphoton."

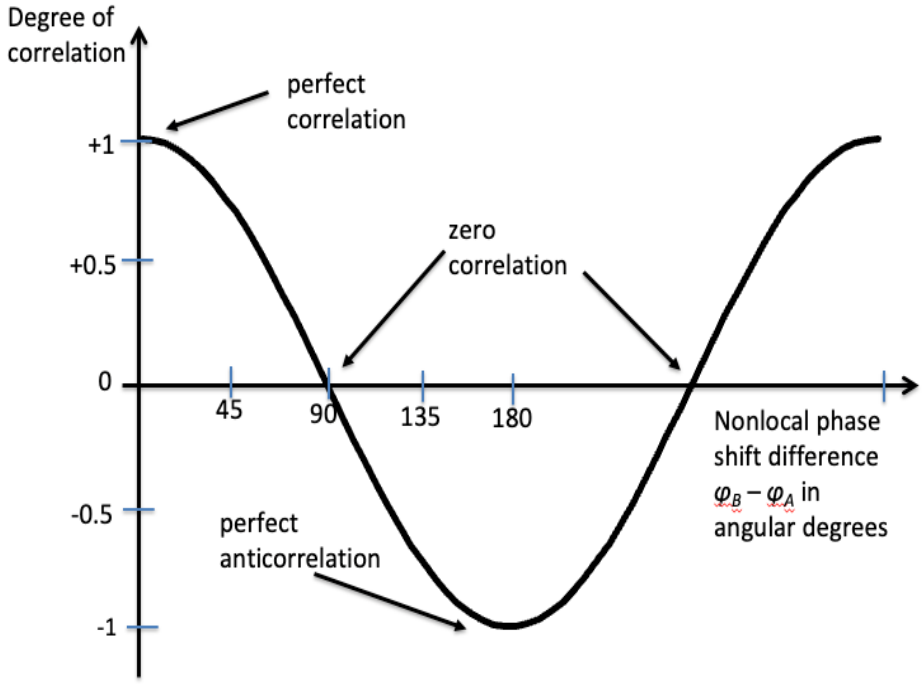

Figure 3. Nonlocal interference of RTO's bi-photon: Remarkably, the *degree of correlation* between RTO's two entangled photons varied sinusoidally with the nonlocal phase difference f_B-f_A.

Independently of violations of Bell's inequality, Fig. 3 provides straightforward evidence of nonlocality: Assume the phase shifters satisfy fA=fB, (note that pre-collaboration between the two detection stations would be required to establish this). According to Fig. 3, the two outcomes are then 100% correlated so that either observer can instantly read off the other observer's outcome simply by glancing at her own detector. Yet the two stations could be in separate galaxies (see the alternative set-up, Fig. 4)!

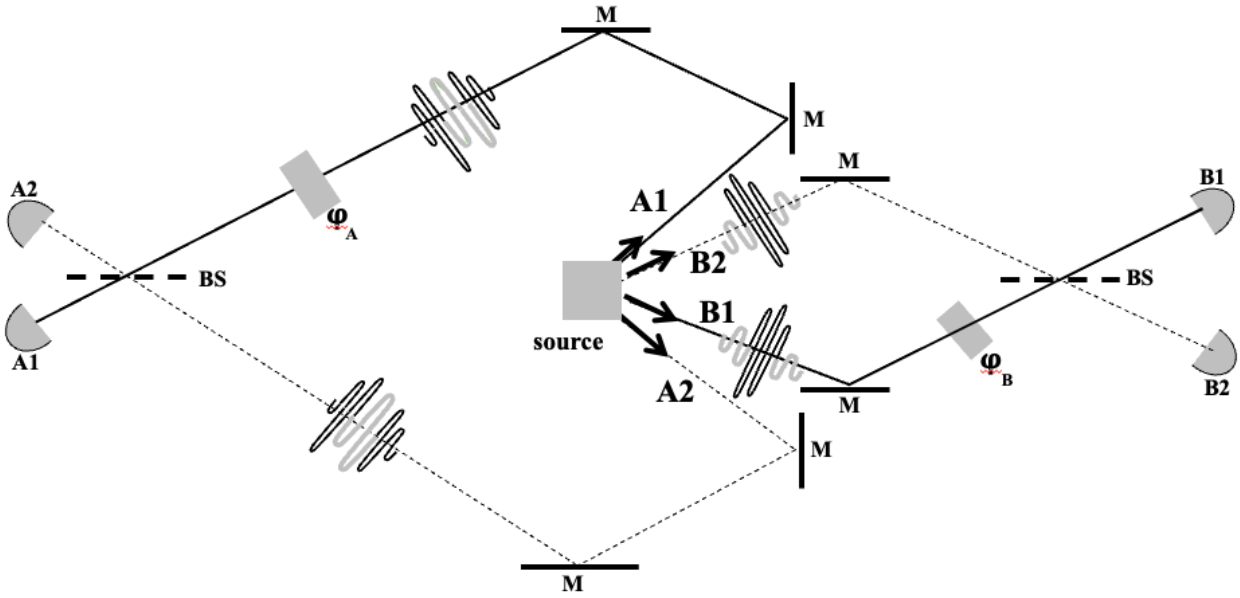

Figure 4. The RTO experiments, designed for widely separated detectors. (Compare Fig. 2)

Solution of the Problem of Outcomes

The RTO experiments found that, when two quantum objects A and B are entangled, the correlations between them become nonlocal: Regardless of their separation distance, alterations of the nonlocal phase difference fA-fB resulted in instantaneous alterations of their correlations. If we now return to the premeasurement state (4), we see that the problem of outcomes is solved: Simply allow subsystem B in (6) to be a macroscopic detector such as a Geiger counter or a cat. This creates no monstrous macroscopic superposition because B is incoherent and does not go through phases. Only the correlation between A and B goes through phases, as described above. If, for example, B is Schrodinger's cat, the cat is not coherent or "smeared" (as Schrodinger put it).

Conclusion: The entangled premeasurement state (4) is not an absurd macroscopic superposition. Neither subsystem is "smeared" (coherently phase-dependent). Only the correlations between the subsystems are coherent, and this is just what we want. The controversial premeasurement state of a quantum object and its detector is not an absurd superposition of detector states; it is instead a perfectly plausible superposition of correlations between detector states and quantum states of the object. This resolves the problem of outcomes.

Let's summarize the above analysis using the two-slit experiment as an example. The physical meaning of entanglement has been misunderstood. Consider the entangled premeasurement state (4) which we reproduce here:

$$\frac{|A1\rangle|D1\rangle + |A2\rangle|D2\rangle}{\sqrt{2}} \qquad (9)$$

where subsystem *A* is a single electron passing through a 2-slit experiment, and subsystem *D* is a pair of which-slit detectors. The $|Ai\rangle$ and $|Di\rangle$ *(i=1 or 2)* are, respectively, the states of the electron at the two slits and the states of the two detectors.

The following interpretation of (9) is **INCORRECT**:

A and *D* are respectively in states $|A1\rangle$ and $|D1\rangle$
AND *A* and *D* are respectively in states $|A2\rangle$ and $|D2\rangle$ (10)

where "AND" indicates superposition. According to (10), the single electron is detected at both slits. This "superposition of paired states" is absurd and paradoxical.

Instead, the entangled state (9) represents a perfect *correlation between* states of *A* and states of *D.* That is,

A is in state $|A1\rangle$ **IF AND ONLY IF** *D* is in state $|D1\rangle$
AND *A* is in state $|A2\rangle$ **IF AND ONLY IF** *D* is in state $|D2\rangle$ (11)

where "AND" again represents superposition. This "superposition of correlations" is what we want.

As another way of summarizing the present paper's key idea, let's compare Equations (2) and (4). (2) represents a coherent (i.e. phase-dependent) superposition *of states* of *A.* The problem of outcomes arises from viewing the entangled state (4) as a coherent superposition of the compound system *AB*. Instead, (4) represents a coherent (i.e. phase-dependent) and non-local superposition of *correlations between A* and *B.*

Solution of the Problem of Wave Function Collapse

Returning to Einstein's thought experiment, Fig. 1: The screen is an array of many small detectors such as photographic grains. As a single electron approaches the screen, we can describe its quantum state as an N-fold superposition over these detectors

$$|y\rangle = \int |\mathbf{r}\rangle\, y(\mathbf{r})\, d\mathbf{r} = C_N S_j \int_j |\mathbf{r}\rangle\, y(\mathbf{r})\, d\mathbf{r} \qquad (12)$$

where $\int$ represents an integral over the two-dimensional screen, $|\mathbf{r}\rangle$ represents the electron's position eigenstate, $y(\mathbf{r}) = \langle \mathbf{r}|y\rangle$ is the electron's wave function, C_N is a suitable normalization constant, S_j is a sum over all detection regions, and $\int_j$ represents an integral over the jth detection region. (HOBSON, 2013). Equation (12) is analogous to the superposition (2) above. This state of the electron then entangles with the screen in a process analogous to Equation (3). The resulting entangled state is analogous to Equation (4):

$$|Y\rangle = C_N S_j |j\rangle \int_j |\mathbf{r}\rangle\, y(\mathbf{r})\, d\mathbf{r} \qquad (13)$$

where $|j\rangle$ represents the state of the jth detection region. As in Section 4, the measurement process therefore results in an entangled state that is analogous to the premeasurement state (4). Specifically, at the instant of detection, there is a perfect nonlocal correlation between the electron being in detection region j and the detector registering detection region j, for all j. The argument of Section 5 (above) then applies to this entangled premeasurement state.

This resolves the problem of wave function collapse.

Disproof of a Proposed Resolution of the Measurement Problem

One attempt to resolve the detection problem appears in Kurt Gottfried's popular graduate-level textbook (GOTTFRIED, 1966, 1991; GOTTFRIED *et al*., 1991). The analysis employs the density operator formulation of quantum physics (SCHLOSSHAUER, 2007) It begins by forming the density operator for the entangled state (4),

$$r = |Y_{AD}\rangle\langle Y_{AD}| = r_{diag} + r_{off\text{-}diag} \tag{14}$$

where the "diagonal" and "off-diagonal" parts of the density operator are defined by

$$r_{diag} = \{|A1\rangle|D1\rangle\langle D1|\langle A1| + |A2\rangle|D2\rangle\langle D2|\langle A2|\} / 2 \tag{15}$$

$$r_{off\text{-}diag} = \{|A1\rangle|D1\rangle\langle D2\langle A2 + |A2\rangle|D2\rangle\langle D1|\langle A1|\} / 2. \tag{16}$$

r_{diag} can be interpreted as an "ignorance mixture" in which the composite system is *either* in the state $|A1\rangle\,|D1\rangle$ *or* in the state $|A2\rangle\,|D2\rangle$ but nobody knows which. Thus, r_{diag} rather than r is often (but incorrectly, as we shall soon see) regarded as the desired solution to the detection problem. Replacing r with r_{diag} is thus a goal for Gottfried and seven other prospective solvers of the measurement problem (WIGNER, 1963; D'ESPAGNAT, 1966; FINE, 1970; SHIMONY, 1974; BROWN, 1986; BUSCH and SHIMONY, 1996; BACCIAGALUPPI, 2013).

Gottfried and Yan argue that $r_{off\text{-}diag}$ can, for all practical purposes, be neglected. This is because the expected value of any observable $\boldsymbol{O}$ is

$$\langle \boldsymbol{O} \rangle = \mathrm{Tr}(r\,\boldsymbol{O}) = S_j\, S_k\, r_{jk}\, O_{kj} \tag{17}$$

where the off-diagonal terms (having $j \neq k$) contain matrix elements such as $O_{12} = \langle D1|\langle A1|\boldsymbol{O}|A2\rangle\,|D2\rangle$. Gottfried and Yan argue that such matrix elements are nonzero only for a "fantastic" observable $\boldsymbol{O}$ because |D1> and |D2> represent radically distinct detector states such as "dead cat" and "alive cat," or because the detectors *D1* and *D2* are separated by macroscopic distances. Thus, Gottfried and Yan assume that such non-diagonal matrix elements must be undetectably small and can, for all practical purposes, be neglected. This would imply that the "butchered" (John Bell's term) density operator r_{diag} can, for all practical purposes, replace r. [10]

However, this attempted resolution was doomed from the start. This is because the ignorance mixture (15) *cannot* be the desired premeasurement state because *it is not entangled and thus has no nonlocal characteristics*, while Einstein's thought experiment shows that non-local characteristics are *required*. The full density operator (14) *does* however have non-local characteristics. Thus $r_{off\text{-}diag}$ must incorporate the nonlocal aspects of detection *and cannot be neglected*.

Disproof of Seven "Proofs" of the Insolvability of the Measurement Problem

At least seven other "detection problem Insolvability proofs" make a similar mistake (WIGNER, 1963; D'ESPAGNAT, 1966; FINE, 1970; SHIMONY, 1974; BROWN, 1986; BUSCH and SHIMONY, 1996; BACCIAGALUPPI, 2013). These analyses differ, however, from Gottfried and Yan's analysis. These seven analyses assume that the ignorance mixture r_{diag} is the desired outcome of the measurement process. The initial state of A for all these analyses is assumed to be a pure state superposition (not a mixture) such as (2). The analyses then investigate whether a suitable post-measurement mixed state of the composite system can be reached via some unitary process. To achieve this, the detector must be represented initially by a mixed state because a unitary process cannot transform a pure state into a mixed state. All seven analyses

regarded such an initial mixed state of the detector as appropriate because the detector is a macroscopic object.

Thus, the mathematical problem of all seven analyses was as follows: Find (i) an initial mixed-state density operator r_{ready} representing the detector D and find (ii) a unitary process U, such that U transforms the initial composite density operator $|Y_A\rangle\langle Y_A| r_{\text{ready}}$, with $|Y_A\rangle$ defined by (2), into the desired final state. This desired final state was a composite mixed state analogous to r_{diag}.

Each of the seven insolubility proofs showed, in different ways using different assumptions, that this mathematical problem has no solution: There is no initial mixed state r_{ready} and unitary process U that transforms $|Y_A\rangle\langle Y_A| r_{\text{ready}}$ into the desired final state. This presumably demonstrated the detection problem to be insolvable.

But again, this approach was doomed from the start because a composite mixed state analogous to r_{diag} has no nonlocal characteristics, so Einstein's analysis in 1927 tells us that it *cannot* correctly represent the desired solution of the detection problem.

Summary: Previous attempts to solve the detection problem, and previous supposed insolvability proofs, failed because they were looking in the wrong place. They assumed that the desired premeasurement state should be a mixture of non-entangled local states, while Einstein's remark shows that *the premeasurement state must be an entangled state* because it must have non-local characteristics.

CONCLUSIONS

This paper resolves the problem of definite outcomes that arise during the detection (or "measurement") process when a superposed quantum system interacts with a macroscopic detector to establish the entangled "premeasurement state" or "Schrodinger's cat state." The problem is that this state appears to be an absurd macroscopic superposition of every possible outcome. Experimental evidence arising from experiments with entangled photons demonstrates, however, that this state is not a coherent superposition of possible outcomes but rather a coherent superposition of all possible *correlations between* the possible outcomes and the corresponding states of the detector. This is precisely what we expect in a quantum measurement process. In the case of Schrodinger's cat, this premeasurement state reads as follows: "The cat is dead if and only if the nucleus decayed, AND the cat is alive if and only if the nucleus did not decay", where "AND" indicates a coherent (phase-dependent) superposition of correlations. This is what we want.

This resolves the problem of definite outcomes. It also resolves the related problem of wave function collapse that arises from the instantaneous nature of the transition from the premeasurement state to a single outcome – a transition that appears to violate special relativity. The resolution lies in the entangled, and hence non-local, nature of the premeasurement state.

We have also shown that one previously published presumed resolution of the measurement problem (GOTTFRIED, 1966, 1991; GOTTFRIED *et al*., 1991) has a fatal flaw. That analysis suggests that the entangled premeasurement state can, for all practical purposes, be replaced by a non-entangled ignorance mixture. But such a mixture cannot represent the actual premeasurement state because it is not entangled and thus lacks non-local characteristics. Similarly, we disprove seven previously published presumed proofs of the insolvability of the measurement problem because they assume the desired premeasurement state is an ignorance mixture that lacks non-local characteristics, and this assumption is incorrect.

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PHYSICAL ORIGINS AND LIMITATIONS OF CANONICAL QUANTUM MEASUREMENT BEHAVIOR

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ABSTRACT. I review and augment my work of the last few years on the physical origins and limitations of canonical quantum measurement behavior. Central to this work is a detailed analysis of the microstructure of real measurement devices. Particular attention is paid to the Mott problem, which addresses a simpler version of canonical quantum measurement behavior: It asks why an alpha particle emitted in nuclear decay produces one and only one track in a cloud chamber. My analysis – entirely consistent with unitarity – leads to an emergent, approximate Born rule supported by experiment, with possible breakdown at very small probability density. I argue that a similar picture applies to other measurement scenarios, including Geiger counters, the Stern-Gerlach experiment and superconducting qubits.

Keywords: Quantum measurement, Mott problem, cloud chamber, Geiger counter, Stern-Gerlach, qubit.

INTRODUCTION

The purpose of this paper is to review and augment my work of the last few years (SCHONFELD, 2021; 2022a; 2023; 2025a) on the physical origins and limitations of canonical quantum measurement behavior. By canonical quantum measurement behavior, I mean, basically, the Born rule. I use the word "canonical" to highlight that the Born rule and related theoretical machinery are widely held to be axioms of physical law, on a level with canonical commutation relations and the gauge-field structure of electromagnetism. My results militate against this view. My work involves mathematical derivation, but it also involves mathematical conjecture. Agreement with experimental data would seem to reinforce the essential correctness of my argumentation, but I am determined to expose even the weak points so others might further advance this line of inquiry.

This is of much more than academic interest because, today, vast resources are being devoted to developing quantum computing technologies, and these appear to make heavy use of the quantum measurement axioms. As well, considerable resources are also being devoted to searching for extremely rare fundamental processes (most notably, proton decay) and it's

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important to know if we really can rely on canonical quantum measurement expectations when probabilities get too small.

It has been almost one hundred years since Born (BORN, 1926) proposed that the square of the absolute value of the Schroedinger wavefunction of an object being measured is proportional to the probability density of measurement. Several years later this was refined and formalized as the projection postulate (VON NEUMANN, 2018) and has been taken for granted as exact physical law ever since. Qualitatively, the gist of the postulate is that a quantum wavefunction evolves according to Schroedinger's equation (unitarity) as long as it's not being measured; but at the moment of measurement, it changes discontinuously and non-unitarily ("collapses") according to application of a single, randomly manifested projection operator (with probability given by the Born rule). This puzzling dichotomy between unitary and non-unitary evolution, which has been an abiding challenge to physical intuition, is referred to as the quantum measurement problem. The effort to understand this problem in an intuitively satisfying way has given rise to voluminous literature, very recently reviewed in this journal (DUGIC *et al*., 2024) and also in (NEUMAIER, 2025). Common approaches involve interpretations of quantum ontology, or epistemology of measurement, or modifications to Schroedinger's equation. But they all have in common the assumption that Nature conforms to the projection postulate, in one form or another, to infinitely many decimal places.

To be sure, nearly a century of experimental data supports the Born rule. Every comparison between a measured scattering cross section and an ab-initio calculation tests the Born rule. Every comparison between a measured decay lifetime and Fermi's golden rule tests the Born rule. Every comparison between idealized theory and the measured pattern in a single-particle interference experiment – whether it involves photons, electrons, neutrons or large molecules (see (SCHONFELD, 2023) for references) – tests the Born rule. And yet, there is no definitive evidence that the process by which quantum mechanics selects measurement outcomes is *intrinsically* random (as opposed to reflecting the vast atomic complexity of real measurement instruments). Nor is there conclusive evidence for projection per se. Nor does the physics community maintain a systematic record of just how well the Born rule actually works quantitatively: For example, there is no tabulation of experiments by the number of decimal places in the fit to the Born rule; or by how many samples are in each measured probability bin; or by the smallest nonzero measured probabilities that are compared with the Born rule. Indeed, there are no generally agreed-upon figures of merit for quantifying the accuracy of the Born rule in any given situation, nor is there any reasoned intuition about where and how best to look for Born rule violations. There have been attempts to search for trilinear contributions to three-slit interference (JIN *et al*., 2017), or for anomalies in high-volume quantum computer calibration (BIALECKI *et al*., 2021), but these do not appear to be guided by any underlying rationale or strategy for optimizing the search.

These are important reasons why scientists must look beyond fundamental ideas about quantum measurement that take the Born rule or the projection postulate as a boundary condition. Another important reason is that both the Born rule and the projection postulate are formulated without any regard for the definition of measurement itself, much less for the internal structure of the actual measurement apparatus. This seems absurd on its face. I received my first inkling that the detailed microstructure of the apparatus cannot be disregarded when I analyzed the statistics of an over-idealized fluorescence photodetector (SCHONFELD, 2019) and found that the concept of Born's rule only makes sense at the discrete locations of the detector's individual molecules. In the present review we will go much further.

It is fair to say that all theoretical approaches that take the Born rule or the projection postulate as a given have this in common: They focus on the wavefunction of the object being measured; more succinctly, they are "object centric." They idealize, or abstract away, or – in the language of density matrices – "trace away" the microscopic details of the measurement apparatus. It seems clear to me that to really understand canonical quantum measurement

behavior, and where it breaks down, one must pursue an "apparatus centric" approach that assumes neither the Born rule nor the projection postulate as axiomatic, but rather derives what an observer actually sees directly from the apparatus's microstructure. That is what I have done. In the future, comprehensive reviews of quantum foundations should cover not just object centric approaches, but apparatus centric approaches as well.

It is important to distinguish between the work reviewed here and the well-known apparatus-centric work of Allahverdyan et al. (ALLAHVERDYAN *et al*., 2013). At the heart of that work is an analysis of the density matrix for a measured object (a spin). I eschew density matrices because I want to understand explicitly how a single measurement trial results in an apparently single measurement outcome.

Most of my work has focused on the cloud chamber, because it is arguably the simplest particle detector ("the 'hydrogen atom' of quantum measurement"); and because its version of the quantum measurement problem – the Mott problem – is also particularly simple.

The next section presents a theory of cloud chamber detection. Section 3 addresses experimental tests of this theory. Section 4 extends the thought process developed for cloud chambers to more sophisticated measurement scenarios involving charged particle detection. Section 5 considers possible implications for uncharged-particle measurement. Section 6 concludes with a summary and some comments on further prospects. An appendix contains a few mathematical details.

THEORY OF CLOUD CHAMBER DETECTION

A cloud chamber is an enclosure containing air supersaturated with condensable vapor, which can be water but is more typically ethyl alcohol. When a charged particle passes through the chamber, it ionizes air molecules, and the resulting ions nucleate visible vapor droplets, which line up in a track along the particle's path. But this is only part of the story, as we shall see.

The cloud chamber's particular version of the quantum measurement problem – the "Mott problem" – refers to a very particular detection scenario: A single atomic nucleus that decays by s-wave alpha emission is placed in a cloud chamber. Everything quantum mechanical about the nuclear decay in isolation is spherically symmetric, but only one alpha detection is observed in the cloud chambers, and that's in the form of a decidedly non-spherically-symmetric track. The Mott problem asks how a spherically symmetric initial state gets manifested as a single linear track. The problem is named for N. F. Mott, who attempted to explain in quantum mechanical terms why a linear track is the generic manifestation of a charged particle in a cloud chamber (MOTT, 1929). What Mott actually showed was that the second-order perturbation-theory contribution to the wavefunction of an alpha decaying from an unstable nucleus into a gas of separated ionizable atoms is dominated by terms in which two ionized atoms line up with the source nucleus. Each such term suggests a linear track, but there are many such terms, so Mott's analysis doesn't explain why decay manifests as a single track, much less what particular feature of the detector is responsible for selecting that particular track direction. And Mott's analysis is silent about another striking feature of alpha tracks emanating from nuclear decay: Visible tracks do not originate at the nucleus itself, but rather at some nontrivial offset, on the order of centimeters (see Fig. 1). What explains that, and what particular feature of the detector is responsible for selecting that particular offset?

The remainder of this section describes my findings about what really happens when an atomic nucleus decays in a cloud chamber. The picture is more complicated than previously realized. [One might suppose the picture would be similar for a bubble chamber, another track-based charged particle detector that exploits a liquid-gas phase transition. That may be correct but the energetics are quite different. See (SCHONFELD, 2021).]

The key physical ingredients that determine how, when and where a track starts – and how close it comes to any semblance of "canonical" – in the Mott scenario are as follows.

1. The alpha particle wavefunction and square-norm flux.
2. The constitution of the cloud chamber medium.
3. Singularities in ionization cross sections.

We discuss each of these in turn.

The alpha particle wavefunction and square-norm flux

We begin with the apparatus-free alpha wavefunction. This is important because it defines the ab initio physical interface between the object being measured (the alpha) and the measurement apparatus (the cloud chamber). Under other circumstances, it is very common for a theorist to model an initial particle state as, say, a Gaussian wavepacket; this guess-as-idealization is made entirely for the theorist's convenience. But I am very uncomfortable relying on something as arbitrary as a wavepacket concocted for my convenience when analyzing something as foundational as quantum measurement behavior. This is one reason to give research priority to the Mott problem. In the Mott scenario – a single heavy nucleus decaying to another heavy nucleus by emitting only a single alpha – one does not have to guess, one knows the apparatus-free alpha wavefunction a priori. It is a Gamow state (GARCIA-CALDERON and PEIERLS, 1976), given by (up to a time-dependent but irrelevant phase)

$$\psi(x,t) = \theta(t - r/v)\frac{1}{r}\left(\frac{\gamma}{4\pi v}\right)^{1/2} exp\left(\left(\frac{r}{v} - t\right)\left(\frac{\gamma}{2} + i\frac{pv}{\hbar}\right)\right), \quad (1)$$

where θ is the step function, t is time, r is distance from the nucleus, γ is the decay e-folding rate, v is alpha speed and p is alpha momentum. [This corrects a sign error in (SCHONFELD, 2021).] [Gamow states can be generalized to multi-particle decays (SCHONFELD, 2022b).] If one ignores interaction with the apparatus, then the wavefunction of the entire system is the outer product of Expression (1) and the many-degree-of-freedom wavefunction of all the cloud chamber molecules. Using the language of scattering theory (TAYLOR, 1972), it is more productive to say that this outer product is the interaction-free wavefunction of the entire system *in the un-ionized channel*. As we shall see, a detection track happens when the total square-norm of the un-ionized channel is, essentially, altogether depleted. Square-norm of an individual particle is the spatial integral of the square-norm density |wavefunction|^2; the total square-norm of Expression (1) – and therefore the square-norm of the interaction-free system wavefunction in the un-ionized channel – is normalized to unity, but inelastic collisions with cloud chamber molecules will tend to transfer that channel's square-norm to the ionized channel. The heart of my analysis is a detailed analysis of that square-norm transfer process.

I use the terms "square-norm density" and "square-norm" rather than the more conventional "probability density" and "probability" because I want strictly to avoid even the hint of assuming a priori that quantum mechanics is intrinsically random or probabilistic. Regardless of what one calls it, the total square-norm of a system's wavefunction is finite and conserved under unitary evolution, so the total square-norm of the un-ionized channel is a finite resource and it is entirely legitimate to examine whether and how it can be depleted.

I highlighted that Expression (1) is a Gamow state because such a state, although not stationary (up to phase), bears important formal similarity to a bound state in the discrete spectrum, and I exploit that similarity. Just as the propagator (Green's function) of a quantum particle with bound states includes a discrete term for each bound state, the propagator for a particle that can be emitted in a very slow radioactive decay includes a discrete term for the

decay's Gamow state (GARCIA-CALDERON and PEIERLS, 1976). With that in mind, I have conjectured that the following property of bound states generalizes to slow-decay Gamow states: When a bound state is eroded over time by a radiative transition (could be radiation of light or emission of an ionization electron into the continuum), the resulting wavefunction is the sum of a radiative state whose square norm increases over time, plus the original bound state wavefunction multiplied overall by a factor of magnitude < 1 that decreases with time (i.e. the bound state's square norm is not debited by eating away the bound state wavefunction piecemeal according to a spatially nontrivial pattern). This enables me to say that if the alpha wavefunction triggers ionization in the cloud chamber, then the post-ionization state gets its square-norm by debiting the entire Gamow-state wavefunction, including the part of the wavefunction that extends beyond the boundaries of the cloud chamber. I see no way around this conjecture, but it requires a more rigorous treatment than I have been able to provide. [Perhaps it relies on the limit of extremely large cross-section discussed in the last part of this Section 2.]

The post-ionization alpha wavefunction is very different from the apparatus-free Gamow state and is another important part of the overall cloud chamber picture. When an alpha ionizes a molecule, the outgoing alpha wavefunction is basically a de-Broglie-wavelength beam radiating from an aperture of roughly molecular size [this is essentially what happens in (MOTT, 1929)]. For cases of practical interest, this beam is very narrow: For a 5 MeV alpha, the de Broglie wavelength is ~$5\text{x}10^{-15}$m, while a molecule has diameter a few $\text{x}10^{-10}$m; so the outgoing beam is a cone with opening angle < $5\text{x}10^{-5}$ radians. For all practical purposes, this means the outgoing alpha wavefunction is perfectly collimated, because, over the typical distance – a fraction of a micron (MORI, 2014) – between subsequent droplets in a cloud chamber track, the alpha beam spreads ~10^{-11}m, a small fraction of its molecular-diameter width; and the next ionization will reset the beam width back to molecular diameter. Clearly, once the entire alpha wavefunction is channeled into a narrow cone emanating from a single ionization event, subsequent ionizations will keep it collimated along the same direction. So we may restate the Mott problem: What is the event that first directs (nearly) all the square-norm of the un-ionized-channel apparatus-free alpha wavefunction into a narrow cone in the ionized channel emanating from a single ionization site?

Mathematically, without identifying square norm with probability, the rate at which an interaction draws square-norm out of the un-ionized channel is determined by the cross section σ of the interaction and the square-norm flux **J** within the channel in the vicinity of the interaction. Specifically, the rate is $\sigma\|\mathbf{J}\|$ (TAYLOR, 1972). A typical molecular cross-section is small, but, for a collimated wavefunction, square-norm is drawn from the un-ionized channel very quickly (square-norm flux is very large because the wavefunction packs a lot of square-norm into a narrow volume). In this way, ionization is perceived to take place with certainty when collimated beam and molecular ionization target are roughly within σ of one another, and we are able to conceptualize a collimated wavefunction as a classical point particle. But square norm is not large for the apparatus-free decay wavefunction, so the interaction that collimates it must be exceptional rather than typical. We shall see shortly that the exceptions result from the dynamic constitution of the cloud chamber medium.

It will be helpful later to note here that for slow decays (small γ), high-momentum alpha particles, and times much longer than the alpha's chamber transit time, the outward square-norm flux of the apparatus-free wavefunction inside the cloud chamber at radius r from the source nucleus is

$$\mathbf{J} = \frac{\hbar}{2mi}[\psi^*\nabla\psi - \psi\nabla\psi^*] \sim \mathbf{r}(p/m)|\psi|^2 \sim \mathbf{r}(\gamma/4\pi r^2)e^{-\gamma t}, \qquad (2)$$

where **r** is the unit vector pointing away from the nucleus, m is alpha particle mass and, obviously, $p=mv$.

The constitution of the cloud chamber medium

The supercooled cloud chamber medium consists of well-separated air molecules (mostly O_2 and N_2), and vapor molecules in varying degrees of clustering. These are all targets for ionization by an alpha particle emitted by nuclear decay, and they all have similar local potential-energy environments for an electron destined to be ejected by ionization. But a cluster possesses a reservoir of energy in the form of collective molecular polarization that can offset single-molecule ionization potential. This has a major impact on the kinematics of ionization, which in turn can have a profound impact on ionization cross section, and that is what makes the difference between a "typical" ionization encounter and the exceptional one that collimates the entire apparatus-free wavefunction into a single track.

In particular, when an ion appears, say, in the center of a spherical vapor cluster, the ion's unscreened charge induces polarization in the surrounding cluster medium. The polarization response has energy

$$\frac{Q^2}{2}\left(1-\frac{1}{\varepsilon}\right)\left(\frac{1}{R}-\frac{1}{R_i}\right), \tag{3}$$

where Q is ion charge, ε is cluster dielectric constant, R is cluster radius and R_i is an effective radius of the volume that the ion itself occupies in the cluster. The dielectric constant may be close to unity for open air but is much greater than one for a vapor cluster. Therefore, Expression (3), manifestly a negative number, is easily large enough to compete with the binding energy of the electron that had to get ejected to produce the ion in the first place. For appropriate values of R, or for an analogous criterion in a differently shaped cluster, Expression (3) can even offset the binding energy exactly. In that case an alpha particle can ionize a vapor molecule with no energy loss. As we discuss below, this is a singular case in quantum Coulombic scattering, and leads to anomalously large ionization cross sections that can indeed collimate apparatus-free wavefunctions

Of course we must be quantitative about what makes an ionization cross section "anomalously large enough." For this reason, in (SCHONFELD, 2021) I introduced a parameter τ to represent the evaporation time of a vapor cluster that initiates a track. Ionization cross section σ for a molecule in a cluster is "large enough" when square-norm flux $\mathbf{J}$ flowing through σ drains nearly all the square-norm from the apparatus-free wavefunction before the cluster in question can evaporate. Mathematically, for unit overall normalization, that amounts to $\sigma\|\mathbf{J}\|\tau > 1$.

[In (SCHONFELD, 2021) I stated the following puzzle: If there's a collection of nuclei all close to one another in a cloud chamber, why don't they all produce alpha decay tracks at the same time when "the right" subcritical cluster comes along? I.e. why don't we see multiple tracks issuing from the same starting point at the same time? There are several factors working against this. First, even if the nuclei in the collection are close to one another, they're not at exactly at the same location, and therefore $\|\mathbf{J}\|$ won't be the same for all of them at the cluster in question. And second, once a first electron is emitted to form the first ion in a given cluster, the next emitted electron – if there is going to be one – would experience a different binding environment because of the ionic charge exposed by the first emitted electron.]

It is convenient to talk about clusters as if they are randomly distributed in a continuous sample space with probability ρ per unit radius R, per volume of location and per unit time of occurrence. But continuity cannot be strictly correct, because a cluster is built out of finitely many molecules. Indeed, I have estimated (SCHONFELD, 2025a) that a cluster at the starting points of a cloud chamber track has ~25 molecules. This will become important below when we talk about limits to the Born rule. Probabilistic randomness also cannot be strictly correct, but it must be a pretty good idealization (with or without unitarity) because there are so many

molecules of all kinds in a macroscopic cloud chamber. Certainly, the reader must not make the mistake of thinking that I am somehow assuming *quantum* randomness a priori.

Singularities in ionization cross sections

A tendency toward singularity is built into quantum Coulombic cross sections because of the long-range nature of the Coulomb potential (TAYLOR, 1972). Certainly the cross section singularity of elastic Coulomb scattering is well known. Singularity is also generic in inelastic Coulomb scattering if there is another state that is degenerate with the initial state of the target molecule (TAYLOR, 1972). That is not the case in typical laboratory experiments, but it happens at a vapor cluster when polarization energy (Expression (3)) exactly cancels the binding energy of an electron that would be expelled from a molecule by ionization and that would be emitted at zero kinetic energy. Thus, as the radius R of a cluster approaches a value R_c for which cancellation is exact, total ionization cross section approaches the singular form $A/(R_c\text{-}R)$ for some coefficient A. [This echoes another Coulombic singularity discussed much earlier in (FEINBERG *et al*., 1986), although never verified experimentally, to my knowledge.]

From this expression, and the distribution ρ of cluster radii, we immediately obtain a statistical distribution of track starting points in space and time (SCHONFELD, 2021). Specifically, we arrive at the expression $\rho_c A v \tau |\psi(\mathbf{x},t)|^2$ for the spatial-temporal probability density (per unit volume and unit time) for track initiation at detector location $\mathbf{x}$ and time t, where ψ is the apparatus-free wavefunction and ρ_c is the value of ρ at $R=R_c$. This is a Born rule, in that it's a probability density proportional to the absolute-value squared of a wavefunction. This particular rule for cloud chambers is completely novel. For it to really be a Born rule in the full sense of the quantum measurement axioms, one would have to reframe cloud chamber detection as measurement of alpha particle position, and to accept that the definitive signature of alpha position is the starting point of its track. Such a reorientation of perspective is entirely unanticipated in the literature. It's not clear to me if or how it relates to the projection postulate, because it's not at all clear whether projection operators exist that could select for track starting points. In any event, this Born rule can be turned into a particular functional form by applying Equation (1), for times much longer than the alpha's chamber transit time:

$$\rho_c A v \tau |\psi(\mathbf{x},t)|^2 = \frac{1}{r^2}\frac{\rho_c A \gamma \tau}{4\pi} e^{-\gamma t}. \qquad (4)$$

This is what we will compare with experiment in Section 3. [See (SCHONFELD, 2021) for a discussion of how this is consistent with Bell's theorem.]

It is very important to highlight why this Born rule can only be approximate: First, because it refers to a wavefunction at a particular spatial position $\mathbf{x}$ even though the anomalous cross section is undoubtedly large enough to encompass a considerable range of other positions. Second, because not all clusters are spherical and not every vapor molecule that is a target for ionization is located at the center of a cluster. Third, because the expression for ionization cross section near critical radius assumes a continuum idealization for the cluster medium, whereas a real cluster is a kind of "stick figure" consisting of a relatively small number of vapor molecules. Fourth, because it neglects possible effects of many small-cross-section elastic interactions with air and vapor molecules that can accumulate over the long time that elapses for a slow decay, and modify the wavefunction in the no-ionization channel.

It is especially important to highlight that this Born rule is obtained without explicit reference to any non-unitary process. Indeed, the argumentation is built around the continuous flow of conserved square-norm, which is a necessary (but not sufficient) signature of unitarity. Nevertheless, I am sometimes asked whether there might be other ways in which my argumentation is circular, i.e. whether I somehow implicitly assume quantum measurement axioms in trying to explain physically how apparently axiomatic behavior comes about.

Clearly, I assume that condensed matter exists (otherwise there could be no cloud camber), and that, at a microscopic (or at least mesoscopic) level, it exhibits statistical behavior characterized by stable distributions. However, I do not derive these assumptions themselves from the most basic unitary first principles. So I suppose there may be some opening for circularity. Still, it is a highly nontrivial result to deduce a previously unknown, very specific distribution (4) from other assumptions that are based on what we know actually does happen, and that do not seem even to foreshadow, let alone resemble anything like the Born rule. Perhaps it is too early to say that I have *derived* a Born rule, but I think I can fairly claim to have *explained* one.

EXPERIMENTAL TEST OF CLOUD CHAMBER THEORY

No one has ever conducted a cloud chamber experiment with the express purpose of measuring the distribution of starting points of tracks from decaying nuclei. In view of the Born rule prediction in Equation (4), this is a glaring gap in the literature and needs addressing. Perhaps this gap is to be expected, since there had previously been little awareness that a track *doesn't* start right at the decaying nucleus itself.

However, since the advent of the Internet, educators have posted many pedagogical videos of cloud chambers in operation, and some of these videos contain images that are relevant to testing Equation (4). For reasons explained in (SCHONFELD, 2022a), the most suitable such video [24] was produced by Jefferson Lab in 2010.

This video shows 90 seconds of alpha decay tracks materializing in a cloud chamber containing a needle source of ^{210}Pb. A needle source is literally a sewing needle whose tip has been thinly plated with a radioactive species. ^{210}Pb is itself a beta emitter, but decays to ^{210}Po, an alpha emitter with half-life of several months. The chamber is a Petri dish, supercooled by sitting on a bed of dry ice. The camera is placed directly above the flat lid of the dish. I examined every video frame and measured the coordinates at which every track started. From that data I compiled the cumulative distribution function (CDF) of track start positions as a function of distance from the source in the plane of the image. I also modeled what the same CDF would turn out to be if the Born rule (4) governed the statistics of track start locations in three-dimensional space. This also involved data fitting in order to fix the unknown parameter $\rho_c A \tau$ in Equation (4). The details of this modeling and fitting can be found in (SCHONFELD, 2022a).

Figure 1 shows a representative frame from the Jefferson Lab video, in which the reader can see that tracks originate away from the tip of the needle. Figure 2 shows the measured CDF and the best fit model based on the Born rule prediction.

For radii up to ~20mm, the quality of the fit ranges from mediocre to good. For radii beyond ~20mm there is a marked deficit of detections in the measured data compared with the model. In (SCHONFELD, 2022a) I explored several candidate explanations for this apparent deficit, primarily based on considering the distribution of heat in and around the cloud chamber. I was able to rule out some and found none of the rest compelling. [There also seems to be a shortfall in detections at radius below roughly 10mm; this may or may not be an artifact of the fitting procedure. I considered and rejected the possibility that it came about because of local heating by the radioactive source itself.] I speculated that the deficit beyond ~20mm might indicate a breakdown of the Born rule at small wavefunction. Detection for very small wavefunction might require a vapor cluster with |R-Rc| much smaller than could actually be achieved with a stick-figure made of finitely many vapor molecules. I have not been able to exclude this possibility.

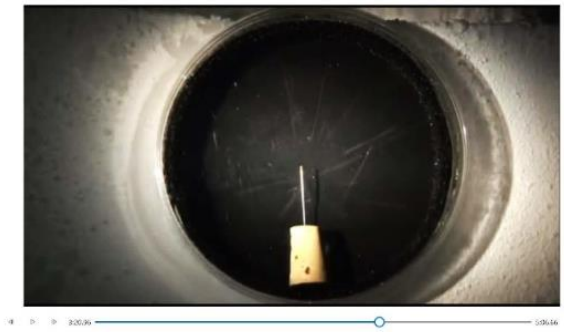

Figure 1. Frame #6030 from [24].

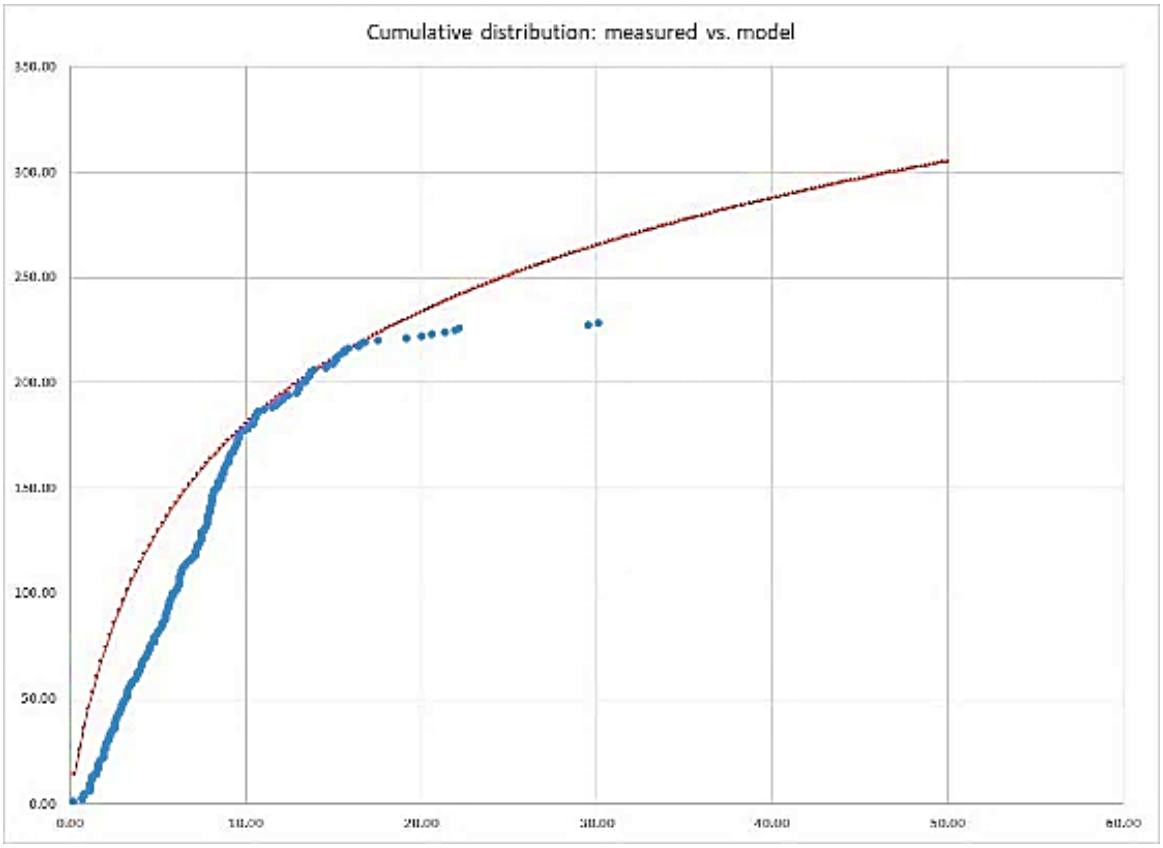

Figure 2. Measured (blue) and Born-rule modeled (red) CDF.
Vertical axis calibrated in total counts, horizontal axis calibrated in mm.

The quality of the fit in Figure 2 is a test of the functional form of the Born rule (4), and the apparent lack of detections beyond ~20mm is a possible signature of the underlying microphysics. The normalization of the fit would also provide a test if one could draw on a robust a priori theory of the coefficient $\rho_c A \tau$ for comparison. There is a literature aimed at quantitatively predicting the statistical distribution of cluster sizes in a supercooled vapor, but it is not developed enough to enable a really robust comparison with our experimental data. In (SCHONFELD, 2025a) I adapted results from (BAUER *et al*., 2001) to validate the measured value of $\rho_c A \tau$ to within a factor of 1-2. This is impressive when one considers how the source tables in (BAUER *et al*., 2001) range over many orders of magnitude.

The analysis of opportunistic video data in this section provides some encouragement that the cloud chamber theory in Section 2 is on the right track. Clearly, there is a strong need for much more careful and more fine-grained experimentation. We also require a much more robust quantitative understanding of the transient cluster population in supercooled vapors.

GENERALIZING FROM CLOUD CHAMBERS

Ideally, we should immediately apply lessons from the cloud chamber to other, more standard measurement scenarios. However, I proceeded more cautiously, first considering an alternative charged-particle track detector in order to learn how to adapt the cloud chamber thought process to different media. In particular, it occurred to me that a Geiger counter detecting a nuclear decay might be productive as an incremental step up in sophistication, because it has strong unappreciated commonality with cloud chambers. First, both rely on alpha particles making ionization tracks. In a cloud chamber, the tracks are directly visible when we see nucleated vapor droplets; in a Geiger counter, the tracks are indirectly visible when we see voltage pulses at the internal anode. Second, both involve media in which ionization cross sections are small. In a cloud chamber, that's the air between vapor clusters; in a Geiger counter, that's the air outside the Geiger-Muller tube, and also the buffered noble gas inside. So, both cloud chamber and Geiger counter have a Mott-like problem: determining precisely where the apparatus-free alpha wavefunction gets collimated. As we have seen, the answer for a cloud chamber is that collimation takes place at exceptional vapor clusters that come and go due to thermal fluctuation. It seems intuitively obvious that, for a Geiger counter, collimation has no choice but to take place at or inside the very thin mica window where particles enter the metallic tube, because none of the gases inside or outside the Geiger-Muller tube support clustering of any kind, let alone exceptional clusters with very large ionization cross sections (and the metal surface of the tube is too far away and the thin-wire anode is too narrow). I conducted an experiment to test this hypothesis (SCHONFELD, 2023).

There are actually three hypotheses here: Collimation takes place (i) at the interface between window and air, (ii) at the interface between window and buffered noble gas, and (iii) in the interior of the window. Since writing (SCHONFELD, 2023), I have learned that my experiment can provide critical discrimination between the three cases. This is important because the three cases have very different microphysical implications. In case (iii), collimation must take place at conjectured localized interior structures (voids or crystal defects) where collective polarization produces energetics very similar to Equation (3) (although now the molecule to be ionized must be at the edge of a void rather than somewhere in the interior of a cluster). In cases (i) and (ii), Equation (1) is replaced by basically the same thing (up to overall scale) without the $1/R$ term (like the electrostatic potential of a point charge over a conducting plane). In these cases, the value of R_i is still related to the radius of the ionization target, but is also sensitive to the topographical scale of surface roughness.

The three hypotheses also differ significantly in another way that one can exploit for experimental analysis. In case (i), an alpha particle collimated at the air-window interface experiences slowing all the way through the window due to interaction with mica before it comes out the other side, in the interior of the tube, where ions can create charge avalanches at the anode. In case (ii), an alpha particle collimated at the buffered-ideal-gas-window interface experiences no slowing due to mica. In case (iii), the amount of slowing depends on precisely where in the mica the collimation takes place. I have modeled the experiment under these three pictures and find that only case (i) appears to track the data satisfactorily. [In (SCHONFELD, 2023), I hadn't thought through this diversity of cases and unwittingly modeled only case (i) (and I did so with an unrelated error that turned out not to have a significant impact on the results).]

Of course all these cases aren't mutually exclusive and in reality could operate in tandem. But the agreement of case (i) with the data does seems not to cry out for blending with the other cases. This makes some intuitive sense, because as the alpha wavefunction propagates from the decaying nucleus, it encounters the air-window interface first, and then the interior of the window, and finally the buffered-ideal-gas-window interface. I.e. we can at least satisfy

ourselves that a winner-take-all case (i) is consistent with causality, because it comes first in the propagation sequence

In my experiment (see Fig. 3), I mounted a needle source of the alpha emitter ^{210}Po on a manual linear stage. I dialed the stage until the "hot" end of the needle just touched the center of the mica window of a commercial Geiger-Muller tube. I then dialed the stage back through equally spaced stops, and at each stop I recorded the Geiger counter count rate. (See (SCHONFELD, 2023) for experimental details, including data conditioning.)

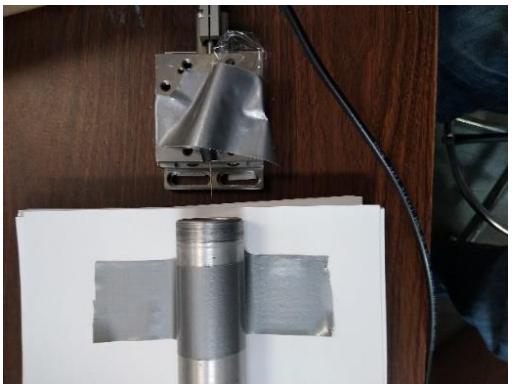

Figure 3. Geiger counter experiment. The Geiger-Muller tube is the cylinder in the bottom half of the photograph. One can make out the very thin source needle issuing from the plug at the lower edge of the movable stage in the top half of the photograph. From (SCHONFELD, 2023).

Figures 4-6 compare the experimental data with models based on cases (i)-(iii), as well as with a naive "geometric" model that assumes collimation takes place at the decaying nucleus itself. [This latter model is basically geometric flux through the window, moderated by attenuation in air and mica.] The central fact of each model is that alphas only make it into the Geiger-Muller tube if the total slowing distance (in air and window for geometric model, and in window only for cases (i)-(iii)) is equivalent to less-than-complete stopping in air. The equations for these models are described in the Appendix. In the model for case (i), I set the value of window thickness (in equivalent slowing-distance in air) to optimize fit to the data. The value that I got, 16mm, is reassuringly close to the manufacturer's estimate. I assumed the same value for the other cases, but I performed some numerical variation to satisfy myself that I couldn't improve fit meaningfully. All curves are normalized to give the same value of counts per minute for zero separation between source and window.

So, from this experiment – which needs to be repeated in a much more controlled setting – we learn that a solid state surface can collimate a single-particle wavefunction. With this recognition, it is a relatively modest step from Mott-like scenarios to more familiar quantum measurement situations. In the remainder of this section, we summarize how this applies to two specific such scenarios, the Stern-Gerlach experiment and measurement of a superconducting qubit.

In the original Stern-Gerlach experiment (GERLACH and STERN, 1922), a beam of neutral spin-1/2 silver atoms passed through a spatially varying magnetic field. The beam was then detected as two very small and close but distinct smears deposited on a glass plate. Here we assume the spin-1/2 beam particles are charged, because we are generalizing from the theory of charged particle detection in a cloud chamber set out in Section 2. Actually, this scenario is a bit hypothetical, because the Stern-Gerlach experiment is in fact much more difficult with charged than neutral particles, and as late as 2019 had not been carried out definitively (HENKEL *et al*., 2019). But it is a good steppingstone to the second scenario – superconducting qubit measurement – which is an object of active engineering development and is not at all hypothetical.

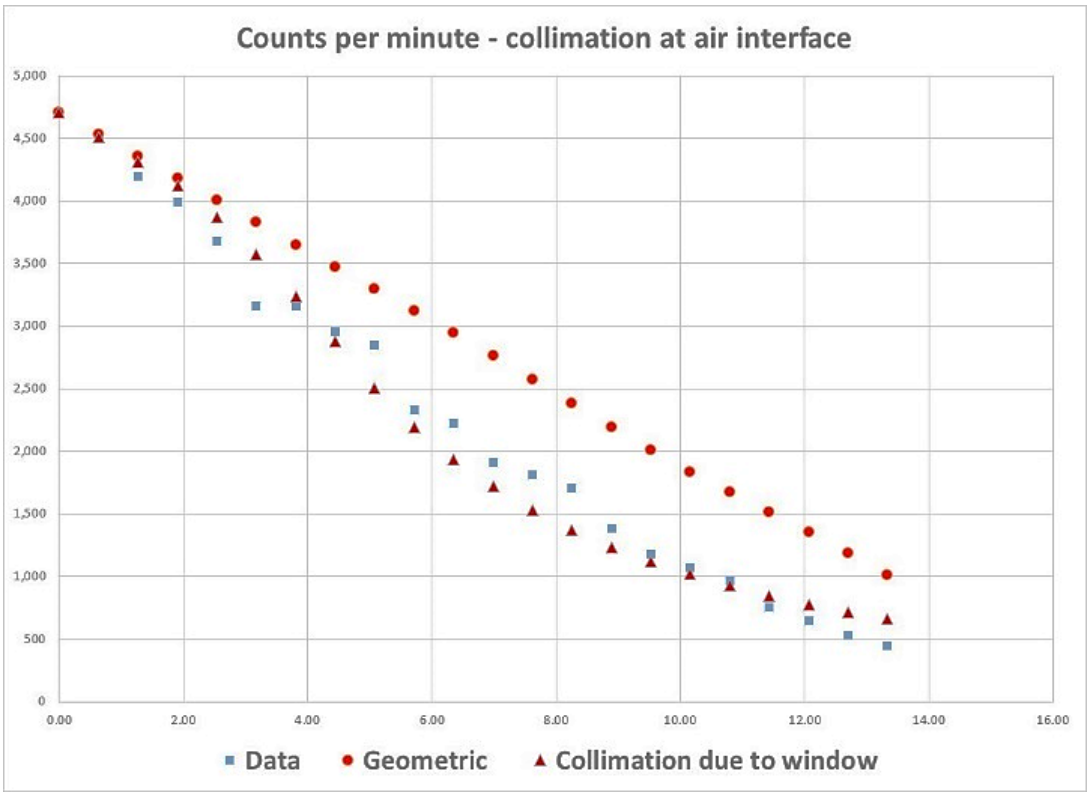

Figure 4. Data and models for Geiger counter experiment. Red circles correspond to geometrical model, purple triangles to case (i) model, and blue squares to data. Radioactive source is modeled as extending over a few millimeters.

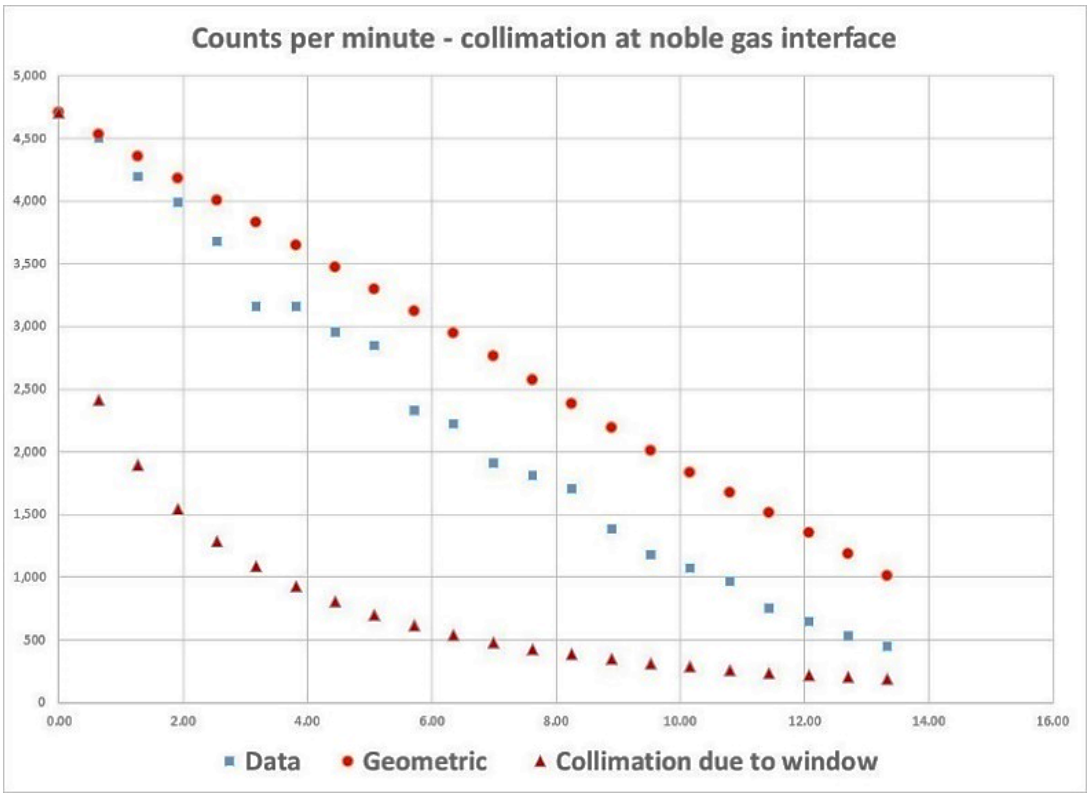

Figure 5. Data and models for Geiger counter experiment. Red circles correspond to geometrical model, purple triangles to case (ii) model, and blue squares to data. Radioactive source is modeled as extending over a few millimeters.

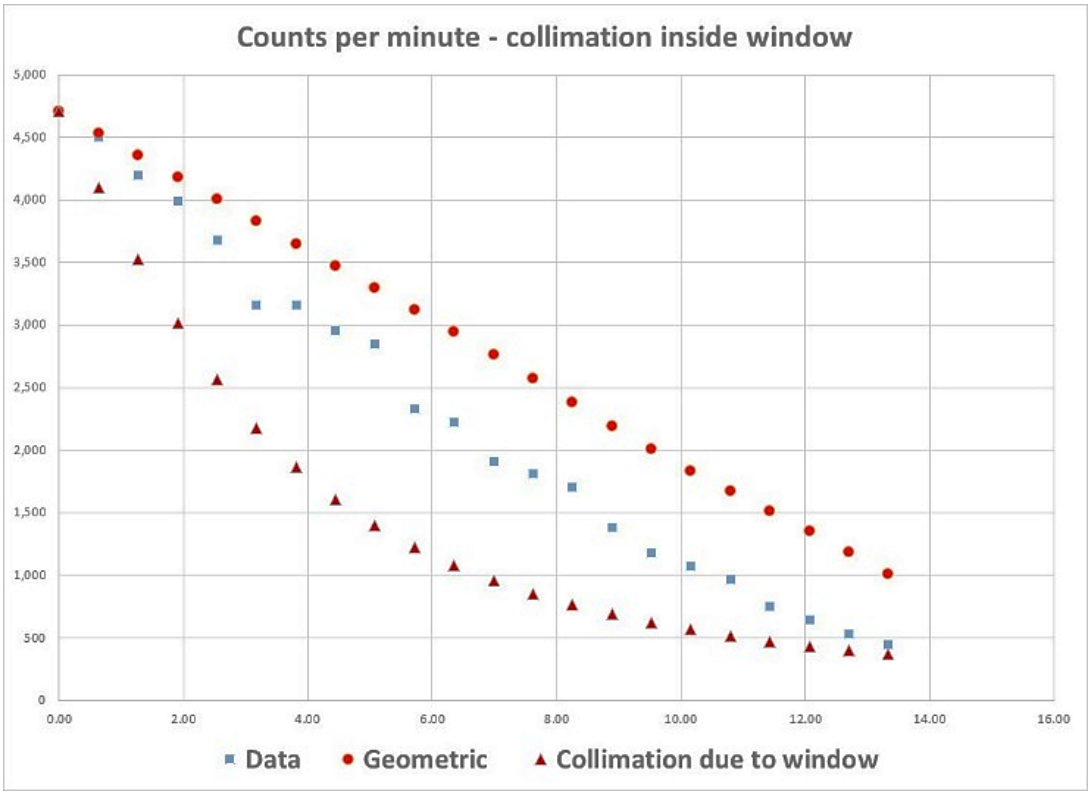

Figure 6. Data and models for Geiger counter experiment. Red circles correspond to geometrical model, purple triangles to case (iii) model, and blue squares to data. Radioactive source is modeled as extending over a few millimeters.

For a spin-1/2 charged particle in such a beam, the magnetic field as usual splits its wavefunction into two very small and close but distinct branches corresponding to the two cardinal spin states (up/down) of which the particle is a superposition. Both branches propagate towards an ionizing detector with a solid acceptance window. If, as my Geiger counter results indicate, the entrance interface of this window contains atoms or molecules with anomalously large ionization cross sections, then a detection probability density analogous to $\square_c A v \square |\square(\mathbf{x},t)|^2$ applies here as well, where **x** is now position in the plane of the detector. And since the two wavefunction branches should be shaped identically but separately scaled by the complex weights of the spin superposition, this immediately turns into the Born rule for spin measurement (with all the caveats about approximate validity that we saw in the cloud chamber case).

[As discussed in SCHONFELD (2023), this adaptation from cloud chamber theory involves some nuance. In the cloud chamber case, the Gamow state of the decay provided a single repository of square-norm available to flow in its entirety into the ionized channel. In the Stern-Gerlach case the concept of Gamow state doesn't necessarily apply. Instead, we have to assume that the anomalous ionization cross-section, wherever it occurs, is large enough to encompass the combined transverse spreads of the two closely-spaced wavefunction branches. With this in mind, it might be interesting to do a Stern-Gerlach experiment with the two branches allowed to drift very far apart before detection. Perhaps that would produce a violation of the Born rule.]

As discussed in SCHONFELD (2023), we can understand the Born rule in superconducting qubit measurement via the same mechanism, because there is an implicit Stern-Gerlach apparatus embedded deeply in the qubit readout system. In detail, a superconducting qubit is an artificial atom made from Josephson junctions coupled to a radio frequency (RF) resonating cavity, typically configured so that the lowest two excited states are close in energy and can be

treated together as a self-contained two-level system. In dispersive readout, the state of this two-level system is measured by sending a microwave pure tone at the cavity via a transmission line, and recording the reflected signal (BLAIS *et al*., 2004). If the frequency of the pure tone is chosen appropriately, the signal reflected from one qubit basis state (up or down) has a phase shift that is detectably different from the phase shift due to reflection from the orthogonal basis state. The reflected signal goes through several stages of amplification and then passes through an analog-to-digital converter (A/D), after which it is recorded as a digitized voltage time series. The phase shift is extracted from the time series via traditional I/Q processing, and the measured state is inferred directly from the result.

All along this signal chain, except for the very last step, there is simply no opportunity for a large-cross-section event to rapidly divert square-norm into an ionization channel or something similar. It's different at the A/D converter. An A/D is basically a succession of elementary solid-state devices that determine whether an input voltage is above or below a pre-set threshold. Each such device is basically a layered semiconductor. One layer is a source of electrons, and the other layers pull these electrons one way or another depending on whether voltage is above or below the threshold. When an electron is drawn into one of the layers, it promotes another electron in the same layer into the conduction band (a sort of ionization process), and that in turn produces a kind of charge cascade observed as a voltage pulse, much as happens in a Geiger counter. In other words, the A/D is basically a set of embedded Stern-Gerlach apparatuses, and so if the Born rule applies to Stern-Gerlach because of wavefunction collimation at the detector interface, then it should apply equally to superconducting qubit measurement because of wavefunction collimation at the interfaces between semiconductor layers (again with all the caveats about approximate validity that we saw in the cloud chamber case). In a recent paper (SCHONFELD, 2025b) I extrapolated from cloud chamber experimental results to estimate the scale of expected Born rule violation in superconducting qubit measurement. I concluded that this violation might be very difficult to observe.

DETECTION OF UNCHARGED PARTICLES

So far we have focused on detection of charged particles, but of course famous signatures of canonical quantum measurement behavior are also observed with detectors of uncharged particles. These include the glass plate used to detect the neutral silver atoms in the original Stern-Gerlach experiment; photomultiplier tubes, CCDs and photographic film used to detect photons in optical slit experiments; and BF_3 detectors used to detect neutrons in neutron slit experiments. I am unable to comment on fogging of glass plates. In (SCHONFELD, 2023) I speculated that the boundary collimation that seems to take place at a Geiger counter window also operates in CCDs and photographic grains. In (SCHONFELD, 2021) I speculated that wavefunctions of liberated electrons are collimated at conducting surfaces in photomultiplier tubes, where the energetics resembles Equation (3). Presumably something similar applies to the charged fragments that result from the fission of a boron nucleus after it absorbs an incoming neutron in a BF_3 detector.

SUMMARY AND FURTHER PROSPECTS

In this paper I have reviewed work of the last few years – both theoretical and experimental – that supports the following picture of what physicists have come to think of as canonical quantum measurement behavior.

- In a cloud chamber, a visible track (and therefore a detection) appears from a charged particle with a diffuse wavefunction (such as a nuclear decay product) where and when there is an exceptional condensed vapor cluster with extremely large ionization cross section. The cross section is large because the energy of induced polarization in the cluster nearly compensates for the binding energy of the ejected electron. The statistics of track origination follows a Born rule, at least approximately.
- In a Geiger counter, an internal track (and therefore a detection) appears from a charged particle with a diffuse wavefunction (such as a nuclear decay product) where and when there is an exceptional feature with extremely large ionization cross section on the near surface of the mica entrance window. The cross section is large because the energy of induced polarization in the mica nearly compensates for the binding energy of the ejected electron. Analysis of experimental data on count rate as a function of distance from a nuclear source indicates that the statistics of track origination follows a Born rule, at least approximately.
- In a charged particle Stern-Gerlach experiment, spin measurement – with the Born rule (at least approximately) – happens when there is an exceptional feature with extremely large ionization cross section on the near surface of the entrance window to an ionizing detector. The cross section is large because the energy of induced polarization in the window nearly compensates for the binding energy of the ejected electron.
- In a superconducting qubit system, state measurement – with the Born rule (at least approximately) – happens when there is an exceptional feature with extremely large ionization cross section at a boundary between semiconductor layers in an electronic A/D converter. The cross section is large because the energy of induced polarization in the semiconductor nearly compensates for the binding energy of the ejected electron.

The common themes are clear: large ionization cross sections at exceptional features in apparatus media, related to balance between induced polarization and electron binding energy, and emergence of an approximate Born rule. I have suggested that the same themes are at play in scenarios involving measurement or detection with uncharged particles.

In SCHONFELD (2023), I suggested that these themes could possibly help us understand a bigger question: Why do almost all particles we observe in everyday life seem to follow tracks as if they were classical? Perhaps, in the primordial past, the wavefunctions of particles we deal with every day first became collimated by interacting with exceptional interface features of emerging condensed matter.

APPENDIX: WAVEFUNCTION COLLIMATION AT GEIGER COUNTER WINDOW

In this appendix, I explain the equations that underline the model curves in Figures 4-6. To do this I extend calculations that first appeared in Section 3 of (SCHONFELD, 2023). To start, refer to Figure 7.

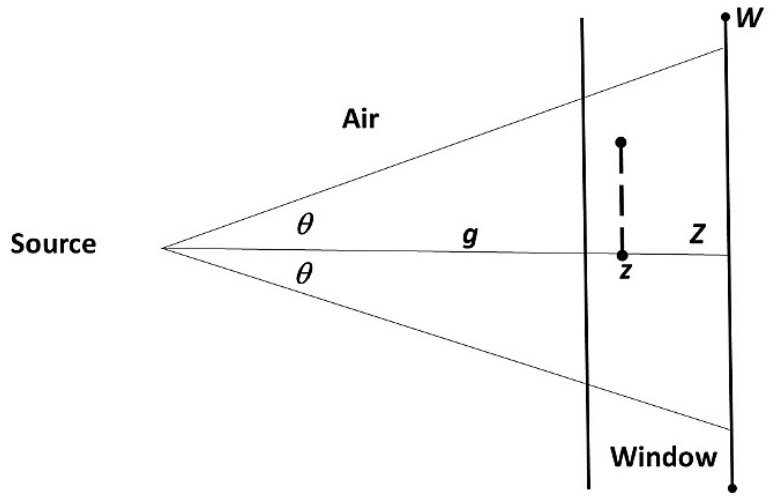

Figure 7. Geiger counter reference diagram for alpha stopping calculations.

In this diagram, g is distance from radioactive source to the window's near surface, Z is window thickness, z is horizontal coordinate of an arbitrary point in the window measured from the near surface (y, length of dashed line, not labeled, is its radial coordinate [vertical in the plane of the diagram), , W is window radius, and θ is the smaller of the angle of a ray which just touches the radius of the window's far surface, or (for geometric and case (i)-(ii) models) along which an alpha is just barely stopped due to a combination of slowing in air and in the window medium. For a very thin window, z and Z are negligible when compared to g or W. Let L be the stopping distance of an alpha particle in air, and let S be a scale factor so that one unit of distance inside the window results in the same slowing as S units of distance in air.

For a geometric model, in which collimation takes place at the source, alpha flux through the window is proportional to the solid angle subtended by a cone of opening angle θ, i.e. proportional to $(1-\cos\theta)$. And θ itself is the smaller of $\arctan(W/g)$ (neglecting Z relative to g) and $\arccos((g+SZ)/L)$.

For the case (i) collimation model, θ is the smaller of $\arctan(W/g)$ and $\arccos(SZ/L)$. [I assume alpha slowing doesn't happen until the wavefunction is collimated (I assumed the opposite in (SCHONFELD, 2023)). Otherwise, there would be no tracks in video [24] that terminate more than ~40mm from the source, regardless of where they start. But in fact, some such tracks can be seen.] For the case (ii) model, θ is simply $\arctan(W/g)$ because there is no slowing until the alpha has fully entered the Geiger-Muller tube. Following Equation (4), the alpha flux into the detector for cases (i) and (ii) is proportional to the integral of $1/((g+z)^2+y^2)$ over the relevant window surface, i.e. proportional to $\ln(\cos\theta)$.

For case (iii), alpha flux into the detector is the integral of $1/((g+z)^2+y^2)$ over the window interior, but only including any point (z,y) for which the ray that traces back to the source then exits the window and satisfies the constraint that distance to the far window surface along the same ray has length less than L/S. Calculating alpha flux into the detector in this model is elementary and only the end result is given here: For $g>W(SZ/L)/(1-(SZ/L)^2)^{1/2}$, flux is proportional to $(SZ/L)\ln((g^2+W^2)/g^2)$. For $g<W(SZ/L)/(1-(SZ/L)^2)^{1/2}$, flux is proportional (with the same multiplier) to

$$\left[\frac{SZ}{L}-\frac{g}{(g^2+W^2)^{1/2}}\right]-\frac{SZ}{L}\ln\frac{SZ}{L}. \tag{5}$$

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QUANTUM PHYSICS: ORIGINS AND MODERN SHAPE

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ABSTRACT. We emphasize and shortly discuss direct link between the basics of quantum mechanics and modern quantum physics and technology.

Keywords: quantum physics, quantum foundations, open quantum systems, quantum information and computation, quantum technology.

INTRODUCTION

"Quantum information" and "quantum computing/computers" (NIELSEN and CHUANG, 2000), "quantum metrology" (NAWROCKI, 2019), "open quantum systems" (BREUER and PETRUCCIONE, 2006; RIVAS and HUELGA, 2012) and "quantum thermodynamics" (BINDER *et al*., 2019) are just some of the names of modern quantum sciences that are usually included in the broad field of "Quantum physics". Above all is "Quantum technology" as a future technology – the technology of the 21st century (MILBURN, 1997).

The development of modern quantum physics and quantum technologies is in complete disharmony with the, still sometimes present, prejudice that prevailed in the middle of the 20th century, which implied that quantum mechanics was completed as a scientific field and regarded merely as a basis of applications. Therefore, it is appropriate to give a certain overview of the development of modern quantum sciences and technology and their connection with the standard, non-relativistic quantum theory – quantum mechanics.

In this paper, special emphasis is placed on the direct connection between the very foundations (basic postulates) of quantum mechanics (MESSIAH, 1961) and new quantum sciences, as well as quantum technology that is under development. From a scientific point of view, all new quantum sciences and technological developments arise from the field of Foundation and Interpretation of Quantum Mechanics (for a brief overview see DUGIĆ *et al*., 2024).

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AN OLD PREJUDICE ON QUANTUM MECHANICS

The development and formulation of quantum mechanics at the beginning of the 20th century was followed by a series of advice given to their successors by founders such as Albert Einstein, Erwin Schrödinger, Werner Heisenberg, Johann von Neumann, Louis de Broglie and others. These giants of world thought, and science gave direct advice related to the foundation and understanding of quantum mechanics. For some reason, for nearly fifty years, the development of physics has gone beyond these tips. A truly interesting situation which, as will be presented below, deserves a separate historical, methodical, and perhaps even philosophical review and analysis which remains a task for future physicists and historians/philosophers of science.

In the period, approximately 1930–1980, there was a widely accepted prejudice that quantum mechanics was a finished science whose deeper development could not lead to deeper and wider scientific breakthroughs, and it was believed that quantum mechanics as a methodical field was suitable only as the basis of numerous scientific fields such as atomic, molecular, nuclear and condensed matter physics. Moreover – in sharp contrast to the advice of the aforementioned giants of science – research in the field *of Foundations of quantum mechanics* were considered second-rate and sometimes forbidden.

The state of affairs in this sense is evidenced by the following description of research practice by David Mermin:
"[*This research was characterized by*] *a head-in-the-sand sentiment to 'shut up and calculate'*."

Even more drastic is the testimony of H.-D. Zeh, one of the founders of the quantum theory of decoherence:
"*However, it was absolutely impossible at that time to discuss these ideas with colleagues, or even to publish them. An influential Heidelberg Nobel prize winner frankly informed me that any further activities on this subject would end my academic career*!"

The 2022 Nobel Prize in Physics winner John Clauser testifies to the same academic atmosphere:
"I thought it was important at the time, even though I was going to ruin my career by doing it, and in some sense, I did: I've never been a professor!"

Young generations who grow up surrounded by a multitude of quantum sciences and the imperative to develop new technologies will not be able to easily interpret the above quotes, for example, how research that can lead to results worthy of the Nobel Prize can be "forbidden" – a true curiosity of sociological and psychological, not only scientific-historical, value.

In contrast to the old practice, Vlatko Vedral gives the following advice to young researchers:
"*If there is going to be some new theory, I don't think it's going to come from solid state physics, where the majority of physicists work. Second, working in a self-imposed box also means that new applications of quantum theory are unlikely to emerge. The many perspectives we can take on quantum mechanics can be the catalyst for new ideas. If you're solving different problems, it's useful to be able to think in terms of different interpretations*."

PROGRESS IN THE FIELD OF FOUNDATION OF QUANTUM MECHANICS

In the above-mentioned period of approximately 50 years in the middle of the last century, only individuals with a certain authority engaged in the questions established by the founders of quantum mechanics. It was not until the early 1980s that the field of Quantum Mechanics began to return on a very broad scale.

Interpretations of Quantum Mechanics and New Quantum Science

On the fingers of one hand, one can count important contributions to the foundations of quantum mechanics in the period around the middle of the 20th century. For the most part, research has been reduced to "philosophical" interpretations of quantum formalism, or to mathematical generalizations and extensions. It turns out, however, that such research, carried out "here and there", step by step, paved the way for the development of new physical sciences – some of them are listed at the very beginning of this paper. Instead of a broader view that would require a lot of space, the following illustration shows a few lines of research from that period and points down with the down arrows to the main steps in the emergence of new quantum sciences.

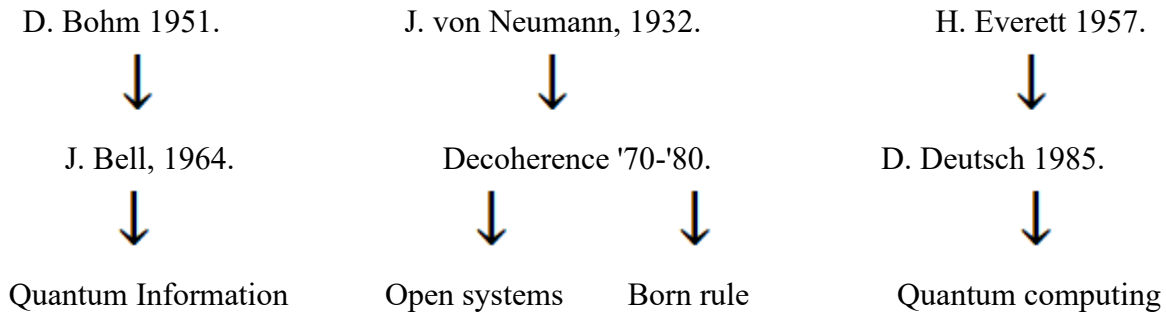

Figure 1. The course of development of some quantum sciences.

Figure 1 shows some of the steps in the development of new quantum sciences starting with the corresponding quantum mechanical foundations. At the top are the theories of Bohm, von Neumann and Everett as the basis for the description of the process of quantum measurement and a deeper interpretation of the physical content of the "wave function". At the bottom are some of the quantum sciences that emerged in the late 1990s and early 2000s (including the "derivation" of the so-called "Born rule".

The importance of the very foundations of quantum mechanics for the emergence of new quantum sciences – which will be emphasized below – is also stated by the following quote from Nobel Prize laureate Anton Zeilinger:

"*This field [quantum informatics and computing] would not exist if humans were not engaged in the founding of quantum mechanics*."

Return to quantum basics

The beginning of the 1980s marked a rapid return to the fundamentals of quantum mechanics, that is, the field of the Foundation of Quantum Mechanics. Questions of interpretation of quantum states, quantum entanglement, and alternatives to standard quantum mechanics are again in focus. Perhaps the key support in this regard was the return to quantum mechanics of some Nobel laureates, such as Murray Gell-Mann, Gerard t'Hooft, Roger Penrose, Anthony Leggett, as well as the ubiquitous doyen of world physics, John Archibald Wheeler, and Bernard d'Espagnat. Some of the major contributions to the first, roughly 15 years, came thanks to Heinz-Dieter Zeh, Wojciech H. Zurek, David Deutsch and Charles H. Bennett. Thanks to them, we have new quantum sciences – quantum information (NIELSEN and CHUANG, 2000), quantum computing (NIELSEN and CHUANG, 2000), decoherence theory (JOOS *et al*., 2003) and the more general theory of open quantum systems (BREUER and PETRUCCIONE, 2006; RIVAS and HUELGA, 2012)–with quantum mechanics at the core of a new field of Quantum physics. Existing textbooks (BREUER and PETRUCCIONE, 2006; NIELSEN and CHUANG, 2003; RIVAS and HUELGA 2012) establish new standards for physicist education, including new views on quantum mechanics.

PROGRESS IN THE FIELD OF FOUNDATION OF QUANTUM MECHANICS

It would be worth highlighting the basic concepts of quantum mechanics in the light of the development of new quantum sciences.

Double splits in quantum mechanics

Standard quantum mechanical theory is characterized by double splits. In fact, this is where the sources of all the problems lie in deeper understanding and interpretation of quantum mechanics. These splits are unknown in classical physics, in which physical state in one instant of time uniquely determines values of all variables of the system and the state in every later instant of time.

Quantum mechanics begins with the independent *kinematic* concepts of quantum state and quantum quantities ("observables"). Quantum states are elements of Hilbert space, while observable quantities are Hermitian operators acting on a Hilbert state space. No quantum state carries unique values of all observables – in *stark contrast to the classical analogue* (see above). This fundamental quantum uncertainty leads to the conclusion that there is *a fundamental quantum uncertainty* of the values of the observables in every quantum state. *Hence,* the determination of the values of observables by means of the measurement procedure inevitably ("irreducibly") requires randomness ("stochasticity") expressed by the probability of the result occurring in each individual act of measurement. One aspect of quantum uncertainty concerns quantum states and is contained in state superpositions. The other aspect of quantum uncertainty is represented by uncertainty relations that have no direct connection with the measurement.

The second type of split in quantum mechanics concerns *Dynamics* of quantum systems, that is, their "evolution" in time. On the one hand, there is unitary (Schrödinger) dynamics, which is linear and reversible, and hence deterministic, in the sense that if the state is known for one instant of time, the state of the system is unambiguously known at every subsequent moment. On the other hand, the process of measurement is typically stochastic– the unpredictable occurrence of individual measurement results in each individual act of measurement.

The departure of quantum mechanics from classical analogues is inevitable within the framework established by the basic concepts of standard quantum mechanical theory – states, observable, measurement, and unitarity of dynamics. So, at the very beginning, quantum mechanics destroys the simple and elegant conceptual scheme of classical physics at its very foundation. Hence, and only from there arise a multitude of "quantum puzzles", that is, problems in understanding, perceiving and interpreting quantum mechanical formalism.

CONCEPTUAL FOUNDATIONS OF THE QUANTUM INFORMATION PROCESSING

Linear superpositions of quantum states introduce non-orthogonality of quantum states. E.g., an orthonormalized basis of states $|\varphi_n\rangle$ gives a superposition $|\varphi\rangle = \sum_n c_n|\varphi_n\rangle$ that is nonorthogonal to every state from the basis. This is in sharp contrast to the classical state space (e.g. the “phase space”) in which all states are mutually orthogonal and therefore cannot be confused in any measurement. Intuitively, one may conclude that appearance of the classical world in quantum theory might require dealing exclusively with the (at least approximately) orthogonal states.

Quantum uncertainty relations introduce the limits of measurability of quantum observables on a system in each state. In some situations, non-commuting observables can

be jointly measured, while commuting ones cannot as long as measurement should provide “sharp” values instead of intervals on the real axis. Thus, deducing the classical-physics rules from the quantum ones may require exclusion of quantum uncertainty.

Interestingly, quantum uncertainty (superposition of states and uncertainty relations) can, in turn, be recognized as the new instances of the information-theoretic merits. To this end, we give a few basic examples.

(No-cloning) *Quantum superpositions* imply (require) the existence of non-orthogonal states that cannot be distinguished from each other by any measurement in a single act of measurement. The formal description of this is known as *the* no-cloning theorem (NIELSEN and CHUANG, 2000; WOOTERS and ZUREK, 1982). *This means that the "copy" operation cannot be performed in a single act, that is, in a single step of any procedure ("protocol").*

(Quantum cryptography) *Non-commutativity of quantum observables* distinguishes, in the general case, the impossibility of simultaneous measurements of such observables in one step; like state cloning, it requires a lot of repetition, that is, measurements on an ensemble. In practice, this means that measurement, typically, changes the state of the object of measurement and thus introduces a change that can be considered a kind of "*error*" due to external influences (due to a procedure, i.e., a process of measurement). Hence, it is only one step to noticing: if the two parties in the communication A(lice) and B(ob) exchange quantum systems and make measurements, errors are inevitable. But, if a covert spy E(va) is inserted between them, then it is intuitively expected (and easily proven) that the error is magnified – *it is easy to spot the presence of Eve*. This is the basis of all "secret key exchange" procedures within the framework of quantum cryptography (BREUER and PETRUCCIONE, 2006).

(Quantum parallelism) *State superpositions are linear*. Therefore, any application of linear (e.g., unitary) operation preserves the linearity of the dynamics of the system. Formally, the linear operator preserves the linear superposition, $\hat{V}$

$$\hat{V}\sum_n c_n|\varphi_n\rangle = \sum_n c_n\hat{V}|\varphi_n\rangle \equiv \sum_n c_n|\chi_n\rangle. \quad (1)$$

Unlike a single step in an expression (1), the classical operation V must be repeated n times:

$$\begin{aligned} V\varphi_1 &= \chi_1, \\ V\varphi_2 &= \chi_2, \\ V\varphi_n &= \chi_n. \end{aligned} \quad (2)$$

If there are N classical bits in the register, the classical processing (2) has exponentially many steps $n = 2^N$ than quantum, which is given by expression (1). Quantum processing given by expression (1) is done in one step, "in parallel", and is called *quantum parallelism*.

Correlations between subsystems A multi-particle system provides information about correlated subsystems. Classical correlations are represented by mixed states in quantum formalism and are absent in pure quantum states of a complex whole. The pure quantum states of the whole carry *Quantum entanglement*, which is a classically unknown, actually forbidden type of correlation. Hence, manipulations of quantum entanglement can lead to classically unattainable manipulations of quantum subsystems. Thus, quantum entanglement ceases to be a curiosity of "philosophical" interest in the Foundation of Quantum Mechanics and becomes an informational-computational resource for procedures (protocols/algorithms) that can be both classically unachievable and more useful than their classical analogues – "Quantum Supremacy". In doing so, linear operations on the whole system or on subsystems preserve quantum parallelism, the expression (2), as a fundamental feature of all quantum systems.

Mixed states of a whole always carry classical correlations. It turns out that there are also non-classical, quantum correlations that can also include quantum entanglement and are collectively referred to as "*Quantum Discord*". It turns out that a quantum discord can be recognized with quantum entanglement at its core (DUGIĆ *et al.,* 2013) – which is consistent with the fact that a quantum discord (as far as is known at the moment) does not provide a "quantum advantage".

Bell's inequalities are direct consequence of the quantum (non-classical) correlations and are often interpreted as *a measure of quantum nonlocality* (quantum nonseparability) in bipartite structures of multiparticle systems. For virtually all pure states, violation of some of Bell's inequalities can be observed. Only a certain class of mixed states can lead to the violation of Bell's inequalities, and such states are called entangled (mixed) states. That is why quantum information processing and computation is usually based on specially prepared pure states of quantum hardware, which usually consists of registers – *quantum bits* (qubits).

The following table shows the direct relationship between the very foundations of quantum mechanics and the field of quantum information and computation.

Table 1. The Relationship between the Fundamentals of Quantum Mechanics and Some Quantum Protocols and Algorithms

Quantum-mechanical basis	Protocols and algorithms
Quantum superpositions	Ban on cloning quantum states
	Quantum parallelism
Uncertainty relations	Quantum cryptography
	Quantum Superdense Coding
Quantum entanglement	Quantum teleportation
	Quantum cryptography
	Quantum computational algorithms

QUANTUM STRUCTURES AND QUANTUM TELEPORTATION

The manipulation of quantum correlations provides new possibilities for quantum computing processing, and therefore they are considered classically unknown – classically non-existent – resources for communication. As an example of this, we will briefly present the quantum teleportation protocol below. Before that, new concepts and views on quantum correlations and their relationship to pure quantum states should be introduced.

Relativity of quantum correlations

All real physical systems are complex – they are made up of parts, physical subsystems. As is known from classical analytical mechanics, various sets of "generalized coordinates" can be used for a set of material points. In quantum formalism, this leads to different forms of the same quantum state, and hence different "quantities" of quantum correlations in a complex whole – relativity of correlations (DUGIĆ *et al*., 2013).

The paradigmatic, and certainly the simplest in this sense, is the example of the hydrogen atom (JEKNIĆ-DUGIĆ *et al.,* 2013, JEKNIĆ-DUGIĆ *et al*., 2014). By definition, a hydrogen atom is an electron + proton pair (e+p). These two quantum particles interact with each other in a Coulomb manner, so solving the Schrödinger equation for the atom is not easy. The standard quantum theory of hydrogen atoms starts from a completely different description–a completely different structure of atoms–through linear canonical

transformations (taken from classical analytical mechanics) by introducing new, non-interacting, subsystems, the center of mass of atoms (CM) and relative particles (R), i.e., the internal degrees of freedom of atoms. So, e+p= atom =CM+R. The absence of interaction in the structure is the very basis of solving the problem of internal energies of hydrogen atoms – achieved by separating variables, i.e., removing interaction. Each structure redefines the tensor factorization of the Hilbert state space of the atom:

$$\mathcal{H}_e \otimes \mathcal{H}_p = \mathcal{H}_{atom} = \mathcal{H}_{CM} \otimes \mathcal{H}_R. \tag{3}$$

On the other hand, the state of the hydrogen atom adapted to the above factorizations:

$$|\vec{k}\rangle_{CM} \otimes |nlm_l m_s\rangle_R = |\Psi\rangle_{atom} = \sum_i c_i |i\rangle_e \otimes |i\rangle_p, \tag{4}$$

where the well-known notation from the quantum theory of hydrogen atoms were used (MESSIAH 1961). Physically, non-interaction in the CM+R atomic structure suggests the absence of any correlations (for an isolated atom), while the interaction of electrons and protons implies correlations – quantum entanglement represented by Schmidt's canonical form on the right side of the term (4), from which we draw the following conclusions.

First, expression (4) clearly states that quantum correlations do not concern the quantum state, but the structure of a complex system – correlations are not an invariant of canonical transformations. Expression (4) states that, *typically, every state of a complex system carries correlations* – the repeatedly discovered *relativity of quantum entanglement* (DUGIĆ and JEKNIĆ, 2006), which equally concerns the quantum discord (DUGIĆ *et al.,* 2013).

Second, in order to use correlations in a system, one must carefully select the local observables on which the manipulation (including quantum measurement) would be performed (DUGIĆ and JEKNIĆ-DUGIĆ, 2008). For example, no manipulation of a center of mass system can provide a "quantum advantage". Conversely, any manipulation on a proton could have consequences for correlations in the e+p structure of hydrogen atoms like any other atom, molecules, etc. Therefore, the manipulation of correlations is also a matter of structure, not of quantum states, thus every manipulation *is achieved by the convenient choice of local operations* – in the sense of equation (3).

Third, the expression (4) relaxes the tasks of state preparation and the recognition of observations that should be measured in order to use quantum computing resources. When it comes to state preparation, the left-hand state of the expression (4) can also be prepared for a pair of "continuous systems" (1 and 2), since the same state carries quantum entanglement for some other structure of a complex system 1 + 2.

A description of quantum teleportation

A quantum bit (qubit) is formally a two-dimensional unitary vector (Hilbert) space that can be physically realized in many ways. That is, the formalism of one qubit is actually a formalism of spin 1/2.

Quantum teleportation is the transfer of quantum information, that is, *the unknown quantum state* of one qubit to another qubit (BENNETT *et al*., 1993; NIELSEN and CHUANG 2000). The teleportation procedure is accomplished by preparing a quantum-entangled pair of qubits, denoted 2 + 3, where qubit 3 is sent to side B, and qubit 2 is sent to side A which also possesses qubit 1 in an unknown quantum state that should be transferred ("teleported") to qubit 3. By measuring on the pair 1 + 2, based on this information, party B performs a certain unitary operation on qubit 3, which guarantees the state of qubit 3 in which qubit 1 is at the beginning – which proves the teleportation procedure.

Formally, let the state of the first qubit, and the initial entangled state of the qubit pair be 2 + 3, $|\Psi\rangle = |\psi\rangle_1 \otimes |\Phi\rangle_{2+3}$ [9,21]. Then the structure of the three-qubit whole is 1 +(2 + 3), and in relation to this structure the initial state is in the form of a tensor product – without any correlations of the subsystems 1 and 2 + 3. However, due to the measurements made by side A, the structure (1 + 2) + 3 is of interest. Thus, by analogy with the expression (4), the state of the whole carries the correlations between the subsystems 1+2 and 3:

$$|\psi\rangle_1 \otimes |\Phi\rangle_{2+3} = |\Psi\rangle = \sum_i c_i |i\rangle_{1+2} \otimes |i\rangle_3, \quad (5)$$

which is not the form of Schmidt's canonical form, because the states of qubit 3 are not orthogonal to each other. Thus the "local" (von Neumann) measurement on the pair 1 + 2, performed by A gives for the final state of the whole 1+2:

$$|k\rangle_{1+2} \otimes |k\rangle_3 \leftrightarrow b_k. \quad (6)$$

Then the corresponding local transformation, unambiguously determined by the value b_k, gives the desired result for the state of the third qubit: $|\psi\rangle_3 = \hat{V}_k |k\rangle_3$ (BENNETT *et al.* 1993, NIELSEN and CHUANG 2000). Note also that the grouping of the tripartite system 1 + 2 + 3 as emphasized above–1 +(2 + 3), or (1 + 2) + 3 – is a trivial type of linear canonical transformation.

OPEN QUANTUM SYSTEMS AND BEYOND

Quantum measurement makes the object of measurement an open quantum system—indescribable by unitary dynamics (BREUER and PETRUCCIONE, 2006; RIVAS and HUELGA, 2012). Historically, the related state changes have been termed "quantum jumps"—that includes the (de)excitation of atoms and molecules. However, those semi-phenomenological descriptions have been reformulated within the Open quantum systems theory on both mathematical and conceptual levels.

As far as it is currently known, behavior of every open system can be described as a "reduced" description of a subsystem (S) in interaction with its environment (E), such that the total S+E system is unitary. This is a unifying picture for quantum physics: the open system's state is obtained by "tracing out" the environmental degrees of freedom. The related differential equation of the "reduced state" (open system's state) is called "master equation".

The open systems theory encapsulates the standard unitary quantum mechanics and quantum optics, describes quantum decoherence and dissipation, thermalization, and sets a basis for various fields and applications, such as quantum thermodynamics, mesoscopic and materials physics and the related technologies. *All that is based on the hypothesis that the total S+E system is quantum unitary*. Thence a basis for sharpening and deepening the foundations of the alternative approaches to the problem of quantum measurement and its different aspects and ramifications (see, e.g., DUGIĆ *et al*., 2024).

MOLECULAR GEARS AS OPEN QUANTUM SYSTEMS

In this section we briefly present some recent results of the present authors on application of the open system theory to investigating dynamical stability of the molecular gears (cogwheels).

Molecular gears are recognized as one of the basic elements of molecular machinery. Typically, they are treated as classical-physics systems. However, expected fast operations and their quick repetition raise the question of the possible quantum contributions to efficient performance of the gears in short time intervals—much before the eventual relaxation (e.g. thermalization). That is, accumulation of quantum contributions may be expected to decrease efficiency in performing the gears rotations.

Of particular interest are the propeller-shaped molecular gears described by the number N of blades. Inclusion of the number N in the proper master equation for the rotation introduces the "size" of the molecular species in nontrivial way.

Augmenting the so-called Caldeira-Leggett master equation by the new parameter N for both the moment of inertia and the damping factor provides a basis for investigating dynamical stability of the one-dimensional (planar) molecular gears and application of the different statistical-inference methods.

The models of the harmonic and weakly non-harmonic rotator have been considered for the different parameter ranges and dynamical regimes (JEKNIĆ-DUGIĆ *et al*., 2018; PETROVIĆ *et al.,* 2020; JEKNIĆ-DUGIĆ *et al.,* 2025). Dynamics of the standard deviations of the angle and the angular momentum observables, the method of the first passage time and dynamics of both linear and differential entropy have been used and linked with some realistic physico-chemical situations. The conclusions are rather physically rich and require *optimization* in regard of the numerous parameters of the considered model of molecular gears. It is remarkable that one of the simplest models of open quantum systems cannot be presented in simple terms and general recipes. Rather, the need for optimization goes hand in hand with the tasks of optimization in the classical engineering—another, somewhat unexpected, lesson from the modern quantum physics theory and its applications.

Although the role of geometric parameters is evident in the case of molecular gears, similar effects are encountered across a broad range of quantum systems. In general, the geometry of a system—its dimensionality, spatial boundaries, and internal structure—enters the Hamiltonian and thereby determines the spectrum of energy levels, transition probabilities, and stability of quantum states. In open quantum systems, geometric features also modulate the coupling to the environment, influencing decoherence rates and dissipative dynamics. Examples can be found in quantum dots, superconducting qubits, optical cavities, and topological materials, where the shape and configuration of the system critically affect coherence and entanglement properties. Hence, the inclusion of structural parameters such as the number of blades in molecular propellers can be viewed as a specific realization of a more general principle: the dynamical behavior of quantum systems is intrinsically conditioned by their geometry.

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THE TOTAL π-ELECTRON ENERGY SAGA - CONTINUATION

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ABSTRACT. The total π-electron energy, as calculated within the Hückel molecular orbital approximation, is a much studied quantum chemical characteristics of unsaturated conjugated compounds. Its theory, together with that of its modification called "graph energy", was outlined in a review published in 2017 (GUTMAN and FURTULA, 2017). In the present paper, we present the main features of these theories, with emphasis on what happened after 2017. We also mention a few data that are not found in the mentioned review.

Keywords: total π-electron energy, graph energy, Hückel molecular orbital theory

GENESIS

Erich Hückel (1896-1980) is a German physicist, one of the pioneers of quantum chemistry. In the 1920s, working with Peter Debye, he developed a revolutionary theory of strong electrolytes, nowadays known as the Debye-Hückel theory. In the 1930s, in order to get a physics professor position at the Marburg University, he was required to present a new habilitation thesis in the field of physics. He decided to apply quantum theory to some chemical problem. Erich's brother Walter was an organic chemist, and he suggested to Erich to try to resolve the century-old "Benzolproblem". To do this, Erich elaborated an approximative approach towards the solution of the Schrödinger equation pertaining to the π-electrons of benzene. The paper (HÜCKEL, 1931) is just the first in a long series of Hückel's publications in this field, and provides the basis of what nowadays is called Hückel molecular orbital (HMO) theory.

The initial success of the HMO theory was remarkable. According to it, the six π-electrons of benzene form a closed-shell system. The same happens with 4n+2 circularly arranged π-electrons (as in cyclopentadienyl anion, cyclopropenyl cation, …) in stark contrast to 4n circularly arranged π-electrons (as in cycloplentadieny cation, cyclobutadiene, cyclopropenyl anion, …), that form an open-shell system. In addition, the total π-electron energy of benzene is $6\alpha+8\beta$, whereas the π-electron energy of three isolated double bonds is $3(2\alpha+2\beta) = 6\alpha+6\beta$. The energy difference, equal to 2β, would be the stabilization caused by

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cyclic delocalization of the π-electrons in benzene, resulting in its outstanding chemical stability. The predictions of HMO theory with regards to other monocyclic polyenes was eventually found to be in excellent agreement with experimental facts, but only for those species that have a planar geometry (*e.g.*, violation occurs in the case of cyclooctatetraene).

It was found that HMO theory can be applied also to other conjugated π-electron systems, both acyclic and polycyclic, both hydrocarbons and heteroatom-containing (COULSON *et al.,* 1978; KUTZELNIGG, 2007). HMO theory gained much of its popularity after the publication of the book (STREITWIESER, 1961), in which numerous correlations between experimentally determined values and those calculated by HMO were presented. The chemical applicability of the HMO model was especially convincing in the case of benzenoid hydrocarbons, and especially in the case of their total π-electron energies (GUTMAN and POLANSKY, 1986; GUTMAN, 1992).

After the appearance of more powerful computers, and more accurate quantum-chemical methods, HMO theory gradually lost its importance. Nowadays it is used solely for teaching purposes.

However, the HMO total π-electron energy survived, and is nowadays a much studied mathematical object with surprisingly many applications. This will be fully documented in what follows and is the main message of this paper.

BASIC FACTS ON HMO TOTAL π-ELECTRON ENERGY

The molecular orbitals in HMO theory are formally assumed to be a linear combination of the wave functions of p-electrons, each located on a particular carbon atom (or heteroatom). Let the number of such basis functions be n (in the case of benzene: $n = 6$). Then the respective Hamiltonian operator $\boldsymbol{H}$ is a square matrix of order n. For conjugated hydrocarbons, the elements of this matrix are given by

$H_{ii} = \alpha$ for all $i = 1,2,\ldots,n$,

$H_{ij} = \beta$ whenever there is a sigma covalent bond between the i-th and j-th atoms,

$H_{ij} = 0$ whenever the i-th and j-th atoms are not covalently bonded.

The parameter α is called Coulomb integral; in most applications its actual value is irrelevant. The parameter β is referred to as the resonance integral; it is important that its value is negative. In the case of heteroatom-containing conjugated molecules, the parameterization of $\boldsymbol{H}$ is somewhat more complicated, see (STREITWIESER, 1961).

According to the above definition, in HMO theory the matrix $\boldsymbol{H}$ can be written as

$$\boldsymbol{H} = \alpha \boldsymbol{I} + \beta \boldsymbol{A}$$

where $\boldsymbol{I}$ is the unit matrix of order n, whereas $\boldsymbol{A}$ is a symmetric (0,1)-matrix that can be interpreted as the adjacency matrix of a graph, namely of the molecular graph of the underlying conjugated molecule; for details see (GUTMAN and POLANSKY, 1986). Recall that

$A_{ii} = 0$ for all $i = 1,2,\ldots,n$,

$A_{ij} = 1$ whenever there is an edge between the i-th and j-th vertices,

$A_{ij} = 0$ whenever the i-th and j-th vertices are not connected by an edge.

Then the molecular orbital energy levels are equal to

$$E_i = \alpha + \beta \lambda_i \ , \ i = 1,2,...,n \qquad (1)$$

where $\lambda_i, \quad i = 1,2,\ldots,n$, are the eigenvalues of the adjacency matrix, forming the spectrum of the molecular graph. For details of the theory of graph spectra see, for instance, (CVETKOVIĆ *et al.,* 2010).

This connection between HMO and spectral graph theory was formally recognized in 1956 (GÜNTHARD and PRIMAS, 1956) but was certainly known earlier. Surprisingly, the first mathematical paper on spectral graph theory appeared a year later (COLLATZ and SINOGOWITZ, 1957).

It can be conjectured that Collatz and Sinogowitz, and possibly other scholars, read Hückel's papers from 1930s, and recognized their graph-theoretical mathematical connection. The time gap between Hückel's molecular orbital model (in the 1930s) and graph spectral theory (in the late 1950s) may be explained by World War II and the destruction that happened in Germany during and after it. Anyway, extensive application of spectral graph theory in HMO theory started in the 1970s and is ongoing ever since; see (GUTMAN and FURTULA, 2017) and the references quoted therein.

Using Eq. (1), the total energy of the π-electrons is

$$E_\pi = \sum_{i=1}^{n} g_i E_i = \sum_{i=1}^{n} g_i [\alpha + \beta\lambda_i]$$

where g_i is the occupation number of the i-th molecular orbital. Usually, if n is even ($n = 2k$), then

$$g_1 = g_2 = \cdots = g_k = 2 \ , \ g_{k+1} = g_{k+2} = \cdots = g_n = 0$$

whereas if n is odd ($n = 2k+1$), then

$$g_1 = g_2 = \cdots = g_k = 2 \ , \ g_{k+1} = 1 \ , \ g_{k+2} = g_{k+3} = \cdots = g_n = 0$$

which results in

$$E_\pi = \begin{cases} n\alpha + \beta\left[2\sum_{i=1}^{n/2} \lambda_i\right] & \text{if } n \text{ is even} \\ n\alpha + \beta\left[\lambda_{(n+1)/2} + 2\sum_{i=1}^{(n-1)/2} \lambda_i\right] & \text{if } n \text{ is odd} \end{cases} \tag{2a}$$

or, using the standard β-units:

$$E_\pi = \begin{cases} 2\sum_{i=1}^{n/2} \lambda_i & \text{if } n \text{ is even} \\ \lambda_{(n+1)/2} + 2\sum_{i=1}^{(n-1)/2} \lambda_i & \text{if } n \text{ is odd} \end{cases} \tag{2b}$$

GRAPH ENERGY

Formulas (2a) and (2b) have an important special case. Namely, for a large class of molecular graphs (including those of benzenoid hydrocarbons and acyclic polyenes), the relation (3)

$$E_\pi = n\alpha + \beta \sum_{i=1}^{n} |\lambda_i| \qquad \text{i. e.,} \qquad E_\pi = \sum_{i=1}^{n} |\lambda_i| \tag{3}$$

holds; details can be found in (GUTMAN and POLANSKY, 1986; GUTMAN and FURTULA, 2017) and elsewhere. Formula (3) holds for conjugated π-electron systems in which all bonding MO energy levels are doubly occupied, and all antibonding MO energy levels are empty.

The special case (3) was known to many early authors, in particular to Charles Coulson and Bernard McClelland (COULSON, 1940; MCCLELLAND, 1971).

Formula (2a) and its simplified version (2b) are so awkward and complicated that it is not to be expected that mathematically oriented scholars will be willing to spend their time and attention to their investigation. On the other hand, formula (3), especially its right-hand side, could be expected to be sufficiently attractive to mathematicians. This expectation motivated the present author to define the energy of a graph G (of any graph) as

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i| \tag{4}$$

where n is the number of vertices of G, and $\lambda_1, \lambda_2, ..., \lambda_n$ are the eigenvalues of the graph G, *i.e.*, the eigenvalues of the adjacency matrix of the graph G. This definition was published in 1976 in an insignificant journal (GUTMAN, 1978), which later became a citation classic.

As will be seen below, this chemically motivated graph-spectral concept had a great impact on the development of the studies of the HMO total π-electron energy and, equally, on research in spectral graph theory. Therefore, the following should be made clear:

1) **In the time of publication of the paper (GUTMAN, 1978), its author was Assistant Professor at the Faculty of Science of the University of Kragujevac.**
2) **Therefore, the concept of graph energy should be (in fact: must be) considered as a result obtained at the Faculty of Science and at the University of Kragujevac.**
3) **So far, the concept of graph energy is the greatest (or, at least: one of the greatest) scientific achievements of people working at the University of Kragujevac, including its Faculty of Science.**
4) **Graph energy belongs among the most influential and world-wide accepted scientific concepts created in Serbia, in the second half of the 20th century.**
5) **In the time of writing of the present paper, the members of the scientific community of Serbia, including the people at the University of Kragujevac and its Faculty of Science, are not prepared to accept the claims 1)-4) and to act accordingly. It may be that a time comes when they will be.**

In what follows, a few data will be presented, justifying claims 3) and 4). More can be found in (GUTMAN and FURTULA, 2017) and in the books (GUTMAN, 2017; GUTMAN and FURTULA, 2019).

GRAPH ENERGY – CHEMICAL BACKGROUND

In the time when the concept of graph energy was put forward, several results in the theory of HMO total π-electron energy were known. Of these, we mention here the Coulson integral formula (COULSON, 1940)

$$E_\pi = \frac{1}{\pi}\int_{-\infty}^{\infty}\left[n - \frac{ix\phi'(G,ix)}{\phi(G,ix)} \right] dx$$

and the McClelland upper bound (MCCLELLAND, 1971)

$$E_\pi \le \sqrt{2mn}$$

together with McClelland's approximation

$$E_\pi \approx a\sqrt{2mn} \;\; ; \;\; a \approx 0.9 \, .$$

In these formulas, the conjugated molecule considered is assumed to possess n carbon atoms and m carbon-carbon bonds (*i.e.*, the respective molecular graph G possesses n vertices and m edges). $\phi(G,\lambda)$ denotes the characteristic polynomial of the molecular graph, $\phi'(G,\lambda)$ is its first derivative, and $i = \sqrt{-1}$. All these results hold if and only if the total π-electron energy satisfies the condition (3). Consequently, the above results would automatically hold also for graph energy.

Thus, at the moment when the concept of graph energy was introduced, several significant mathematical results were known to hold for it (GUTMAN, 1978). The author hoped that because of the simplicity of the expression (4), some mathematicians will start to study it, thus enhancing the theory of HMO total π-electron energy, thus helping chemists to get a deeper insight into the quantum-theoretical description of conjugated π-electron-containing molecules. This indeed happened, but to an extent that the author did not anticipate.

GRAPH ENERGY – PER ASPERA

In spite of the author's great expectations, after the publication of the paper (GUTMAN, 1978) nothing happened. Not a single colleague showed any interest in graph energy, not a single paper on this topic (except a few authored or coauthored by I.G.) was published. This appeared to become I.G.'s scientific fiasco.

This lasted for 20 years. In 1999 things started to change, first slowly and then explosively, see Table 1.

GRAPH ENERGY – AD ASTRA

After a twenty-years of silence, in 1999 the first papers produced independently of I.G. were published. Their authors were from China (LI, 1999; ZHANG and LI, 1999) and India (WALIKAR *et al.,* 1999). Of other early researches on graph energy, we mention here those from Canada (CAPOROSSI *et al*., 1999), Germany and Sweden (KOOLEN and MOULTON, 2001), and Columbia (RADA and TINEO, 2003).

In the book (GUTMAN and FURTULA, 2019), all published papers on graph energy were collected (known to the authors in April 2019), together with the names and countries of all involved researchers. These data were mainly generated by internet search. In (GUTMAN and RAMANE, 2020), this census was completed for 2019. After that time no systematic bibliographic research along these lines was done. Therefore, the data displayed in Table 1 for the time after 2019 are certainly and grossly incomplete.

In Table 1 we give the number of papers published in a given year and add some short comments. These numbers slightly differ from those in the book (GUTMAN and FURTULA, 2019), because in the meantime a few more relevant publications were discovered.

Table 1. Published papers on graph energy.

year	papers	comment
1999	6	of these 3 authored or coauthored by I.G.
2000	4	of these 3 coauthored by I.G.
2001	14	of these 7 authored or coauthored by I.G.
2002	3	of these 1 coauthored by I.G.
2003	5	of these 1 coauthored by I.G.
2004	10	
2005	16	
2006	11	
2007	37	
2008	56	more than one per week
2009	72	
2010	69	
2011	63	
2012	65	
2013	68	
2014	82	
2015	116	more than two per week
2016	124	
2017	152	almost three per week
2018	139	
2019	156	three per week
2020	113	no internet search done, yet more than two per week
2021	100	incomplete
2022	85	incomplete
2023	77	incomplete
2024	58	incomplete, yet more than one per week

It may safely be said that in our time, scientific investigations of graph energy are enormous, resulting in well over 2000 publications, and quite a few books. No individual could follow the published production in this area (which nowadays is about 2-3 papers each week). Preparing a complete or nearly complete bibliography is also beyond a person's ability and would require the work of a larger team. Maybe AI could help?

It may safely be said that in our time, scientific investigations of graph energy are done worldwide. Authors all over the world were and are involved in such research. They are from the following countries:

Afghanistan, Argentina, Austria, Australia
Bahrain, Belarus, Belgium, Benin, Bosnia and Herzegovina, Brazil
Canada, Chile, China, Columbia, Croatia, Czech
Denmark
Egypt, Ethiopia
Finland, France
Georgia, Germany, Great Britain, Greece
Hungary

India, Indonesia, Iran, Iraq, Ireland, Israel, Italy
Japan
Kuwait
Lebanon
Malaysia, Malta, Mexico, Morocco
Netherlands, Nigeria, Norway
Oman
Pakistan, Philippines, Poland, Portugal
Ruanda, Rumania, Russia
Saudi Arabia, Serbia, Singapore, Slovakia, Slovenia, Somalia,
South Africa, South Korea, Spain, Sudan, Sweden
Taiwan, Thailand, Turkey
Ukraine, United Arab Emirates, United States of America, Uruguay, Uzbekistan
Venezuela
Yemen

As seen, scholars from almost all continents participate in research of graph energy. To our great dismay, Antarctica is missing from our list. So far.

Most numerous researchers come from China and India, followed by Pakistan and Iran. In Serbia, graph-energy-related studies were done in Belgrade, Kragujevac, Niš, Novi Pazar, Novi Sad, Sombor, and some other smaller places.

We end this section by reminding the reader that the origin of this enormous work is in Kragujevac, at the University of Kragujevac. Not many scientific achievements of this caliber have their origin in Serbia.

THE GRAPH ENERGY DELUGE

The mathematics of the Hückel molecular orbital theory is necessarily based on the adjacency matrix of the underlying molecular graph, cf. Eq. (1). Therefore, also the graph energy was originally defined in terms of the eigenvalues of the adjacency matrix, cf. Eq. (4). It was soon recognized that as far as graph energy is concerned, there is no necessity to use the adjacency matrix, *i.e.*, the eigenvalues of other matrices could also be employed.

The first such modification of graph energy was based on the Laplacian matrix – the "Laplacian energy" (GUTMAN and ZHOU, 2006). The Laplacian matrix $\boldsymbol{L}$ of a graph G with n vertices and m edges is defined via its elements as:

$L_{ii} = d_i$ for $i = 1,2,\ldots,n$,

$L_{ij} = -1$ whenever there is an edge between the i-th and j-th vertices,

$L_{ij} = 0$ whenever the i-th and j-th vertices are not connected by an edge,

where d_i is the degree (= number of first neighbors) of the i-th vertex. Then the Laplacian energy of G is

$$LE = \sum_{i=1}^{n} \left| \frac{2m}{n} - \mu_i \right| \tag{5}$$

where $\mu_1, \mu_2, ..., \mu_n$ are the eigenvalues of the Laplacian matrix. Recall that for these eigenvalues the relation $\mu_1 + \mu_2 + \cdots + \mu_n = 2m$ holds.

Soon followed the "distance energy", based on the eigenvalues of the distance matrix (INDULAL *et al.*, 2008). After some time, mathematicians (especially from India) recognized that a graph-energy-like quantity can be defined by using any real and symmetric square matrix, especially those that are somehow related to graphs. This resulted in arbitrarily many "graph energies". Their production was further enhanced after the American mathematician Vladimir Nikiforov showed how such energies can be defined also for non-square matrices (NIKIFOROV, 2007).

The "graph-energy deluge" began. In the book (GUTMAN and FURTULA, 2019), more than 170 different "graph energies" are recorded. In (GUTMAN and RAMANE, 2020), pertaining to the year 2019, additional 13 such "graph energies" were registered. Nowadays, their number may exceed 300, although no census after 2019 was made.

Needless to say that in almost all cases, the new "graph energies" are mathematically trivial and worthless, whereas their applicability in any area of human activity is questionable and unproved. In order to stop the deluge, efforts have been made to elaborate a general theory of graph energies, that would include – as special cases – the results for each particular "graph energy" (GUTMAN, 2012; DAS *et al.*, 2018; LI and YANG, 2024). Nevertheless, at the present moment, there is no sign that the deluge is ceasing.

APPLICATIONS OF GRAPH ENERGY

The obvious application of graph energy is in chemistry, where it coincides with the HMO total π-electron energy for the vast majority of conjugated molecules. The most direct application is for calculating standard enthalpy and other enthalpy-related thermodynamic quantities. Details can be found in (GUTMAN and POLANSKY, 1986; GUTMAN, 1992; GUTMAN and SOLDATOVIĆ, 2001; GUTMAN and FURTULA, 2017) and elsewhere.

What came as a surprise, a very pleasant surprise indeed, was the finding that graph energy has got a large number of other applications, in areas far from organic chemistry. In what follows we list a few of them. The present author did not participate in these applications and, therefore, the interested readers are directed to the references quoted.

Crystalography (YUGE, 2017; YUGE, 2018)
Macromolecules (DHANALAKSHMI *et al.,* 2015; PRAŽNIKAR *et al*., 2019)
Proteins (WU *et al*., 2015; DI PAOLA *et al.,* 2016; SUN *et al*., 2016; YU *et al*., 2017; XU *et al.,* 2020)
Mechanics (GÜNDÜZ, 2009)
Biology (GIULIANI *et al*., 2014; GAO *et al*., 2022; GONG *et al.,* 2022)
Biochemistry (BATHS *et al.,* 2014)
Medicine (BOLANOS and AVIYENTE, 2011; DAIANU *et al*., 2015; DASGUPTA *et al.,* 2015; NITHIN *et al*., 2021; BANDYOPADHYAY *et al*., 2024; OUDJER *et al.,* 2024; NAZ *et al.*, 2025; TANG *et al.,* 2025)
Psychology (SOLOVIEV, 2020; PALUMBO *et al.,* 2024; SUBRAMANI *et al.,* 2025)
Linguistics (VIERLBOECK *et al.,* 2025)
Air Traffic (JIANG *et al*., 2016)
Satellite Communication (AKRAM and NAZ, 2018)
Process Analysis (MUSULIN, 2014a; MUSULIN, 2014b)
Climate Change (PHILLIPS, 2019)
Pattern Recognition (XIAO *et al*., 2011; XIAO and HALL, 2018)
Image Analysis (SONG *et al.,* 2010; BAI *et al*., 2014; POURNAMI and GOVINDAN, 2017; SHI *et al.,* 2025; ZHAO and CAI, 2025)
Satellite Image Classification (MENG and XIAO, 2011; ZHANG *et al*., 2013)

Face Recognition (ANGADI and HATTURE, 2019)
Complex Systems Design (SINHA and DE WECK, 2013; IANDOLI *et al*., 2018; SINHA and SUH, 2018; EDWARDS *et al*., 2024)
Spacecrafts (PUGLIESE and NILCHIANI, 2017)
Electric automobiles (ATHEEQUE and BASHA, 2024)
Terrorism (QI *et al*., 2013).

It should be noted that in most of these applications, the Laplacian energy is employed; see Eq. (5) for its definition.

For instance, the application described in (QI *et al.,* 2013) assumes that by surveillance of telephone conversations of terrorist suspects, a network (multigraph) is created. Then the change of the Laplacian energy of this network, upon the deletion of a vertex is to be calculated (for each vertex). The greatest such change indicates the expected leader of the terrorist group.

In an analogous manner, Laplacian energy serves to recognize the most important features on an image. In complex systems design (including construction of spacecrafts), the aim is to ensure that the system will continue to function if some of its components fail. By means of Laplacian energy, one pinpoints the most critical components.

CONCLUDING REMARKS

Half a century ago, the present author studied the Hückel molecular orbital theory. Then he proposed a minor modification of the HMO total π-electron energy - the *graph energy.* The sole purpose of the graph energy concept was to make the total π-electron energy more attractive to mathematically trained colleagues. It was hoped that the examination of graph energy will lead to a deeper insight into the structure-dependency of total π-electron energy, thus helping chemist to better understand the properties of conjugated molecules. Nothing more was in mind of the present author when he published his paper (GUTMAN, 1978). What happened later went far beyond of his expectations.

First: Thousands of scholars started to do, and are currently doing, research on graph energy. This most pleasing fact shows that the idea was well chosen and fell on fertile scientific ground. Let's ignore the detail that twenty years was needed until somebody understood the idea.

Second: The other most pleasing fact is that graph energy found applications in areas fully outside of the field of chemistry of unsaturated conjugated compounds, equally outside of any quantum theory. Such phenomena several times occurred in the history of science. Scientific concepts, that initially appear to be purely theoretical and of no practical value, sometimes become useful where nobody could have expected.

Third: The total π-electron energy saga does not end in 2025. He who lives long enough will see what follows.

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QUADRATIC ACID AS A STRUCTURAL MOTIVE IN A LEHN-TYPE CRYPTAND - PREDICTION OF ION SELECTIVITY BY QUANTUM CHEMICAL CALCULATIONS. XX😊

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ABSTRACT. The ion selectivity of [$2_{Qua}.2_{Qua}.2_{Qua}$] was investigated based on descriptors derived from quantum chemical calculations (B3LYP/LANL2DZp), including structural aspects and model reaction energies. The results clearly show that the cryptand [$2_{Qua}.2_{Qua}.2_{Qua}$] demonstrates the same ion selectivity as the earlier investigated cryptands [$2_{Oxa}.2_{Oxa}.2_{Oxa}$] and [2.2.2]. There is a clear preference for K^+ (over Rb^+) and Ba^{2+} (over Sr^{2+}). The substitution of the oxalic acid or ethyl moieties by the quadratic acid block, with its sp^2-carbon cycle, makes the cryptates [$M \subset 2_{Qua}.2_{Qua}.2_{Qua}$]$^{m+}$ less flexible in comparison to [$M \subset 2_{Oxa}.2_{Oxa}.2_{Oxa}$]$^{m+}$ and [$M \subset 2.2.2$]$^{m+}$. To compensate for the quadratic acid-based inflexibility, the cryptand [$2_{Qua}.2_{Qua}.2_{Qua}$] utilizes twisting the CN···NC angle to improve the coordination of guest cations and nest them in a better way in [$2_{Qua}.2_{Qua}.2_{Qua}$].

Keywords: selective ion complexation, cryptand, DFT-study.

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INTRODUCTION

One of the reasons why supramolecular chemistry is so appealing to many scientists is that it encompasses a diverse range of chemical sub-disciplines, each of which can make valuable and significant contributions. In addition, the inclusion of a variety of interaction concepts can effectively achieve new binding motifs and new properties in supramolecules.

In the year 1969, 55 years ago, Jean-Marie Lehn and his team presented the first cryptands today known as the [2.2.2] (see Fig. 1). To obtain the intriguing molecule, the researchers employed a conventional, classical organic synthesis approach (DIETRICH *et al.*, 1969a, DIETRICH *et al.*, 1969b).

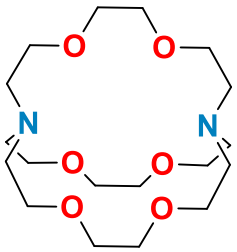
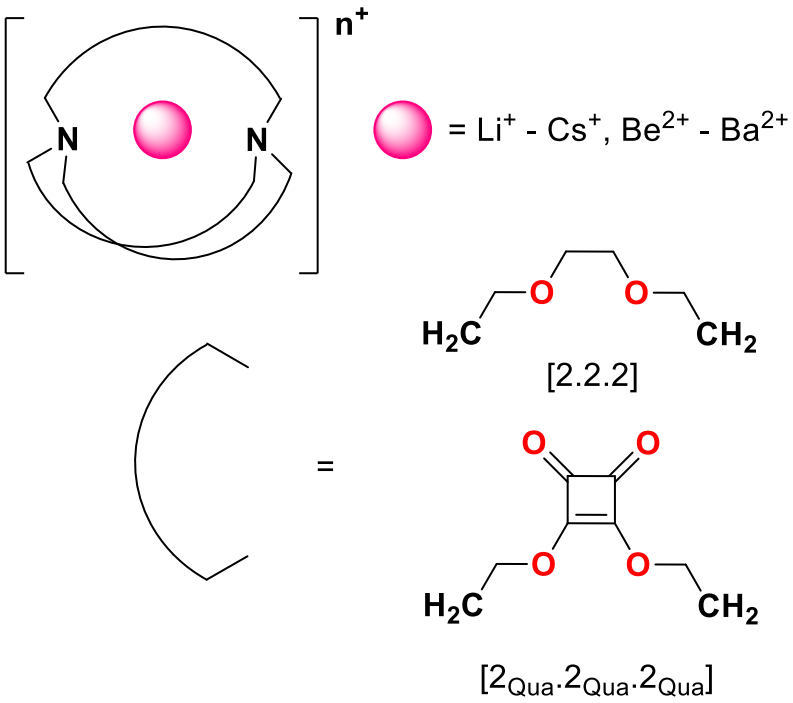


Figure 1. Lehn's original cryptand, best known by Lehn's notation [2.2.2] – system name 4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane.

Three decades later, scientists around the world, including Prof. Rolf W. Saalfrank and his team here in Erlangen, developed the concept of metallo-topomers and established metallo-supramolecular chemistry as a consistent and logical continuation of Lehn's cryptands. While Lehn's cryptands are based on classical organic synthesis, in metallo-supramolecular chemistry the cages are constructed from ligands and metal ions and can then form themselves utilizing the lability of complex bonds for repairing and forming the most stable structure (SAALFRANK *et al.*, 2000, 2008). The field of dynamic chemistry, which is based on the concept of labile covalent bonds, is currently contributing new knowledge, as evidenced e.g. by the work of Max von Delius and his team at Ulm (SHYSHOV *et al.*, 2017 and HOLLSTEIN *et al.*, 2024).

Lehn's classic cryptand [2.2.2] is an unparalleled blueprint for cryptands with new assemblies, and analogous donor properties (two as bridgeheads and six in the bridging groups), and it will continue to inspire new developments in this field. Computational chemistry is the ideal tool for designing and evaluating already before synthesis new cryptands derived from Lehn's classic cryptand [2.2.2]. An incomplete list of systems derived from [2.2.2] is e.g. i) [bpy.bpy.bpy] (PUCHTA *et al.*, 2007) and its mixed [2.2.bpy], [2.bpy.bpy] cryptands, (BEGEL *et al.*, 2013) ii) [phen.phen.phen] and the mixed ryptands [2.2.phen], [2.phen.phen], (PUCHTA *et al.*, 2008) iii) [TriPip222] (BEGEL *et al.*, 2016), iv) [bfu.bfu.bfu] (PALMER and PUCHTA, 2020) or v) the 2.2'-bioxazole-based isomeric bicyclic Lehn-type cryptands (ĆOĆIĆ *et al.*, 2020).

Extending our research on the Lehn-type cryptands derived from [2.2.2], we present in this manuscript a quantum chemical study on the selective alkali and alkaline earth metal ion complexation by a new Lehn-type cryptand, in which the 1,2-diethoxyethane moiety is replaced by a quadratic acid ester group, resulting in [2_{Qua}.2_{Qua}.2_{Qua}]. (See Scheme 1).



Scheme 1. In this study investigated systems with the oxalic acid group and [2.2.2] as a reference.

APPLIED COMPUTATIONAL METHODS

All calculations were performed at the hybrid B3LYP (LEE *et al.*, 1988; BECKE, 1993; STEPHENS *et al.*, 1994). theory level in combination with the LANL2DZ (DUNNING and HAY, 1977; HAY and WADT, 1985a; HAY and WADT, 1985b; WADT *et al.*, 1985;). basis set with effective core potentials, augmented with polarization functions on non-hydrogen atoms, to utilize an uniform and coherent basis set. This combination of the hybrid functional and basis set (further denoted as B3LYP/LANL2DZp), was selected since in earlier studies on selective ion complexation and related topics, we obtained results that were consistent with experimental values. The special challenge in these studies is the missing of experimental complexation energies. Comparison of published experimental values of the complex formation constant $\log K_S$ for $[M \subset 2.2.2]^{m+}$ with our gas-phase calculations showed a good correlation and predicted the correct ion selectivity on a relative scale (GALLE *et al.*, 2006). The success of calculations at this level has been documented (ILLNER *et al.*, 2005; SCHEURER *et al.*, 2005; WEBER *et al.*, 2005; PUCHTA *et al.*, 2006; CAPPONI *et al.*, 2024a, CAPPONI *et al.*, 2024b) and additionally permits comparison of the results of the current study with our earlier work. By carrying out calculations of vibrational frequencies, all structures were characterized as minima on the potential energy surface with no imaginary frequencies. All calculations were performed without any implicit solvent model. Presented relative energies were corrected for zero-point vibrational energy. The calculations were performed using the GAUSSIAN16 suite of programs (FRISCH *et al.*, 2016).

RESULTS AND DISCUSSION

Two descriptors are particularly suitable for determining the ion selectivity of different cryptands:

1. Investigation of the reaction energies of suitable model reactions.

2. Comparison of bond lengths, specifically the distances between the guest cation and the cryptand donor atoms.

This simple and straightforward approach has proven to be very useful and reliable in many of our previous studies (PUCHTA *et al.*, 2019) as well as those conducted by other teams (DANKERT *et al.*, 2021).

Energetic criteria

To gain insight into the complexation energies of the investigated metal cations in the [$2_{Qua}.2_{Qua}.2_{Qua}$] cryptand, we apply the simple equation 1 (n = 6):

$$[M(H_2O)_n]^{m+} + [2_{Qua}.2_{Qua}.2_{Qua}] \longrightarrow [M \subset 2_{Qua}.2_{Qua}.2_{Qua}]^{m+} + n\ H_2O \qquad (1)$$

The idea is based on the solvation of the investigated ionic metal centre by a standardised first solvation shell. This reduces the complexation energy compared to pure metal ion complexation in a clear and comprehensible way without the crude approximations of an implicit solvents model. The reliability of this approach has been proven in a couple of investigations. In former studies, we showed that the selected solvent does not affect the predicted ion selectivity, only the absolute energy values change (PUCHTA *et al.*, 2019). Our initial study on this topic yielded clear results that the calculated complexation energy for the [2.2.2]-cryptand aligns perfectly with the experimentally determined complexation constants, suggesting identical ion selectiveness (GALLE *et al.*, 2006).

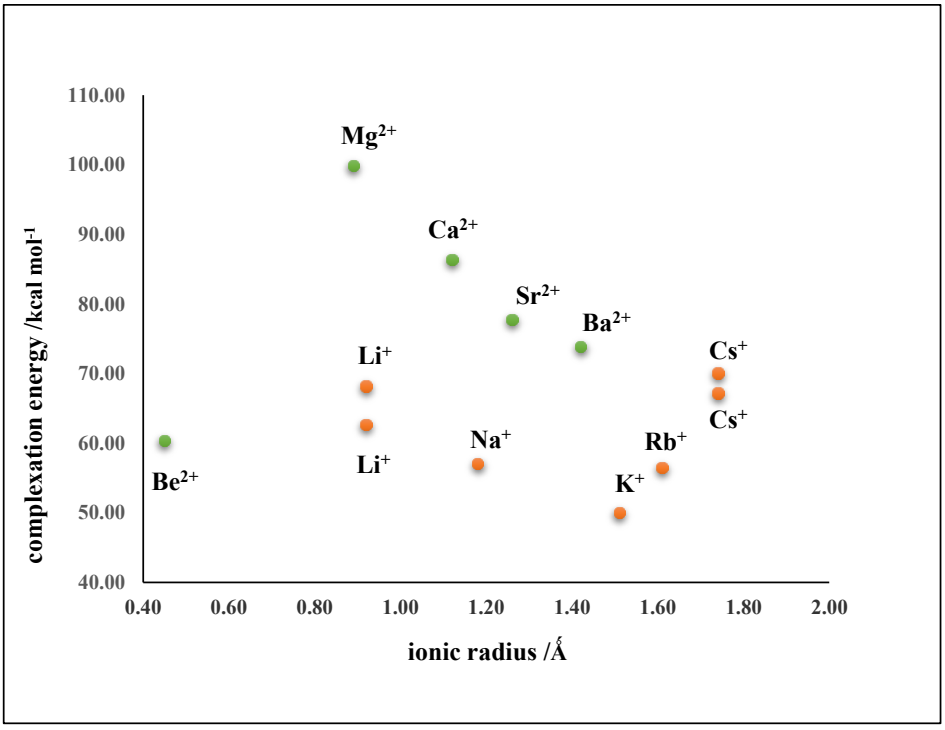
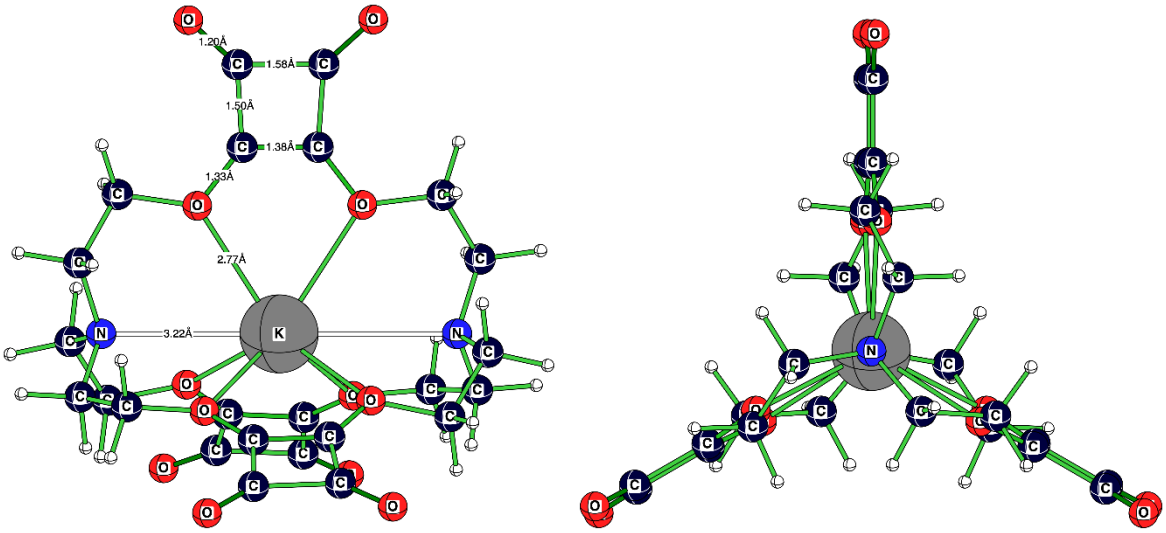


Figure 2. Calculated (RB3LYP/LANL2DZp) complexation energies of [$M \subset 2_{Qua}.2_{Qua}.2_{Qua}$]$^{m+}$ [kcal/mol] according to model reaction equations (1) in correlation with the alkaline (orange) and alkaline earth cations (green) ionic cations.

Figure 2 and Table 1 clearly show that the potassium monocation has the lowest complexation energy of all alkali metal ions (see Scheme 2). The Rb^+ ion is more than 5 kcal/mol less stable. The complexation of the Na^+ ion is only 0.5 kcal/mol less stable than Rb^+ and can therefore be most accurately described as isoenergetic to the Rb^+-cation. The alkaline

earth metal ions demonstrate a clear pattern. The barium dictation is the most stable, followed by the Sr^{2+} ion. This same ion selectivity is evident in the classic Lehn cryptand [2.2.2] and in [2_{Oxa}.2_{Oxa}.2_{Oxa}].[Error! Bookmark not defined.,i] A closer look at the three systems immediately reveals that [2_{Qua}.2_{Qua}.2_{Qua}] has even higher energy values than [2_{Oxa}.2_{Oxa}.2_{Oxa}]. This can be seen as a first indication that the cryptand presented here could be even less flexible than [2_{Oxa}.2_{Oxa}.2_{Oxa}] due to its cyclic assembly of the square acid and the four sp^2-hybridized carbon atoms in the square of the quadratic acid.



Scheme 2. Calculated (B3LYP/LANL2DZp) structure of cryptate [K ⊂ 2_{Qua}.2_{Qua}.2_{Qua}]$^+$.

On examination of the structures, it would appear that the six-oxygen donor-atom-metal cation interactions are of central importance. Table 2 and Figure 3 clearly show that the O-cation distances can be interpreted simply. Cations above the bisection line are too small to fit in the cavity. This is because the reference bonds of an undisturbed reference system are shorter, which means the cation cannot stabilize itself in the cage. The ions below are too big for the cavity. The reference bonds are longer, and the cation is compressed in the cavity. Ions on the bisection line have the ideal bond length compared to the reference system $[M(H_2O)_m]^{n+}$, fitting it perfectly. It is evident that the largest cation, Cs^+, is unable to fit within the cavity due to its considerable size, as it lies below the bisection lines. Lithium, the smallest alkaline cation, shows two bond lengths. It stabilizes itself by three M-O-interactions and one M-N-interaction, sitting in one corner of the cage. One bond length is ideal, while the other Li-O distance is too long for a stabilizing interaction. The *D_3* structures can be calculated as transition states, despite the local minima of [Cs ⊂ 2_{Qua}.2_{Qua}.2_{Qua}]$^+$ and [Li ⊂ 2_{Qua}.2_{Qua}.2_{Qua}]$^+$. However, analysis shows that these structures offer no useful stabilization. Sodium as well as beryllium, magnesium, calcium, and strontium are too small. The beryllium dictation is a special case, as always, it is shifted along the *C_3*-axis to one side, similar to the lithium cation, and stabilizes itself elegantly by a Be-N interaction and three Be-O interactions. As anticipated, the potassium and barium cations are perfectly positioned on the bisection line, with the Rb^+ cation just a short distance away. It is important to note that the next stable cations, sodium, and strontium, are significantly further away from the bisection line than the Rb-cation.

The same concept was also applicable to the metal ion bridgehead nitrogen atoms interaction (see Fig. 4). The reference complexes are the metal ions, which show a complete first coordination sphere of ammonia ligands ($[M(NH_3)_n]^{m+}$). As already addressed above (*vide supra*) we find two distances between the Be^{2+}- cation and the bridgehead N-atoms, a binding one at 1.71 Å (nearly ideal on the angle bisector) and one not interacting at 5.25 Å.

Consequently, we observe the same situation in the cryptate [Li ⊂ $2_{Qua}.2_{Qua}.2_{Qua}$]$^{+}$, as mentioned already while discussing the Li-O interaction. As we discussed before, the ions Li^{+} and Be^{2+} are too small to fit. Similarly, Mg^{2+}, Ca^{2+}, $Sr^{2+,}$ and Na^{+} do not fit and cannot benefit from a proper ion-nitrogen interaction because they are also above the bisection line. Special interest is given to the ions K^{+} and Ba^{2+}. According to the energetic criteria, they fit best in [$2_{Qua}.2_{Qua}.2_{Qua}$] but do not receive good stabilization from the N-bridge head atoms. The rubidium ion is close to the bisection line and is the second best among alkaline metal ions. The last and largest ion, cesium, is close to the bisection line, whether in D_3- or C_1-symmetry.

Table 1. Calculated complexation energies [kcal mol^{-1}] (B3LYP/LANL2DZp) calculated according to equation (1) for [M ⊂ $2_{Qua}.2_{Qua}.2_{Qua}$]$^{m+}$ and related systems.

	Li^{+}	**Na^{+}**	**K^{+}**	**Rb^{+}**	**Cs^{+}**
Ionic radius [Å]	0.92	1.18	1.51	1.61	1.74
[$2_{Qua}.2_{Qua}.2_{Qua}$] [kcal/mol]	62.63 (C_3)	57.08 (D_3)	50.01 (D_3)	56.46 (D_3)	67.21 (C_1)
[$2_{Oxa}.2_{Oxa}.2_{Oxa}$]* [kcal/mol]	61.81	48.11	38.78	43.76	54.69
[2.2.2]** [kcal/mol]	4.86	24.04	-5.00	-1.22	8.26
	Be^{2+}	**Mg^{2+}**	**Ca^{2+}**	**Sr^{2+}**	**Ba^{2+}**
Ionic radius [Å]	0.45	0.89	1.12	1.26	1.42
[$2_{Oxa}.2_{Oxa}.2_{Oxa}$] [kcal/mol]	60.35 (C_1)	99.92 (C_1)	86.32 (D_3)	77.74 (D_3)	73.93 (D_3)
[$2_{Oxa}.2_{Oxa}.2_{Oxa}$]* [kcal/mol]	33.14	91.08	69.08	63.70	60.12
[2.2.2] ** [kcal/mol]	3.36	17.14	-11.48	-16.59	-20.18

*Ref. (DANKERT *et al*., 2021) ** **Ref.** (CAPPONI *et al*., 2024a) **values in brackets: Point group of the cryptate complex**

Table 2. Calculated bond length (B3LYP/LANL2DZp) of [M ⊂ $2_{Qua}.2_{Qua}.2_{Qua}$]$^{m+}$ and the references [$M(H_2O)_n$]$^{m+}$ and [$M(NH_3)_n$]$^{m+}$.

Ion	**Point group**	**[$M(H_2O)_n$]$^{m+}$ d(M-O) [Å]**	**[$M(NH_3)_n$]$^{m+}$ d(M-N) [Å]**	**[M ⊂ $2_{Qua}.2_{Qua}.2_{Qua}$]$^{m+}$ d(M-O) [Å]**	**[M ⊂ $2_{Qua}.2_{Qua}.2_{Qua}$]$^{m+}$ d(M-N) [Å]**
Li^{+}	C_3	2.11$^{♦}$	2.13$^{♦}$	2.03; 3.62	2.10; 4.84
Li^{+} (ts)	D_3			2.28	3.31
Na^{+}	D_3	2.40	2.67	2.63	3.35
K^{+}	D_3	2.76	3.01	2.77	3.22
Rb^{+}	D_3	2.97	3.21	2.85	3.20
Cs^{+}	C_1	3.20	3.45	3.04	3.16; 3.13
Cs^{+} (ts)	D_3			2.94	3.20
Be^{2+}	C_1	1.85$^{♦}$	1.77$^{♦}$	1.64; 4.06; 3.70; 4.44	1.71; 5.25
Mg^{2+}	C_1	2.10	2.29	2.22	3.17; 3.12
Ca^{2+}	D_3	2.43	2.63	2.65	2.93
Sr^{2+}	D_3	2.60	2.80	2.74	3.08
Ba^{2+}	D_3	2.80	3.00	2.82	3.12

$^{♦}$: n =4 all other values n =6

These observations indicate that, for these ions, the metal ion-oxygen interaction is the determining factor. Additionally, we attribute the differences in behaviour to the lower flexibility of [$2_{Qua}.2_{Qua}.2_{Qua}$] compared to [2.2.2] and even to [$2_{Oxa}.2_{Oxa}.2_{Oxa}$]. The reason is that N-donors can move more easily towards the guest cation, which, in addition to the importance of the M-O interactions, affects the behaviour.

The cause of the mentioned behaviour can be identified by examination of CN···NC and O-C-C-O angles in the cryptate complexes (see Tab. 3 and Fig. 5).

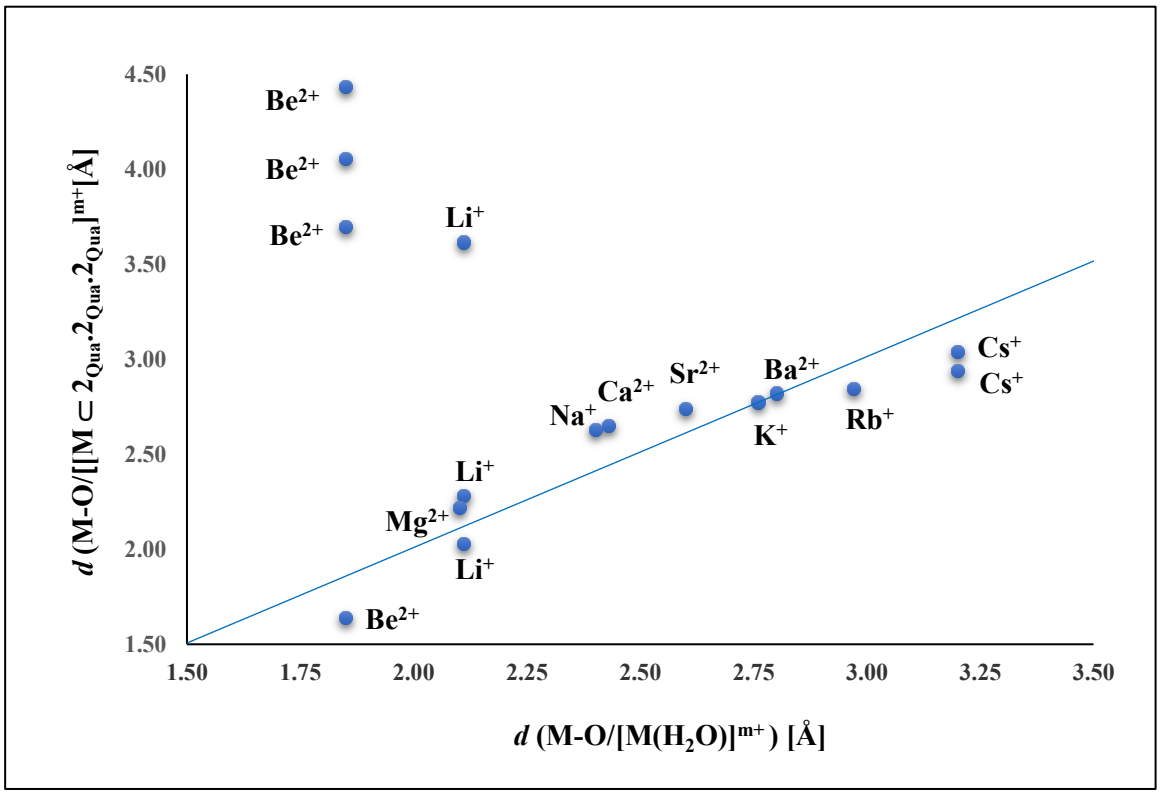


Figure 3. Comparison of the calculated M-O bond lengths [Å] in $[M \subset 2_{Qua}.2_{Qua}.2_{Qua}]^m$ and in $[M(H_2O)_n]^{m+}$ (RB3LYP/LANL2DZp).

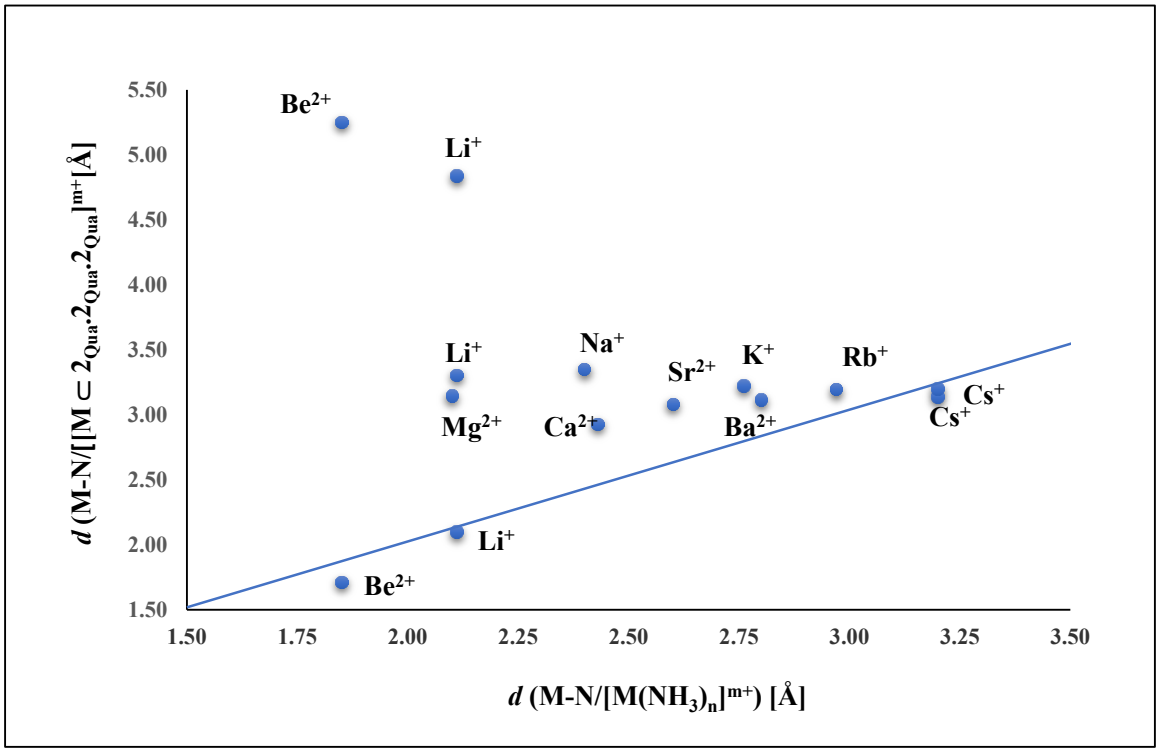


Figure 4. Comparison of the calculated M-N bond lengths [Å] in $[M \subset 2_{Qua}.2_{Qua}.2_{Qua}]^m$ and in $[M(NH_3)_n]^{m+}$ (RB3LYP/LANL2DZp).

Table 3. Calculated dihedral angle (B3LYP/LANL2DZp) O-C-C-O and CN···NC of

$[M \subset 2_{Qua}.2_{Qua}.2_{Qua}]^{m+}$.

Ion	Point group	O-C-C-O [°]	CN···NC [°]
Li^+	C_3	4.31	-20.17
Li^+ (ts)	D_3	-3.64	35.32
Na^+	D_3	2.99	-15.78
K^+	D_3	4.45	-40.50
Rb^+	D_3	6.25	-40.40
Cs^+	C_1	-0.02	-31.50
Cs^+ (ts)	D_3	9.72	-36.91
Be^{2+}	C_1	2.22; 8.85; -3.86	-20.93; -21.93; -26.40
Mg^{2+}	C_1	3.72	-43.82
Ca^{2+}	D_3	2.47	-87.24
Sr^{2+}	D_3	2.76	-57.85
Ba^{2+}	D_3	3.57	-45.57

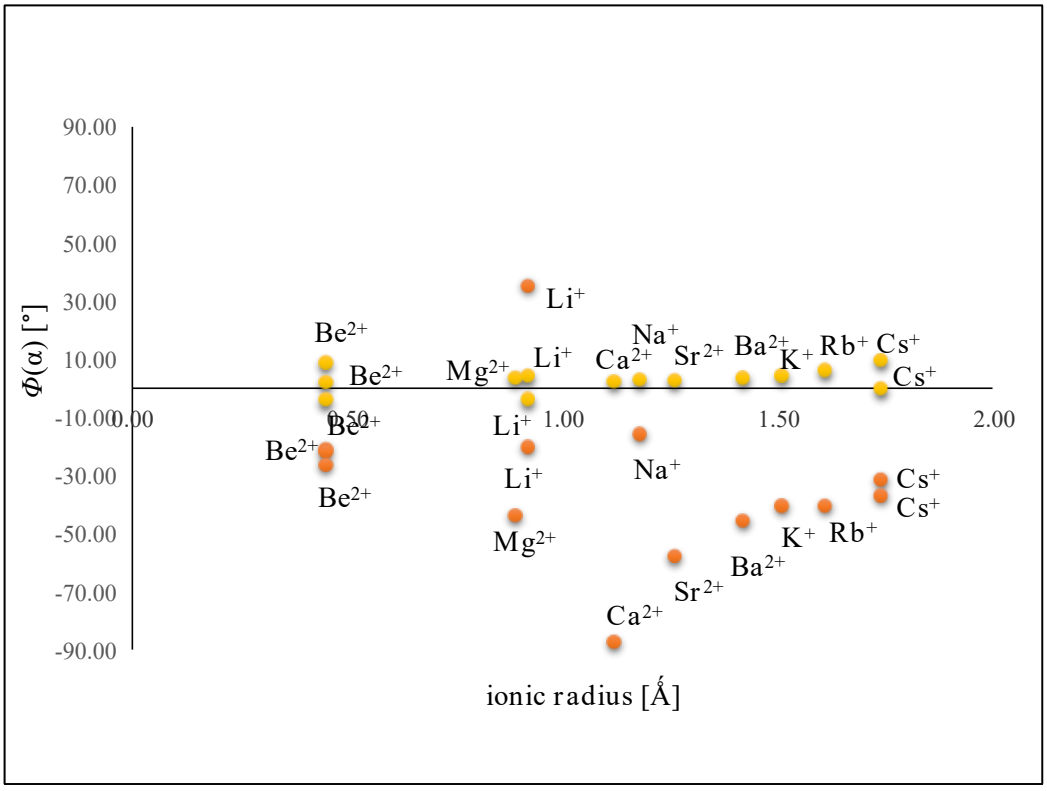


Figure 5. Calculated dihedral angles $\Phi(\alpha)$ O-C-C-O (yellow) and C-N···N-C (orange) of $[M \subset 2_{Qua}.2_{Qua}.2_{Qua}]^{m+}$ plotted against the ionic radius of M^{m+} (RB3LYP/LANL2DZp).

The CN···NC angles cover a value range of more than 70°, while the OC-CO angles only cover around 10° (15%). A comparison of these values with the CN···NC angles of $[2_{Oxa}.2_{Oxa}.2_{Oxa}]$ (a bit over 100°) and the OC-CO angles (around 70°) clearly shows that $[2_{Qua}.2_{Qua}.2_{Qua}]$ is even more inflexible than $[2_{Oxa}.2_{Oxa}.2_{Oxa}]$. This leads to poorer adaptability to the guests and less stabilization of the guest cations, as expressed in the high energies of our model equation 1 compared to $[2_{Oxa}.2_{Oxa}.2_{Oxa}]$ and much more [2.2.2].

The constant outlier, beryllium, was not considered because the system has already been shown to stabilize itself uniquely and independently. Even if the dihedral angles fall within the expected range, this does not affect the conclusion.

The sevenfold larger range of dihedral angles irrefutably demonstrates the superior flexibility of the CN···NC structural motif compared to the O-C-C-O moiety. This was attributed to the sp^2-hybridization of the moiety and the rectangular cyclic shape of the quadratic acid carbon core, which is inherently more rigid than other structures, dominated by sp^3-hybridization and by non-cyclic cores.

CONCLUSION

Quantum chemical studies have revealed that the cryptand system [$2_{Qua}.2_{Qua}.2_{Qua}$] exhibits the same ion selectivity as [$2_{Oxa}.2_{Oxa}.2_{Oxa}$] and [2.2.2], with a marked preference for K^+ (over Rb^+) and Ba^{2+} (over Sr^{2+}). The substitution of the oxalic acid or ethyl-moiety by the quadratic acid-moiety which contains sp^2-carbon cycles makes [M ⊂ $2_{Qua}.2_{Qua}.2_{Qua}$]$^{m+}$ less flexible compared to the two previously investigated systems. This reduced flexibility results in higher relative complexation energies and necessitates the use of the CN···NC angle to enhance the coordination of guest cations in [$2_{Qua}.2_{Qua}.2_{Qua}$].

Dedicated in memoriam to our friend and colleague **Dr. Jürgen Limmer** (05.01.1943 – 06.08.2024)

☺ for part XIX please see:
Host-guest complexes of two imine based isomeric {2}- Lehn-type cryptands: prediction of ion selectivity by quantum chemical calculations XIX
Alan Adel, Ralph Puchta, Dušan Ćoćić, Majda Kolenović Serezlić, Tanja Soldatović, Rudi van Eldik J. Coord. Chem., 2025, 78, 152 - 164.

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EXPLORING THE NATURE OF NONCOVALENT INTERACTIONS BETWEEN ARENES AND IONS USING QUANTUM CHEMICAL APPROACH: IS THERE ONLY ONE WAY?

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ABSTRACT. Quantum chemical approach was used to study four different types of interactions of electron-rich and electron-deficient arenes with alkali cations and halide anions. Cation-π and C-H···anion interactions of benzene, as well as anion-π and C-F···cation interactions of hexafluoro benzene, were studied by the means of two methods of energy decomposition analysis – Symmetry Adapted Perturbation Theory (SAPT) and Extended Transition State – Natural Orbitals for Chemical Valence (ETS-NOCV). Thorough analysis showed that these decomposition methods identify induction/orbital interactions as the most dominant component of interactions with cations, while electrostatic component is the dominant one in the systems containing anions. Minor disagreements were observed in the cases of interactions with larger ions (K^+ and Br^-). Overall, SAPT and ETS-NOCV are in good agreement for interactions that include cations. Caution is needed when analyzing the nature of arene-anion interactions, where ETS-NOCV can give unusually large individual components in some cases.

Keywords: cation-π interaction, anion-π interaction, Density Functional Theory, Symmetry Adapted Perturbation Theory, Extended Transition State, Natural Orbitals for Chemical Valence, Electrostatic Potentials

INTRODUCTION

Noncovalent interactions are the interactions that hold the world together. Being hydrogen bonds, ion-π, stacking, host-guest interactions, or the hydrophobic effects, to name a few, they are present in all molecular systems, and show great importance in many fields,

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ranging from catalysis and materials (ALKORTA *et al.*, 2020; SCHNEIDER, 2022), to their biological relevance in drug design, protein folding, and DNA structure (JENA *et al.*, 2022).

Noncovalent interactions of aromatic molecules are essential for chemical and biological recognition (SALONEN *et al.*, 2011). Particular importance is that of interactions of aromatic moieties with ions. The most important ones are cation-π and anion-π interactions. Cation-π interactions have shown their outstanding relevance in many chemical and biological systems, as they are among the strongest noncovalent interactions (DOUGHERTY, 2025). Among the cation-π interactions of benzene with alkali cations, the strongest one is with Li^+, with interaction energy of about -38 kcal/mol (ĆERANIĆ *et al.*, 2025). On the other hand, anion-π interactions were considered to be counterintuitive, but were shown to be feasible for arenes containing heteroatoms and/or electron-withdrawing substituents (RATHER *et al.*, 2020). These interactions can also be very strong, e.g. anion-π interaction between hexafluorobenzene and F^- has interaction energy of about -18 kcal/mol (RATHER *et al.*, 2020). Aside from ion-π interactions, where ions are situated above the aromatic rings, arenes can interact with ions via their edges, forming, among others, C-H···anion and C-F···cation interactions (PAPP *et al.*, 2017). These interactions are somewhat weaker than ion-π interactions; C-H···anion hydrogen bond between benzene and F^- has the energy of about -16 kcal/mol, while C-F···cation interaction between and hexafluorobenzene and Li^+ has the interaction energy of about -22 kcal/mol (PAPP *et al.*, 2017).

We have analyzed and compared the nature of the four different arene-ion interactions by using the methods of quantum chemistry. Quantum chemical approach was shown to be very reliable in analyzing geometries, strengths and nature of noncovalent interactions on a molecular level (PASTORCZAK and CORMINBOEUF, 2017; HAJJI *et al.*, 2021). The usual way of studying the nature of noncovalent interactions is by decomposing the total interaction energies into physically meaningful terms (STASYUK *et al.*, 2018). In this work we have used two energy decomposition analyses. Older and more popular method is based on Symmetry Adapted Perturbation Theory – SAPT (JEZIORSKI *et al.*, 1994; HOHENSTEIN and SHERRILL, 2010; HOHENSTEIN *et al.*, 2011). On the other hand, newer method used herein to study ion-arene interactions is Extended Transition State – Natural Orbitals for Chemical Valence (ETS-NOCV) (ZIEGLER and RAUK, 1977; MICHALAK *et al.*, 2008; MITORAJ *et al.*, 2009). Although conceptually different in obtaining the results, SAPT and ETS-NOCV have terms which are complementary. This means that the results of these decompositions can be easily compared, but also that one of these approaches can serve as the confirmation of the results of the other one. Using these two quantum chemical approaches, we were able to determine the influence of electrostatic, orbital and dispersion effects on arene-ion interactions.

METHODOLOGY

In this work we have studied ion-arene dimers consisting of alkaline cations (Li^+, Na^+, K^+) or halide anions (F^-, Cl^-, Br^-) and benzene or hexafluorobenzene. Full optimizations of all dimers were done in the Gaussian 09 (version D.01) program package (FRISCH *et al.*, 2009) using the B3LYP density functional (LEE *et al.*, 1988; MIEHLICH *et al.*, 1989; BECKE, 1993; STEPHENS *et al.*, 1994) with the Grimme D3 empirical dispersion (GRIMME *et al.*, 2010) and def2-TZVP basis set (WEIGEND and AHLRICHS, 2005). Frequency calculations were done and all studied systems were shown to be true minima, since no imaginary frequencies were found. The same level of theory was used to calculate the interaction energies according to the following formula:

$$\Delta E = E_{DIMER} - (E_{ARENE} + E_{ION}) \quad (1)$$

The interaction energy was corrected for basis set superposition error using the counterpoise method by Boys and Bernardi (BOYS and BERNARDI, 1970).

Electrostatic potentials of benzene and hexafluorobenzene were obtained from Gaussian wavefunctions and were mapped on the molecular surface defined by 0.001 a.u. electron density isosurface using the WFA-SAS program (BULAT *et al.*, 2010). The local minima and maxima of electrostatic potentials were found and calculated in the MultiWFN program package (LU and CHEN, 2012; LU, 2024) using the efficient ESP evaluation algorithm adopted by this program (ZHANG and LU, 2021).

The nature of interactions was studied by decomposing the B3LYP-D3/def2-TZVP interaction energies in obtained dimers within the ETS-NOCV methodology implemented in the ORCA 6.1.0 software (NEESE, 2025). This method decomposes the total interaction energy into four components:

$$\Delta E_{ETS\text{-}NOCV} = \Delta E_{ELST} + \Delta E_{EXCH\text{-}REP} + \Delta E_{ORB} + \Delta E_{DISP} \quad (2)$$

where ELST (electrostatic), EXCH-REP (exchange-repulsion) and ORB (orbital) terms are explicitly calculated, while DISP (dispersion) energy component is D3 empirical dispersion correction.

Another method used to gain insight into the nature of these interactions was SAPT, which was performed in the PSI4 (version 1.10) program (SMITH *et al.*, 2020). These calculations were done at the SAPT0 level using the def2-TZVP basis set, since the total interaction energies derived by it showed very good agreement with the B3LYP-D3/def2-TZVP interaction energies. This method calculates four individual terms, the sum of which gives the total interaction energy:

$$E_{ELST} + E_{EXCH} + E_{IND} + E_{DISP} = E_{SAPT} \quad (3)$$

where ELST is electrostatic, EXCH is exchange energy, IND denotes induction, and DISP stands for dispersion.

RESULTS AND DISCUSSION

With the help of electrostatic potential maps of benzene and hexafluorobenzene (Fig. 1), we can explain the possibility of the four different interactions with ions. Benzene is the prototype of electron-rich aromatic ring, as evidenced by its negative electrostatic potential above the entire ring, meaning it can form cation-π interactions. Because of its positive potential on the edges in the hydrogen atom region, it can also form C-H···anion interactions. Hexafluorobenzene is the prototype of electron-deficient aromatic ring, since the six fluorine atoms pull the electron density towards them, leaving the area above the ring with positive electrostatic potential. This makes hexafluorobenzene suitable for anion-π interactions, while the negative potential around the fluorine atoms enables C-F···cation interactions.

Based on the observations of electrostatic potentials of benzene and hexafluorobenzene, 12 systems were constructed for this work (Fig. 2) to study the interactions of arenes and ions, namely alkali cations and halide anions. The optimizations yielded interactions between benzene and alkali cations exactly above the arene ring center (Fig. 2a), with cation-π distances increasing with the increase in cation size (Tab. 1), as observed in our previous study (ĆERANIĆ *et al.*, 2025). The obtained C-H···anion interaction with fluoride is linear and very short (Table 1), while the interactions with larger halides were bifurcated (Fig. 2a), which is similar to dimers obtained previously using different methodologies (PAPP *et al.*, 2017; MALENOV and ZARIĆ, 2021). Anion-π interactions have

anions exactly above the arene ring center (Fig. 2b), which is similar to hexafluorobenzene-anion dimers obtained by employing Moller-Plesset Perturbational Theory of the Second Order (RATHER *et al.*, 2020). It can be, however, noted that anion-π distances of hexafluorobenzene are longer than cation-π distances of benzene (Tab. 1), which can be indicative of weaker interactions. Finally, C-F···cation interactions between hexafluorobenzene and alkali cations were all bifurcated (Fig. 2b), with increasing distance by going from Li^+ to K^+ (Table 1). Similar dimers were obtained previously using the Focal-Point Analysis method for Li^+ and Na^+ ions (PAPP *et al.*, 2017).

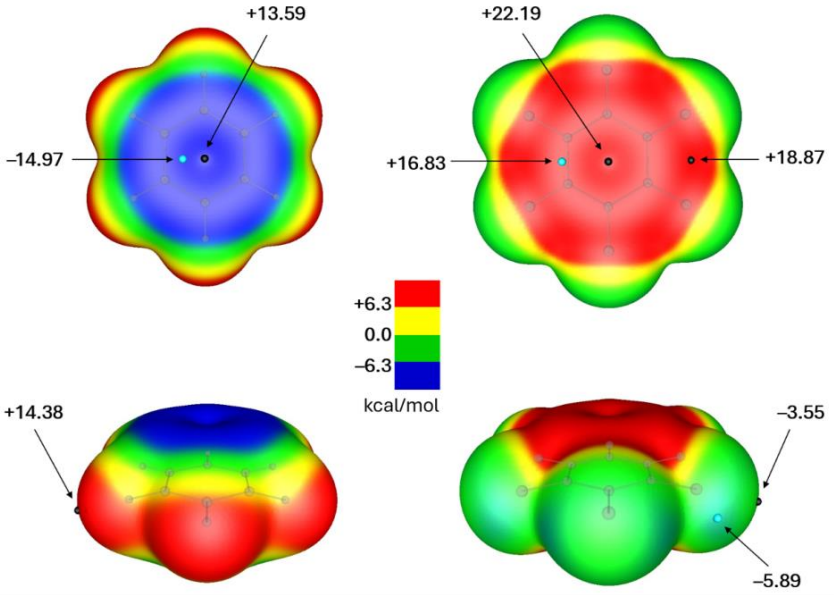

Figure 1. Electrostatic potential maps of benzene (left) and hexafluorobenzene (right) calculated at the B3LYP-D3/def2-TZVP level and mapped on the surface defined by the electron density of 0.001 a.u. The values of minima (light blue dots) and maxima (black dots) are shown in kcal/mol.

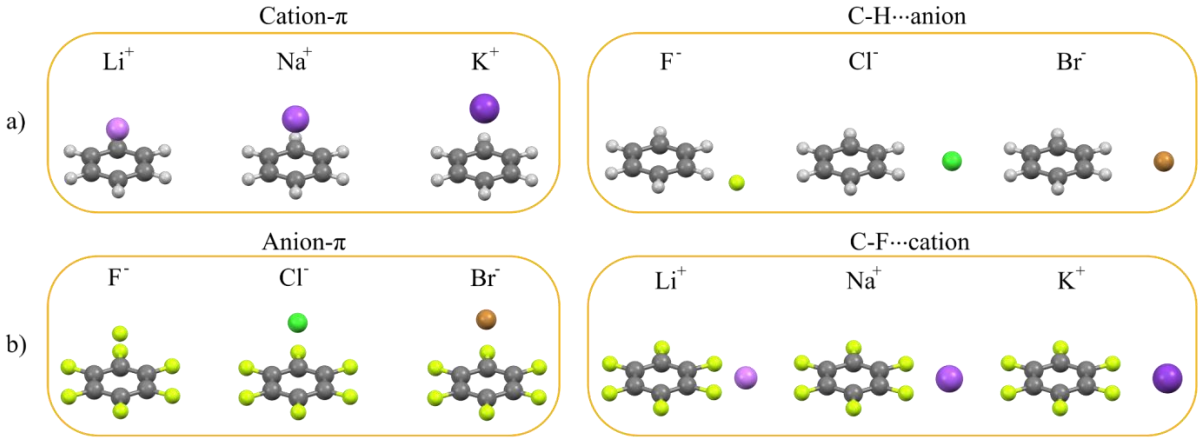

Figure 2. Optimized geometries of interactions of benzene (a) and hexafluorobenzene (b) with alkali cations and halide anions. The calculations were performed at the B3LYP-D3/def2-TZVP level of theory.

The strongest of all interactions studied in this work are cation-π, the strongest being benzene-Li^+ interaction (-39.13 kcal/mol, Tab. 1). Interactions of benzene with anions are significantly weaker, since the strongest one is less than 50% of the strength of cation-π (benzene-F^-, -18.80 kcal/mol, Tab. 1). Interactions of hexafluorobenzene with cations are

weaker than those of benzene. Namely, hexafluorobenzene-Li^+ is moderately strong, with interaction energy of -26.75 kcal/mol (Tab. 1). On the other hand, hexafluorobenzene forms stronger interactions with anions than benzene, in particular with larger anions (Tab. 1). Overall, the general trend is observed – larger ions form weaker interactions with arenes, whether or not the interaction is formed above the ring or with the atoms on the edge (Tab. 1). Interestingly, all interactions obtained herein using the B3LYP-D3/def2-TZVP level of theory are stronger than similar interactions obtained in previous works using different quantum chemical approaches (PAPP *et al*., 2017; MALENOV and ZARIĆ, 2021; ĆERANIĆ *et al.*, 2025).

Table 1. Interaction energies (ΔE) and the observed arene-ion distances (d) for all studied systems. The distance d represents the distance from the ion to the center of the ring in the case of ion-π interactions; in the case of C-H···anion and C-F···cation, it represents the average distance from the ion to the H/F atoms.

Interaction type	Arene system	Ion	ΔE kcal/mol	d Å
Cation—π	**Benzene**	Li^+	-39.13	1.851
		Na^+	-25.39	2.419
		K^+	-18.25	3.027
C-H···anion	**Benzene**	F^-	-18.80	1.561
		Cl^-	-9.14	2.728
		Br^-	-7.72	2.927
Anion-π	**Hexafluorobenzene**	F^-	-20.27	2.543
		Cl^-	-14.37	3.156
		Br^-	-12.94	3.345
C-F···cation	**Hexafluorobenzene**	Li^+	-26.75	1.946
		Na^+	-17.61	2.385
		K^+	-12.61	2.844

Two different approaches of energy decomposition analysis were employed to study the nature of these interactions – perturbative approach known as SAPT, as well as the ETS-NOCV approach, as the decomposition of an energy obtained by the means of variational principles. These two approaches are complementary, since their individual terms can be compared and used to describe the physically meaningful components of the total interaction energies.

Strictly speaking, the B3LYP-D3/def2-TZVP interaction energies reported in Table 1 were decomposed into physically meaningful terms only within the ETS-NOCV framework. The SAPT part was more challenging, since we initially had to determine the SAPT level which is capable of reproducing the B3LYP-D3/def2-TZVP interaction energies. This level turned out to be SAPT0 with the same basis set, which shows very good agreement with obtained DFT energies for benzene-ion interactions (particularly, C-H···anion, Fig. 3), while for hexafluorobenzene-ion interactions the SAPT and DFT energies show less agreement (Fig. 4), although it is quite satisfying. It is worth noting that SAPT in some cases cannot reproduce the total interaction energy for interactions of some arenes with anions (MALENOV and ZARIĆ, 2021).

Both SAPT and ETS-NOCV show that induction/orbital is a highly dominant energy component in benzene-Li^+ cation-π system (Fig. 3a). However, for cation-π interactions of benzene with larger cations, induction effects are significantly less pronounced, and electrostatic attraction becomes more important (Fig. 3a). Interestingly, the two decomposition methods disagree on the dominant energy component for benzene-Na^+ system, since SAPT favors electrostatic, while ETS-NOCV predicts orbital as the more important contribution. Both methods agree that in benzene-K^+ system electrostatic contribution is more

important than induction/orbital interactions. This can be expected based on the significantly larger cation-π distance in this system (Tab. 1), which prevents significant orbital overlap. Another SAPT analysis of cation-π systems was previously reported, with similar conclusions regarding the electrostatic and induction balance in these systems (SOTERAS *et al.*, 2008). Overall, for cation-π interactions SAPT always predicts stronger electrostatics and weaker induction effects than ETS-NOCV (Fig. 3a).

C-H···anion interactions are dominated by electrostatic effects, regardless of the applied decomposition method (Fig. 3b). A similar trend in SAPT components for benzene-anion interactions was previously reported (MALENOV and ZARIĆ, 2021). However, it can be observed that ETS-NOCV electrostatics is significantly more pronounced than SAPT electrostatics (Fig. 3b). A particularly interesting system is benzene-F^-, where both electrostatic and induction/orbital energies surpass the total interaction energy (Fig. 3b). However, this system also suffers from a very strong exchange-repulsion term, due to the very short distance between hydrogen and fluorine atoms (1.561 Å, Table 1). Although the dispersion interactions are overall very weak in benzene-ion interactions, they are somewhat more pronounced in interactions with anions, primarily on the SAPT level (Fig. 3).

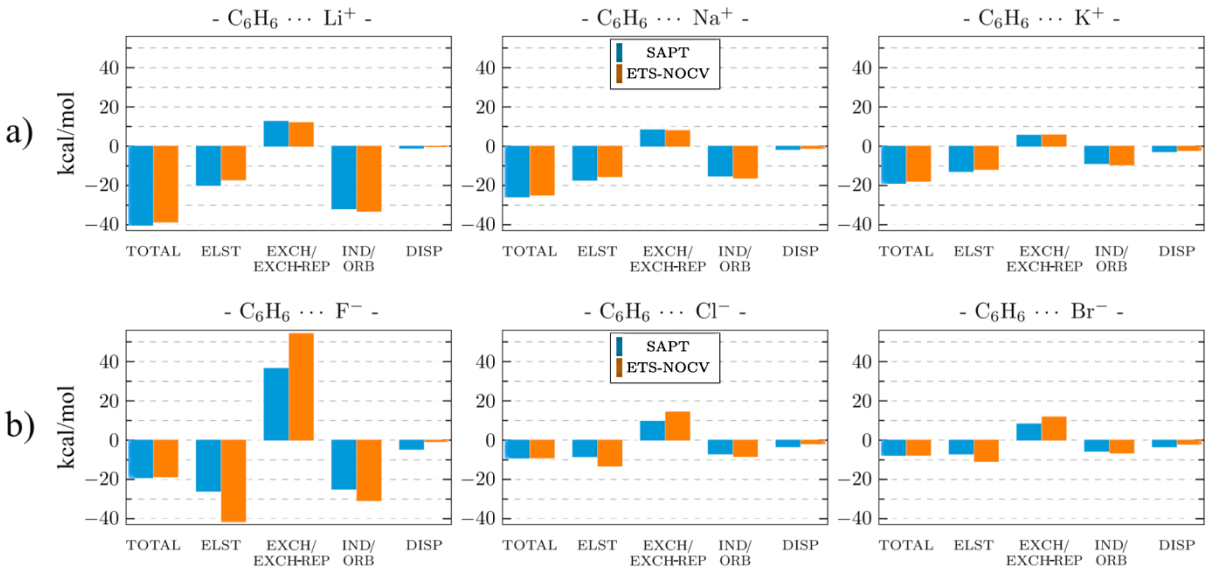

Figure 3. SAPT and ETS-NOCV decomposition analysis of energies of interactions of benzene with (a) cations and (b) anions. SAPT calculations were performed at SAPT0/def2-TZVP level of theory, while ETS-NOCV energy decomposition was performed on the B3LYP-D3/def2-TZVP interaction energies.

As previously observed in the SAPT study of hexafluorobenzene-anion systems (MALENOV and ZARIĆ, 2021), anion-π interactions are highly dominated by electrostatic effects; here we report that electrostatics are even more pronounced in the terms of ETS-NOCV decomposition (Fig. 4a). Two decomposition methods disagree on the importance of induction and dispersion in hexafluorobenzene-Br^- system; while SAPT favors dispersion, ETS-NOCV prefers orbital interactions (Fig. 4a). However, while ETS-NOCV does not address dispersion effects directly, but instead adds Grimme empirical dispersion, SAPT explicitly calculates dispersion and in all systems with anions gives larger dispersion contribution than herein applied D3 (Figs. 3b and 4a).

The least studied type of interactions presented in this work are C-F···cation interactions. Similar to cation-π interactions with Li^+ and Na^+, induction/orbital effects are more pronounced than electrostatic in hexafluorobenzene-Li^+ and hexafluorobenzene-Na^+ systems (Fig. 4b). Again, similar to benzene-K^+, hexafluorobenzene-K^+ system shows

similarities in electrostatic and induction/orbital components (Fig. 4b), which can also be attributed to the larger distance between fluorine and potassium atoms (2.844 Å, Table 1).

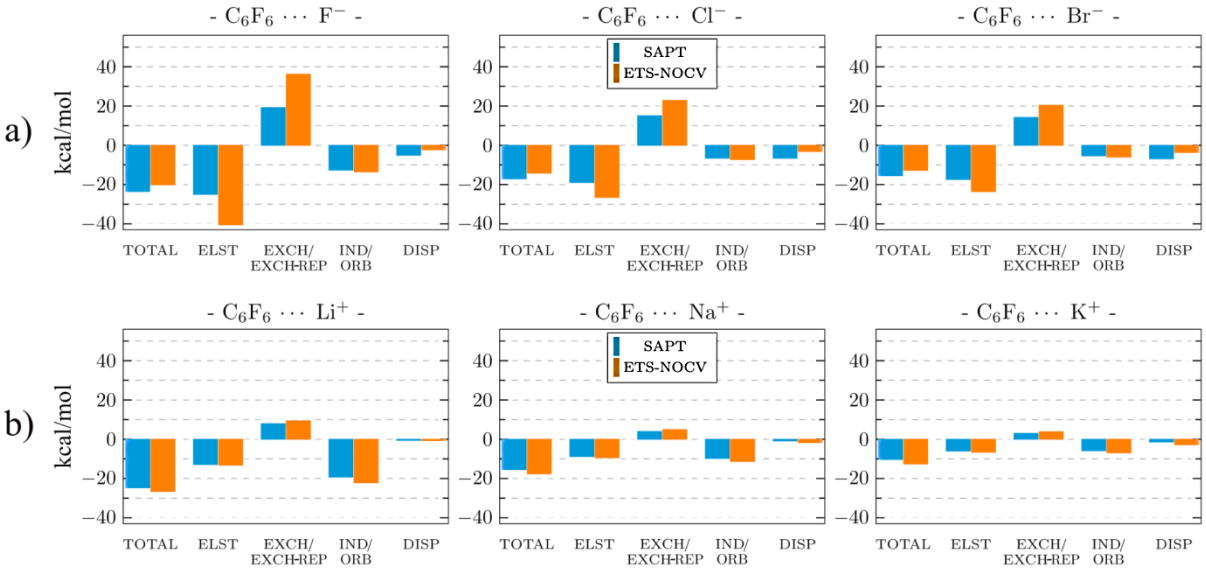

Figure 4. SAPT and ETS-NOCV decomposition analysis of energies of interactions of hexafluorobenzene with (a) anions and (b) cations. SAPT calculations were performed at SAPT0/def2-TZVP level, while ETS-NOCV decomposition was performed on the B3LYP-D3/def2-TZVP interaction energies.

When comparing the SAPT and ETS-NOCV approaches for arene-ion interactions, these methods are in both qualitative and quantitative agreement when it comes to interactions of cations (Figs. 3a and 4b). However, for interactions with anions, ETS-NOCV tends to overestimate all explicitly calculated terms, when compared to SAPT (Figs. 3b and 4a). One should therefore be careful when analyzing the nature of anion-π interactions using different energy decomposition schemes.

CONCLUSIONS

Quantum chemical methods are among the most important methods used today to study noncovalent interactions. In this paper, two of the many available quantum chemical approaches for energy decomposition analysis – perturbative SAPT and variational ETS-NOCV – were employed to study arene-ion interactions. These methods are conceptually different, but give complementary energy terms which are physically meaningful and provide insight into nature of these interactions.

Based on electrostatic potential maps of benzene and hexafluorobenzene as prototypes of electron-rich and electron-deficient arenes, we have identified four different types of interactions, namely cation-π and C-H···anion (for benzene), and anion-π and C-F···cation (for hexafluorobenzene). Density functional theory calculations on B3LYP-D3/def2-TZVP level obtained 12 dimers consisting of benzene/hexafluorobenzene and alkali cations/halide anions. Generally, both SAPT and ETS-NOCV identify induction/orbital interactions as the most dominant in cation-π and C-F···cation interactions, while anion-π and C-H···anion interactions are governed by electrostatic effects. The only notable exception to these rules among the studied systems is benzene-K^+, for which both decomposition methods indicate that electrostatics is the most dominant attractive force.

The two decomposition methods show some disagreements in their analysis of arene-ion interactions. The disagreements are mostly related to interactions with larger ions, namely K^+ and Br^-, which have larger intermolecular distances and are more challenging to assess. Overall, both SAPT and ETS-NOCV perform similarly for arene-cation interactions. However, for arene-anion interactions ETS-NOCV tends to give significantly larger individual contributions than SAPT, particularly for very small fluoride ions. These observations imply that particular caution is needed when interpreting the nature of noncovalent interactions of anions using the methods of quantum chemistry.

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UNVEILING THE BONDING IN NHBECO: A VALENCE BOND THEORY APPROACH

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ABSTRACT. In this study, the bonding and electronic structure of the HNBeCO molecule were investigated using high level classical Valence Bond (VB) theory. Starting from a full-structure calculation involving 175 VB structures, we identified and selected only seven dominant VB structures to describe the bonding between nitrogen and beryllium in HNBeCO. Our results showed that the employed set of VB structures accurately predicts the bond dissociation energy, closely matching the reference values obtained from CCSD(T) calculations. This study highlights the importance of both static and dynamic correlation in describing multiple bonding in beryllium-containing compounds. Notably, we confirmed that the N-Be bond in HNBeCO exhibits a triple bond character.

Keywords: valence bond theory, bonding, quantum chemistry.

INTRODUCTION

The year 2025 has been declared the International Year of Quantum Science and Technology. This year marks 100 anniversaries of Heisenberg's matrix mechanics, one of the foundational developments in quantum mechanics. Quantum mechanics has substantially influenced the development of theoretical chemistry throughout the 20th century, and it transformed chemistry from a phenomenological discipline into a fundamental science. The foundational work of Heisenberg and Schrödinger provided chemists with two theoretical frameworks for understanding chemical bonding: Valence Bond (VB) theory and Molecular Orbital (MO) theory (SHAIK and HIBERTY, 2008). Although both theories emerged around the same time, they soon became competing approaches. VB theory initially dominated the field of theoretical chemistry until the 1950s, after which MO theory gained prominence. Since the 1980s, however, VB theory has experienced a renaissance. While MO theory remains dominant today, VB theory offers the unique advantage of expressing the wavefunction as a linear combination of chemically intuitive Lewis structures. This contribution presents a case study that highlights the interpretative power of modern VB methods.

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Multiple bonding is a well-established phenomenon among *p*-, *d*-, and *f*-block elements, whereas its occurrence in *s*-block chemistry remains rare (CHIRIK, 2019). Within the *s*-block, beryllium is a notable exception, owing to its small atomic radius and high ionization energy, which favors the formation of covalent bonds (HAWTHORNE and HUMINICKI, 2002). Experimental and theoretical investigations have provided evidence for Be–Be multiple bonding in carbonyl complexes, as well as partial multiple bond character in heteronuclear Be–Fe species (WANG *et al.,* 2021; PURKAYASTHA *et al*., 2024). In addition to metal–metal interactions, beryllium has demonstrated the ability to form multiple bonds with carbon and nitrogen (NIEMEYER and POWER, 1997). Several structurally characterized organoberyllium compounds exhibit significantly shortened Be–C and Be–N bond lengths, suggesting the presence of π-bonding contributions (ARROWSMITH *et al*., 2016).

The recent paper reported the synthesis and characterization of a novel HNBeCO complex, formed by reacting beryllium with HNCO in a solid neon matrix (WANG *et al*., 2022). Spectroscopic observations, complemented by computational analyses, reveal that the molecule adopts a linear geometry and exhibits an unusual Be–N triple bond (WANG *et al*., 2022). It has been proposed that this bonding interaction consists of two strong π bonds and a weaker dative σ bond, representing a rare example of multiple bonding involving beryllium (WANG *et al*., 2022). These findings provide new insights into the bonding capabilities of electron-deficient main group elements and highlight the potential of beryllium to engage in complex bonding scenarios previously considered exclusive to *p*- and *d*-block elements.

Motivated by these findings, we sought to examine the nature of bonding in the HNBeCO complex using VB theory (SHAIK and HIBERTY, 2008). While MO approaches have been widely applied to such systems, VB theory offers a complementary perspective, particularly well-suited for analyzing the resonance structures and the role of orbital hybridization in bond formation (HIBERTY and BRAÏDA, 2018; GALBRAITH *et al*., 2021). Our aim was to gain a deeper understanding of the electronic structure of this unusual complex, with a focus on the bonding interactions between beryllium and neighboring atoms.

COMPUTATIONAL METHODS

The structure of HNBeCO was optimized at the B3LYP level of theory in combination with the 6-31G* basis set using the Gaussian 09 program (FRISCH *et al*., 2009). The calculation of vibrational frequencies validated that this structure corresponds to a minimum on the potential energy surface.

Valence bond theory provides a localized and chemically intuitive description of molecular electronic structure, representing the wavefunction as a linear combination of spin-coupled electron-pairing structures (SHAIK and HIBERTY, 2008). The VBSCF method is the standard classical VB method that includes static electron correlation only. The breathing orbital valence bond (BOVB) method extends this framework by allowing each VB structure to employ its own optimized set of orbitals, thereby capturing dynamic correlation associated with orbital relaxation (SHAIK and HIBERTY, 2008).

The Chirgwin–Coulson weights of seven VB structures were computed at four different theoretical levels: VBSCF, BOVB, S-BOVB, and SD-BOVB. These weights reflect the importance of each structure in the total VB wavefunction and provide insight into the electronic structure and resonance character of HNBeCO.

The split-BOVB (S-BOVB) method further improves the flexibility of the VB wavefunction by allowing active two-electron bonding orbitals to be split into separately optimized orbitals, each single occupied (SHAIK and HIBERTY, 2008). Hence, at this “S” level, all active electron pairs are described as two-electron singlet coupled into a pair of orbitals. Splitting the electron pairs basically includes radial dynamical correlation into the active

space. The highest level of BOVB variants, known as the SD-BOVB level, combines the S-BOVB approach with delocalization of the inactive orbitals across multiple centers (SHAIK and HIBERTY, 2008). Thus, the SD-BOVB basically reduces the Pauli repulsion between inactive pairs in comparison to the S-BOVB level. Together, BOVB, S-BOVB, and SD-BOVB provide a progressively refined hierarchy of valence bond methods suitable for multi-reference systems with both localized and delocalized bonding features. In this study all VB calculations were performed using the XMVB 3.0 program (SONG *et al.*, 2005; CHEN *et al.*, 2015).

RESULTS AND DISCUSSION

The optimized structure of HNBeCO investigated in this study was obtained using a significantly smaller basis set compared to that used by Wang and coauthors (WANG *et al.*, 2022). However, the chosen level of theory was found to be capable of accurately reproducing subtle geometric features such as critical bond length alternation (Fig. 1), consistent with the findings reported in the previous paper (WANG *et al.*, 2022).

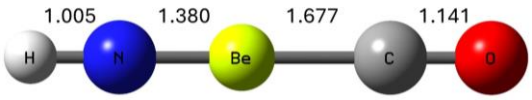

Figure 1. Optimized structure of HNBeCO with bond distances (in Å).

The reference bond dissociation energy (BDE) was obtained at the CCSD(T)/6-31G* level of theory. Generally, the CCSD(T) is widely accepted as the gold-standard in quantum chemistry. To describe the N-Be bonding within the VB framework, we selected an active space of 6 hybrid orbitals (sp_z, p_x and p_y on both N and Be atoms) populated by a total of 6 electrons. From a full structure VBSCF calculation, which involving 175 possible VB structures, only 7 structures with Chirgwin–Coulson weights larger than 4.5% were selected. These VB structures are shown in Figure 2.

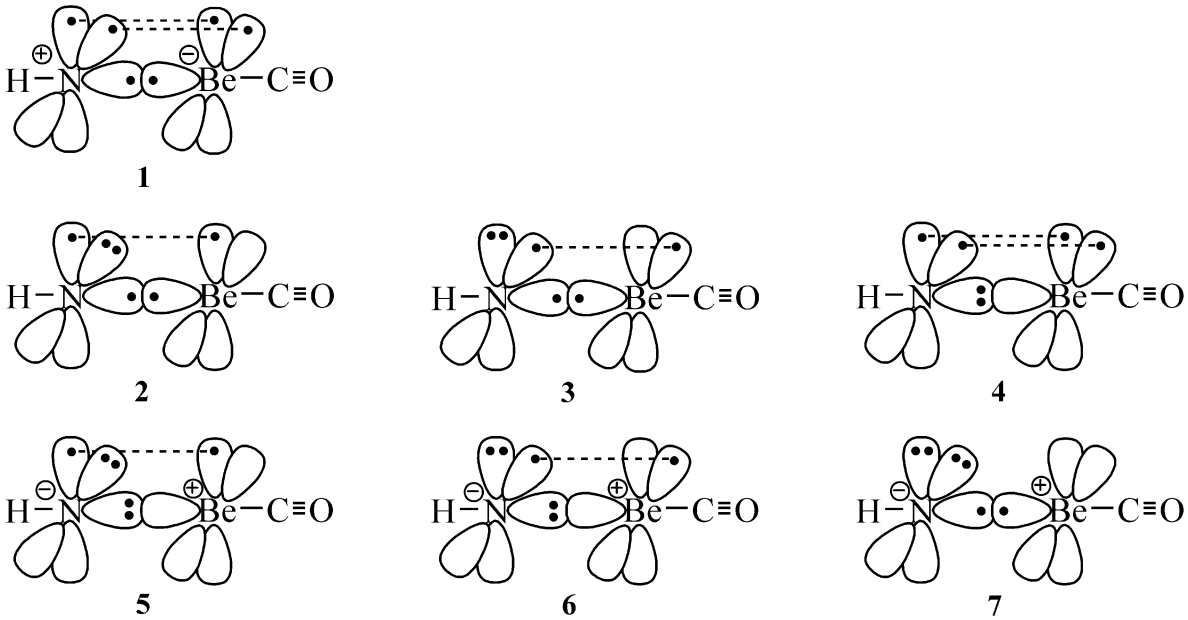

Figure 2. Set of 7 VB structures.

The selected 7 VB structures yield a BDE approximately 11 kcal/mol lower than that obtained with all 175 VB structures (Table 1). When including the breathing orbital effect at the BOVB level, this reduced set of 7 VB structures provides very similar results to the full-structure VBSCF calculation. In the next step, at the S-BOVB level, all active orbitals occupied with 2 electrons were split in all selected VB structures. Including radial dynamical correlation at the S-BOVB level improved the BDE by ~ 6 kcal/mol relative to the BOVB result. At the SD-BOVB level, the BDE is further improved, and the obtained value is about 9 kcal/mol less than the reference CCSDT energy. Considering that the VB description relies on a relatively small subset of VB structures, this discrepancy is acceptable. Based on these results, the SD-BOVB wavefunction can be confidently used for further bonding analysis in the molecule.

Table 1. Calculated BDE energies

	BDE [kcal/mol]
CCSD(T)	165.53
VBSCF (175 structures)	147.23
VBSCF (7 structures)	136.53
BOVB	146.88
S-BOVB	152.87
SD-BOVB	156.19

Previous discussion reveals that seven VB structures are relevant to describe the bonding in HN–BeCO. Structures **2** and **3** represent the dominant neutral covalent forms, featuring σ-bonding between N–Be, and contribute the most across all computational levels. Structure **1** is an ionic form (N^+–Be^-), while structure **4** involves partial π-donation from nitrogen to beryllium. Structures **5**, **6** and **7** are ionic forms with varying charge distributions (e.g., N^-–Be^+). All these VB structures confirmed previous results that the N-Be bond in HNBeCO exhibits a triple bond character.

The most significant contributions across all levels arise from structures **2** and **3**, with each maintaining a weight close to or slightly above 25% (Table 2). This consistency across all computational levels suggests that these two structures dominate the resonance hybrid. In contrast, structure **1**, which carries a relatively minor weight at the VBSCF level (2.48%), gains substantial importance at the BOVB level (11.02%) and retains a higher weight in subsequent models. This increase is a clear manifestation of the importance of orbital relaxation: BOVB allows for separate orbital optimization for each VB structure. Structures **4**–**7** exhibit intermediate weights, and their contributions slightly vary with the inclusion of dynamic correlation. Notably, the weight of structure **4** decreases when going from VBSCF (21.49%) to BOVB (15.57%), likely due to competition with more stabilized structures upon orbital relaxation. However, its contribution increases slightly in SD-BOVB (16.31%), indicating that dynamic correlation partially recovers its energetic significance. Within the VB framework, the "Charge Shift resonance energy" (RE_{CS}), is defined as the difference between the energies of the full-VB-structure wavefunction and the wavefunction consisting of the most stable VB structure. In our case, the most stable structure is **2**, which is isoenergetic with structure **3**. At the SD-BOVB level, we found that RE_{CS} equals 66.25 kcal/mol. This reveals that nearly one third of the BDE originates from charge shift resonance stabilization.

Table 2. Chirgwin-Coulson weights of structures at different levels.

	VBSCF	BOVB	S-BOVB	SD-BOVB
1	2.48	11.02	10.17	8.84
2	25.34	24.84	25.11	25.72
3	25.34	24.76	24.73	25.10
4	21.49	15.57	15.31	16.31
5	8.68	7.18	6.79	6.43
6	8.68	7.27	7.29	7.04
7	8.00	9.36	10.60	10.56

CONCLUSIONS

In this study,Valence Bond (VB) theory was employed to investigate the bonding and electronic structure of HNBeCO. The bonding between nitrogen and beryllium in HNBeCO can be described as a resonance among seven dominant VB structures, all displaying multiple bonding interactions between N and Be. Two neutral covalent structures play a dominant role, collectively contributing nearly 50% of the total wavefunction. These structures highlight a dative σ-bond alongside two π bonds between N–Be atoms. Overall, the bonding in HNBeCO cannot be captured by a single classical structure, but rather emerges from a delicate balance of covalent, ionic, and delocalized interactions. Furthermore, our study revealed that the charge shift resonance stabilization significantly influences the bonding between N and Be atoms.

Acknowledgments

The authors would like to dedicate this paper to students and teachers who stood against corruption and the collapse of the educational system in Serbia during the 2024–2025 academic year. The authors thank the Serbian Ministry of Science, Technological Development, and Innovation (Agreement No. 451-03-137/2025-03/200122).

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STRESS & ANTI-STRESS: HOLISTIC QUANTUM-INFORMATIONAL FRAMEWORK

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ABSTRACT. In the report of United Nations at the beginning of 1990s *stress* was marked as a disease of 20th century, as its role in the development of numerous psychosomatic disorders was undoubtedly confirmed. On these lines, contemporary investigations of *psychosomatic diseases* imply the necessity of application of *holistic methods*, oriented to *healing the person as a whole* and not disease as a symptom of disorder of the whole, suggesting their *macroscopic quantum origin*. In the focus of these quantum-holistic methods are body's *acupuncture system & consciousness* – which (within the Feynman propagator version of quantum mechanics) have *informational structure of quantum-holographic* Hopfield-like associative neural network – with very significant quantum-holographic psychosomatic implications. So, all holistic acupuncture-based & consciousness-based approaches and techniques can be treated as *quantum-informational therapies*, by *imposing new healing boundary conditions in the energy-state space* of EM quantum-field-related *acupuncture system/(individual and collective) consciousness*. The above mentioned quantum-holographic psychosomatic framework provides better understanding of the *nature of psychosomatic diseases*, which might help in *developing strategies for psychosomatic complementary and integrative medicine in the 21st century*.

Keywords: stress, anti-stress, psychosomatics, integrative medicine, acupuncture system, consciousness, quantum-holographic informatics.

INTRODUCTION

Stress is inevitable consequence of life. To some extent, which is individual, stress contributes to a better adaptation to daily life and work: stress itself is the life salt (SELYE, 1974). However, when this boundary is crossed, prolonged stress becomes harmful and causes numerous psychosomatic diseases. This is the reason why stress has come into the focus of science and medicine since the beginning of 1960s, when Hans Seley, director of the Institute for Experimental Medicine and Surgery of the University of Montreal, introduced the notion of *general adaptation syndrome* as a group of mutually connected *non-specific stress-reactions* of the organism (SELYE, 1974; LINDEMAN, 1982; BLAGAJAC, 1992; GROUP OF AUTHORS 1999; RAKOVIĆ *et al*., 2009; RAKOVIĆ, 2025).

The different causes of stress (hate, anger, fear, frustration, noise, nicotine etc.) were named by Seley as *stressors*, to which an organism reacts always equally: injecting sugars, fats, and adrenaline (stress-realized hormone) into the blood, followed by growth of blood pressure, narrowing of blood vessels and increasing secretion of gastric acid – as a preparatory physiological reaction of the organism for the second phase of stress, of intense muscular strain for "fight or flight". As in contemporary life and work conditions the *"fight or flight"* as a normal reaction to stressful situations is missing, thus mobilized energetic and physiological potentials are returning against the organism, and with continuing (chronic) action can cause numerous *psychosomatic disorders*.

Although the problem of stress is now especially important in the Balkans, because of the increased interpersonal, interethnic, and interreligious conflicts the whole Balkan region has been facing on the crossroad of the two millennia, it is not less important in industrially most developed countries. At the end of 1980s the famous American magazine *Time* chose for its headline "Stress: Epidemic of Eighties", and Paul Rosch, president of the *American Institute of Stress*, pointed out that numerous studies showed that the problem was even amplified, and that 75-90% visits to physicians are related to stress. Also, the *World Health Organization* has recently described job stress as a *world epidemic*, and in report of *United Nations* at the beginning of 1990s it was marked as a *disease of 20th century*; at the same time, it was estimated that 60-80% job accidents were caused by stress. Finally, recent investigations undoubtedly confirmed important role of the stress in development of different psychosomatic disorders: cardiovascular, gastrointestinal, dermatological, rheumatic, immunologic, neurological, and psychiatric.

Further on the quantum-informational framework of psychosomatics will be presented, which enables better understanding of the *nature of psychosomatic disorders* from the fundamental viewpoint, as well as the *limits and methods of their prevention and healing*, including *optimization of the existing transpersonal programs within the family environment.*

QUANTUM-INFORMATIONAL FRAMEWORK OF PSYCHOSOMATICS

Contemporary medicine has put its emphasis on the *alopatic-dosed non-economic highly pharmaceutic-oriented* medicine technologies. On the contrary, in the past years more attention is payed to bioadequate *homeopatic-dosed economic* bioresonant *quantum-informational medicine* technologies, related to usage of such values of the field energy, appearing in normal functioning of human organism (VOLL, 1975; ZHANG, 1987; DEVYATKOV and BETSKII, 1994;SIT'KO and MKRTCHIAN, 1994; GROUP OF AUTHORS, 1999; BELLAVITE and SIGNORINI, 2002; STAMBOLOVIĆ, 2003; TODOROVIĆ, 2005; RAKOVIĆ *et al*., 2006; SAMOHIN and GOTOVSKI, 2007; DJORDJEVIĆ, 2008; POTEHINA *et al*., 2008; RAKOVIĆ, 2008; RAKOVIĆ, 2009; RAKOVIĆ *et al*., 2009; GOTOVSKIZ *et al*., 2010; JOVANOVIĆ-IGNJATIĆ, 2010; RAKOVIĆ, 2011; RAKOVIĆ *et al*., 2011; RAKOVIĆ, 2025; https://www.imconsortium.org; http://www.issseem.org.) On these lines, contemporary investigations of *psychosomatic diseases* imply the necessity of application of *holistic methods*, oriented to *healing the person as a whole* and not disease as a symptom of disorder of the whole, suggesting their *macroscopic quantum origin* (VOLL, 1975; ZHANG, 1987; DEVYATKOV and BETSKII, 1994; SIT'KO and MKRTCHIAN, 1994; GROUP OF AUTHORS, 1999; RAKOVIĆ *et al*., 2006; SAMOHIN and GOTOVSKI, 2007; POTEHINA *et al*., 2008; RAKOVIĆ, 2008; RAKOVIĆ, 2009; RAKOVIĆ *et al*., 2009; GOTOVSKIZ *et al*., 2010; JOVANOVIĆ-IGNJATIĆ 2010; RAKOVIĆ, 2011; RAKOVIĆ *et al*., 2011; RAKOVIĆ, 2025).

In the focus of these quantum-holistic methods are body's *acupuncture system and consciousness* – which (within the Feynman propagator version of quantum mechanics) have *quantum-informational structure of quantum-holographic* Hopfield-like associative neural network PERUŠ (1996) – with very significant quantum-holographic psychosomatic implications (GROUP OF AUTHORS, 1999; RAKOVIĆ *et al*., 2006; RAKOVIĆ, 2008; RAKOVIĆ, 2009; RAKOVIĆ *et al*., 2009;

JOVANOVIĆ-IGNJATIĆ, 2010; RAKOVIĆ, 2011; RAKOVIĆ *et al*., 2011; RAKOVIĆ, 2025). In this context, it should be noted that Resonant Recognition Model (RRM) of biomolecular recognition implies that on the biomolecular level information processing is going on in the *inverse space* of Fourier spectra of the primary sequences of biomolecules (ĆOSIĆ, 1994; ĆOSIĆ, 1997; KEKOVIĆ *et al*., 2010), similarly to (quantum) holographic ideas that cognitive information processing is going on in the *inverse space* of Fourier spectra of the perceptive stimuli (PRIBRAM, 1971; PRIBRAM, 1991), thus supporting idea on *quantum-holographic fractal coupling* of various hierarchical levels in biological species (ZHANG, 1987).

In the context of *acupuncture-based and consciousness-based approaches and techniques of quantum-informational medicine* (YOGANANDA, 1946; LINDEMAN, 1973; VOLL, 1975; ORME-JOHNSON and FARROW, 1977; FISHMAN and GRINIMS, 1979; SARASWATI, 1982; CHIA, 1983; HAZ, 1984; BRENNAN, 1987; ZHANG, 1987; CHOPRA, 1989; JOHARI, 1989; MARKIDES, 1990; TART, 1992; DOSSEY, 1993; DEVYATKOV and BETSKII, 1994; SIT'KO and MKRTCHIAN, 1994; VUJIČIN, 1995; CALLAHAN and CALLAHAN, 1996; MILENKOVIĆ, 1997; JEROTIĆ, 1998; VLAHOS, 1998; COHEN, 1999; GROUP OF AUTHORS, 1999; HARRIS *et al*., 1999; HELLINGER and TEN HEVEL, 1999; KAMP, 1999; MIHAJLOVIĆ SLAVINSKI, 2000; PETROVIĆ, 2000; PEARL, 2001; BELLAVITE and SIGNORINI, 2002; STAMBOLOVIĆ, 2003; TODOROVIĆ, 2005; RAKOVIĆ *et al*., 2006; STIBAL, 2006; SUI, 2006; HEW LEN and VITALE, 2007; MURPHY, 2007; SAMOHIN and GOTOVSKI, 2007; TIRTHA, 2007; DJORDJEVIĆ, 2008; KINSLOW, 2008; POTEHINA *et al*., 2008; RAKOVIĆ, 2008; BARTLETT, 2009; OVERBYE, 2009; RAKOVIĆ, 2009; RAKOVIĆ *et al*., 2009; GOTOVSKIZ *et al*., 2010; GROF and GROF, 2010; JOVANOVIĆ-IGNJATIĆ, 2010; MILENKOVIĆ, 2010; BEDRIČIĆ, 2011; HADŽI-NIKOLIĆ, 2011; PANAJOTOVIĆ, 2011; RAKOVIĆ, 2011; RAKOVIĆ *et al*., 2011; SIMONOVSKA, 2011; TOMŠIĆ AKENGEN, 2011; GRABOVOI *et al*., 2012; RAKOVIĆ, 2025; http://www.atpweb.org; https://www.imconsortium.org; http://www.issseem.org;) their goal would be a bioresonant excitation of the electromagnetic (EM) microwave (MW) / ultralowfrequency (ULF)-modulated or radiofrequency (RF) / lowfrequency (LF)-modulated psychosomatically disordered state (acupuncture palpatory-painful or psychologically traumatic, as one of hundreds possible disordered states) thus enabling that its initial memory attractor is bioresonantly excited (similar to annealing procedure in artificial neural networks Hecht-Nielsen (1990) becoming more shallower and wider on the account of deepening of the (energy-dominating) attractor of healthy (acupuncture palpatory painless or psychologically traumatic-free) state – which is then altogether *quantum-holographically projected* on the lower quantum-holographic *cellular level*, thus changing the *expression of genes* (GROUP OF AUTHORS 1999; RAKOVIĆ *et al*., 2006; RAKOVIĆ, 2008; RAKOVIĆ, 2009; RAKOVIĆ *et al*., 2009; RAKOVIĆ, 2011; RAKOVIĆ *et al*., 2011; RAKOVIĆ, 2025). Thus, all these acupuncture-based and consciousness-based holistic approaches and techniques might be considered as *quantum-informational therapies*, via *imposing new boundary conditions in the energy-state space of the acupuncture system / consciousness.*

However, when this process is hindered by *transpersonally entangled blockages* in the EM field-related energy-state space of the acupuncture system / consciousness (on numerous laboratory tests revealing the evidence of entangled minds i.e. *extrasensory experiences* in a quantum reality, see refs (JAHN and DUNE, 2011)) – then memory attractors of quantum-holographic network of field-related *collective consciousness* should be removed as well (via *prayer* or *circular (psycho / energy) therapies* from all relevant meta-positions included in the problem (MARKIDES, 1990; TART, 1992; DOSSEY, 1993; VUJIČIN, 1995; MILENKOVIĆ, 1997; JEROTIĆ, 1998; VLAHOS, 1998; GROUP OF AUTHORS 1999; HARRIS *et al*., 1999; HELLINGER and TEN HEVEL, 1999; KAMP, 1999; MIHAJLOVIĆ SLAVINSKI, 2000; PETROVIĆ, 2000; RAKOVIĆ *et al*., 2006; HEW LEN and VITALE, 2007; RAKOVIĆ, 2008; OVERBYE, 2009; RAKOVIĆ, 2009; RAKOVIĆ *et al*., 2009;GROF and GROF, 2010; BEDRIČIĆ, 2011; RAKOVIĆ, 2011; RAKOVIĆ *et al*., 2011; TOMŠIĆ AKENGEN, 2011; HADŽI-NIKOLIĆ, 2011; RAKOVIĆ, 2025; http://www.atpweb.org;), thus providing *spiritual integration of personality* which *initiates the process of permanent healing* as suggested by experiences of clients in *post-hypnotic regressions* (NEWTON, 1974). These

transpersonal holistic procedures, alongside with working on all levels of *EM bioresonant (MW / ULF-modulated or RF / LF-modulated) therapies* (VOLL, 1975; ZHANG, 1987; DEVYATKOV and BETSKII, 1994; SIT'KO and MKRTCHIAN, 1994; GROUP OF AUTHORS, 1999; SIGNORINI, 2002; STAMBOLOVIĆ, 2003; BELLAVITE and TODOROVIĆ, 2005; RAKOVIĆ *et al*., 2006; SAMOHIN and GOTOVSKI, 2007; DJORDJEVIĆ, 2008; RAKOVIĆ, 2008; POTEHINA *et al*., 2008; RAKOVIĆ, 2009; RAKOVIĆ *et al*., 2009; GOTOVSKIZ *et al*., 2010; JOVANOVIĆ-IGNJATIĆ, 2010; RAKOVIĆ, 2011; RAKOVIĆ *et al*., 2011; RAKOVIĆ, 2025; https://www.imconsortium.org; http://www.issseem.org) and *non-circular (psycho / energy) therapies* (YOGANANDA, 1946; LINDEMAN, 1973; ORME-JOHNSON and FARROW, 1977; FISHMAN and GRINIMS, 1979; SARASWATI, 1982; CHIA, 1983; HAZ, 1984; BRENNAN, 1987; CHOPRA, 1989; JOHARI, 1989; MARKIDES, 1990; TART, 1992; DOSSEY, 1993; VUJIČIN, 1995; CALLAHAN and CALLAHAN, 1996; MILENKOVIĆ, 1997; JEROTIĆ, 1998; VLAHOS 1998; COHEN, 1999; KAMP, 1999; HARRIS *et al*., 1999; HELLINGER and TEN HEVEL, 1999; MIHAJLOVIĆ SLAVINSKI 2000; PETROVIĆ, 2000; PEARL, 2001; STIBAL, 2006; SUI, 2006; HEW LEN and VITALE, 2007; MURPHY, 2007; TIRTHA, 2007; KINSLOW, 2008; BARTLETT, 2009; OVERBYE, 2009; GROF and GROF, 2010; MILENKOVIĆ, 2010; HADŽI-NIKOLIĆ, 2011; PANAJOTOVIĆ, 2011; SIMONOVSKA, 2011; TOMŠIĆ AKENGEN; 2011; GRABOVOIC *et al*., 2012; http://www.atpweb.org), might be the holistic clue for imposing healing boundary conditions in the energy-state space of the acupuncture system / consciousness of the patients, cf. Fig. 1.

ON MACROSCOPIC QUANTUM NATURE OF ASUPUNCTURE SYSTEM AND CONSCIOUSNESS

It should be pointed out that on all quantum-holographic hierarchical levels of biological macroscopic open quantum systems S_k (local cell's biomolecular protein / target, local acupuncture system / consciousness, or nonlocal out-of-body consciousness / collective consciousness), there exist *two* (interacting) macroscopic quantum subsystems (RAKOVIĆ *et al*., 2006; RAKOVIĆ, 2008; RAKOVIĆ, 2009; RAKOVIĆ *et al*., 2009): first with *modifying many-electron hypersurface* $E_e(\phi_e^{(k)})$ and second with *modifying EM multi-phonon hypersurface* $E_v(\phi_v^{(k)})$, as in Fig. 1.

It should be added that an energy hypersuface of multi-phonon quantum state might also include low-energy long-range coherent MW Frohlich excitations (created as a result of interaction of electronic and phonon subsystems (FROHLICH, 1968; KEKOVIĆ *et al*., 2005), of particular significance in microwave resonance therapy (MRT) of a dynamic modification of the EM multi-phonon (and related many-electron) acupuncture macroscopic quantum subsystem (DEVYATKOV and BETSKII, 1994; SIT'KO and MKRTCHIAN, 1994; GROUP OF AUTHORS, 1999; RAKOVIĆ *et al*., 2006; POTEHINA *et al*., 2008; RAKOVIĆ, 2008; RAKOVIĆ, 2009; RAKOVIĆ *et al*., 2009; JOVANOVIĆ-IGNJATIĆ, 2010; RAKOVIĆ, 2011; RAKOVIĆ *et al*., 2011; RAKOVIĆ, 2025;).

The mentioned quantum-holographic picture implies that quantum-holographic hierarchical parts carry information on wholeness, enabling subtle *quantum-holographic fractal coupling* between various hierarchical biophysical levels – including numerous acupuncture projection zones and corresponding organs and cells, with underlying *macroscopic quantum-informational control mechanisms of embryogenesis / ontogenesis and morphogenesis* and their backward epigenetic influence on the *expression of genes*, starting from the first fertilized cell division which initializes differentiation of the acupuncture system of non-threshold electrical GJ-synapses ("gap-junctions") (ZHANG, 1987; GROUP OF AUTHORS, 1999; RAKOVIĆ *et al*., 2006; RAKOVIĆ, 2008; RAKOVIĆ, 2009; RAKOVIĆ *et al*., 2009; JOVANOVIĆ-IGNJATIĆ, 2010; RAKOVIĆ, 2011; RAKOVIĆ *et al*., 2011; RAKOVIĆ, 2025;).

This underlying quantum-coherent nonlocality might be of fundamental importance in understanding epigenetic macroscopic (quantum) holistic very nature of *psychosomatic health and diseases* as well – implying also a *fuzzy borderline* between quantum coherent (nonstationary) and

semi-classical decoherent (stationary) manifestations of the macroscopic quantum-informational *acupuncture system* and *consciousness* (as well as any macroscopic condensed-state physical (sub)system), and their *close relationship* with significant psychosomatic-cognitive implications (RAKOVIĆ *et al*., 2006; RAKOVIĆ, 2008; RAKOVIĆ, 2009; RAKOVIĆ *et al*., 2009; RAKOVIĆ, 2011; RAKOVIĆ *et al*., 2011; RAKOVIĆ, 2025;).

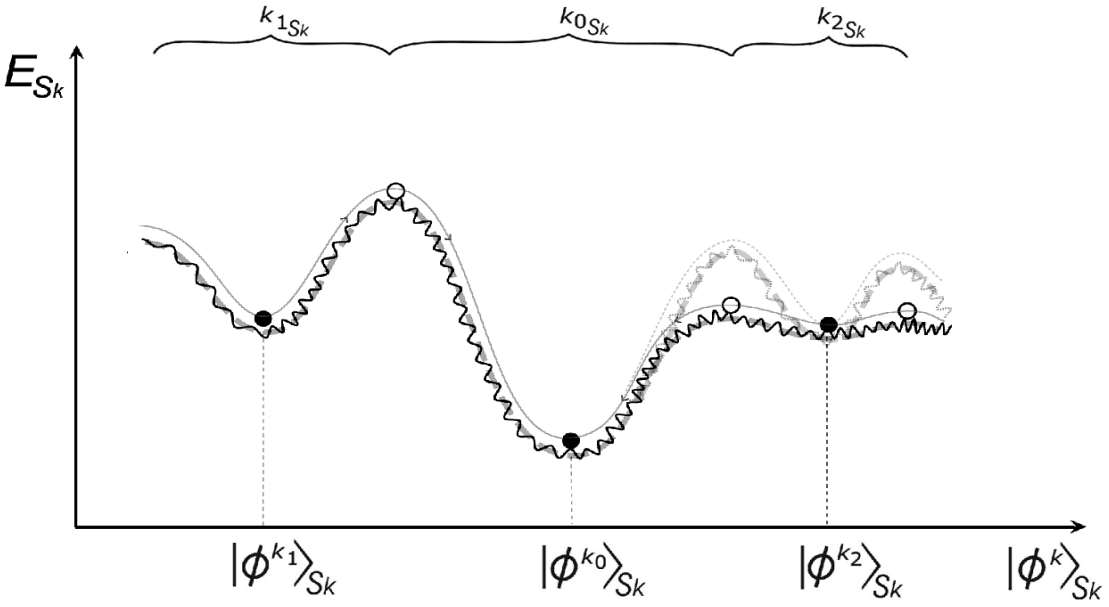

Figure 1. Schematic presentation of the adaptation of memory attractors in the energy-state ($E_{S_k}(\phi^k)$) hypersurface of the quantum-holographic memory / propagator of various hierarchical levels of biological macroscopic open quantum systems S_k (local cell's biomolecular protein / target, local acupuncture system / consciousness, or nonlocal out-of-body consciousness / collective consciousness):

$$G(r_2,t_2;r_1,t_1)=\sum_{i=1}^{P}\phi^{k_i}(r_2,t_2)\phi^{k_i}{}^{*}(r_1,t_1)\ =\sum_{i=1}^{P}A_{k_i}(r_2,t_2)A_{k_i}{}^{*}(r_1,t_1)e^{\frac{i}{\hbar}(\alpha_{k_i}(r_2,t_2)-\alpha_{k_i}(r_1,t_1))}$$

It should be pointed out that Nature presumably has chosen elegant room-temperature solution for quantum-holographic information processing, permanently fluctuating between quantum-coherent states $\left|\phi^k(t)\right\rangle_{S_k}=\sum_i c_{k_i}(t)\left|\phi^{k_i}\right\rangle_{S_k}$ and classically-reduced states $\widehat{\rho}^{k}_{S_k}(t)=\sum_i\left|c_{k_i}(t)\right|^2\left|\phi^{k_i}\right\rangle_{S_kS_k}\left\langle\phi^{k_i}\right|$ of the biological macroscopic open quantum system S_k, via non-stationary bioresonance interactions with out-of-body farther environment and through decoherence by bodily closer environment. Thus quantum neural holography combined with quantum decoherence might be very significant element of the feedback bioinformatics, from the level of cell – to the level of organism – and further to the level of collective consciousness, with epigenetic backward dynamic influence on the expression of genes. This implies necessity of quantum-informational successive bioresonant balansing of all unwilling side memory attractors (like ϕ^{k_2} in Figure), which would cause development of psychosomatic diseases on the individual level, and interpersonal fights in this and further generations on the collective level.

The above problem is of fundamentally theoretical physical significance, as it tackles the question of *universality of quantum mechanics*, i.e. the question of general validity of the quantum-physical laws for *macroscopic phenomena* as well, mostly treated by the methods of classical physics. Although this question was raised in the early phase of founding of quantum-mechanical theory (and temporarily put aside for very different reasons, being considered as a difficult scientific problem), in this respect the situation is not much better today, and it can be said freely that the

problem of universal validity of quantum mechanics is still open (GHIRARDI *et al*., 1986; ZUREK, 1991; PENROSE, 1996; RAKOVIĆ and DUGIĆ, 2002; ZUREK, 2003; DUGIĆ, 2004; RAKOVIĆ *et al*., 2004; KOFLER and BRUKNER, 2007; KOFLER and BRUKNER, 2008; VEDRAL, 2010; RAKOVIĆ *et al*., 2014).

On this line, it should be pointed out that Sit'ko with coauthors have revealed *necessary and sufficient conditions* for existence of *macroscopic selfconsistent potentials* (of so called Landau-Haken type) alongside acupuncture meridians, with EM MW *eigenfrequencies* of healthy and disordered states of the *acupuncture system* (ANDREYEV *et al*., 1982; SIT'KO *et al*., 1988; SIT'KO and GRIZHKO, 1991; SIT'KO and MKRTCHIAN, 1994; SIT'KO, 2012), pointing out that living systems are the fourth level of quantum ladder of Nature (nuclear-atomic-molecular-biological), governed by specific macroscopic quantum laws of the *Physics of the Alive*.

Also, it is worth pointing out that Umezawa with coauthors and Del Giudice with coauthors, by applying fundamental quantum-field theoretical formalism of *spontaneous symmetry breaking*, have pointed to biological room-temperature macroscopic condensates of virtual quasiparticles of the effective mass and charge, so called *evanescent photons in water* (nonpropagated / tunneling longitudinal modes of quantum EM field embedded by biological macroscopic ordered locallizations of the electric dipole field of water), as a possible quantum basis of functioning of *cells* in general (RICCIARDI and UMEZAWA, 1967; STUART *et al*., 1978; STUART *et al*., 1979; GIUDICE *et al*., 1982; GIUDICE *et al*., 1986; GIUDICE *et al*., 1988; GIUDICE *et al*., 1989; UMEZAWA, 1993; PREPARATA, 1995; MONTANGNIER *et al*., 2010), while Jibu and coauthors have pointed to them as a possible quantum basis of *consciousness* in brain (JIBU *et al*., 1994; JIBU and YASUE, 1995; JIBU *et al*., 1996; JIBU and YASUE, 1997).

According to such a theoretical concept, as evanescent photons in water are not related to propagating waves (in EM RF range (GIUDICE *et al*., 1982; GIUDICE *et al*., 1986; GIUDICE *et al*., 1988; GIUDICE *et al*., 1989; PREPARATA, 1995; MONTANGNIER *et al*., 2010)), they cannot be detected externally – so in the region of biological macroscopic ordered localizations of the electric dipole field of water special probes must be inserted, to enable embedded quanta of non-propagating modes of the EM RF field to be scattered in detectable propagating modes, which were detected experimentally in the EM RF region (Ho *et al*., 1994).

On the other hand, Popp and coauthors have conducted EM optical measurements in darkness by specially designed detector and discovered that *biological systems*, from bacteria to biological tissues, *continuously emit ultra-weak photon emission* (mainly in the *visual range of* EM spectrum, of non-exponential attenuation and specific frequency and phase and amplitude modulation for all basic biological and physiological activities), so photons of such non-standard characteristics are called *biophotons* (COMPLETE ISSUE, 2003). It was discovered that biophoton emission reflects the following *important characteristics*: health as a symmetry between left and right sides of body; illness via disordered symmetry between left and right sides of body; light channels within body which regulate transfer of energy and information between different parts; biological rhythms such as 14-days, 1-month, 3-months i 9-months.

Especially, SIT'KO *et al*. (2010) have conducted EM MW measurements via specially designed radiometric system (on the level of inherent noises $\sim 5 \cdot 10^{-23}$ W/Hz·cm^2), which enabled obtaining of the following *important characteristics of the acupuncture channels and points* (COMPLETE ISSUE, 1998): *channels* have diameter of 3÷5 mm in their surface exits in the acupuncture points; *refraction index* within channels is $n = 1$ as in the air, while being 5÷6 in the body outside channels; in case of functional disorders of channels, upon external EM MW flux of $10^{-21} \div 10^{-20}$ W/Hz·cm^2 the corresponding *acupuncture points* completely absorb radiation, while upon flux greater than 10^{-19} W/Hz·cm^2 acupuncture points completely reflect external EM MW radiation (so in natural conditions the effects of solar radiation on biological systems are neglecting in the very sensitive EM MW regulatory region, being intensely absorbed by atmosphere, which was presumably of evolutional significance in natural selection of biological species).

Based on the principles of *photonic crystals* and *photonic bandgap guiding* (where the confinement of photons in some low-index hollow-core 3D defect might be achieved by exploiting photonic bandgap reflectivity of the surrounding higher-index (quasi) periodic medium (LOURTIOZ *et al*., 2008)), it seems that the above mentioned EM MW experiments suggest an interesting possibility (RAKOVIĆ, 2014; RAKOVIĆ, 2015) to consider the *low-index* $n = 1$ *acupuncture channels* as 3D *photonic crystal channel waveguides of propagated EM MW photons* (influencing backward the structure and ionic conductivity of the channels), *confined* by the surrounding higher-index (quasi) periodic cellular body medium outside channels (of $n = 5 \div 6$ in the cellular cytoplasm and $n \gg 1$ in the cellular membranes of metabolic depending striking polarization of the volume ion density (ADEY, 1981)) *with non-propagated EM MW evanescent photons*.

Exotic aspect of acupuncture channels (of strange vacuum-like refractive index) *may be a relic of the external inflow of vital energy / prana / chi / uncreated light* (via miniature *quantum-gravitational tunnels* stabilized by exotic nature of *vital energy* as the quantum vacuum fluctuations in these tunnels (RAKOVIĆ *et al*., 2004; RAKOVIĆ, 2008; RAKOVIĆ, 2009; RAKOVIĆ, 2014; RAKOVIĆ, 2015)), indicating that this type of exotic transpersonal communications provides *continuously-refreshing interaction* between two mentally-addressed persons and thereby *trans-personal stabilize quantum-entanglement* of their acupuncture systems / consciousnesses, i.e. *prevents decoherence* of their macroscopic quantum-entangled states by interaction with their local bodily environments (*in contrast to the situation in the microworld* where there are no such stabilizing mental-transpersonal addressing exotic effects, and hence laboratory formed quantum-entangled particle-pairs must be *well isolated from the environment* in order to prevent their quantum-decoherence (DUGIĆ, 2004)).

In this context, it should be pointed out that the *healing effects* upon acupuncture system / consciousness of the patient are *often blocked* by quantum-holographic *spiritual coded self-acceptance* of the disease as a form of *(self) punishment* (as suggested by the respondents in the *post-hypnotic regressions* (NEWTON, 1974)), when *prayers and love* for yourself and others with the aim of ceasing (self) punishment are necessary – thus *effecting a spiritual integration of personality*, i.e. *unfolding transpersonal energy blockages*, which *triggers a process of ongoing healing* (RAKOVIĆ *et al*., 2004; RAKOVIĆ, 2008; RAKOVIĆ, 2009; RAKOVIĆ, 2014; RAKOVIĆ, 2015; RAKOVIĆ, 2016A; RAKOVIĆ, 2016B; RAKOVIĆ, 2017; RAKOVIĆ, 2018; RAKOVIĆ, 2019; RAKOVIĆ, 2022; RAKOVIĆ, 2023; RAKOVIĆ, 2024A; RAKOVIĆ, 2024B)

THREE FRONT LINES OF COMPLEMENTARY AND INTEGRATIVE PSYCHOSOMATIC MEDICINE

The presented integrative quantum-holographic framework for psychosomatics might have significant holistic implications, providing fundamental quantum-informational framework for better understanding of the *epigenetic nature of psychosomatic diseases* as well as *limitations and methods of their prevention and healing*, which might help in *developing strategies for complementary and integrative psychosomatic medicine in the 21st century.*

Thus, on the basis of integrative quantum-holographic framework it might be said that *three front lines of complementary and integrative psychosomatic medicine do exist* (RAKOVIĆ *et al*., 2009; RAKOVIĆ, 2011; RAKOVIĆ, 2025): (1) *Spirituality and circular (psycho / energy) therapies from all relevant meta-positions*, with possibility of permanent erasing of mutual memory attractors on the *level of collective consciousness*; (2) *(Quantum) holistic medicine and non-circular (psycho / energy) therapies*, whose efforts temporary erase memory attractors on the *level of acupuncture system / individual consciousness*, and prevent or alleviate their somatization, as a consequence of the indolence on the first level; and (3) *Conventional symptomatic medicine*, whose activities on the *somatic level* via immunology, pharmacology, biomedical diagnostics and surgery hinder or soothe somatized consequences of the carelessness on the first two levels.

Hence, it should be pointed out that *necessary activities* on the second and third front lines, with *neglect of the first front line*, might have a consequence of *further epigenetic transfer of memory attractors* on the level of individual and collective consciousness in this and further generations, thus *accumulating epigenetic quantum-holographic loads* which afterwards might cause not only illnesses, but also inter-personal fights, wars, and other troubles.

CONCLUSION

The presented *integrative quantum-holographic framework for psychosomatics* might have significant holistic implications, providing fundamental quantum-informational framework for better understanding of the *nature of stress-induced psychosomatic diseases* as well as *limitations of methods of anti-stress prevention and healing*, which might help in *developing strategies for integrative psychosomatic medicine in the 21st century.*

Within this framework, it appears that all holistic acupuncture-based & consciousness-based approaches and techniques can be treated as *quantum-informational therapies*, by *imposing new healing boundary conditions* in the energy-state space of EM quantum-field-related *acupuncture system / (individual and collective) consciousness*.

On this line, the extended *overview* RAKOVIĆ (2025) of holistic recommendations for *regular balancing* of the acupuncture system / (individual and collective) consciousness might be of significance for improvement of *psychosomatic status of wider population*.

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[126] https://www.imconsortium.org; official website of the Consortium of Academic Medical Centers for Integrative Medicine, founded by the end of 1990s, which includes over 70 highly esteemed US academic health centers and affiliate institutions, in order to transform medicine and healthcare through rigorous scientific studies, new models of clinical care, and innovative educational programs that integrate biomedicine, the complexity of human beings, the intrinsic nature of healing, and the rich diversity of therapeutic systems.

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ENTANGLEMENT OF FORMATION DYNAMICS OF A TWO-MODE SYSTEM IN A COMMON GAUSSIAN NOISY CHANNEL

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ABSTRACT. Entanglement of formation is a measure that has a clear physically motivated definition, namely, it provides a lower bound over all pure-state entanglement decompositions required to create a given state. We investigate the open system dynamics of entanglement of formation of a two-mode Gaussian state interacting with a common bosonic environment. In the framework of the theory based on completely positive dynamical semigroups, the open system dynamics leads to a master equation in Lindblad form, which preserves the positivity and the Gaussian form of an initially Gaussian state at all times. For an initially separable state we witness the generation of entanglement, and its preservation in the limit of asymptotic times.

Keywords: entanglement of formation, common environment, Gaussian states.

INTRODUCTION

Quantum information theory has obtained remarkable achievements in the last decades, and as the second quantum revolution occurs, it promises even more groundbreaking advances. Important proposals in quantum cryptography ADESSO *et al.* (2014), teleportation and quantum computing have been already demonstrated in numerous experiments and have now entered the phase of technological applications and explorations. However, even though the processing and transmission of quantum information is currently very successful, one of the most pressing matters regarding the practical implementation of quantum communication and computation, represented by the fact that any physical quantum system is affected by a surrounding environment, is still intensely studied JEKNIC-DUGIC *et al.* (2016), JEKNIC-DUGIC *et al.* (2024). This is due to the fact that any quantum system must be regarded as an open system, that is subjected to interaction with an uncontrollable environment, which has a non-negligible influence on it. The theory of open quantum systems plays a major role in the study and application of quantum information. Quantum dynamics of open systems cannot be described in terms of a unitary time evolution, as opposed to the case of closed system, but by using a suitable equation of motion for its density operator, called quantum master equation (BREUER and PETRUCCIONE, 2006).

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In the last years, in-depth research has been conducted on the dynamics of Gaussian continuous-variable states embedded in an environment ARSENIJEVIC *et al*. (2018), MIHAESCU and ISAR (2018), STOICA and ISAR (2023), based on the fact that these states are readily generated and transformed using beam splitters, homodyne measurements, and squeezers in the laboratory XIANG *et al.* (2011a, 2011b). However, attempting to exploit these states for quantum information and computation purposes faces the obvious difficulty that they are unavoidably altered by the interaction with the environment GOYAL and GHOSH (2010). Therefore, investigation of the effects of quantum decoherence on the evolution of Gaussian continuous-variables states and, consequently, on their quantum correlations in noisy channels, is of great importance PRAUZNER-BECHCICKI and JAKUB (2004), TANG *et al.* (2005).

In JEONG *et al.* (2000) the authors studied the evolution of the nonlocality for an initial two-mode squeezed vacuum (TMSV) state in a thermal environment and have shown that the larger the initial squeezing parameter, the faster the squeezed state loses its nonlocality. For a similar initial TMSV state, but interacting with an uncorrelated squeezed environment, in TANG *et al.* (2005) it was revealed that squeezing the environment does not increase the lifetime of the entanglement of the initial two-mode squeezed state. In BENATTI and FLOREANINI (2006) the authors investigated two non-interacting harmonic oscillators interacting with a common bath and showed that starting from an initially separated Gaussian state, entanglement can be created during the interaction with the noisy environment. Regarding the generation of entanglement, the problem was studied further in XIANG *et al.* (2008), where two initial states were considered: a single-mode squeezed state and a squeezed vacuum state, interacting with a squeezed thermal environment. It was found that not only this type of environment can generate entanglement when starting with an uncorrelated state, but it can even amplify the existing entanglement, when the squeezing parameters are suitable chosen.

In this paper we investigate the entanglement of formation in Gaussian two-mode squeezed vacuum states, and its dynamics during the interaction with a common squeezed thermal bath. Entanglement of formation is a measure designed to quantify entanglement in mixed states in analogy to Schmidt decomposition criterion for pure states, whereby a separable global pure state can be factorized into local pure states. Otherwise, if the reduced states with respect to a given bipartition are mixed, then the global pure state is entangled and the von Neumann entropy represents a well-defined measure of entanglement. Entanglement of formation measure arises from the extension of the above concept to globally mixed states, where one has to evaluate the lower bound on entanglement given by the infimum over all possible pure-state decompositions WOOTTERS (2001). Thus, entanglement of formation is a generalized measure based on a well-motivated physical definition, which can be readily extended to multipartite states. Previously it was studied in Gaussian states undergoing the open system dynamics given by independent Gaussian noisy channels DUMITRU and ISAR (2015).

This paper is organized as follows. After the introduction to the microscopic derivation of the Lindblad master equation, we present the master equation tailored to optical systems, such as two bosonic modes interacting with a common bosonic environment. Then the time differential equation is solved for an initially separable two-mode Gaussian state, and the entanglement of formation is evaluated, highlighting the role of this setup on the entanglement generation processes. Then we present the results and discussions, altogether with the concluding remarks.

OPEN QUANTUM SYSTEMS: MASTER EQUATION

The theory of open quantum systems arose out of the need to describe the diffusion and dissipation in optical systems, for instance, and it deals with various quantum-statistical methods intended to describe the underlying physical processes governing the evolution. The

master equation approach leads to an effective equation of motion for a subsystem that belongs to a composed system: the system under investigation and the environment. Let us consider a system evolving according to a total Hamiltonian H composed of the free Hamiltonian H_0 and the interaction Hamiltonian H_1:

$$H = H_0 + H_1. \tag{1}$$

This decomposition is rather arbitrary, depending on the physical situation, where one may choose to highlight the physical process which is more influential on the dynamics of the system, compared to other underlying processes. The Schrödinger equation for a state $|\psi(t)\rangle$ describes the time evolution of the system:

$$\frac{d}{dt}|\psi(t)\rangle = -\frac{i}{\hbar}H|\psi(t)\rangle \tag{2}$$

where the solution subject to the initial time constraint $|\psi(0)\rangle = |\psi(t=0)\rangle$ is given by $|\psi(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\psi(0)\rangle$. This is the Schrödinger picture representation, where the time dependence is entirely carried by the state vector. Yet, a change of reference frame can highlight the contribution of the interaction Hamiltonian to changes in the state, $|\tilde{\psi}(t)\rangle = e^{-\frac{i}{\hbar}H_I t}|\psi(0)\rangle$, or equivalently $|\tilde{\psi}(t)\rangle = e^{-\frac{i}{\hbar}H_0 t}|\psi(t)\rangle$. In terms of the density operator the von Neumann equation governs the composite system evolution:

$$\frac{d}{dt}\rho(t) = -\frac{\mathrm{i}}{\hbar}[H, \rho(t)], \tag{3}$$

whereas the relation to the interaction picture representation $\tilde{\rho}(t)$ is given by: $\rho(t) = U_0(t)\,\tilde{\rho}(t)\,U_0^{\dagger}(t)$, where $U_0(t) = \mathrm{e}^{-\mathrm{i}H_0 t/\hbar}$ denotes the unitary transformation due to H_0. Combining this with Eqs. (1) and (3) one obtains:

$$\begin{aligned}\frac{d}{dt}U_0(t)\,\tilde{\rho}(t)\,U_0^{\dagger}(t) &= -\frac{\mathrm{i}}{\hbar}[H_0, U_0(t)\,\tilde{\rho}(t)\,U_0^{\dagger}(t)] + U_0(t)\,\frac{d}{dt}\tilde{\rho}(t)\,U_0^{\dagger}(t) \\ &= -\frac{\mathrm{i}}{\hbar}[H, U_0(t)\,\tilde{\rho}(t)\,U_0^{\dagger}(t)],\end{aligned} \tag{4}$$

arriving at the von Neumann equation in the interaction picture:

$$\frac{d}{dt}\tilde{\rho}(t) = -\frac{\mathrm{i}}{\hbar}[H_I, \tilde{\rho}(t)], \tag{5}$$

where H_I denotes the interaction Hamiltonian, defined as:

$$H_I = U_0^{\dagger}(t)\,H_1\,U_0(t), \tag{6}$$

and we used the relations $[H_0, U_0(t)] = 0$ and $U_0^{-1}(t) = U_0^{\dagger}(t)$. A formal solution to Eq. (5) is given by

$$\tilde{\rho}(t) = \rho(0) + \frac{1}{\mathrm{i}\hbar}\int_0^t dt'\,[H_I(t'), \tilde{\rho}(t')], \tag{7}$$

which now can be substituted into Eq. (3), arriving at the von Neumann equation in the integro-differential form in the interaction picture:

$$\frac{d}{dt}\tilde{\rho}(t) = \frac{1}{i\hbar}[H_I(t), \rho(0)] - \frac{1}{\hbar^2}\int_0^t dt' \, [H_I(t), [H_I(t'), \tilde{\rho}(t')]]. \tag{8}$$

Born and Markov approximations

From Eq. (8) we see that the evolution of the composite system is governed by the exact master equation, determined by the Hamiltonian that couples the system to the environment. However, one is interested in the information about the system, while the reservoir is known usually only through its general characteristics, such as temperature and energy density of states. One recovers the evolution of the system of interest through tracing out the degrees of freedom of the environment. By denoting $\tilde{\rho}_S(t) = \mathrm{Tr}_R[\tilde{\rho}(t)]$, we obtain

$$\frac{d}{dt}\tilde{\rho}_S(t) = \frac{1}{i\hbar}\mathrm{Tr}_R\{[H_I(t), \rho(0)]\} - \frac{1}{\hbar^2}\int_0^t dt' \, \mathrm{Tr}_R\{[H_I(t), [H_I(t'), \tilde{\rho}(t')]]\}, \tag{9}$$

where the subscripts S and R stand for the system and reservoir, respectively.

In addition, the following assumptions are required in order to achieve the well-known Lindblad master equation.

1. ***Born approximation I.*** We consider that at the initial time $t_0 = 0$ the system and the environment are uncorrelated:

   $$\rho(0) = \rho_S(0) \otimes \rho_R(0). \tag{10}$$

   Additionally, one can assign $\mathrm{Tr}_R\{[H_I(t), \rho_R(0)]\} = 0$ if the reservoir operators coupled to the system have zero mean value in the state $\rho_R(0)$, which can be adjusted by including these average values in the system Hamiltonian.
2. ***Born approximation II.*** Inevitably the system and environment become correlated in time, yet this effect can be neglected if one considers a weak coupling between them, along with the assumption that the environment is much larger than the system. In this case, the reservoir initially considered in thermal equilibrium state, stays unperturbed by the interaction with the system, so that the factorization in Eq. (9) applies also at later times: $\rho(t) = \rho_S(t) \otimes \rho_R(0)$.
3. ***Markovian approximation.*** Finally, in the axiomatic approach, the most general generator of the Markovian dynamics is obtained on the base of completely positive quantum dynamical semigroups, assuring that the memory effects from the previous times are neglected. Similarly, in Eq. (9), where the time dependent state of the system depends on its past history through the integration of $\rho_S(t')$, it is replaced by $\rho_S(t)$. In addition, the time evolution of the reduced density operator still depends upon an explicit choice for the initial preparation at time $t = 0$, and, therefore, this dynamics is not yet represented by a dynamical semigroup. Therefore, a change of integration variable and of the limits of integration, respectively

   $$t' \to t - t', \qquad \int_0^t \to \int_0^\infty, \tag{11}$$

will restore the equivalence with the Lindblad master equation obtained in the framework of completely positive quantum dynamical semigroups.

Finally, the Lindblad master equation in the interaction picture reads:

$$\frac{d}{dt}\tilde{\rho}_S(t) = -\frac{1}{\hbar^2}\int_0^\infty dt'\ \mathrm{Tr}_R\{[H_I(t),[H_I(t-t'),\tilde{\rho}_S(t)\otimes\rho_R(0)]]\}. \tag{12}$$

Nowadays the Lindblad master equation is a foundational tool for the open quantum system dynamics modeling, in various research areas. Detailed discussions on the validity boundaries of Eq. (12) are offered in Refs. CARMICHAEL (1999) and (BREUER and PETRUCCIONE, 2006).

OPTICAL MASTER EQUATION: DAMPED HARMONIC OSCILLATORS

The two basic building block systems in quantum optics are the damped harmonic oscillator and the damped two-level atom. The investigation here covers two bosonic modes interacting with a common environment, which is treated as a reservoir composed of an infinite number of bosonic modes. Commonly, the infinite collection of environmental bosonic modes is considered to be in thermal equilibrium state, however a more general environment is obtained once we consider the phase sensitive states, i.e. squeezed thermal states. The free Hamiltonian in this case gives the free evolution of the system and the thermal bath

$$\begin{aligned} &H_0 = H_S + H_B, \\ &H_S = \hbar\sum_{i=1}^{2}\omega_i a_i^\dagger a_i, \qquad\qquad H_B = \hbar\sum_k \Omega_k b_k^\dagger b_k, \end{aligned} \tag{13}$$

where a_i and b_k denote, respectively, the annihilation operators of the two bosonic modes of the system with frequencies ω_i and the reservoir with mode frequencies Ω_k, while the sum over k accounts for the infinite number of bosonic modes in the environment. For defining the interaction Hamiltonian, we have to include the terms that describe two bosonic modes interacting with a common environment. This setup emerges from the following interaction Hamiltonian:

$$H_1 = \sum\nolimits_k g_k b_k (a_1^\dagger + a_2^\dagger) + h.c. \tag{14}$$

It is important to note that we assumed the Rotating Wave Approximation (RWA) in the interaction Hamiltonian, which essentially neglects the fastly oscillating terms. The contribution of these terms to the dynamics of the system is negligible, since they perform in different time scales CARMICHAEL (1999).

Using the Hamiltonian (14) in the master equation (12), we arrive at the Lindblad master equation in interaction picture ($\hbar = 1$) XIANG *et al.* (2011a):

$$\begin{aligned} \frac{d}{dt}\rho_S = \frac{\gamma}{2}\sum_{i,j=1,2}\{&(N+1)\left(2a_i\rho a_j^+ - a_j^+ a_i\rho - \rho a_j^+ a_i\right) + N\left(2a_j^+\rho a_i - a_i a_j^+\rho - \rho a_i a_j^+\right) \\ &+ M\left(2a_i^+\rho a_j^+ - a_j^+ a_i^+\rho - \rho a_j^+ a_i^+\right) + M^*\left(2a_i\rho a_j - a_j a_i\rho - \rho a_j a_i\right)\}, \end{aligned} \tag{15}$$

where γ is the dissipation parameter and the coefficients N and M are related to the correlation functions of the environment, once the time integral and partial trace on the environment

degrees of freedom are performed in Eq. (12), and the resonant terms survive SCULLY *et al.* (1997):

$$\begin{aligned}
&\left\langle b^{+}(\Omega_i)\, b(\Omega_j) \right\rangle = N(\Omega_i)\, \delta(\Omega_i - \Omega_j)\,, \\
&\left\langle b(\Omega_i)\, b^{+}(\Omega_j) \right\rangle = \left(N(\Omega_i) + 1 \right) \delta(\Omega_i - \Omega_j)\,, \\
&\left\langle b(\Omega_i)\, b(\Omega_j) \right\rangle = M(\Omega_i)\, \delta(\Omega_i - \Omega_j)\,.
\end{aligned} \tag{16}$$

These parameters satisfy the relation $|M|^2 \leq N(N+1)$, which assures the complete positivity condition of the Lindblad master equation above. In particular, for a squeezed vacuum bath $|M|^2 = N(N+1)$, and the coefficients are given by:

$$N = \sinh^2 s, \qquad M = -e^{i\theta} \cosh s \sinh s, \tag{17}$$

where s is the squeezing parameter of the reservoir, and θ is the squeezing angle. From here on we consider $\theta = 0$, and therefore, M is a real number.

Gaussian states

The system of two uncoupled harmonic oscillators pertains to the class of continuous variable (CV) states described in an infinite dimensional Hilbert space by pairs of ladder operators for each mode or, alternatively, in terms of position and momentum operators, related as $a_k = (x_k + p_k)/\sqrt{2}$. Arranged in a vector of operators $R^{\mathrm{T}} = (x_1, p_1, x_2, p_2)$, the canonical commutation relation has the following form, where J_1 is the one mode symplectic matrix:

$$[R_k, R_l] = \mathrm{i}\, J_{kl}, \qquad J = J_1 \oplus J_1, \quad \text{with} \quad J_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{18}$$

The CV states commonly encountered in physical setups are Gaussian states defined as the eigenstates of a quadratic Hamiltonian, an example of which is the Hamiltonian of harmonic oscillators. In phase space Gaussian states are fully characterized by a characteristic function of Gaussian form SERAFINI *et al.* (2004):

$$\chi_G(\xi) = e^{-\frac{1}{2}\xi^{\mathrm{T}}\sigma\xi - \mathrm{i}\xi^{\mathrm{T}}d}, \tag{19}$$

which is completely described by the first and second statistical moments, namely, the displacement vector d and the covariance matrix σ, respectively, given by:

$$d = \mathrm{Tr}[\rho_G R], \qquad \sigma = \mathrm{Tr}[\{(R-d)\,, (R-d)^{\mathrm{T}}\}_{+} \rho_G], \tag{20}$$

where ρ_G is the density operator of the Gaussian state. While the displacements can be adjusted to zero, the covariance matrix encodes all the information on quantum correlations, such as entanglement. The block decomposition of a bipartite covariance matrix is defined as:

$$\sigma = \begin{pmatrix} A & C \\ C^{\mathrm{T}} & B \end{pmatrix}, \tag{21}$$

where A and B are the covariance matrices of the first and second mode, respectively, and C is the correlation matrix between the bosonic modes.

The initial Gaussian state evolving in time under the Lindblad master equation will remain Gaussian at all times, since Eq. (15) involves only terms which are utmost quadratic

PARIS *et al.* (2003). Typically, in this case one has to rewrite the master equation for the characteristic function through the standard operator correspondence, leading to the so-called Lyapunov equation for the covariance matrix.

Initial single-mode squeezed state

The two-mode covariance matrix of the single-mode squeezed state is given by $\sigma_{\mathrm{SMSS}}=\sigma_s\oplus\sigma_s$, where σ_s is the single-mode covariance matrix:

$$\sigma_s=\frac{1}{2}\begin{pmatrix}\cosh 2r & \sinh 2r\\ \sinh 2r & \cosh 2r\end{pmatrix}, \tag{22}$$

where r is the squeezing parameter of the state. The time-depending solution for the covariance in this case can be brought to the form XIANG *et al.* (2008), XIANG *et al.* (2009):

$$\sigma^{I}_{\mathrm{SMSS}}(t)=\frac{1}{2}\begin{pmatrix}n_1 & 0 & c_1 & 0\\ 0 & n_2 & 0 & c_2\\ c_1 & 0 & n_1 & 0\\ 0 & c_2 & 0 & n_2\end{pmatrix}, \tag{23}$$

with the following matrix elements:

$$\begin{aligned} n_1&=\frac{1}{2}\left[\left(2N+1-e^{2r}+2M\right)\tau+2e^{2r}\right], \quad n_2=\frac{1}{2}\left[\left(2N+1-e^{-2r}-2M\right)\tau+2e^{-2r}\right],\\ c_1&=\frac{1}{2}\left[2N+1+2M-e^{2r}\right]\tau, \qquad\qquad c_2=\frac{1}{2}\left[2N+1-2M-e^{-2r}\right]\tau, \end{aligned} \tag{24}$$

where the time parametrization is encoded in the dimensionless time variable $\tau=1-e^{-2\gamma t}$.

ENTANGLEMENT OF FORMATION

Entanglement of formation is a measure of entanglement that is based on an operational definition, namely, the quantification of how much pure state entanglement is required to create a given state. Its physical motivation relies on defining a reliable mixed state entanglement quantifier based on the fact that any given state ρ can be decomposed in the basis of pure maximally entangled states as

$$\rho=\Sigma_j p_j\,|\psi_j\rangle\langle\psi_j|, \quad \text{with} \quad \sum_j p_j=1. \tag{25}$$

Then, entanglement of formation is given by the infimum pure state decompositions, i.e as a weighted sum over the von Neumann entropy $E(\Psi_j)$ of the maximally entangled pure state Ψ_j WOOTTERS (2001):

$$E_f(\rho)=\inf\sum_j p_j E(\Psi_j)\,. \tag{26}$$

Calculating all such possible decompositions is a daunting task, however, for the class of symmetric Gaussian states, which do not change after interchanging the two modes, a generic formula has been deduced GIEDKE *et al.* (2003):

$$E_f = h_+(\Delta)\log_2[h_+(\Delta)] - h_-(\Delta)\log_2[h_-(\Delta)], \tag{27}$$

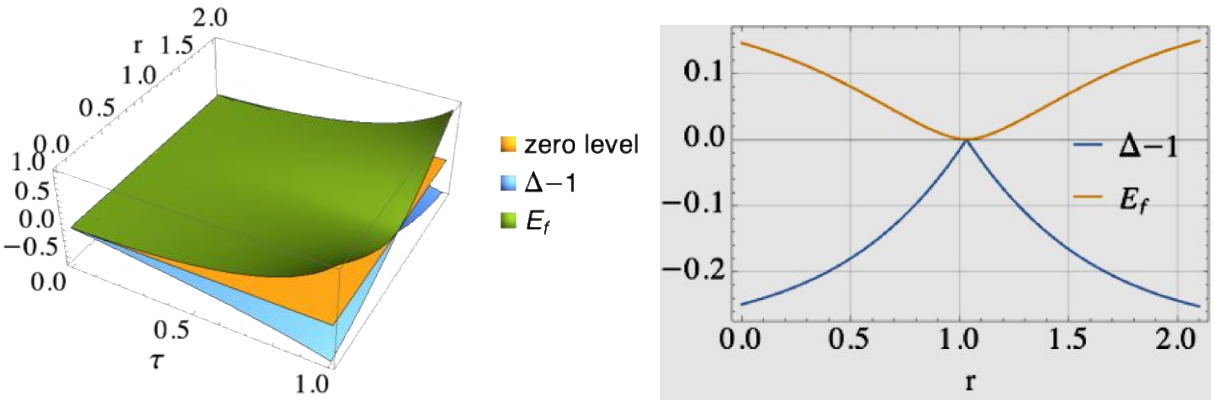
where $h_\pm(\Delta) = (\Delta^{-1/2} \pm \Delta^{1/2})^2/4$, and the function Δ can be expressed in terms of the block matrices of the covariance matrix (21), as follows RIGOLIN *et al.* (2004):

$$\Delta = 2\sqrt{\det A - \det C - \sqrt{\mathrm{Tr}(AJCJBJC^TJ) - 2\det A \det C}}\,. \tag{28}$$

This measure of entanglement represents a positive definite function and a reliable quantifier however, it must be checked together with the actual witness of entanglement, which is the function Δ. Thus, a given state is entangled if and only if $\Delta < 1$, while in the case of $\Delta \geq 1$ the value of E_f is no longer representative for the presence of quantum entanglement.

RESULTS AND DISCUSSIONS

In Figs. 1-3 it is shown the function $\Delta - 1$ together with the entanglement of formation measure E_f for the initial bipartite single mode squeezed state, which is a separable state. As discussed in the previous subsection, the presence of entanglement is certified whenever $\Delta - 1 < 0$, and in this case E_f quantifies the amount of entanglement. Thus, a notable result of these assertions is that the initially separable bipartite state can acquire entanglement due to the interaction with a common squeezed vacuum environment or squeezed thermal environment, depending on the interplay between bath parameters, such as squeezing and temperature, and squeezing of the initial state.



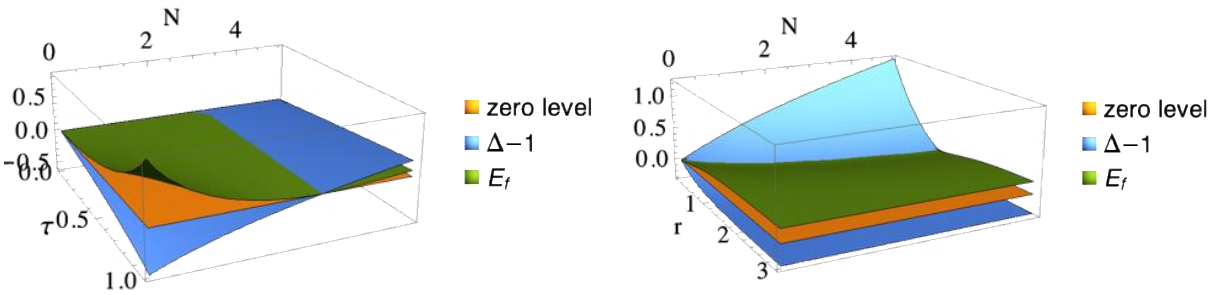
(a) (b)

Figure 1. Dependence of the entanglement of formation and function $\Delta - 1$ on the squeezing parameter r for an initial single-mode squeezed state in a squeezed vacuum bath with $N = 1.5$. In (a) it is shown also the time dependence, where $\tau = 1 - e^{-2\gamma t}$ is the dimensionless time parameter, and in (b) the instant of time is fixed to $\tau = 0.5$.

Fig. 1 (a) depicts the time evolution of entanglement of formation, and its dependence on the initial state squeezing for a squeezed vacuum environment (temperature $T = 0$), while Fig. 1 (b) captures an instance of dimensionless time for the same parameters as in Fig. 1 (a). The central point in the plot, where $E_f = \Delta - 1 = 0$ always, corresponds to equal squeezing parameters s of the bath and r of the system and, therefore, these two opposed contributions counter compensate each other. Entanglement is generated, it increases monotonically in time and evolves non-monotonically around this equal squeezing point, where $\Delta - 1 < 0$ and the difference between the two mentioned squeezing parameters determines the values of the

created. One can see that E_f is a positive function achieving its maximum in the limit of asymptotic time ($\tau = 1$).

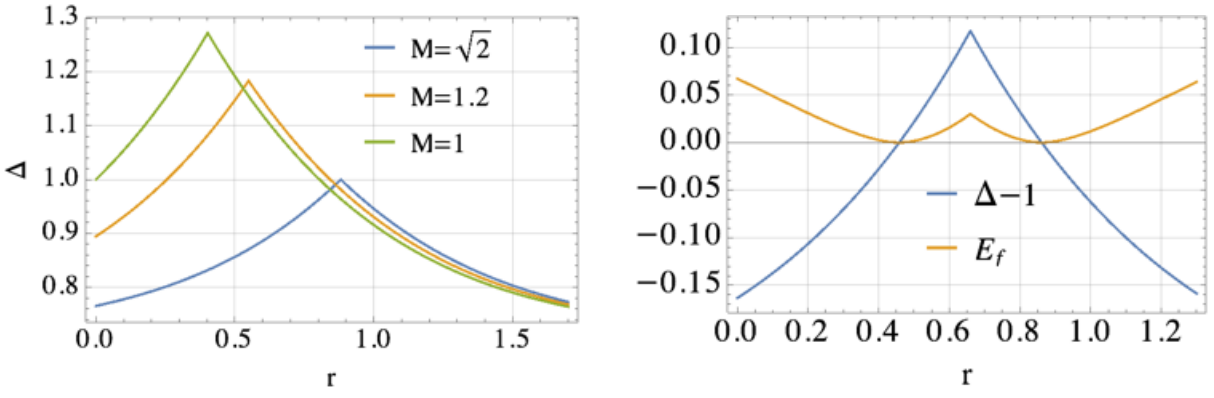
Figs. 2 (a) and (b) depict the time evolution of entanglement for a thermal bath as a function of the thermal photon number of the environment, which in this case depends only on the temperature of the environment, since the bath squeezing is zero. Similarly, as in the previous pictures, one can see that entanglement generation takes place, due to the effective communication established between the two modes, where the environment plays the role of a mediator. This mechanism operates on the resources of the initial state, as the single mode squeezing in our case. However, the creation of entanglement is impeded, for relatively large temperatures, by the quantum decoherence due to interaction with the bath. One can see in Fig. 2 (b) that higher the initial state squeezing mitigates the destruction effect of the high thermal photon number in the reservoir and leads to the preservation of entanglement.



(a) (b)

Figure 2. Dependence of the entanglement of formation and function $\Delta - 1$ on the thermal photon number N for an initial single-mode squeezed state interacting with a thermal bath ($M = 0$).
(a) Time dependence for a fixed squeezing parameter $r = 1$, and
(b) dependence on the initial squeezing at a fixed instance of time $\tau = 0.5$, where $\tau = 1 - e^{-2\gamma t}$ is the dimensionless time parameter.

Fig. 3 (a) shows the dependence of the function Δ and Fig. 3 (b) shows the dependence of the function $\Delta - 1$ and of the entanglement of formation on the initial state squeezing for different temperatures of the squeezed thermal reservoir.



(a) (b)

Figure 3. Dependence on squeezing parameter r of the initial single-mode squeezed state in a squeezed thermal bath with $N = 1$, at the instance of dimensionless time $\tau = 0.5$, (a) of the function Δ for different values of bath squeezing M, and (b) of the entanglement of formation and function $\Delta - 1$ for $M = 1.3$.

In this case $|M|^2 < N(N+1)$, and higher is the gap in this inequality, higher is the temperature of the environment, which can be detrimental to the creation and preservation of entanglement. Thus, compared to the squeezed vacuum bath (Fig. 1 and the blue line in Fig. 3 (a)), a non-zero value of the temperature of the bath leads to the appearance of a gap in the region where $\Delta < 1$ and where entanglement is created, around the point where the squeezing parameters of the initial state and of the bath are equal, corresponding to the peak on the blue line in Fig. 3 (a).

This region becomes larger by increasing the temperature, so that for temperatures high enough, the entanglement can be generated only for stronger initial squeezing parameter than some critical value, which is close to the equal squeezing value. In Figs. 3 (a) and (b) we can observe that even though entanglement of formation measure has positive values, it is not representative of entanglement if $\Delta - 1 > 0$.

CONCLUSIONS

We investigated the open system dynamics of a bipartite Gaussian state interacting with a common squeezed thermal bath, focusing on the time evolution of quantum entanglement quantified by the entanglement of formation measure. We briefly outlined the microscopic derivation method leading to the Markovian master equation in Lindblad form, and presented the optical master equation corresponding to two bosonic modes interacting with a common squeezed bosonic environment.

Compared to the previously studied evolution of entanglement of formation in Gaussian states coupled to two independent environments, the common reservoir, being a particular case of two correlated baths, plays the role of a communication mediator between the two modes of the system, which amounts to generation of entanglement in an initially separable state. Yet, the interaction with the environment tends to impede the entanglement creation and preservation. This was revealed by the opposing actions provided by the squeezing of the initial state and the squeezing parameter of the environment, as well as by the influence of the non-zero temperature of the bath. In Ref. XIANG *et al.* (2008) there were presented similar results for the behaviour of the logarithmic negativity measure of entanglement in the common reservoir setup. This similarity is not surprising, given that both measures, logarithmic negativity and entanglement of formation, are viable quantifiers of entanglement. Compared to logarithmic negativity, entanglement of formation has an operational definition with a clear physically motivated derivation, which could be straightforwardly investigated for multi-mode states, and therefore, we appreciate that it can present an interesting and important subject of future studies.

Acknowledgments

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A SHORT REVIEW ON QUANTUM MACHINE LEARNING

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ABSTRACT. Quantum Machine Learning (QML) integrates two prosperous scientific fields: quantum computing and artificial intelligence. We will review recent developments in QML-based methods, their theoretical foundations, algorithmic progress, practical applications, and remaining issues. By analyzing contemporary QML literature, we will identify its main strengths and weaknesses that guide the pursuit of achieving quantum advantage in machine learning tasks.

Keywords: quantum computing, machine learning, quantum advantage, quantum-inspired algorithms.

INTRODUCTION

Machine learning and neural networks have been the focus of intensive scientific research for several decades. A noticeable advancement of computing power has enabled the practical implementation of theoretical frameworks established in the 20th century, driving significant advancements in artificial intelligence in recent years. In recognition of the pioneering work that laid the foundation for modern machine learning models, John J. Hopfield and Geoffrey Hinton were awarded the 2024 Nobel Prize in Physics.

Quantum physics has fundamentally altered our understanding of Nature, where quantum computing is a computational paradigm based on the principles of quantum mechanics. The basic idea for using physical systems in efficiently simulating some complex tasks was introduced by Richard Feynman (FEYNMAN, 1999). His proposal was inspired by the limitations of classical computational methods in modeling quantum systems. Key quantum phenomena such as superposition and entanglement are the basis for exotic quantum algorithms, which enable quantum computers to perform complex parallel computations and encode information in fundamentally new ways. From theoretical point of view, these unique properties offer potential advantages in computational speed and efficiency, particularly for problems intractable for classical computers due to their exponential complexity. Quantum Machine Learning (QML) aims to leverage these capabilities to improve or redefine classical learning algorithms, promising faster and more efficient data processing integrated into advanced artificial intelligence systems.

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CLASSIFICATION OF QUANTUM MACHINE LEARNING APPROACHES

Most literature usually recognizes four characteristic approaches on which QML is based. These approaches differ according to whether the data or the algorithms for their processing are classical (C) or quantum (Q). A traditional schematic view of combining quantum computing and machine learning is displayed in Fig. 1.

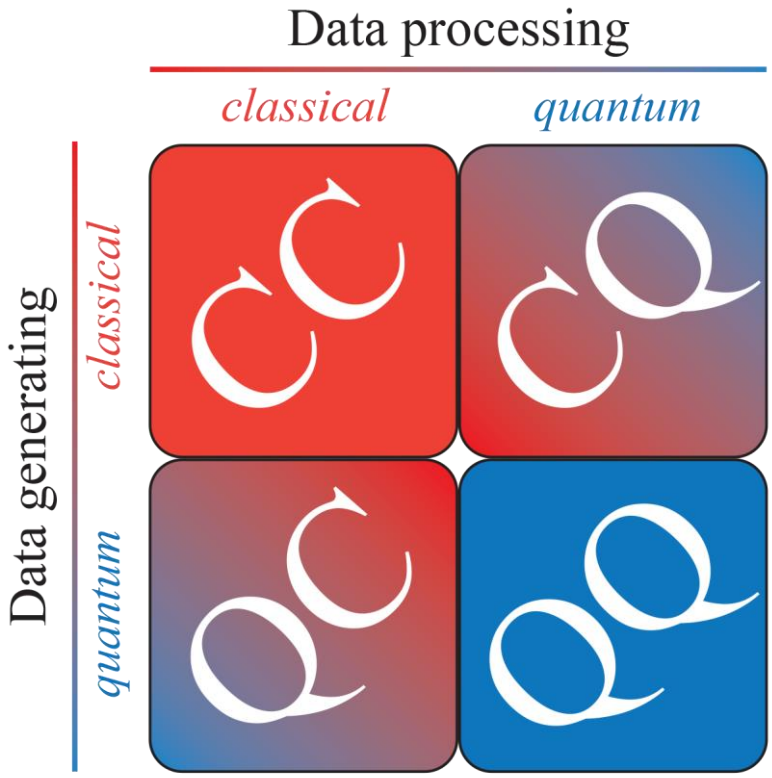

Figure 1. A schematic view of combining quantum computing and machine learning
(The figure is adapted from https://commons.wikimedia.org/wiki/File:Qml_approaches.tif?page=1 (CC BY-SA 4.0) by Maria Schuld).

The CC approach relies on both classical data and computational techniques. In this context, machine learning is based on quantum mechanical principles, hence, it is commonly referred to as 'quantum-inspired' (or 'quantum-like') machine learning algorithms. The idea of utilizing quantum mechanics in classical computing was introduced by MOORE and NARAYANAN (1995). First successful quantum-inspired (Qi) algorithms include optimization techniques such as evolutionary algorithms (QiEA) (HAN and KIM, 2013), genetic algorithms (QiGA) (NARAYANAN and MOORE, 1996; HAN *et al.*, 2001), Particle Swarm Optimization (QiPSO) (SUN *et al.*, 2004) and Quantum Simulated Annealing (QSA) (SOMMA *et al.*, 2007). A detailed review of such quantum-inspired metaheuristic algorithms can be found in (GHAREHCHOPOGH, 2022). In recent years, several quantum-inspired techniques have been developed beyond optimization. Most found inspiration in quantum algorithms, imposing classical counterparts to quantum-based machine learning methods. These methods, implemented on classical hardware, circumvent some main drawbacks of genuine quantum computing, such as limited number and connectivity of noise-prone physical qubits and costly requirements for quantum state preparation. Consequently, a few quantum-inspired algorithms harvesting benefits of quantum speedup are developed, such as *dequantized algorithms* (SCHULD and PETRUCCIONE, 2021; TANG, 2022), *tensor networks* (CARRASQUILLA, 2020; ALCHIERI *et al.*, 2021), *classical simulations of quantum variational algorithms* and

alternative methods that incorporate quantum phenomena and adapt it to classical settings (HUYNH *et al.*, 2023).

The QC methods use quantum data and classical processing. They are usually utilized to analyze the measurement data employing conventional machine learning (AARONSON, 2007). These are particularly useful for manipulating data obtained via quantum experiments (SASAKI and CARLINI, 2002; BISIO *et al.*, 2010).

The CQ systems explore classical data using quantum systems. The most common objective of this methodology is to use existing or create new quantum algorithms to be used in data mining. Classical input data originating from text or images is appropriately encoded and fed to the quantum computer for further evaluation and analysis (ZEGUENDRY *et al*., 2023).

Finally, the QQ techniques use algorithms and data, which are both quantum in nature. This category examines the processing of quantum data using quantum devices, either by inputting experimental measurements into a quantum computer or by employing a quantum computer to simulate and analyze the behavior of quantum systems. In the former case, a quantum computer simulates the behavior of analyzed quantum system and uses its state as input for a quantum machine learning algorithm executed on the same computer (JIANG, 2023).

Due to the progressive evolution of QML in many practical areas, a more suitable contemporary categorization scheme is proposed (ABOHASHIMA *et al*., 2020; HUYNH *et al.*, 2023):

- **Quantum Machine Learning** that includes various quantum adaptations of classical machine learning algorithms that require quantum computation for their execution.
- **Quantum-inspired Machine Learning**, which integrates quantum computing concepts to enhance traditional machine learning algorithms, without the actual necessity for quantum computation.
- **Hybrid Classical-Quantum Machine Learning**, which combines classical and quantum algorithms to optimize performance and minimize learning costs by exploiting the strengths of both approaches.

To explain the benefits of this new classification, let us consider the CQ and QQ systems. Here, CQ uses classical input data that should be encoded and fed into a quantum circuit. In this case, QQ can be seen as part of the CQ system. Moreover, some conventional algorithms may be executed before data encoding, thus making this approach hybrid. Using similar arguments and examples, one may show that the traditional classification does not make a clear boundary between ML models based on quantum mechanics. Therefore, an overview of QML methods will be given according to the above contemporary categorization.

QUANTUM MACHINE LEARNING ALGORITHMS

Quantum machine learning mainly leverages the inherent parallelism of quantum computing to enhance the efficiency and performance of classical machine learning algorithms. The basic principle of this approach is translating information (data) into quantum states, followed by applying unitary transformations to perform computational tasks. Realizing the potential speedups offered by quantum mechanics demands systematically adapting conventional algorithms to conform with fundamental constraints and operational principles of quantum computation.

Data encoding is a critical process in machine learning since it transforms "raw data" into a format that can be easily, precisely, and effectively processed by an algorithm. This is crucial in cases where the initial data format is unsuitable for direct use in computations or applications (e.g., for categorical variables). Instead of a conventional data fed to the input of an algorithm and generated at the output in classical machine learning, quantum machine learning deals with quantum states (data). Therefore, QML requires more intricate encoding. There are several strategies to encode conventional data into quantum (SCHULD and KILLORAN, 2019), where the three most important are (ZEGUENDRY *et al*., 2023):

- *Basic encoding* is the traditional bit-wise conversion of a binary string into equivalent state of a quantum system. One may use quantum superposition of a few (or all) states to perform parallel computing on all of them.
- *Amplitude encoding* is an approach in which normalized input vectors of dimension $N=2^n$ are associated with the amplitudes of a n qubit state.
- *Qsample encoding* is a hybrid quantum data representation that integrates amplitude and basis encoding, combining real-valued amplitude vectors with classical binary probability distributions.

More complex quantum QML circuits are based on elementary algorithms, such as Grover's (GROVER, 1997), Quantum Phase Estimation (KITAEV, 1995; NIELSEN and CHUANG, 2000), Harrow-Hassidim-Lloyd (HHL) algorithm (HARROW *et al.*, 2009), and Variational Quantum Circuit (VQC) (CEREZO *et al.*, 2021). The notable examples of QML applications are Quantum Support Vector Machines (QSVM) (ANGUITA *et al.*, 2003; REBENTROST *et al.*, 2014), Quantum Principal Component Analysis (QPCA) (LLOYD *et al.*, 2014), Quantum Linear Regression (SCHULD *et al.*, 2016), and Quantum Neural Network (DA SILVA *et al.*, 2016).

Quantum Support Vector Machines

Support Vector Machines (SVM) are a class of supervised learning algorithms commonly employed to address problems involving linear classification. The fundamental principle of SVM lies in constructing an optimal hyperplane that separates two distinct classes within a feature space. This hyperplane acts as a decision boundary for classifying new data points and its position in hyperspace is based on the principle of maximizing the margin between the hyperplane and the nearest data points from each class, known as support vectors. The optimization objective in SVM varies in convexity depending on the choice of the kernel function. In cases involving non-convex objective functions, optimization may converge to local optima, potentially compromising both efficiency and classification accuracy.

Quantum Support Vector Machines (QSVM) integrate Grover's algorithm (GA) as a quantum subroutine for optimization, enabling convergence to global optima even in the presence of non-convex cost functions (ANGUITA *et al.*, 2003). Therein, GA reduces the temporal (time) complexity of the SVM optimization task, particularly in the computation of the kernel matrix, which is typically among computationally the most expensive tasks. In this quantum framework, the objective function is assumed to be accessible via a quantum oracle. Additionally, an alternative quantum SVM method proposed in REBENTROST *et al.* (2014) exhibits exponential speedup over classical counterparts, without imposing constraints on the optimization problem.

Quantum Principal Component Analysis

Classical Principal Component Analysis (C-PCA) is one technique for dimensionality reduction in machine learning tasks. It performs the transposition of the covariance matrix into diagonal form. The covariance matrix summarizes the relations between various data elements. Principal components refer to the few relatively large eigenvalues (that are, *primary* or *principal*) compared to the rest, which are selected as the new feature vectors.

Conventional PCA exhibits a runtime complexity of $O(d^2)$, where d denotes the dimensionality of the Hilbert space. In contrast, the quantum PCA algorithm (LLOYD *et al.*, 2014) offers a significant improvement in computational efficiency. The procedure begins by encoding classical data into quantum states via Quantum Random Access Memory (QRAM), which allows the preparation of quantum states corresponding to randomly sampled data vectors. Subsequently, a density matrix is constructed from the ensemble of quantum states. Applying density matrix exponentiation in conjunction with quantum phase estimation and continuous data sampling, the quantum algorithm executes the decomposition of input data into its principal components. That is, this approach enables the extraction of dominant eigenvectors associated with the data's covariance structure. The quantum PCA algorithm achieves a runtime complexity of $O((\log d)^2)$, which is an exponential speedup as a function of dimensionality over its classical counterpart.

Quantum Linear Regression

Quantum Linear Regression (QLR) is a quantum algorithm that aims to perform linear regression using quantum computing principles, potentially offering speed advantages over classical methods. It leverages the quantum analog of classical linear regression, typically solving the equation $w = (X^TX)^{-1}X^Ty$, where X is the input matrix and y is the output vector. Data points are encoded into amplitude-encoded quantum states, which allows the processing of exponentially large datasets using few qubits.

The core component of QLR often involves the HHL algorithm (HARROW *et al.*, 2009) to solve linear systems efficiently on a quantum computer. HHL outputs a quantum state proportional to the solution vector rather than the explicit classical values. Inner products are then computed via quantum techniques such as the Hadamard test. QLR assumes efficient quantum access to data via quantum RAM, which is a strong and currently impractical requirement. It can achieve exponential speedups in theory but only under specific and restrictive conditions such as low-rank data matrices and well-conditioned systems. Practical use remains limited due to current hardware constraints and overhead in preparing quantum states when applying algorithms to a genuine quantum device. However, QLR is an important theoretical step in exploring the power of quantum machine learning.

Quantum Neural Networks

Quantum Neural Networks (QNNs) represent an emerging paradigm that combines principles of quantum theory with the properties of an artificial neural network (NN). The main advantage over classical neural networks that operate on binary data is that QNNs employ qubit superposition, which enables exponentially larger state spaces for information processing. This allows QNNs to outperform classical models in complex pattern recognition, optimization, and similar machine learning tasks in high-dimensional spaces. Another key advantage of QNNs is their ability to explore multiple computational paths simultaneously through quantum parallelism, which may lead to significant speedups for specific classes of problems. Additionally, quantum entanglement can be used to model complex correlations between inputs in ways that classical networks cannot replicate efficiently (SCHULD *et al.*, 2014).

However, the practical implementation of QNNs is also limited by the quantum hardware constraints that significantly restrict real-world applications. Moreover, QNN usually suffers from vanishing gradient problems, when the gradient tends to zero during supervised training. This problem is known as *barren plateau* (BP) and its dominance in quantum architectures makes it a key factor in choosing appropriate circuit (McClean *et al.*, 2018). In contrast to conventional NN, where gradients vanish exponentially with the number of layers, in QNN similar trend of gradient disappearance happens with an increase in the number of qubits. However, recent research has shown that deep QNN circuits, although employing only a few qubits, can flatten the loss landscape due to noise accumulation in deep circuits (Wang *et al.*, 2021). Nevertheless, designing effective quantum circuits that can generalize like classical deep learning models remains a fundamental research challenge.

QUANTUM-INSPIRED MACHINE LEARNING TECHNIQUES

Quantum-inspired machine learning (QiML) refers to a broad class of machine learning algorithms inspired by quantum phenomena or quantum computing. However, it is founded on the principles of classical machine learning and incorporates the ability to simulate quantum hardware using classical representation and computation techniques. Three distinctive categories have been identified based on underlying methodologies, such as *dequantized algorithms*, *tensor networks*, and *simulation of quantum variational algorithms*. One should note that some methods do not fall into either category, although they are classified as quantum-inspired (Huynh *et al.*, 2023).

Dequantized algorithms aim to determine if the QML algorithms' speedups are attributed to the power of quantum computation or are the consequence of specific input and output encoding/decoding inherent to the underlying quantum counterpart. A seminal work in this area was presented by Ewin Tang (Tang, 2019). Analyzing a state-of-the-art quantum recommendation system (Kerenidis and Prakash, 2017), the authors devised a classical algorithm with an execution runtime approaching the quantum one. They showed that the specific data structure used to quickly prepare quantum states also fulfills the classical L_2-norm sampling assumption, thus allowing efficient SQ ("sample and query") access to the data. An extension of this work is formalized to dequantize quantum algorithms for supervised clustering (SC) and principal component analysis (PCA) (Tang, 2021). A benefit of the dequantization approach for solving linear systems is demonstrated by the low-rank inversion algorithms (Gilyén *et al.*, 2018; Chia *et al.*, 2018). Significant results are also achieved for the Least Squares Support Vector Machine (LS-SVM) optimizations (Ding *et al.*, 2021), Linear Discriminant Analysis (LDA) (Cong and Duan, 2016), Hamiltonian simulations (Chia *et al.*, 2022), and similar quantum-related algorithms (Huynh *et al.*, 2023).

Contemporary QiML research focuses on *tensor networks* (TN) applications as powerful machine learning models. This direction builds on years of classical research, both inside and outside the machine learning field, that can be easily adapted to quantum problems. It was demonstrated that tensor networks provide a principled framework that bridges classical neural network methodologies and quantum computing. A recent study (Huggings *et al.*, 2019) implies a formal correspondence between specific tensor network structures and quantum circuits, wherein many TN architectures admit direct mappings to equivalent quantum circuits. One of the main motivations for employing TNs is their proven efficiency in classically simulating many-body quantum wavefunctions, which are based on higher-order tensor decompositions and representations (Ran and Su, 2023).

The effective emulation of quantum computations on classical hardware critically depends on the ability to simulate qubits and their associated capacity for exponential information encoding. Resources needed for classical simulations scale exponentially with the

number of qubits and the depth of the quantum circuit. Some classical strategies, such as data compression, optimized circuit parametrization, and batching methods, can reduce emulation complexity. However, these methods are effective only for simulations of a system composed of up to ten qubits, which defines the current lower limit for supremacy of quantum algorithms over classical. The most typical emulated quantum algorithms are quantum kernels and quantum variational methods (GUJJU *et al.*, 2023). A detailed study of the significant challenges in simulating these quantum algorithms is provided in XU *et al.*, (2023).

Miscellaneous quantum-inspired methods such as classifiers, quantum-based feature representation in machine learning tasks etc., are overviewed in HUYNH *et al.*, (2023). Understanding contemporary advancements in QiML techniques requires mastering the theoretical foundations of key algorithms such as Quantum-inspired Binary Classifier (TIWARI and MELUCCI, 2019), Helstrom Quantum Centroid (SERGIOLI *et al.*, 2019) which is a Quantum-inspired Binary Supervised Learning Classification, Quantum-inspired Support Vector Machines (DING *et al.*, 2021), Quantum Nearest Mean Classifier (SERGIOLI *et al.*, 2018), Quantum-inspired K Nearest-Neighbor (CHEN *et al.*, 2015), quantum algorithms for ridge regression (YU *et al.*, 2019), and Quantum-inspired Neural Networks (SAGHEER, *et al.*, 2019).

HYBRID CLASSICAL-QUANTUM MACHINE LEARNING

Hybrid classical-quantum machine learning is the approach that merges classical and quantum algorithms to improve performance and reduce the cost of learning. Using this combined approach, novel methods are proposed, such as a variational quantum classifier (ADHIKARY *et al.*, 2020), variational quantum SVM and SVM supported by quantum kernel-based algorithm (HAVLÍČEK *et al.*, 2019), hybrid K Nearest-Neighbor algorithm (RUAN *et al.*, 2017), a hybrid quantum computer-based quantum version of nonlinear regression (ZHANG *et al.*, 2018), hybrid quantum-classical neural networks (LIANG *et al.*, 2021; ARTHUR and DATE, 2022), and many others.

In recent study (ADHIKARY *et al.*, 2020), the advantages of hybrid variational quantum classifiers (hVQCs) over purely quantum classifiers are explored. The authors demonstrated that a hybrid approach, which combines quantum circuits with classical optimization techniques, can outperform a purely quantum classifier in terms of accuracy and efficiency. Their experiments on the MNIST dataset show that the hybrid model achieves a test accuracy of 96.05%, significantly higher than the 67% achieved by the purely quantum classifier with a small bond dimension. This indicates that integrating classical components can enhance the performance of quantum classifiers by leveraging the strengths of both quantum and classical computing.

Variational Quantum SVMs (VQ-SVMs) and Quantum Kernel-based SVMs (QK-SVMs) combine quantum feature encoding with classical optimization or classification, offering advantages over purely classical or purely quantum approaches. VQ-SVMs use parameterized quantum circuits to map data into complex quantum spaces, while QK-SVMs grasps on quantum circuits to compute kernel functions that capture rich data correlations. Compared to classical SVMs, these methods can potentially access higher-dimensional feature spaces more efficiently, and unlike fully quantum models, they are more resilient to hardware limitations due to their hybrid structure (HAVLÍČEK *et al.*, 2019).

A hybrid quantum-classical k-nearest neighbors (KNN) algorithm combines quantum computing techniques with classical methods to enhance performance over purely classical approaches. The quantum enhancement is based on the circuit that calculates the Hamming distance, while classical methods are used for preparing datasets. By leveraging potentials of

classical and quantum computations, this algorithm outperforms quantum Centroid and QNN approach on time performance and classification accuracy (RUAN *et al.*, 2017).

Recently proposed hybrid quantum-classical approach to nonlinear regression offers distinct advantages over existing classical or quantum methods. Utilizing quantum computing's ability to encode and process high-dimensional data efficiently, this hybrid model can capture highly complex patterns in data more effectively than state-of-the-art classical systems alone (ZHANG *et al.*, 2018). Additionally, integrating classical optimization techniques allows for more practical and scalable implementations, circumventing current constraints in quantum hardware.

Hybrid quantum-classical neural networks (hQCNNs) integrate quantum computing's high-dimensional feature mapping with classical optimization techniques, thus outperforming conventional or quantum models. Usually, classical components handle tasks like data preprocessing and optimization, making the hybrid model more scalable and adaptable to larger datasets (LIANG *et al.*, 2021). On the other hand, quantum circuits can encode data into high-dimensional Hilbert spaces, enabling the capture of complex patterns that classical networks might miss or disregard (LIANG *et al.*, 2021; ARTHUR and DATE, 2022). By integrating quantum and classical components, hQCNNs can be deployed on existing quantum hardware, bridging the gap between the theoretical potential of quantum computing and its practical applications on current noisy intermediate-scale quantum hardware.

CHALENGES AND FUTURE DIRECTIONS

Despite the promising future of QML, several significant challenges for full potential in practical applications remain. Quantum hardware is still in an early developmental stage, with issues like qubit coherence times and error rates hindering practical implementations. Developing algorithms that can outperform classical counterparts in real-world applications is a very tedious task. Currently, there are only a few useful quantum algorithms and finding new efficient algorithms is in focus of an ongoing area of research. Future directions include improving quantum hardware, developing error-correction techniques, and creating hybrid quantum-classical algorithms to bridge the gap between theoretical potential and practical application. Combining the strengths of both paradigms could lead to more practical and efficient solutions. Finally, the criteria proving the advantage of quantum over classical machine learning are *open topics*. Establishing standardized benchmarking for QML algorithms will facilitate more realistic and sustainable progress in the QML field.

CONCLUSIONS

Quantum Machine Learning represents a frontier in computational science, offering the possibility of transforming how machines learn from data. It stands at the confluence of quantum computing and artificial intelligence, offering transformative potential across various domains. While significant challenges persist, ongoing research and advancements in quantum technology hold promise for significant breakthroughs in various domains, including artificial intelligence, data analysis, and beyond. A concerted effort across various disciplines will be crucial in unlocking the full capabilities of current QML techniques. Moreover, it may happen in the future that a novel approach that diverges from classical machine learning background may potentially elevate QML to an entirely new level.

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MARKOVIAN MASTER EQUATION FOR THREE INTERACTING QUBITS IN WEAK COUPLING LIMIT: PEDAGOGICAL EXAMPLE

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ABSTRACT. While models of one qubit and two qubits open quantum systems are widely used in contemporary physical literature, especially one dealing with the problems of quantum information and computation, model of three qubits is rarely exploited. One reason, regarding dynamics of open quantum systems, lays in the fact that adding one qubit to state space complicates considerably computational tasks. By computational tasks here is meant obtaining analytical details of dynamics, which are preferable for fundamental physical considerations. In this paper, ab initio derivation of Markovian master equation, in regime of the weak coupling limit, for three interacting qubits is presented in pedagogical manner. In this way, it will become clearer what challenges in dealing with seemingly innocuous three-qubits model are. Master equation in hand can serve for further physical inquiries, not limited to the field of quantum information and quantum computation.

Keywords: qubit, open quantum systems, Markovian dynamics

INTRODUCTION

Open quantum systems are nowadays of wide interest in both fundamental research and quantum technologies and various applications (NIELSEN and CHUANG, 2000; DEJPASAND and SASANI GHAMSARI, 2023; CHAE and CHOI, 2024). The theory of open quantum systems is still in development, with main hallmark: it is not possible to formulate canonical equation of motion, also known as quantum master equation, for open quantum system's dynamics (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011). This is in sharp contrast with quantum mechanics of isolated quantum systems where Schrodinger equation governs the unitary dynamics (MESSIAH, 1962).

It turned out that it is useful to borrow concept of Markovian dynamics from classical statistical physics to single out one possible kind of dynamics of open quantum systems– quantum Markovian dynamics. Such approach is based on notion of Markovian semigroup which is related to Chapman-Kolmogorov equation of classical Markovian processes (BREUER

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and PETRUCCIONE, 2002). The result of that approach is well-known Gorini-Kossakowski-Sudarshan-Lindblad quantum master equation which is now acknowledged as one of cornerstones of open systems quantum theory (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011).

While mathematical reasoning provides the basis for rigorous proof of the existence of GKSL master equation, the physical conditions surrounding the dynamics stay secondary. Over time, mathematical physicists have developed various approaches to overcome lack of physical details, starting from microscopic picture, i.e., model Hamiltonian. One of the most prominent methods in this regard is Nakajima-Zwanzig projection technique (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011). Following this route, it is possible to obtain master equation which is in GKSL form with insight into physical details at the same time.

Besides being Markovian, here we will be interested in finite-dimensional, open quantum systems, exclusively. From perspective of fundamental physics and quantum technology application, models of one and two qubits are quite well studied as a representative of finite-dimensional systems (NIELSEN and CHUANG, 2000). But realistic physical situations for sure welcome models of more than two-qubits systems, such as e.g., model of three interacting qubits as open quantum system.

So, the goal of this paper is derivation of Markovian master equation, starting from microscopic picture, for the model of three interacting qubits in contact with thermal (bosonic) bath.

This paper is structured as follows. Section *General setting* presents sketch of thinking in open quantum system theory with the aim of highlighting what is most important, starting from microscopic picture and introducing proper set of assumptions and approximations. In this way, the reader gets rough idea about what the goal is and how to reach it. Section *The model* introduces the Hamiltonian of interest revealing details which shape dynamics of open quantum system. The subsequent section, *The Algorithm*, outlines all essential computational steps in a concise form. In *Computational Details*, the procedure for obtaining the desired quantum master equation is presented. The last section is *Conclusion* of the paper. Additional details are shared in the subsequent *Appendices*.

GENERAL SETTING

Open quantum system (A) is system in unavoidable contact with another quantum system (typically with many degrees of freedom) called environment (B) (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011). Basic assumption of open quantum systems theory is that A+B composite system is isolated and that dynamic of composite system is unitary. Generator of unitary dynamics is Hamiltonian of composite system:

$$H = H_A \otimes I_B + I_A \otimes H_B + \alpha H_{AB}; \tag{1}$$

H_A and H_B are self-Hamiltonians of open system and environment, respectively, while H_{AB} stands for interaction Hamiltonian which explicit form is given as

$$H_{AB} = \sum_l A_l \otimes B_l \, . \tag{2}$$

Hermitian operators A_l and B_l act on to Hilbert space of open system and environment, respectively. Coupling constant α accounts for the strength of interaction between systems A and B.

In further analysis it is convenient to introduce interaction picture with respect to the free Hamiltonian of open system and environment: $H_0 = H_A + H_B$: tilde will be used to denote operators with respect to interaction picture.

The corresponding differential form of composite system unitary dynamics is given by equation:

$$i\hbar \frac{d\tilde{\rho}_{AB}}{dt} = \left[\tilde{H}_{AB}, \tilde{\rho}_{AB}\right], \tag{3}$$

known as von Neumann-Liouville equation, where $\tilde{\rho}_{AB}$ is density operator for the whole A+B. The reduced dynamics of open system A follows by tracing out environmental degrees of freedom in Eq. (3):

$$i\hbar \frac{d\tilde{\rho}_A(t)}{dt} = tr_B\left[\tilde{H}_{AB}, \tilde{\rho}_{AB}\right], \tag{4}$$

which is starting place for further mathematical considerations (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011).

The standard approach in theory of open quantum systems consists of applying Nakajima-Zwanzig projection operator technique on Eq. (4) which leads to the following time non-local master equation (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011):

$$\frac{d\tilde{\rho}_A(t)}{dt} = \int_{t_0}^{t} \mathcal{K}(t-s)\,\tilde{\rho}_A(s)ds,\ \tilde{\rho}_A(t_0) = \rho_{A0}\,, \tag{5}$$

where $\mathcal{K}(t)$ is so called memory kernel which tells how the change of $\tilde{\rho}_A(t)$ depends on its history. In other words, dynamic of open quantum system is non-Markovian. Eq. (5) is, from mathematical point of view, intractable if proper assumptions and approximations are not invoked. For the sake of completeness, it is important to note that it is possible (and desirable) to describe quantum non-Markovian processes through local in time master equation (via technique of time-convolutionless forms or TCL for short (BREUER and PETRUCCIONE, 2002) which is perfectly equivalent to results obtained by Nakajima-Zwanzig technique (CHRUŚCIŃSKI and KOSSAKOWSKI, 2012). General form of this TCL master equation is given by:

$$\frac{d\tilde{\rho}_A(t)}{dt} = \mathcal{L}(t-t_0)\tilde{\rho}_A(t), \tilde{\rho}_A(t_0) = \rho_{A0}, \tag{6}$$

where $\mathcal{L}$ is superoperator known as (time dependent) Liouvillian of master equation.

The question(s) of open system's non-Markovianity quantification and description is tightly connected with the notion of quantum Markovianity (BREUER, 2012). Quantum Markovianity of open system dynamics is reflected in the fact that corresponding dynamical map fulfill semigroup and divisibility property. Divisibility property is analogous to Chapman-Kolmogorov equation which defines the notion of classical Markovianity (BREUER and PETRUCCIONE, 2002).

By dynamical map here is meant mapping $\Lambda(t, t_0)$:

$$\rho(t) = \Lambda(t, t_0)\rho(t_0) \tag{7}$$

i.e. integral form of dynamical law. In other words, $\Lambda(\mathrm{t}, \mathrm{t}_0)$ for Markovian dynamics satisfies equation

$$\frac{d\Lambda(t,t_0)}{dt} = \mathcal{L}_M \Lambda(t,t_0),\ \Lambda(t_0,t_0) = \mathbb{I}, \tag{8}$$

whose solution is given by:

$$\Lambda(t,t_0) = e^{(t-t_0)\mathcal{L}_M}, \tag{9}$$

where $\mathcal{L}_M$ is generator of the semigroup and M stand for Markovian. Eq. (9) implies that $\Lambda(t,t_0)$ depends only upon the difference "$t-t_0$" and hence $\Lambda(t) \equiv \Lambda(t,0)$ defines one-parameter semigroup satisfying composition law

$$\Lambda(t_1)\Lambda(t_2) = \Lambda(t_1+t_2), \tag{10}$$

which is an instance of map divisibility (BREUER, 2012).

Requests for quantum Markovian (in above sense) and completely positive and trace-preserving (CPTP) dynamics led to mathematical derivation of master equation in the well-known form (RIVAS and HUELGA, 2011):

$$\frac{d\tilde{\rho}_A(t)}{dt} = -\frac{i}{\hbar}[H_{LS},\tilde{\rho}_A] + \sum_k \gamma_k \left(V_k \tilde{\rho}_A V_k^\dagger - \frac{1}{2}\{V_k^\dagger V_k, \tilde{\rho}_A\}\right) = \mathcal{L}_M \tilde{\rho}_A,\ \tilde{\rho}_A(t_0) = \rho_0 \tag{11}$$

which is due to Gorini, Kosakowski, Sudarshan and Lindblad (GKSL). $\gamma_k's$ are decay rates, V_k are Lindblad operators while H_{LS} stands for so called Lamb shift which produces a shift in the energy levels of the open quantum system. $\mathcal{L}_M$, in the context of Eq. (11) is also called Liovillian of master equation. $\{A,B\} = AB + BA$ is standard notation for anticommutator of two operators.

It is known that Liouvillian of Eq. (11) generalizes to (not to be confused with Eq. (6)) (RIVAS and HUELGA, 2011)

$$\mathcal{L}_M(t)\tilde{\rho}_A = -\frac{i}{\hbar}[H(t),\tilde{\rho}_A] + \sum_k \gamma_k(t)\left(V_k(t)\tilde{\rho}_A V_k^\dagger(t) - \frac{1}{2}\{V_k^\dagger(t)V_k(t),\tilde{\rho}_A\}\right), \tag{12}$$

where symbols have the same meaning as in Eq. (11), only now time dependent. Interestingly, Eq. (12) accounts for non-Markovian dynamics if $\gamma_k(t) < 0$, for at least one k. Because of the last feature, Eq. (11) will be of only interest for further considerations.

We will not dwell here on the problems which surround quantification or rigorous definition of quantum Markovianity, question which is not settled, in unambiguous manner, yet (BREUER, 2012). In other words, in this paper, property expressed by Eq. (10) is basic for definition of quantum Markovianity. But it should be kept in mind that it is not the only point of view in contemporary literature, i.e. Eq. (10) is not considered sufficient condition (RIVAS and HUELGA, 2011).

Rather, we would like to emphasize that situations where dynamics is Markovian (in sense of Eq. (11) i.e. Eq. (10)) still offer rich physics from the perspective of fundamentals and applications. In other words, basic quantum phenomena such as quantum dissipation, quantum decay and quantum decoherence (JOOS *et al.*, 2003, SCHLOSSHAUER, 2007, GARDINER and ZOLLER, 2004) can be modeled and studied in framework of Markovianity expressed by Eq. (11). From computational point of view, despite unsettled definition, Markovian dynamics is easier to handle.

At this point, a brief remark is in order. As will be seen, different notations will be used for frequencies. To avoid possible confusion, let us emphasize that ω will be used for the frequencies (and frequency differences) of the open system and will always be a discrete quantity. On the other hand, Ω will be used to denote the frequencies of the environment and may represent either a discrete (as in Eq. (18)) or a continuous (as in Eq. (29)) quantity.

THE MODEL

As open, quantum finite-dimensional system (A) of interest here it will be considered system of three mutually interacting qubits that interact with infinite-dimensional thermal bath of harmonic oscillators, i.e., environment (B).

The free Hamiltonians, cf. Eq. (1), of open quantum system and bosonic bath are $H_A = \omega_0(S_{1z} + S_{2z} + S_{3z}) + \beta S_{1z} \otimes S_{2z} \otimes I_3$ and $H_B = \sum_{\vec{k}} \hbar\Omega_{\vec{k}} b^\dagger_{\vec{k}} b_{\vec{k}}$, respectively. β plays role of intercoupling constant whereby it is assumed that $\beta > \alpha$. Interaction part of Hamiltonian, $H_{AB} = (S_{1x} + S_{2x} + S_{3x}) \otimes \sum_{\vec{k}} g_{\vec{k}} \left(b^\dagger_{\vec{k}} + b_{\vec{k}} \right) \equiv A \otimes B$, stands for interaction between open system and environment with $g_{\vec{k}}$ playing the role of coupling constant α. Operators S_{iz} and S_{ix} are standard spin-1/2 operators, while bosonic operators $b^\dagger_{\vec{k}}$ and $b_{\vec{k}}$ fulfil commutation relations $\left[b_{\vec{k}}, b^\dagger_{\vec{k}'} \right] = \delta_{\vec{k}\vec{k}'}$ (MESSIAH, 1962).

By thermal bath here is meant multimode bosonic environment which separable state is given by reduced density operator (BREUER and PETRUCCIONE, 2002):

$$\rho_B = \prod_{\vec{k}} \left[1 - e^{-\frac{\hbar\Omega_{\vec{k}}}{k_B T}} \right] e^{-\frac{\hbar\Omega_{\vec{k}} b^\dagger_{\vec{k}} b_{\vec{k}}}{k_B T}}, \tag{13}$$

where k_B is Boltzmann constant and T is temperature of the bath. Multimode character is expressed by frequency $\Omega_{\vec{k}}$ where $\vec{k}$ is wave vector taking discrete values. It will turn out that thermal averages of bosonic operators are needed, so for convenience they are listed here:

$$\langle b^\dagger_{\vec{k}} \rangle = \langle b_{\vec{k}} \rangle = 0, \tag{14a}$$

$$\langle b_{\vec{k}} b_{\vec{k}'} \rangle = \langle b^\dagger_{\vec{k}} b^\dagger_{\vec{k}'} \rangle = 0, \tag{14b}$$

$$\langle b^\dagger_{\vec{k}} b_{\vec{k}'} \rangle = \langle n_{\vec{k}} \rangle \delta_{\vec{k}\vec{k}'}, \tag{14c}$$

$$\langle b_{\vec{k}} b^\dagger_{\vec{k}'} \rangle = \left(1 + \langle n_{\vec{k}} \rangle \right) \delta_{\vec{k}\vec{k}'}, \tag{14d}$$

where $\langle n_{\vec{k}} \rangle = \frac{1}{e^{\frac{\hbar\Omega_{\vec{k}}}{k_B T}} - 1}$ stands for thermal average number of bosons in a mode with frequency $\Omega_{\vec{k}}$. Some details concerning averages, Eqs. (14), can be found in Appendix 2.

THE ALGORITHM

Mathematical derivation of Eq. (11) does not say much about the microscopic origin of dynamics and physical limitations of GKSL master equation. To continue further, it is necessary to characterize properties of the environment and strength of the interaction between systems A and B, to begin with. Then using technique of Nakajima-Zwanzig and invoking famous set of approximations–Born, Markov and secular–it is possible to obtain GKSL form of master equation. Interested reader may find appropriate details related to microscopic derivation of GKSL master equation in (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011): for purposes of this paper, we will use only some points of immediate interest.

Following this route of obtaining GKSL master equation it turns out that Eq. (11) can be formulated in the following, unitarily equivalent, form:

$$\frac{d\tilde{\rho}_A}{dt} = -\frac{i}{\hbar}[H_{LS}, \tilde{\rho}_A] + \sum_{\omega}\sum_{kl}\gamma_{kl}(\omega)\left(A_l(\omega)\tilde{\rho}_A A_k^{\dagger}(\omega) - \frac{1}{2}\left\{A_k^{\dagger}(\omega)A_l(\omega), \tilde{\rho}_A\right\}\right). \quad (15)$$

In Eq. (15), $\gamma_{kl}(\omega)$ are matrix elements of positive semidefinite matrix, for all ω, which may be diagonalized by unitary matrix, where elements on diagonal are decay rates from Eq. (11). Using matrix elements, u_{ki}, from unitary transformation, we may write relation $A_i = \sum_{k=1}^{d^2-1} u_{ki} V_k$ between new (A_i) and old (V_k) Lindblad operators, where d stands for dimensionality of open system' Hilbert space. Unitary equivalence means that Eq. (11) and Eq. (15) describe the same dynamics. So, we will refer to Eq. (15) further on.

To be able to write down master equation, Eq. (15), it is necessary to find operators $A_l(\omega)$ and H_{LS} as well as the functions $\gamma_{kl}(\omega)$.

The expressions for $A_l(\omega)$ are obtained by taking interaction part of Hamiltonian, H_{AB}, in interaction picture:

$$\tilde{H}_{AB} = U_0^{\dagger}(\sum_l A_l \otimes B_l)U_0 = \sum_l \tilde{A}_l(t) \otimes \tilde{B}_l(t)\,; \quad (16)$$

$U_0 = U_A \otimes U_B$ stands for unitary operator having in mind standard quantum-mechanics equality $U_m = e^{-\frac{i}{\hbar}tH_m}$ where $m = A, B$. Writing Eq. (16) in explicit form leads to the expression $\tilde{H}_{AB} = \sum_l \sum_{\omega} A_l(\omega)\, e^{-i\omega t} \otimes \sum_{\Omega_m} B_l(\Omega)\, e^{-i\Omega_m t}$ with operators:

$$A_l(\omega) = \sum_{\varepsilon_A - \varepsilon'_A = \hbar\omega} |\varepsilon_A\rangle\langle\varepsilon_A|A_l|\varepsilon'_A\rangle\langle\varepsilon'_A| \quad (17)$$

and

$$B_l(\Omega_m) = \sum_{\varepsilon_B - \varepsilon'_B = \hbar\Omega_m} |\varepsilon_B\rangle\langle\varepsilon_B|B_l|\varepsilon'_B\rangle\langle\varepsilon'_B|. \quad (18)$$

In Eqs. (17) and (18) ω and Ω represent open system and environment frequencies, respectively, while ε_A is running through the discrete spectrum of H_A and ε_B is running through the discrete spectrum of H_B. Operators $A_l(\omega)$ from Eq. (17) are just those from Eq. (15), so Eq. (17) can be considered as defining equation.

The properties of the environment are encapsulated in Fourier transformation of correlation functions which is defined as $\langle\tilde{B}_k^{\dagger}(t)\tilde{B}_l(t-s)\rangle = tr\left[\tilde{B}_k^{\dagger}(t)\tilde{B}_l(t-s)\rho_B\right]$, in general (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011). If the state of the environment is stationary (here thermodynamic equilibrium) and equation $[H_B, \rho_B] = 0$ holds, then previous equality simplifies $\langle\tilde{B}_k^{\dagger}(t)\tilde{B}_l(0)\rangle = tr\left[\tilde{B}_k^{\dagger}(t)B_l\rho_B\right]$. The one-sided Fourier transformation of the correlation functions in this case reads:

$$\Gamma_{kl}(\omega) = \int_0^{+\infty} dt e^{i\omega t}\, tr\left[\tilde{B}_k^{\dagger}(t)B_l\rho_B\right]. \quad (19)$$

It is convenient to decompose Eq. (19) as follows:

$$\Gamma_{kl}(\omega) = \tfrac{1}{2}\gamma_{kl}(\omega) + iS_{kl}(\omega). \quad (19a)$$

For the stationary state (e.g. Eq. (13)) of the environment, functions $\gamma_{kl}(\omega)$ are defined by the following equality in interaction picture:

$$\gamma_{kl}(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t}\, tr\left[\tilde{B}_k^{\dagger}(t)B_l\rho_B\right],$$

while defining equation for Lamb-shift Hamiltonian, H_{LS}, reads (BREUER and PETRUCCIONE, 2002; RIVAS and HUELGA, 2011):

$$H_{LS} = \sum_{\omega} \sum_{k,l} S_{kl}\,(\omega) A_k^{\dagger}(\omega)\, A_l(\omega);$$

so having expressions for $\Gamma_{kl}(\omega)$ and $\gamma_{kl}(\omega)$ automatically yields an expression for $S_{kl}(\omega)$.

For the present model, an interaction Hamiltonian of the form $H_{AB} = A \otimes B$ results in simplified expressions for the decay rates and the Lamb shift:

$$\gamma(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t}\, tr[\tilde{B}(t) B \rho_B], \tag{20}$$

and

$$H_{LS} = \sum_{\omega} S(\omega)\, A^{\dagger}(\omega) A(\omega), \tag{21}$$

which will be of immediate interest further on.

COMPUTATIONAL DETAILS

The first step is solving eigenvalue problem of open system Hamiltonian H_A, i.e. $H_A|\epsilon_i\rangle = \epsilon_i|\epsilon_i\rangle$. It is not hard to check that set of eigenvalues and eigenvectors are those given in Table 1, whence it is noted that eigenvectors are tensor product of eigenstates of the S_z operator, $|g\rangle$ and $|e\rangle$.

From general expression $A(\omega) = \sum_{\omega=\varepsilon_j-\varepsilon_i} |\varepsilon_i\rangle\langle\varepsilon_i|A|\varepsilon_j\rangle\langle\varepsilon_j|$ follows that it is necessary to write down all differences of eigenvalues $\varepsilon_j - \varepsilon_i$. To be more tractable those data are presented in Table 2.

Table 1 Eigenvalues and eigenvectors of open system's Hamiltonian.

Eigenvalues	Eigenvectors
$\epsilon_1 = \frac{\beta}{4} - \frac{3\omega_0}{2}$	$\|\epsilon_1\rangle = \|g\rangle\|g\rangle\|g\rangle$
$\epsilon_2 = \frac{\beta}{4} - \frac{\omega_0}{2}$	$\|\epsilon_2\rangle = \|g\rangle\|g\rangle\|e\rangle$
$\epsilon_3 = -\frac{\beta}{4} - \frac{\omega_0}{2}$	$\|\epsilon_3\rangle = \|g\rangle\|e\rangle\|g\rangle$
$\epsilon_4 = \frac{\beta}{4} + \frac{\omega_0}{2}$	$\|\epsilon_4\rangle = \|g\rangle\|e\rangle\|e\rangle$
$\epsilon_5 = -\frac{\beta}{4} - \frac{\omega_0}{2}$	$\|\epsilon_5\rangle = \|e\rangle\|g\rangle\|g\rangle$
$\epsilon_6 = -\frac{\beta}{4} + \frac{\omega_0}{2}$	$\|\epsilon_6\rangle = \|e\rangle\|g\rangle\|e\rangle$
$\epsilon_7 = \frac{\beta}{4} + \frac{\omega_0}{2}$	$\|\epsilon_7\rangle = \|e\rangle\|e\rangle\|g\rangle$
$\epsilon_8 = \frac{\beta}{4} + \frac{3\omega_0}{2}$	$\|\epsilon_8\rangle = \|e\rangle\|e\rangle\|e\rangle$

A closer look at Table 2 shows that there are mutually equal differences $\varepsilon_j - \varepsilon_i$. For example,
$\varepsilon_1 - \varepsilon_2 = -\omega_0$, $\varepsilon_2 - \varepsilon_7 = -\omega_0$, $\varepsilon_3 - \varepsilon_4 = -\omega_0$, $\varepsilon_3 - \varepsilon_6 = -\omega_0$, $\varepsilon_5 - \varepsilon_4 = -\omega_0$, $\varepsilon_5 - \varepsilon_6 = -\omega_0$, $\varepsilon_7 - \varepsilon_8 = -\omega_0$. For this particular frequency, $-\omega_0$, Eq. (17) takes the form:
$A(-\omega_0) = |\varepsilon_2\rangle\langle\varepsilon_2|A|\varepsilon_1\rangle\langle\varepsilon_1| + |\varepsilon_7\rangle\langle\varepsilon_7|A|\varepsilon_2\rangle\langle\varepsilon_2| + |\varepsilon_4\rangle\langle\varepsilon_4|A|\varepsilon_3\rangle\langle\varepsilon_3| + |\varepsilon_6\rangle\langle\varepsilon_6|A|\varepsilon_3\rangle\langle\varepsilon_3| +$
$+|\varepsilon_4\rangle\langle\varepsilon_4|A|\varepsilon_5\rangle\langle\varepsilon_5| + |\varepsilon_6\rangle\langle\varepsilon_6|A|\varepsilon_5\rangle\langle\varepsilon_5| + |\varepsilon_8\rangle\langle\varepsilon_8|A|\varepsilon_7\rangle\langle\varepsilon_7|$,
bearing in mind that $A = S_{1x} + S_{2x} + S_{3x}$.

All in all, following the Table 2 becomes clear that it is needed to find the following operators: $A(0)$, $A(\pm\omega_0)$, $A(\pm 2\omega_0)$, $A(\pm 3\omega_0)$, $A\left(\pm\frac{\beta}{2}\right)$, $A\left(\pm\frac{\beta-2\omega_0}{2}\right)$, $A\left(\pm\frac{\beta+2\omega_0}{2}\right)$, $A\left(\pm\frac{\beta-4\omega_0}{2}\right)$ and $A\left(\pm\frac{\beta+4\omega_0}{2}\right)$. Having in mind relation $[A(-\omega)]^\dagger = A(\omega)$, it is enough to calculate frequencies with negative signs. With the help of expressions for spin operators (see Appendix 1), after some algebra, follows that non-zero contributions come from operators $A(\pm\omega_0)$, $A\left(\pm\frac{\beta-2\omega_0}{2}\right)$ and $A\left(\pm\frac{\beta+2\omega_0}{2}\right)$, i.e.:

$$A(\pm\omega_0) = I_1 \otimes I_2 \otimes \frac{1}{2} S_{3\mp},$$
$$A\left(\pm\frac{\beta-2\omega_0}{2}\right) = \frac{1}{2} S_{1\pm} \otimes \frac{1}{2}(I_2 + 2S_{2z}) \otimes I_3 + \frac{1}{2}(I_1 + 2S_{1z}) \otimes \frac{1}{2} S_{2\pm} \otimes I_3,$$
$$A\left(\pm\frac{\beta+2\omega_0}{2}\right) = \frac{1}{2} S_{1\mp} \otimes \frac{1}{2}(I_2 - 2S_{2z}) \otimes I_3 + \frac{1}{2}(I_1 - 2S_{1z}) \otimes \frac{1}{2} S_{2\mp} \otimes I_3. \quad (22)$$

Table 2 Eigenvalue differences.

$\varepsilon_1 - \varepsilon_2 = -\omega_0$	$\varepsilon_2 - \varepsilon_1 = \omega_0$	$\varepsilon_3 - \varepsilon_1 = \omega_0 - \frac{\beta}{2}$	$\varepsilon_4 - \varepsilon_1 = -\frac{\beta - 4\omega_0}{2}$
$\varepsilon_1 - \varepsilon_3 = \frac{\beta - 2\omega_0}{2}$	$\varepsilon_2 - \varepsilon_3 = \frac{\beta}{2}$	$\varepsilon_3 - \varepsilon_2 = -\frac{\beta}{2}$	$\varepsilon_4 - \varepsilon_2 = -\frac{\beta - 2\omega_0}{2}$
$\varepsilon_1 - \varepsilon_4 = \frac{\beta - 4\omega_0}{2}$	$\varepsilon_2 - \varepsilon_4 = \frac{\beta - 2\omega_0}{2}$	$\varepsilon_3 - \varepsilon_4 = -\omega_0$	$\varepsilon_4 - \varepsilon_3 = \omega_0$
$\varepsilon_1 - \varepsilon_5 = \frac{\beta - 2\omega_0}{2}$	$\varepsilon_2 - \varepsilon_5 = \frac{\beta}{2}$	$\varepsilon_3 - \varepsilon_5 = 0$	$\varepsilon_4 - \varepsilon_5 = \omega_0$
$\varepsilon_1 - \varepsilon_6 = \frac{\beta - 4\omega_0}{2}$	$\varepsilon_2 - \varepsilon_6 = \frac{\beta - 2\omega_0}{2}$	$\varepsilon_3 - \varepsilon_6 = -\omega_0$	$\varepsilon_4 - \varepsilon_6 = 0$
$\varepsilon_1 - \varepsilon_7 = -2\omega_0$	$\varepsilon_2 - \varepsilon_7 = -\omega_0$	$\varepsilon_3 - \varepsilon_7 = -\frac{\beta + 2\omega_0}{2}$	$\varepsilon_4 - \varepsilon_7 = -\frac{\beta}{2}$
$\varepsilon_1 - \varepsilon_8 = -3\omega_0$	$\varepsilon_2 - \varepsilon_8 = -2\omega_0$	$\varepsilon_3 - \varepsilon_8 = -\frac{\beta + 4\omega_0}{2}$	$\varepsilon_4 - \varepsilon_8 = -\frac{\beta + 2\omega_0}{2}$
$\varepsilon_5 - \varepsilon_1 = -\frac{\beta + 2\omega_0}{2}$	$\varepsilon_6 - \varepsilon_1 = -\frac{\beta - 4\omega_0}{2}$	$\varepsilon_7 - \varepsilon_1 = 2\omega_0$	$\varepsilon_8 - \varepsilon_1 = 3\omega_0$
$\varepsilon_5 - \varepsilon_2 = -\frac{\beta}{2}$	$\varepsilon_6 - \varepsilon_2 = -\frac{\beta - 2\omega_0}{2}$	$\varepsilon_7 - \varepsilon_2 = \omega_0$	$\varepsilon_8 - \varepsilon_2 = 2\omega_0$
$\varepsilon_5 - \varepsilon_3 = 0$	$\varepsilon_6 - \varepsilon_3 = \omega_0$	$\varepsilon_7 - \varepsilon_3 = \frac{\beta + 2\omega_0}{2}$	$\varepsilon_8 - \varepsilon_3 = \frac{\beta + 4\omega_0}{2}$
$\varepsilon_5 - \varepsilon_4 = -\omega_0$	$\varepsilon_6 - \varepsilon_4 = 0$	$\varepsilon_7 - \varepsilon_4 = \frac{\beta}{2}$	$\varepsilon_8 - \varepsilon_4 = \frac{\beta + 2\omega_0}{2}$
$\varepsilon_5 - \varepsilon_6 = -\omega_0$	$\varepsilon_6 - \varepsilon_5 = \omega_0$	$\varepsilon_7 - \varepsilon_5 = \frac{\beta + 2\omega_0}{2}$	$\varepsilon_8 - \varepsilon_5 = \frac{\beta + 4\omega_0}{2}$
$\varepsilon_5 - \varepsilon_7 = -\frac{\beta + 2\omega_0}{2}$	$\varepsilon_6 - \varepsilon_7 = -\frac{\beta}{2}$	$\varepsilon_7 - \varepsilon_6 = \frac{\beta}{2}$	$\varepsilon_8 - \varepsilon_6 = \frac{\beta + 2\omega_0}{2}$
$\varepsilon_5 - \varepsilon_8 = -\frac{\beta + 4\omega_0}{2}$	$\varepsilon_6 - \varepsilon_8 = -\frac{\beta + 2\omega_0}{2}$	$\varepsilon_7 - \varepsilon_8 = -\omega_0$	$\varepsilon_8 - \varepsilon_7 = \omega_0$

Having Eqs. (22), next to be calculated is function $\Gamma(\omega)$. The environment degrees of freedom in interaction Hamiltonian are represented by operator $B = \sum_{\vec{k}} g_{\vec{k}} \left(b^\dagger_{\vec{k}} + b_{\vec{k}}\right)$ which in interaction picture takes the form $\tilde{B}(t) = \sum_{\vec{k}} g_{\vec{k}} \left(b^\dagger_{\vec{k}} e^{i\,t\,\Omega_k} + b_{\vec{k}} e^{-i\,t\,\Omega_k}\right)$. Putting these two into $\Gamma(\omega) = \int_0^{+\infty} dt e^{i\omega t}\, tr[\tilde{B}(t) B \rho_B]$ and making use of Eqs. (14) follows:

$$\Gamma(\omega) = \sum_{\vec{k}} \int_0^{+\infty} dt\ g^2_{\vec{k}} \langle n_{\vec{k}} \rangle e^{it(\omega + \Omega_k)} + \sum_{\vec{k}} \int_0^{+\infty} dt\ g^2_{\vec{k}} (1 + \langle n_{\vec{k}} \rangle) e^{it(\omega - \Omega_k)}. \quad (23)$$

Similarly, the expression for decay rate function read:

$$\gamma(\omega) = \sum_{\vec{k}} \int_{-\infty}^{+\infty} dt \; g_{\vec{k}}^2 \langle n_{\vec{k}} \rangle \, e^{it(\omega+\Omega_k)} + \sum_{\vec{k}} \int_{-\infty}^{+\infty} dt \; g_{\vec{k}}^2 (1 + \langle n_{\vec{k}} \rangle) e^{it(\omega-\Omega_k)}. \quad (24)$$

Integrals $\int_0^{+\infty} dt\, e^{it(\omega\pm\Omega_k)}$ and $\int_{-\infty}^{+\infty} dt\, e^{it(\omega\pm\Omega_k)}$ are not well-defined in sense of improper Riemann integrals, but do make sense in distribution theory–for details see (RIVAS and HUELGA, 2011) and references therein. Here, we are interested in final forms of those integrals, which read:

$$\int_0^{+\infty} dt\, e^{it(\omega\pm\Omega_k)} = \frac{i}{\omega\pm\Omega_k} + \pi\delta(\omega \pm \Omega_k)$$

and

$$\int_{-\infty}^{+\infty} dt\, e^{it(\omega\pm\Omega_k)} = 2\pi\delta(\omega \pm \Omega_k),$$

where δ denotes Dirac delta function.

Making use of these integrals, Eqs. (23) and (24) transform into expressions:

$$\Gamma(\omega) = \sum_{\vec{k}} g_{\vec{k}}^2 \langle n_{\vec{k}} \rangle \left(\frac{i}{\omega+\Omega_k} + \pi\delta(\omega + \Omega_k) \right) + \sum_{\vec{k}} g_{\vec{k}}^2 \left(1 + \langle n_{\vec{k}} \rangle \right) \left(\frac{i}{\omega-\Omega_k} + \pi\delta(\omega - \Omega_k) \right) \quad (25)$$

and

$$\gamma(\omega) = 2\pi \sum_{\vec{k}} g_{\vec{k}}^2 \langle n_{\vec{k}} \rangle \, \delta(\omega + \Omega_k) + 2\pi \sum_{\vec{k}} g_{\vec{k}}^2 (1 + \langle n_{\vec{k}} \rangle) \delta(\omega - \Omega_k), \quad (26)$$

respectively. Comparing last two expressions with Eq. (19a) follows equation for $S(\omega)$:

$$S(\omega) = \sum_{\vec{k}} g_{\vec{k}}^2 \left(\frac{\langle n_{\vec{k}} \rangle}{\omega+\Omega_k} + \frac{1+\langle n_{\vec{k}} \rangle}{\omega-\Omega_k} \right). \quad (27)$$

At this point it is convenient to switch from sums over modes in Eqs. (25) and (26) to integrals. Justification for doing this comes from two reasons. First reason is of formal nature: it is easier mathematically to handle integrals than sums. The second reason is physical: the bath has vast degrees of freedom making the spectrum of H_B practically continuous. Eqs. (26) and (27) now read:

$$\gamma(\omega) = \int_0^{\infty} d\Omega\, J(\Omega) \langle n(\Omega) \rangle \delta(\omega + \Omega) + \int_0^{\infty} d\Omega\, J(\Omega)(1 + \langle n(\Omega) \rangle) \delta(\omega - \Omega), \text{ i.e.}$$

$$\gamma(\omega) = \begin{cases} J(|\omega|)\langle n(|\omega|)\rangle, & \omega < 0 \\ J(|\omega|)(1 + \langle n(|\omega|)\rangle), & \omega \geq 0 \end{cases} \quad (28)$$

and

$$S(\omega) = \int_0^{\infty} d\Omega\, J(\Omega) \left(\frac{\langle n(\Omega) \rangle}{\omega+\Omega} + \frac{1+\langle n(\Omega) \rangle}{\omega - \Omega} \right). \quad (29)$$

In the context of a bosonic bath, negative frequencies correspond to the physical process of the system absorbing energy from the bath, while positive frequencies describe the system emitting energy into the bath. Here, $J(\Omega)$ is the so-called spectral density of the bath and contains information about the strength of coupling per frequency. Basically, $J(\Omega)$ occurs by smoothing $g_{\vec{k}}^2$. Just as an example, the so-called ohmic spectral density is given by the equation:

$$J(\Omega) = 2\pi \sum_{\vec{k}} g_{\vec{k}}^2 \delta(\Omega - \Omega_k) \xrightarrow{yields} J(\Omega) = 2\pi\alpha\Omega e^{-\Omega/\Omega_c} \quad (30)$$

where α is a constant that modifies strength of interaction and Ω_c is cut-off frequency (RIVAS *et al*., 2010). Spectral density, Eq. (29), is well suited for Markovian dynamics, especially for the bath at high temperatures. Nevertheless, other choices of spectral densities can be made but with the caveat that the validity of the master equation itself may be brought into question. We will not pursue further questions about explicit form and properties of spectral density: these questions are important when it comes to analysis of dynamics governed by master equation, whether numerically or analytically.

Using formula Eq. (21) and operators Eqs. (22) it is possible to show (by simple, but tedious algebra) that expression for Lamb shift takes the form:

$H_{LS} = \sum_{i=1}^{7} c_i G_i$,

where

$$c_1 = \frac{\hbar^2(3S(\omega_0)+\hbar^2 S(\omega_0)-2\mathbb{I}\omega_0)}{2\sqrt{2}},\ c_2 = \frac{2\mathbb{I}\hbar^2\omega_0}{\sqrt{2}},\ c_3 = \frac{\hbar^2((1+\hbar)^2 S(\omega_0)-4\mathbb{I}\hbar\omega_0)}{4\sqrt{2}},$$
$$c_4 = \frac{\hbar^2((1+\hbar)^2 S(\omega_0)-4\mathbb{I}\hbar\omega_0)}{4\sqrt{2}},\ c_5 = \frac{-2\hbar^3(\mathbb{I}\beta+S(\omega_0)-2\mathbb{I}\omega_0)}{\sqrt{2}},\ c_6 = \frac{\hbar^2(2\mathbb{I}\beta\hbar+(1+\hbar)^2 S(\omega_0)-4\mathbb{I}\hbar\omega_0)}{4\sqrt{2}},$$
$$c_7 = \frac{\hbar^2(2\mathbb{I}\beta\hbar+(1+\hbar)^2 S(\omega_0)-4\mathbb{I}\hbar\omega_0)}{4\sqrt{2}} \tag{31}$$

and

$$G_1 = \frac{1}{2\sqrt{2}} I_1\otimes I_2\otimes I_3,\ G_2 = \frac{2}{\hbar} I_1\otimes I_2\otimes S_{3z},\ G_3 = \frac{2}{\hbar} I_1\otimes S_{2z}\otimes I_3,\ G_4 = \frac{2}{\hbar} S_{1z}\otimes I_2\otimes I_3,$$
$$G_5 = \frac{\sqrt{2}}{\hbar^2} S_{1z}\otimes S_{2z}\otimes I_3,\ G_6 = \frac{\sqrt{2}}{\hbar^2} S_{1x}\otimes S_{2x}\otimes I_3,\ G_7 = \frac{\sqrt{2}}{\hbar^2} S_{1y}\otimes S_{2y}\otimes I_3. \tag{32}$$

In above expressions, $S(\omega_0)$ is defined by Eq. (29), $\mathbb{I} = \int_0^\infty d\Omega\, J(\Omega)\, \frac{\omega(1+2\langle n(\Omega)\rangle)+\Omega}{\omega^2-\Omega^2}$ and β is intercoupling constant introduced in *The model* section.

The desired master equation for three qubits immersed in thermal, bosonic bath takes the simplified form:

$$\frac{d\tilde{\rho}_A}{dt} = -\frac{i}{\hbar}[H_{LS}, \tilde{\rho}_A] + \sum_\omega \gamma(\omega)\left(A(\omega)\tilde{\rho}_A A^\dagger(\omega) - \frac{1}{2}\{A^\dagger(\omega)A(\omega), \tilde{\rho}_A\}\right), \tag{33}$$

where ω runs through allowed positive and negative frequencies.

In the literature, it is common for master equations concerning qubit systems to be expressed in terms of Pauli operators, $\vec{\sigma}$, bearing in mind that $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$. Therefore, the final form of the master equation will also be written in this way here, considering the identity $\sigma_\pm\sigma_\mp = 2(1 \mp \sigma_z)$. Clearly, it is understood that the Lamb shift is also expressed in terms of Pauli operators. So, interaction-picture quantum Markovian master equation reads:

$$\frac{d\tilde{\rho}_A}{dt} = -\frac{i}{\hbar}[H_{LS}, \tilde{\rho}_A] + \frac{\boldsymbol{\gamma(\omega_0)}}{\mathbf{16}}\left(I_1\otimes I_2\otimes\sigma_{3-}\tilde{\rho}_A I_1\otimes I_2\otimes\sigma_{3+} - \frac{1}{2}\{I_1\otimes I_2\otimes\sigma_{3+}\sigma_{3-}, \tilde{\rho}_A\}\right)$$
$$+ \frac{\boldsymbol{\gamma(-\omega_0)}}{\mathbf{16}}\left(I_1\otimes I_2\otimes\sigma_{3+}\tilde{\rho}_A I_1\otimes I_2\otimes\sigma_{3-} - \frac{1}{2}\{I_1\otimes I_2\otimes\sigma_{3-}\sigma_{3+}, \tilde{\rho}_A\}\right)$$
$$+ \frac{\boldsymbol{\gamma\left(\frac{\beta-2\omega_0}{2}\right)}}{\mathbf{64}}\left(\left(\sigma_{1+}\otimes\frac{\sigma_{2-}\sigma_{2+}}{2}\otimes I_3 + \frac{\sigma_{1-}\sigma_{1+}}{2}\otimes\sigma_{2+}\otimes I_3\right)\tilde{\rho}_A\left(\sigma_{1-}\otimes\frac{\sigma_{2-}\sigma_{2+}}{2}\otimes I_3 + \frac{\sigma_{1-}\sigma_{1+}}{2}\otimes\sigma_{2-}\otimes I_3\right)\right.$$
$$\left. - \frac{1}{2}\left\{\left(\sigma_{1-}\otimes\frac{\sigma_{2-}\sigma_{2+}}{2}\otimes I_3 + \frac{\sigma_{1-}\sigma_{1+}}{2}\otimes\sigma_{2-}\otimes I_3\right)\left(\sigma_{1+}\otimes\frac{\sigma_{2-}\sigma_{2+}}{2}\otimes I_3 + \frac{\sigma_{1-}\sigma_{1+}}{2}\otimes\sigma_{2+}\otimes I_3\right), \tilde{\rho}_A\right\}\right)$$

$$+\frac{\boldsymbol{\gamma\left(-\frac{\beta-2\omega_0}{2}\right)}}{\mathbf{64}}\Big(\Big(\sigma_{1-}\otimes\frac{\sigma_{2-}\sigma_{2+}}{2}\otimes I_3+\frac{\sigma_{1-}\sigma_{1+}}{2}\otimes\sigma_{2-}\otimes I_3\Big)\tilde{\rho}_A\Big(\sigma_{1+}\otimes\frac{\sigma_{2-}\sigma_{2+}}{2}\otimes I_3+\frac{\sigma_{1-}\sigma_{1+}}{2}\otimes\sigma_{2+}\otimes I_3\Big)$$
$$-\frac{1}{2}\Big\{\Big(\sigma_{1+}\otimes\frac{\sigma_{2-}\sigma_{2+}}{2}\otimes I_3+\frac{\sigma_{1-}\sigma_{1+}}{2}\otimes\sigma_{2+}\otimes I_3\Big)\Big(\sigma_{1-}\otimes\frac{\sigma_{2-}\sigma_{2+}}{2}\otimes I_3+\frac{\sigma_{1-}\sigma_{1+}}{2}\otimes\sigma_{2-}\otimes I_3\Big),\tilde{\rho}_A\Big\}\Big)$$
$$+\frac{\boldsymbol{\gamma\left(\frac{\beta+2\omega_0}{2}\right)}}{\mathbf{64}}\Big(\Big(\sigma_{1-}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2-}\otimes I_3\Big)\tilde{\rho}_A\Big(\sigma_{1+}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2+}\otimes I_3\Big)$$
$$-\frac{1}{2}\Big\{\Big(\sigma_{1+}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2+}\otimes I_3\Big)\Big(\sigma_{1-}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2-}\otimes I_3\Big),\tilde{\rho}_A\Big\}\Big)$$
$$+\frac{\boldsymbol{\gamma\left(-\frac{\beta+2\omega_0}{2}\right)}}{\mathbf{64}}\Big(\Big(\sigma_{1+}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2+}\otimes I_3\Big)\tilde{\rho}_A\Big(\sigma_{1-}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2-}\otimes I_3\Big)$$
$$-\frac{1}{2}\Big\{\Big(\sigma_{1-}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2-}\otimes I_3\Big)\Big(\sigma_{1+}\otimes\frac{\sigma_{2+}\sigma_{2-}}{2}\otimes I_3+\frac{\sigma_{1+}\sigma_{1-}}{2}\otimes\sigma_{2+}\otimes I_3\Big),\tilde{\rho}_A\Big\}\Big) \tag{34}$$

Having quantum master equation at hand is half of task: solution of master equation Eq. (34) (to be presented elsewhere) is needed for further use and analysis. We will now briefly comment on possible approaches in this regard.

The obtained master equation is local in time, with time-independent decay rates and Lindblad operators. Nevertheless, solving this equation is associated with some computational challenges.

By the solution of the master equation, we refer to the Kraus decomposition (RIVAS and HUELGA, 2011):

$$\rho(t)=\sum_{i=1}^{d^2}K_i(t)\rho(0)K_i^{\dagger}(t), \tag{35}$$

which follows from Kraus' theorem, which asserts that any CPTP dynamics can be cast in the above form. $K_i(t)$ are so-called Kraus' operators, while d denotes dimension of state space of open quantum system.

The method for obtaining Kraus decomposition when the master equation is known (and vice versa) is presented in (ANDERSSON *et al*., 2007). It turns out that, in the case of three qubits considered in this paper, the method involves the use of 64×64 matrices with highly complex matrix elements, which poses a computational challenge even for specialized mathematical software. In other words, dimension of the problem increases exponentially with the system size. Obtaining Kraus decomposition is preferable whenever an assessment or verification of the algebraic properties of the dynamics of an open quantum system is required, irrespective of the physical aspects of interest — be they thermodynamic, optical, of any other nature.

Otherwise, the quantum master equation can be solved using numerical methods. Let us mention two possibilities. Using the procedure known as *quantum unravelling of the master equation* (BREUER and PETRUCCIONE, 2002) has advantage that instead working with the statistical operator everything shifts to the wave functions (each of them undergoing "quantum trajectory"). In this way, saving in computational resources is quadratic: from $\sim d^2$ parameters for density matrix to $\sim d$ parameters for wave function. This is especially convenient for finite-dimensional quantum systems: it is relatively easy to make computations using methods of numerical linear algebra.

On the other hand, quantum master equation can be expressed by systems of partial differential equations. One of the most popular approaches for solving systems of partial differential equations is the 4th-order Runge-Kutta algorithm. By integrating master equation, the density operator of open quantum system can be obtained at any time t. Some details about this and other numerical algorithms can be found in (PRESS *et al*., 2007), with a discussion of

the advantages and limitations of the methods. Of course, alternative methods and approaches found in contemporary literature also merit investigation; the discussion above is intended merely to illustrate the established procedure in the numerical solution of the master equation.

Formally, the equation Eq. (34) can also be recast in a time-dependent form, where the decay rates are specified *a priori,* based on certain phenomenological considerations, for example. This, in turn, may lead into the realm of non-Markovian dynamics through the lenses of quantum thermodynamics, to name just one possibility.

CONCLUSION

In this paper, a Markovian quantum master equation for three qubits in thermal equilibrium with the environment has been derived. The resulting master equation may be of interest for problems in e.g. quantum thermodynamics or quantum optics, within either an analytical or numerical approach.

Acknowledgments

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Appendix 1:

Dyadic expressions for spin-$\frac{1}{2}$ operators are given by well-known equalities:

$I = |g\rangle\langle g| + |e\rangle\langle e|$,

$S_z = \frac{\hbar}{2}(|g\rangle\langle g| - |e\rangle\langle e|)$,

$S_x = \frac{\hbar}{2}(|g\rangle\langle e| + |e\rangle\langle g|)$ and

$S_y = \frac{i\hbar}{2}(|g\rangle\langle e| - |e\rangle\langle g|)$.

From these equalities, dyadic form of spin raising and lowering operators follows:

$S_+ = S_x + iS_y = \hbar|e\rangle\langle g|$,

$S_- = S_x - iS_y = \hbar|g\rangle\langle e|$,

as well as expressions:

$|g\rangle\langle g| = \frac{1}{2}\left(I + \frac{2S_z}{\hbar}\right)$,

$|e\rangle\langle e| = \frac{1}{2}\left(I - \frac{2S_z}{\hbar}\right)$.

To meet specific requirements of calculations in this paper, it is useful to have in mind relations:

$\left(I + \frac{2S_z}{\hbar}\right)^2 = \frac{2}{\hbar}(\hbar I + 2S_z) = 4|g\rangle\langle g|$,

$\left(I - \frac{2S_z}{\hbar}\right)^2 = \frac{2}{\hbar}(\hbar I - 2S_z) = 4|e\rangle\langle e|$,

$S_-S_+ = \hbar^2|g\rangle\langle g| = \frac{\hbar^2}{2}\left(I + \frac{2S_z}{\hbar}\right)$ and

$S_+S_- = \hbar^2|e\rangle\langle e| = \frac{\hbar^2}{2}\left(I - \frac{2S_z}{\hbar}\right)$.

Appendix 2

The aim of this Appendix is to outline the derivation of expressions Eqs. (14). Having in mind that ρ_B is separable state, i.e. tensor product of density operators for each of m modes

$\rho_B = \rho_1 \otimes \rho_2 \ldots \otimes \rho_{\vec{k}} \ldots \otimes \rho_{mB}$,

it follows $\langle b^\dagger_{\vec{k}} \rangle = tr\left[b^\dagger_{\vec{k}} \rho_B\right] = tr\left[b^\dagger_{\vec{k}} \rho_1 \rho_2 \ldots \rho_{\vec{k}} \ldots \rho_{mB}\right] = tr\left[b^\dagger_{\vec{k}} \rho_{\vec{k}}\right]$, where the identity $tr[A_1 \otimes A_2 \ldots \otimes A_m] = trA_1 trA_2 \ldots trA_m$ is used and the fact that $tr\left[\rho_{B_{\vec{k}}}\right] = 1, \forall \vec{k}$.

With use of the explicit form of density operator for mode with frequency $\omega_{\vec{k}}$:

$\rho_{\vec{k}} = \sum_{k=0}^{\infty} e^{-\frac{\hbar \omega_{\vec{k}} n_{\vec{k}}}{k_B T}} |n_{\vec{k}}\rangle \langle n_{\vec{k}}|$,

the average value is:

$$\langle b^\dagger_{\vec{k}} \rangle = \sum_{k=0}^{\infty} \langle n_{\vec{k}} \left| b^\dagger_{\vec{k}} e^{-\frac{\hbar \omega_{\vec{k}} n_{\vec{k}}}{k_B T}} \right| n_{\vec{k}} \rangle = 0, \quad \text{(A2.1)}$$

by virtue of creation operator properties. In similar way it is possible to show that $\langle b_{\vec{k}} \rangle = 0$.

By definition, $\langle b^\dagger_{\vec{k}} b_{\vec{k}'} \rangle = tr\left[b^\dagger_{\vec{k}} b_{\vec{k}'} \rho_B\right]$ and using separability of state ρ_B follows:

$$\langle b^\dagger_{\vec{k}} b_{\vec{k}'} \rangle = tr\left[b^\dagger_{\vec{k}} b_{\vec{k}'} \rho_1 \rho_2 \ldots \rho_{\vec{k}} \rho_{\vec{k}'} \ldots \rho_{mB}\right] = tr\left[b^\dagger_{\vec{k}} \rho_{\vec{k}} b_{\vec{k}'} \rho_{\vec{k}'}\right] = \langle b^\dagger_{\vec{k}} \rangle \langle b_{\vec{k}'} \rangle = 0.$$

In case of $\vec{k} = \vec{k}'$:

$\langle b^\dagger_{\vec{k}} b_{\vec{k}} \rangle \stackrel{\text{def}}{=} \langle n_{\vec{k}} \rangle = tr\left[b^\dagger_{\vec{k}} b_{\vec{k}} \rho_B\right] = \frac{1}{Z} \sum_{k=0}^{\infty} n_k e^{-\frac{\hbar \omega_k n_k}{k_B T}} = \frac{1}{e^{\frac{\hbar \omega_{\vec{k}}}{k_B T}} - 1}$, so, in one place:

$$\langle b^\dagger_{\vec{k}} b_{\vec{k}'} \rangle = \langle n_{\vec{k}} \rangle \delta_{\vec{k}\vec{k}'}. \quad \text{(A2.2)}$$

Using commutator relation $\left[b_{\vec{k}}, b^\dagger_{\vec{k}'}\right] = \delta_{\vec{k}\vec{k}'}$ with (A2.2) follows the equality: $\langle b_{\vec{k}} b^\dagger_{\vec{k}'} \rangle = \left(1 + \langle n_{\vec{k}} \rangle\right) \delta_{\vec{k}\vec{k}'}$.

The rest of identities can be obtained by similar line of reasoning.

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NONCOMMUTATIVE SCALAR FIELDS: QUANTUM SYMMETRIES AND BRAIDED BV QUANTIZATION

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ABSTRACT. It is strongly believed that the fully consistent quantum gravity theory should lead to a quantum spacetime. The continuous description of spacetime in terms of differential manifolds is no longer adequate at the quantum gravity energies. Although the full quantum gravity is still unknown, there are several physical theories/models that incorporate the idea of a quantum spacetime. Some of them are: string theory, loop quantum gravity, noncommutative (NC) geometry. In this short paper we address the properties of scalar fields on noncommutative spacetimes. We will discuss the deformed symmetries and quantization of the ϕ^4-theory in four dimensions for two different NC deformations: Moyal or θ-constant NC spacetime and the λ-Minkowski spacetime. Using the newly developed braided BV quantization, we will show that there are no non-planar diagrams and no UV/IR mixing for both NC deformations. However, a nontrivial deformation of the momentum conservation law appears in the λ-Minkowski spacetime.

Keywords: NC scalar field, Drinfel'd twist, braided L_∞-algebra, BV quantization

INTRODUCTION

Following the successful formulation of Quantum Mechanics (QM) and the growing experimental results in particle physics, in the late 1920s the development of Quantum Field Theory (QFT) began. In the early days of Quantum Electrodynamics, the problem of calculating electron self-energy appeared: the UV limit of the obtained results was divergent. Motivated by the success of his uncertainty relations, Heisenberg (HEISENBERG, 1930) suggested imposing noncommutativity between coordinate operators

$$[x_i, x_j] \sim \theta^{ij}\,, \tag{1.1}$$

resulting in the uncertainty relations between coordinates

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$$\Delta x_i \, \Delta x_j \geq \theta^{ij} \, . \tag{1.2}$$

However, Heisenberg soon gave up this idea, regarding it as too radical. In the attempt to eliminate the ultra-violet (UV) divergences in QFT, in 1947, Snyder proposed a way to obtain a discrete space-time replacing the usual coordinates by the operators satisfying nontrivial commutation relations (SNYDER, 1947). This was the first time that noncommutative (NC) spaces appeared in physics. However, Snyder's idea was not accepted at that time. One reason was that the renormalization theory came out to be very successful in eliminating divergences in QFT. The second reason was the mathematical complexity of NC spaces. It took some time until the mathematical structure was formulated, and the first physical models were derived. The mathematical structure of NC spaces became clearer in the 1980s and the 1990s. One of the main results was the Gelfand-Naimark theorem (GELFAND and NAIMARK, 1947). It states that it is possible to describe a manifold by an (appropriately restricted) algebra of functions on the manifold. The space behind can be ignored completely since all the important information are now contained in the algebra of functions. This theorem can be generalized in different ways. For example, the algebra of functions does not have to be commutative, it can be a deformation of the commutative one. If the deformation is continuous, then there exists a set of continuous parameters that control the noncommutativity. The usual commutative space-time (manifold) is obtained for special values of these parameters. The deformed algebra of functions is not the algebra of functions on a manifold but on a "noncommutative space". The main notion that is lost in this generalization is that of a point: Noncommutative geometry is pointless geometry.

In this short paper we address the properties of scalar fields on noncommutative spacetimes using the formalism of the Drinfel'd twist and the homological perturbation theory. In the next section we review the construction of NC ϕ^4-theory scalar field theory via the Drinfel'd twist and the briaded L_∞-algebra. In Sections 3 and 4 we then discuss the deformed symmetries and quantization of the ϕ^4-theory in four dimensions for two different NC deformations: Moyal or θ-constant NC spacetime and the λ-Minkowski spacetime respectfully.

Noncommutative scalar field theory

Nowadays there are different approaches to noncommutative geometry (CONNES, 1994, LANDI, 1997; MADORE, 1999; ASCHIERI *et al*., 2008). A well-defined way to introduce noncommutative deformations of spacetime and the corresponding symmetries (Lorentz, Poincaré, conformal...) is via Drinfel'd twist (DRINFEL'D, 1985). The twist deforms the symmetry (Hopf) algebra by changing the comultiplication, that is the Leibniz rule of the symmetry generators when they act on products of representations changes. In this way some of the standard conservation laws become deformed. To have modules algebras (functions, differential forms, tensors...) consistent with the deformed symmetries, the twist operator has to be applied to deform them as well. In particular, the new multiplication in module algebras, $\star$-multiplication, is introduced via the inverse of the given twist operator.

Abelian twist – In this paper we will focus on a particular class of Drinfel'd twist operators, the Abelian Drinfel'd twists. They are defined using the set of commuting vector fields

$$\mathcal{F} = \exp\left(-\frac{\mathrm{i}\theta^{AB}}{2}(X_A \otimes X_B)\right) . \tag{2.1}$$

The set of commuting vector fields X_A, X_B are chosen between the generators of the Poincaré algebra. The twist operator can in generally be constructed from a more general set of vector fields. Our choice ensures that the standard Poincaré symmetry of (quantum field

theory on) Minkowski spacetime is replaced by a deformed/twisted Poincaré symmetry. The matrix θ^{AB} is antisymmetric and constant. It is considered as a small deformation parameter[2].

The pointwise product between functions $\mu(f \otimes g) = f \cdot g$ is replaced by the noncomutative $\star$-product, defined via

$$\begin{aligned} f \star g &= \mu \circ \mathcal{F}^{-1}(f \otimes g) \\ &= f \cdot g + \frac{\mathrm{i}\theta^{AB}}{2}(X_A \mathrm{f} \cdot X_B g) + \boldsymbol{O}(\theta^2)\,. \end{aligned} \tag{2.2}$$

The noncommutativity in the space of functions is expressed via triangular $\mathcal{R}$ matrix so that the following relations hold

$$\begin{aligned} f \star g &= \mathcal{R}^{-1}(g \star f) = \mathrm{R}_\alpha g \star \mathrm{R}^\alpha f\,, \\ \mathcal{R}^{-1} &= \mathcal{F}^2 \equiv \mathrm{R}_\alpha \otimes \mathrm{R}^\alpha\,. \end{aligned} \tag{2.3}$$

To define a scalar field theory on the NC spacetime defined by (2.2) and (2.3), we use the formalism of the braided L_∞-algebras. It is well known that the data of any classical field theory are completely encoded in a corresponding L_∞-algebra (HOHM and ZWIEBACH, 2017; JURČO *et al*., 2019). Applying the twist formalism to a classical L_∞-algebra results in the braided L_∞-algebra and the corresponding field theory is referred to as the braided field theory (DIMITRIJEVIĆ ĆIRIĆ *et al*., 2021).

Classical braided scalar field theory – We illustrate this formalism on the simple example of a real massive scalar field ϕ in four dimensions with $\lambda\phi^4$-interaction. The underlying braided L_∞-algebra of this theory is graded vector space $V = V_1 \oplus V_2$, consisting of the space of fields V_1 and the space of antifields V_2, equipped with the set of braided brackets

$$\begin{aligned} \ell_1^\star(\phi) &= (-\Box - m^2)\,\phi\,, \\ \ell_3^\star(\phi_1, \phi_2, \phi_3) &= \lambda\,\phi_1 \star \phi_2 \star \phi_3\,, \\ &= \lambda \mathrm{R}_\alpha \phi_2 \star \mathrm{R}^\alpha \phi_1 \star \phi_3 = \phi_1 \star \mathrm{R}_\alpha \phi_3 \star \mathrm{R}^\alpha \phi_2\,, \end{aligned} \tag{2.5}$$

for $\lambda \in \mathbb{R}$ and all $\phi_i \in V_1$. In the last line of (2.5) we explicitly wrote the braided symmetry of the $\ell_3^\star$ bracket.

The cyclic pairing of degree -3 is taken to be

$$\langle \phi, \phi^+ \rangle_\star = \int \mathrm{d}^4\mathrm{x}\ \phi \star \phi^+ \tag{2.6}$$

where $\phi \in V_1$ and $\phi^+ \in V_2$.

This construction leads to the action functional

---

[2]More precisely, the twist (2.1) is defined as

$$\mathcal{F} = \exp\left(-\frac{\mathrm{i}\kappa\theta^{AB}}{2}(X_A \otimes X_B\right)$$

where θ^{AB} is the constant antisymmetric matrix and the small deformation parameter is labeled with κ. To shorten the notation, κ is usually absorbed in θ^{AB} and we say that θ^{AB} is the small deformation parameter.

$$\begin{aligned} S^{\star}(\phi) &= \frac{1}{2!}\langle \phi, \ell_1^{\star}(\phi)\rangle_{\star} - \frac{1}{3!}\langle \phi, \ell_2^{\star}(\phi,\phi)\rangle_{\star} - \frac{1}{4!}\langle \phi, \ell_3^{\star}(\phi,\phi,\phi)\rangle_{\star} + \cdots \\ &= \int d^4x \ \frac{1}{2}\phi(-\Box - m^2)\phi - \frac{\lambda}{4!}\phi \star \phi \star \phi \star \phi \ , \end{aligned} \tag{2.7}$$

and the equation of motion

$$\begin{aligned} F_{\phi} &= \ell_1^{\star}(\phi) - \frac{1}{2}\,\ell_2^{\star}(\phi,\phi) - \frac{1}{4!}\,\ell_3^{\star}(\phi,\phi,\phi) + \cdots = 0 \\ 0 &= (-\Box - m^2)\,\phi - \frac{\lambda}{4!}\,\phi \star \phi \star \phi \ . \end{aligned} \tag{2.8}$$

The free theory remains undeformed, while the interaction term has a NC contribution.

To better understand the constructed theory, we will choose two different Abelian twists based on the Poincaré algebra of the four dimensional Minkowski spacetime. In the next section we work with the Moyal (θ-constant deformation), while in Section 4 we discuss the λ-Minkowski spacetime.

Braided BV quantization: Moyal spacetime

The Moyal twist is defined as

$$\mathcal{F} = \exp\left(-\,\mathrm{i}/2\ \theta^{ij}\ \partial_i \otimes \partial_j\right) \ , \tag{3.1}$$

where $\left(\theta^{ij}\right)$ is a $(3)\times(3)$ antisymmetric real-valued matrix, and $\partial_i = \frac{\partial}{\partial x^i}$ for $i = 1,2,3$ are vector fields generating spatial translations on $\mathbb{R}^{1,3}$. In order to simplify some of the analysis in the quantum field theory, such as the treatment of time-ordering, as well as avoiding potential issues with unitarity, we restricted the twist (2.1) to spatial translation only. The corresponding $\star$-product of functions and the $\mathcal{R}$-matrix are given by

$$\begin{aligned} f \star g &= \mu \circ \mathcal{F}^{-1}(f \otimes g) \\ &= f \cdot g + \frac{\mathrm{i}\theta^{ij}}{2}\left(\partial_i f \cdot \partial_j g\right) + \ \boldsymbol{O}(\theta^2) \ , \\ \mathcal{R} &= \mathrm{R}^{\alpha} \otimes \mathrm{R}_{\alpha} = \mathcal{F}^{-2} = \exp\left(\mathrm{i}\theta^{ij}\ \partial_i \otimes \partial_j\right) . \end{aligned} \tag{3.2}$$

Braided scalar QFT – Let us now explain how to compute correlation functions of the interacting braided scalar field theory using the braided BV formalism developed in (NGUYEN *et al*., 2021). More details can be found in (BOGDANOVIĆ *et al*., 2024).

We start from the cohomology $H^{\bullet}(V)$ of the abelian L_{∞}-algebra (V, ℓ_1), which describes the classical vacua of the free (braided) scalar field theory on $\mathbb{R}^{1,3}$. The cohomology $H^{\bullet}(V)$ is also an abelian L_{∞}-algebra concentrated in degrees 1 and 2, given by the solution space $H^1(V) = \ker(\ell_1)$ of the massive Klein–Gordon equation $(\Box + m^2)\,\phi = 0$ and the space $H^2(V) = \mathrm{coker}(\ell_1)$ with the trivial differential 0.

The n-point correlation functions in momentum space are defined as

$$\widetilde{G}_n^{\star}(p_1,\dots,p_n)^{\mathrm{int}} = \sum_{m=1}^{\infty} \mathrm{P}((\,\mathrm{i}\hbar\Delta_{\mathrm{BV}}\mathrm{H} + \{S_{\mathrm{int}},-\}_{\star}\mathrm{H})^m(\mathrm{e}^{p_1}\odot_{\star}\cdots\odot_{\star}\mathrm{e}^{p_n}))\ . \tag{3.3}$$

This is a formal power series expansion in $\hbar$ and the coupling constant λ in S_{int} . Let us clarify the operators appearing in this definition.

We start by defining a translation-equivariant projection $\mathrm{p}:\mathrm{V}\to H^{\bullet}(V)$ of degree 0 and a translation-invariant contracting homotopy $\mathrm{h}:V_2\to V_1$. For this, let $\mathsf{G}:C^{\infty}(\mathbb{R}^{1,3})\to C^{\infty}(\mathbb{R}^{1,3})$ denote the scalar Feynman propagator

$$\mathsf{G} = -\frac{1}{\Box + m^2} \qquad \text{with} \qquad \widetilde{\mathsf{G}}(k) = \frac{1}{k^2 - m^2}\ , \tag{3.4}$$

where $\widetilde{\mathsf{G}}(k)$ are the eigenvalues of the Green operator G when acting on plane wave eigenfunctions of the form $\mathrm{e}^{\mathrm{i}\,k\cdot x}$. It satisfies

$$\ell_1\circ\mathsf{G} = -(\Box + m^2)\circ\mathsf{G} = \mathrm{id}_{C^{\infty}(\mathbb{R}^{1,3})}\ . \tag{3.5}$$

ince we are interested in calculating (braided) correlation functions, we take the trivial projection map $\mathrm{p}=0$, or more accurately we restrict the cochain complex of $H^{\bullet}(V)$ to its trivial subspaces. With these choices, the contracting homotopy $\mathrm{h}:V_2\to V_1$ is given by the propagator $\mathrm{h}=\mathsf{G}$. In momentum space representation the contracting homotopy acts as

$$\mathrm{h}(\phi^+)(k) = \frac{\phi^+(k)}{k^2 - m^2}\ . \tag{3.6}$$

Next, we extend the maps p and h to the braided space of functionals $\mathrm{Sym}_{\mathcal{R}}(V[2])$ on V. This space represents the space of obesrvables in QFT. The data given above induce a trivial projection map $\mathsf{P}:\mathrm{Sym}_{\mathcal{R}}(V[2])\to\mathrm{Sym}_{\mathcal{R}}\big(H^{\bullet}(V[2])\big)$ given by

$$\mathsf{P}(1) = 1 \qquad \text{and} \qquad \mathsf{P}\Big(\varphi_1\odot_{\star}\cdots\odot_{\star}\varphi_n\Big) = 0\ . \tag{3.7}$$

The extended contracting homotopy $\mathsf{H}:\mathrm{Sym}_{\mathcal{R}}(V[2])\to\mathrm{Sym}_{\mathcal{R}}(V[2])$ is defined as

$$\begin{aligned} \mathrm{H}(1) &= 0\ , \\ H\Big(\varphi_1\odot_{\star}\cdots\odot_{\star}\varphi_n\Big) &= \frac{1}{n}\sum_{a=1}^{n}\pm\,\varphi_1\odot_{\star}\cdots\odot_{\star}\varphi_{a-1}\odot_{\star}\mathrm{h}(\varphi_a)\odot_{\star}\varphi_{a+1}\odot_{\star}\cdots\odot_{\star}\varphi_n\ , \end{aligned} \tag{3.8}$$

or all $\varphi_1,\dots,\varphi_n\in V[2]$. We used the translation-invariance of h in (3.8) which trivializes the action of $\mathcal{R}$-matrices. Note that on generators $\varphi_a\in V[2]$, the twisted symmetric product $\odot_{\star}$ is braided graded commutative:

$$\varphi_a\odot_{\star}\varphi_b = (-1)^{|\varphi_a|\,|\varphi_b|}\,\mathrm{R}_{\alpha}(\varphi_b)\odot_{\star}\mathrm{R}^{\alpha}(\varphi_a)\ . \tag{3.9}$$

The translation invariant perturbation δ consists of the braided BV Laplacian Δ_{BV} and the braided antibracket with the interaction action $\{S_{\mathrm{int}},-\}_{\star}$

$$\delta = \mathrm{i}\,\hbar\Delta_{\mathrm{BV}} + \{S_{\mathrm{int}},-\}_{\star}\ . \tag{3.10}$$

The braided BV Laplacian is defined by

$$\Delta_{\mathrm{BV}}(1)=0 \quad , \qquad \Delta_{\mathrm{BV}}(\varphi_1)=0 \quad , \qquad \Delta_{\mathrm{BV}}(\varphi_1 \odot_\star \varphi_2)=\langle \varphi_1,\varphi_2\rangle_\star \, ,$$

$$\begin{aligned}\Delta_{\mathrm{BV}}\left(\varphi_1 \odot_\star \cdots \odot_\star \varphi_n\right) = \sum_{a<b} \pm\langle \varphi_a, \mathrm{R}_{\alpha_{a+1}} \cdots \mathrm{R}_{\alpha_{b-1}}(\varphi_b)\rangle_\star \varphi_1 \odot_\star \cdots \odot_\star \varphi_{a-1} \\ \odot_\star \mathrm{R}^{\alpha_{a+1}}(\varphi_{a+1}) \odot_\star \cdots \odot_\star \mathrm{R}^{\alpha_{b-1}}(\varphi_{b-1}) \odot_\star \varphi_{b+1} \odot_\star \cdots \odot_\star \varphi_n \, ,\end{aligned} \tag{3.11}$$

for all $\varphi_1, \ldots, \varphi_n \in V[2]$. The action of the braided BV Laplacian encodes the braided Wick theorem, that is the quantization of the free theory. In particular, the 4-point function in free theory is given by

$$\begin{aligned}\tilde{G}_4^\star(p_1,p_2,p_3,p_4)^{(0)} = \; & (\mathrm{i}\hbar\Delta_{\mathrm{BV}}\mathrm{H})^2 \, \mathrm{e}^{p_1} \odot_\star \mathrm{e}^{p_2} \odot_\star \mathrm{e}^{p_3} \odot_\star \mathrm{e}^{p_4} \\ = \; & (\mathrm{i}\hbar)^2(2\pi)^8 \big(\delta(p_1+p_2)\widetilde{\mathrm{G}}(p_1)\delta(p_3+p_4)\widetilde{\mathrm{G}}(p_3) \\ & +\delta(p_1+p_4)\widetilde{\mathrm{G}}(p_1)\delta(p_2+p_3)\widetilde{\mathrm{G}}(p_3) \\ & +\mathrm{e}^{-\mathrm{i}\,p_2\cdot\theta\,p_3}\,\delta(p_1+p_3)\widetilde{\mathrm{G}}(p_1)\delta(p_2+p_4)\widetilde{\mathrm{G}}(p_4) \, .\end{aligned} \tag{3.12}$$

The NC phase factor in the last term is the consequence of the nontrivial action of $\mathcal{R}$ -matrices in the braided Wick theorem. Unlike the standard NC QFTs (MINWALLA *et al.*, 2000; SZABO, 2003) where the Wick theorem is not deformed, in braided QFTs the free theory is deformed and the deformation is encoded in the braided Wick theorem.

The antibracket in (3.10) is the braided graded Poisson bracket

$$\{-,-\}_\star : \mathrm{Sym}_{\mathcal{R}}(V[2]) \otimes \mathrm{Sym}_{\mathcal{R}}(V[2]) \to \mathrm{Sym}_{\mathcal{R}}(V[2])[1]$$

defined by setting

$$\{\varphi_a,\varphi_b\}_\star = \langle \varphi_a,\varphi_b\rangle_\star = \pm\{\mathrm{R}_\alpha(\varphi_b), \mathrm{R}^\alpha(\varphi_a)\}_\star \tag{3.13}$$

for $\varphi_a \in V[2]$, and extending this to all of $\mathrm{Sym}_{\mathcal{R}}(V[2])$ as a braided graded Lie bracket which is a braided graded derivation on $\mathrm{Sym}_{\mathcal{R}}(V[2])$ in each of its slots; for example

$$\{\varphi_1, \varphi_2 \odot_\star \varphi_3\}_\star = \langle \varphi_1,\varphi_2\rangle_\star \odot_\star \varphi_3 \pm \mathrm{R}_\alpha(\varphi_2) \odot_\star \langle \mathrm{R}^\alpha(\varphi_1), \varphi_3\rangle_\star \, . \tag{3.14}$$

Interaction action For $\lambda\,\phi^4$-theory on $\mathbb{R}^{1,3}$, the interaction action $S_{\mathrm{int}} \in \mathrm{Sym}_{\mathcal{R}}(V[2])$ in (3.10) is defined by

$$S_{\mathrm{int}}^\star \equiv -\frac{1}{4!}\langle \xi, \ell_3^{\star ext}(\xi,\xi,\xi)\rangle_\star^{\mathrm{ext}} \, . \tag{3.15}$$

The contracted coordinate functions $\xi \in \mathrm{Sym}_{\mathcal{R}}(L[2]) \otimes V$ are given by

$$\xi = \int_k (\mathrm{e}_k \otimes \mathrm{e}^k + \mathrm{e}^k \otimes \mathrm{e}_k) \, , \tag{3.16}$$

where $\mathrm{e}_k(x) = \mathrm{e}^{-\mathrm{i}\,k\cdot x}$ is the basis of plane waves for V_1 with dual basis $\mathrm{e}^k(x) = \mathrm{e}_k^*(x) = \mathrm{e}^{\mathrm{i}\,k\cdot x}$ for V_2.

These bases are dual with respect to the inner product (2.6), in the sense that

$$\int_p \langle \mathrm{e}_k, \mathrm{e}^p \rangle_\star \, \mathrm{e}_p = \mathrm{e}_k \qquad \text{and} \qquad \int_k \mathrm{e}^k \, \langle \mathrm{e}_k, \mathrm{e}^p \rangle_\star = \mathrm{e}^p \,, \tag{3.17}$$

where throughout we use

$$\int \mathrm{d}^4 x \; \mathrm{e}^{\pm \mathrm{i} \, k \cdot x} = (2\pi)^4 \, \delta(k) \,. \tag{3.18}$$

The star-products among basis fields are

$$\mathrm{e}_k \star \mathrm{e}_p = \mathrm{e}^{-\frac{\mathrm{i}}{2} k \cdot \theta \, p} \; \mathrm{e}_{k+p} \,, \tag{3.19}$$

while the action of the inverse $\mathcal{R}$-matrix on them is given by

$$\mathcal{R}^{-1}\big(\mathrm{e}_k \otimes \mathrm{e}_p\big) = \mathrm{R}_\alpha(\mathrm{e}_k) \otimes \mathrm{R}^\alpha\big(\mathrm{e}_p\big) = \mathrm{e}^{\,\mathrm{i} \, k \cdot \theta \, p} \; \mathrm{e}_k \otimes \mathrm{e}_p \,. \tag{3.20}$$

Here we introduced the following notation $k \cdot \theta \, p = \theta^{ij} k_i p_j$. The explicit calculation of (3.15) using (2.6), (3.19) and (3.20) results in

$$S^\star_{\mathrm{int}} = \int_{k_1,k_2,k_3,k_4} V_4(k_1,k_2,k_3,k_4) \; \mathrm{e}^{k_1} \odot_\star \mathrm{e}^{k_2} \odot_\star \mathrm{e}^{k_3} \odot_\star \mathrm{e}^{k_4} \,. \tag{3.21}$$

The interaction vertex

$$V_4(k_1,k_2,k_3,k_4) = -\frac{\lambda}{4!} \; \mathrm{e}^{\frac{\mathrm{i}}{2} \sum_{a<b} k_a \cdot \theta \, k_b} \; (2\pi)^4 \, \delta(k_1 + k_2 + k_3 + k_4) \tag{3.22}$$

coincides with the vertex of the standard noncommutative $\lambda \, \phi^4$ -theory. It has the braided symmetry

$$V_4(k_{a+1}, k_a) = \mathrm{e}^{-\mathrm{i} \, k_a \cdot \theta \, k_{a+1}} \; V_4(k_1,k_2,k_3,k_4) \tag{3.23}$$

under interchange of any pair of neighbouring momenta, and also the cyclic symmetry

$$V_4(k_1,k_2,k_3,k_4) = V_4(k_4,k_1,k_2,k_3) \tag{3.24}$$

which follows from momentum conservation in (3.22).

One-loop two-point function – To illustrate both the formalism introduced above and the properties of the braided $\lambda \, \phi^4$-theory with Moyal deformation, we now present the result for the two-point function at one loop. From the definition (3.3) it follows

$$\tilde{G}^\star_2(p_1,p_2)^{(1)} = (\mathrm{i}\hbar \Delta_{\mathrm{BV}} \mathrm{H})^2 \, \{S_{\mathrm{int}}, \mathrm{H}(\mathrm{e}^{p_1} \odot_\star \mathrm{e}^{p_2})\}_\star \,.$$

Inserting the interaction action (3.21) results in

$$\begin{aligned} \tilde{G}^\star_2(p_1,p_2)^{(1)} \;\; = \; & \frac{4}{2} \int_{k_1,k_2,k_3,k_4} V_4(k_1,k_2,k_3,k_4) \\ & \times \big(\langle \mathrm{e}^{k_4}, \mathrm{G}(\mathrm{e}^{p_1}) \rangle_\star \, (\mathrm{i}\hbar \Delta_{\mathrm{BV}} \mathrm{H})^2 \, (\mathrm{e}^{k_1} \odot_\star \mathrm{e}^{k_2} \odot_\star \mathrm{e}^{k_3} \odot_\star \mathrm{e}^{p_2}) \\ & + \langle \mathrm{e}^{k_4}, \mathrm{G}(\mathrm{e}^{p_2}) \rangle_\star \, (\mathrm{i}\hbar \Delta_{\mathrm{BV}} \mathrm{H})^2 \, (\mathrm{e}^{p_1} \odot_\star \mathrm{e}^{k_1} \odot_\star \mathrm{e}^{k_2} \odot_\star \mathrm{e}^{k_3}) \big) \,. \end{aligned}$$

These expressions are evaluated by using the braided Wick expansion (3.12) in momentum space. Adding all contributions we obtain the one-loop contribution to the two-point function as

$$\tilde{G}_2^{\star}(p_1,p_2)^{(1)} = \frac{\hbar^2\,\lambda}{2}\,\frac{(2\pi)^4\,\delta(p_1+p_2)}{(p_1^2-m^2)\,(p_2^2-m^2)}\int_k \frac{1}{k^2-m^2}\ . \tag{3.25}$$

This result is independent of the deformation parameter and coincides with the classical two-point function (at $\theta = 0$), including the correct sign and overall combinatorial factor. It shows that there is no UV/IR mixing in the two-point function at one-loop order, in contrast to the standard noncommutative quantum field theory (MINWALLA *et al*., 2000; SZABO, 2003). It also suggests that there are no non-planar Feynman diagrams in perturbation theory. This appears to be a consequence of the braided symmetries of the interaction vertex due to the braided L_∞-structure, through its interplay with the braided Wick theorem. This result is also consistent with the results in (OECKL, 2000).

Braided BV quantization: λ-Minkowski spacetime

In the previous section we discussed the example of NC deformation of Minkowski spacetime (and Poincaré symmetry) in which the translations remain undeformed. This results in the standard conservation law of momenta, see (3.22). In this section we will discuss another deformation of Minkowski spacetime, but this time with broken translational invariance in the x-y plane. This deformation will result in the deformation of the momentum conservation law.

The λ-Minkowski spacetime is defined by the Drinfel'd twist (DIMITRIJEVIĆ ĆIRIĆ *et al*., 2018a)

$$\mathcal{F} = \exp\left(-\frac{\mathrm{i}\theta}{2}\left(\partial_z \otimes \partial_\varphi - \partial_\varphi \otimes \partial_z\right)\right). \tag{4.1}$$

The commuting vector fields ∂_z and $\partial_\varphi = x\,\partial_y - y\,\partial_x$ are the generators of translations in z direction and rotations around z-axis, respectly. The pointwise product between functions $\mu(f \otimes g) = f \cdot g$ is replaced by the noncomutative $\star$-product, defined via

$$\begin{aligned} f \star g &= \mu \circ \mathcal{F}^{-1}\,(f \otimes g)\,, \\ &= f \cdot g + \frac{\mathrm{i}\theta}{2}\left(\partial_z f \cdot \partial_\varphi g - \partial_\varphi f \cdot \partial_z g\right) + \boldsymbol{O}(\theta^2)\ . \end{aligned} \tag{4.2}$$

The feature of noncommutativity in the space of functions is expressed via triangular $\mathcal{R}$ matrix so that the following relations hold

$$\begin{aligned} f \star g &= \mathcal{R}^{-1}(g \star f) = \mathrm{R}_\alpha g \star \mathrm{R}^\alpha f\,, \\ \mathcal{R}^{-1} &= \mathcal{F}^2 \equiv \mathrm{R}_\alpha \otimes \mathrm{R}^\alpha\,. \end{aligned} \tag{4.3}$$

The underlying braided L_∞-algebra of the $\lambda\phi^4$ scalar field theory is again the graded vector space $V = V_1 \oplus V_2$, consisting of the space of fields V_1 and the space of antifields V_2, equipped with the set of braided brackets. Out of all possible combinations from elements $\phi \in V_1$ and $\phi^+ \in V_2$, the only nontrivial action of braided brackets is when applied on fields $\phi, \phi_i \in V_1$ only and are given by

$$\begin{aligned} \ell_1^\star(\phi) = \ell_1(\phi) &= -(\Box + m^2)\phi\,, \\ \ell_3^\star(\phi_1,\phi_2,\phi_3) &= \lambda\phi_1 \star \phi_2 \star \phi_3\,. \end{aligned} \tag{4.4}$$

In order to get numbers in this formalism, we have to introduce a braided cyclic pairing of degree -3 acting nontrivial only for fields $\phi \in V_1$ and antifields $\phi^+ \in V_2$ nontrivially defined by the integral

$$\langle \phi, \phi^+ \rangle_\star = \int d^4x\, \phi \star \phi^+ = \int d^4x\, \phi \cdot \phi^+ = \langle \phi, \phi^+ \rangle\,. \tag{4.5}$$

Using the given L_∞-algebra data, we can write the classical action and the corresponding equations of motion as

$$\begin{aligned} \mathrm{S}_{\mathrm{cl}} &= \frac{1}{2!}\langle \phi, \ell_1^\star(\phi)\rangle_\star - \frac{1}{4!}\langle \phi, \ell_3^\star(\phi,\phi,\phi)\rangle_\star \\ &= \int d^4x \frac{1}{2}\phi(-\Box - m^2)\phi - \frac{\lambda}{4!}\phi\star\phi\star\phi\star\phi\,, \end{aligned} \tag{4.6}$$

$$\begin{aligned} \mathrm{F}_\phi &= \ell_1^\star(\phi) - \frac{1}{3!}\ell_3^\star(\phi,\phi,\phi) = 0 \\ 0 &= (-\Box - m^2)\phi - \frac{\lambda}{3!}\,\phi\star\phi\star\phi\,. \end{aligned} \tag{4.7}$$

Note that formally, (4.6) has the same form as the corresponding action in the general abelian twist case (2.7).

Interaction action – To illustrate the difference between the Moyal case and the $\boldsymbol{\lambda}$-Minkowski spacetime we calculate again the one loop contribution to the two-point function.

The Feynman propagator G is the inverse of $\ell_1^\star$ given in (4.4). As in the previous section, we restrict to the trivial cohomology via $\mathrm{p} = 0$ and contracting homotopy becomes the actual propagator $h = \mathrm{G}$. In the momentum space representation it is

$$\mathrm{h}(\phi^+)(k) = \frac{\phi^+(k)}{k^2 - m^2} = \phi^+\,\widetilde{\mathrm{G}}(k)\,. \tag{4.9}$$

The interacting action functional $S_{\mathrm{int}}^\star \in \mathrm{Sym}_{\mathcal{R}}(L[2])$ is defined as

$$S_{\mathrm{int}}^\star \equiv -\frac{1}{4!}\langle \xi, \ell_3^{\star ext}(\xi,\xi,\xi)\rangle_\star^{\mathrm{ext}}\,. \tag{4.10}$$

Contracted coordinate functions $\xi \in \mathrm{Sym}_{\mathcal{R}}(L[2]) \otimes V$ used in definition are constructed as combinations

$$\xi = \int_k (\mathrm{e}_k \otimes \mathrm{e}^k + \mathrm{e}^k \otimes \mathrm{e}_k) \tag{4.11}$$

and other objects are naturally extended from acting on V to acting on $\mathrm{Sym}_{\mathcal{R}}(L[2]) \otimes V$ and lending results in $\mathrm{Sym}_{\mathcal{R}}(L[2])$ but being very careful that every time one commutes any neighboring elements, one has to introduce the $\mathcal{R}$ matrix.

In the plane wave basis we have $\mathrm{e}_k(x) = \mathrm{e}^{-\mathrm{i}\,k\cdot x}$ in V_1 and $\mathrm{e}^k(x) = \mathrm{e}^*_k(x) = \mathrm{e}^{\mathrm{i}\,k\cdot x}$ in V_2[3].

These basis vectors are dual with the respect to this pairing

$$\begin{aligned}\langle \mathrm{e}_k, \mathrm{e}^p\rangle &= \int \mathrm{d}^4x\, \mathrm{e}^{-\mathrm{i}\,k\cdot x} \star \mathrm{e}^{\mathrm{i}\,p\cdot x} \\ &= \int d^4x\, \mathrm{e}^{-\mathrm{i}\,(k+_\star \mathrm{p})\cdot x} = (2\pi)^4\delta(p+_\star k) \\ &= (2\pi)^4\delta(p+k)\,.\end{aligned} \tag{4.12}$$

The $\star$-sum of two and three momenta is defined as

$$\begin{aligned}k+_\star p &= R\left(\frac{\theta}{2}p_z\right)k + R\left(-\frac{\theta}{2}k_z\right)p, \\ p+_\star q+_\star r &= R(r_3+q_3)p + R(-p_3+r_3)q + R(-p_3-q_3)r\,,\end{aligned} \tag{4.13}$$

with the rotation matrix R given by

$$R\left(\frac{\theta}{2}p_z\right) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\left(\frac{\theta}{2}p_z\right) & \sin\left(\frac{\theta}{2}p_z\right) & 0 \\ 0 & -\sin\left(\frac{\theta}{2}p_z\right) & \cos\left(\frac{\theta}{2}p_z\right) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

While the $\star$-sum does not affect t and z components (they are summed in the usual, undeformed way), it modifies the sumation of the x and y components. This reflects the deformed momentum conservation law in the xy-plane. The corresponding $\star$-delta functions have the following properties

$$\begin{aligned}\delta^\star(k) &= \int \mathrm{d}^4x\, \mathrm{e}^{\pm\mathrm{i}\,k\cdot x} = \delta(k)\,, \\ \delta^\star(k_1+_\star k_2) &= \int \mathrm{d}^4x\, \mathrm{e}^{-\mathrm{i}\,k_1\cdot x} \star \mathrm{e}^{\mathrm{i}\,k_2\cdot x} = \int d^4x\, \mathrm{e}^{-\mathrm{i}\,(k_1+_\star \mathrm{k}_2)\cdot x} = \delta(k_1+k_2)\,, \\ \delta^\star(k_1+_\star k_2+_\star k_3) &= \int \mathrm{d}^4x\, \mathrm{e}^{-\mathrm{i}\,k_1\cdot x} \star \mathrm{e}^{\mathrm{i}\,k_2\cdot x} \star \mathrm{e}^{\mathrm{i}\,k_3\cdot x} = \delta^\star(k_2+_\star k_3+_\star k_1) \quad, \\ &= \delta^\star\big(k_1+\ (k_2+_\star k_3)\big) = \delta^\star\big((k_1+_\star k_2)+k_3\big)\,. \\ \delta^\star\big((-p_2)+_\star q+_\star(-q)+_\star(-p_1)\big) &= \delta^\star\big((-p_2)+_\star(-p_1)\big) = \delta(p_1+p_2)\,.\end{aligned} \tag{4.14}$$

To simplify calculations, we introduce the following notation

$$\begin{aligned}\partial_z \mathrm{e}^{k_i} &= ik_{iz}\mathrm{e}^{k_i}\,, \\ \partial_z \mathrm{e}_{k_j} &= -ik_{jz}\mathrm{e}_{k_j}\,, \\ \partial_\varphi \mathrm{e}^{k_i}(x) &= i\big(xk_{iy} - yk_{ix}\big)\mathrm{e}^{k_i}(x) = \left(k_{iy}\,\partial_{k_{ix}} - k_{ix}\,\partial_{k_{iy}}\right)\mathrm{e}^{k_i} = L_i\mathrm{e}^{k_i}\,, \\ \partial_\varphi \mathrm{e}_{k_j}(x) &= -i\big(xk_{jy} - yk_{jx}\big)\mathrm{e}_{k_j}(x) = \left(k_{jy}\,\partial_{k_{jx}} - k_{jx}\,\partial_{k_{jy}}\right)\mathrm{e}_{k_j}(x) = L_j\mathrm{e}_{k_j}(x)\,.\end{aligned}$$

The action of the $\mathcal{R}^{-1}$ matrix on the basis vectors can be written as

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[3] We note that the plane waves are not a basis fully adapted to the twist (4.1). A more natural choice would be a symmetry adapted basis obtained by solving the wave equation in the cylindrical coordinates. A detailed discussion in the "symmetry adapted basis" will be presented in (BOGDANOVIĆ *et al*., in preparation) .

$$\mathrm{e}^{k} \star \mathrm{e}^{p} = \mathrm{R}_{\alpha}\mathrm{e}^{p} \star \mathrm{R}^{\alpha}\mathrm{e}^{k} = e^{\theta(p_z L_k - k_z L_p)}(\mathrm{e}^{p} \star \mathrm{e}^{k}) \,, \tag{4.15}$$

and similarly for other basis vectors.

Starting from (4.10) and applying (4.15), we calculate the interaction action

$$S^{\star}_{\mathrm{int}} = \int_{k_1,k_2,k_3,k_4} V_4(k_1,k_2,k_3,k_4)\, \mathrm{e}^{k_1} \odot_{\star} \mathrm{e}^{k_2} \odot_{\star} \mathrm{e}^{k_3} \odot_{\star} \mathrm{e}^{k_4} \,. \tag{4.16}$$

The vertex $V(k_1,k_2,k_3,k_4)$

$$V(k_1,k_2,k_3,k_4) = -\frac{\lambda}{3!} e^{\theta \sum_{a<b}(k_{bz}L_a - k_{az}L_b)} (2\pi)^4 \delta^{\star}\left(k_1 +_{\star} k_2 +_{\star} k_3 +_{\star} k_4\right) \tag{4.17}$$

has the following properties under the permutation of momenta

$$\begin{aligned} V(k_2,k_1,k_3,k_4) = &\quad e^{\theta(k_{1z}L_2 - k_{2z}L_1)} V(k_1,k_2,k_3,k_4) \,, \\ V\big(k_1,k_3,k_2,k_{4,}\big) = &\quad e^{\theta(k_{2z}L_3 - k_{3z}L_2)} V(k_1,k_2,k_3,k_4) \,, \\ V(k_2,k_3,k_1,k_4) = &\quad e^{\theta(k_{1z}(L_2+L_3) - (k_{2z}+k_{3z}L_1)} V(k_1,k_2,k_3,k_4) \end{aligned} \tag{4.18}$$

and similarly for other permutations. We immediately notice that the interaction vertex (4.17) encodes the deformed conservation of momenta!

One-loop two-point function – By definition (3.3), the two-point function in momentum space is

$$\tilde{G}^{\star}_2(p_1,p_2) \quad = \sum_{m=1}^{\infty} \mathrm{P}(\,\mathrm{i}\hbar\Delta_{\mathrm{BV}}\mathrm{H} + \{S_{\mathrm{int}}, -\}_{\star}\mathrm{H})^m(\mathrm{e}^{p_1} \odot_{\star} \mathrm{e}^{p_2})) \,.$$

The first contribution is the free propagator, coming from $m = 1$ step

$$\tilde{G}^{\star}_2(p_1,p_2)^{(0)} = \mathrm{i}\hbar\Delta_{\mathrm{BV}}\mathrm{H}\left(\mathrm{e}^{p_1} \odot_{\star} \mathrm{e}^{p_2}\right) . \tag{4.19}$$

This reduces to

$$\tilde{G}^{\star}_2(p_1,p_2)^{(0)} = (\mathrm{i}\,\hbar)(2\pi)^4 \delta(p_1+p_2)\widetilde{\mathrm{G}}(p_1) \,, \tag{4.20}$$

which is the commutative result. The free theory is unchanged.

The one-loop contribution to $\tilde{G}^{\star}_2(p_1,p_2)$ is given by

$$\tilde{G}^{\star}_2(p_1,p_2)^{(1)} = (\mathrm{i}\hbar\Delta_{\mathrm{BV}}\mathrm{H})^2 \{S_{\mathrm{int}}, \mathrm{H}(\mathrm{e}^{p_1} \odot_{\star} \mathrm{e}^{p_2})\}_{\star} \,.$$

Following the same steps as in the previous section, we obtain

$$\tilde{G}^{\star}_2(p_1,p_2)^{(1)} = \frac{\hbar^2\,\lambda}{2} \frac{(2\pi)^4\,\delta(p_1+p_2)}{(p_1^2-m^2)\,(p_2^2-m^2)} \int_k \frac{1}{k^2-m^2} \,. \tag{4.21}$$

The result (4.21) is the same as (3.25) and it is identical to the result in the commutative case. Unlike in the standard NC QFT approach (DIMITRIJEVIĆ ĆIRIĆ *et al*., 2018b), there are no non-planar diagrams, and no UV/IR mixing appears. The deformed momentum conservation law does not change the two-point function (4.21). To see nontrivial consequences of the deformed momentum conservation law, we need to calculate correlation functions with more then one vertex. This is planned for our future work.

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MODERN COSMOLOGY – 100 YEARS OF QUANTUM SCIENCE

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ABSTRACT. In this article, we contribute to the special issue of the Kragujevac Journal of Science devoted to the International Year of Quantum Science and Technology (IYQ2025). We discuss several connections between Quantum Theory and Modern Cosmology. We begin with a brief overview of the major theoretical discoveries of Quantum Theory and Quantum Mechanics, proceed to Quantum Field Theory (QFT), and conclude with aspects of modern, quantum cosmology.

Keywords: International Year of Quantum Science and Technology, quantum mechanics, quantum field theory, modern cosmology.

INTRODUCTION

On 7 June 2024, United Nations General Assembly adopted Resolution No 78/287 and proclaimed 2025 the International Year of Quantum Science and Technology, IYQ. The Resolution contains two parts emphasizing one of the most important roles of science and its purpose of existence (https://docs.un.org/en/A/RES/78/287):

> *"...Emphasizing that quantum science and technology is vital for economic advancement and that its potential applications could address basic needs such as food, health, sustainable cities and communities, communications, clean water and energy, and support climate action...",*

as well as

> *"...Recognizing that the year 2025 coincides with the 100th anniversary of the development of the methods of quantum mechanics that have led to its prominence in both science and technology today...".*

One of the authors of this article was delighted and very proud when the Resolution was first announced. The other experienced similar emotions once he became aware of the Resolution, the IYQ program, and aspects of its implementation. The entire world recognized the importance and the tremendous, century-long effort of scientists in defining and

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developing this fundamental theory – the essence and one of the cores of what we now call Modern Physics. And not scientists in general, but more explicitly **physicists**. And not physicists in general, but, in particular, **theoretical physicists**.

Of course, as theoretical physicists, we fully acknowledge the great efforts and contributions of experimental physicists and many others. We simply wish to emphasize the fundamental contribution of theoretical physics to the foundations and development of Quantum Theory.

This article is written to celebrate 100 years of Quantum Science, and the narrative we choose, and use is intended primarily for young physicists, students, and all readers interested in various aspects of Quantum Theory and its applications.

The rest of the paper is organized as follows. In the next section, we review the major theoretical discoveries of Quantum Theory and Quantum Mechanics. The following two sections are devoted to the shortcomings of Quantum Mechanics and to Quantum Field Theory, respectively. After that, we discuss a portion of Modern Cosmology that involves the use of QFT in curved spacetime. We conclude with comments on Quantum Theory at the Planck scale, the wave function of the universe, the path-integral formulation of Quantum Theory, and our final thoughts. Throughout the paper, we use natural units i.e. $\hbar = c = 1$.

THANKS TO …

Quantum theory was not created all at once. According to Ball (BALL, 2025), "The creation of modern quantum mechanics was a messy business in which many of the participants did not grasp the significance of their own discoveries."

At the beginning of the 20th century, the limitations of the classical physical approach in describing processes and phenomena in the micro-world were becoming increasingly apparent. It was at this time that the first successful steps toward non-classical, i.e., quantum, descriptions began to emerge.

Thanks to Max Planck, we now know that light can be emitted in discrete quanta, i.e., as particles. This breakthrough occurred in 1900 and was published the following year (PLANCK, 1901).

Thanks to Albert Einstein, we now know that light (waves) can also be absorbed as particles. This discovery was made in 1905 (EINSTEIN, 1905).

Thanks to Louis de Broglie, we now understand that this dual nature of light-behaving as a wave in some circumstances and as a particle in others – is a general property of all micro-objects. This work was completed in 1924 and published in 1925 (DE BROGLIE, 1925).

Thanks to Werner Heisenberg, we now have a formal mathematical framework for the new physics-quantum physics. His work in 1925 (HEISENBERG, 1925) introduced matrix mechanics, which enabled the prediction of quantum properties of micro-objects, such as the emission spectra of atoms.

Thanks to Erwin Schrödinger and the circumstances of the time, we also have an alternative, and ultimately more popular, framework called wave mechanics. Schrödinger was inspired by de Broglie's largely overlooked suggestion. This work was completed in 1926 (SCHRÖDINGER, 1926).

Heisenberg's 1925 work is considered the first published article in which the theoretical foundations of Quantum Mechanics were defined. That is why 2025 marks the celebration of 100 years of Quantum Theory and Quantum Technology, recognized as the International Year of Quantum Science and Technology (IYQ2025).

Thanks to Niels Bohr, Max Born, Wolfgang Pauli, Arnold Sommerfeld, John von Neumann, and many others, we now have a much deeper understanding of the quantum nature of Nature.

BUT …

From the very beginning, Quantum Mechanics was unable to address relativistic phenomena, which are treated at the classical (non-quantum) level by the Special Theory of Relativity (STR). Extending the theory to encompass relativistic phenomena at the quantum level became both necessary and unavoidable. This challenge was ultimately addressed through the development of the Quantum Theory of Fields, now known as Quantum Field Theory (QFT).

How can relativistic considerations be implemented at the quantum level? The first step was achieved using symmetries. A consistent theory must be Lorentz invariant, i.e., invariant under the Lorentz group – or more precisely, the Poincaré group – which ensures that it is relativistic. These symmetries, which form the core of STR, must be incorporated into Quantum Mechanics.

In theory, additional symmetries simplify physical problems. For example, rotational invariance greatly simplifies scattering problems at both the classical and quantum levels. However, the inclusion of relativistic considerations through Lorentz invariance complicates quantum mechanical analysis. The primary reason is that, in relativistic systems, the number of particles need not be conserved.

In standard Quantum Mechanics, the dynamics of a particle are described by its wave function, i.e., the time evolution of the associated wave function, which is governed by the Schrödinger equation.

$$i\hbar \frac{\partial}{\partial t}\psi(t,\vec{x}) = \hat{H}\psi(t,\vec{x}), \tag{1}$$

where Hamiltonian of the system is

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} + V(\hat{\vec{x}}). \tag{2}$$

In order to incorporate Lorentz invariance even for a free-particle system, the first approach is to adopt the relativistic expression for the Hamiltonian.

$$\hat{H} = \sqrt{\hat{\vec{p}}^2 c^2 + m^2 c^4}, \tag{3}$$

However, this is not sufficient. To merge Quantum Mechanics with Lorentz invariance, it is necessary to abandon the single-particle paradigm of Quantum Mechanics. In relativistic phenomena, the number of particles need not be conserved, because the expression for a particle's energy

$$E^2 = \vec{p}^2 c^2 + m^2 c^4, \tag{4}$$

shows that energy can be converted into particles (i.e., mass) and vice versa. This implies that a multi-particle paradigm is required. Another, more mathematically rigorous explanation is that causality and unitarity cannot be simultaneously accommodated within the single-particle framework of Quantum Mechanics. For example, according to standard Quantum Mechanical procedures, the probability amplitude for a particle to propagate from one point to another is given by

$$K(\vec{x}_2,\vec{x}_1)=\left\langle \vec{x}_2\left|\exp\{-i\hat{H}t\}\right|\vec{x}_1\right\rangle, \tag{5}$$

where $\hat{H}$ can be either non-relativistic or relativistic. However, the probability amplitude will have non-zero value even if position 4-vectors $x_1=(ct,\vec{x}_1)$ and $x_2=(ct,\vec{x}_2)$ are space-like separated. This implies a violation of causality, i.e. $K(\vec{x}_2,\vec{x}_1)\neq 0$ is not physically acceptable result for space-like separated points.

In conclusion, there is no consistent quantum theory that is both relativistic and restricted to a single particle. At the quantum level, this has profound implications, as we will revisit. Quantum Field Theory (QFT) is the only framework capable of reconciling Quantum Mechanics with the Special Theory of Relativity (STR).

QUANTUM FIELD THEORY

Quantum Field Theory is necessary to describe nature at its most fundamental level, at the shortest distances accessible to us. The physical phenomena under consideration involve relativistic (fundamental) particles and their interactions, and QFT provides an elegant framework for understanding them (RATTAZZI, 2024).

The unification of Quantum Mechanics with the Special Theory of Relativity was not an easy task. Paul Dirac was among the first physicists to successfully describe the electron using only its quantum behaviour and the basic principles of STR (DIRAC, 1928). This work laid the foundation for Werner Heisenberg and Wolfgang Pauli to extend the description to particles of arbitrary mass, charge, or spin using quantum fields (HEISENBERG AND PAULI, 1929; HEISENBERG AND PAULI, 1930). They also introduced the Lagrangian formulation of Quantum Field Theory. For more details, see a recent reference by BERNARDEZ (2023).

For example, using the Lagrangian formalism the action functional for a real scalar field $\phi(t,\vec{x})$ (in Minkowski spacetime) is

$$S[\phi]=\frac{1}{2}\int dtd^3\vec{x}\left[\dot{\phi}^2-(\nabla\phi)^2-m^2\phi^2\right], \tag{6}$$

where dot denotes partial derivative with respect to time, and dynamical equation for the field is Klein-Gordon equation

$$\ddot{\phi}(t,\vec{x})-\nabla^2\phi(t,\vec{x})+m^2\phi(t,\vec{x})=0. \tag{7}$$

Solving this equation, and after canonical quantization procedure, we end up with quantum field $\hat{\phi}(t,\vec{x})$, whose mode expansion is

$$\hat{\phi}(t,\vec{x})=\frac{1}{\sqrt{2}}\frac{1}{(2\pi)^{3/2}}\int d^3\vec{k}\left[\hat{a}_{\vec{k}}v^*_{\vec{k}}(t)e^{i\vec{k}\cdot\vec{x}}+\hat{a}^\dagger_{\vec{k}}v_{\vec{k}}(t)e^{-i\vec{k}\cdot\vec{x}}\right], \tag{8}$$

where $v_{\vec{k}}(t)$ are mode functions, while $\hat{a}_{\vec{k}}$ and $\hat{a}^\dagger_{\vec{k}}$ are time-independent annihilation and creation operators, respectively. Each of these operators will annihilate or create one-particle state, which means that we now have in our hand tools to describe phenomena in which particles are destroyed or created.

The mode functions satisfy the equation

$$\ddot{v}_{\vec{k}}(t) + \omega_{\vec{k}}^2 v_{\vec{k}}(t) = 0, \tag{9}$$

where $\omega_{\vec{k}}$ is energy of a particle with mass m and momentum vector $\vec{k}$

$$\omega_{\vec{k}} = +\sqrt{\vec{k}^2 + m^2}. \tag{10}$$

Mode functions satisfy normalization conditions

$$W(v_{\vec{k}}, v_{\vec{k}}^*) \equiv \dot{v}_{\vec{k}}(t) v_{\vec{k}}^*(t) - v_{\vec{k}}(t) \dot{v}_{\vec{k}}^*(t) = 2i, \tag{11}$$

where $W(v_{\vec{k}}, v_{\vec{k}}^*)$ is Wronskian. Non-vanishing commutation relation for time-independent annihilation and creation operators is then

$$\left[\hat{a}_{\vec{k}}, \hat{a}_{\vec{q}}^\dagger\right] = \delta^{(3)}(\vec{k} - \vec{q}). \tag{12}$$

Quantum Field Theory thus addresses both challenges by introducing a new paradigm: the fundamental entities are not particles, but fields-abstract objects defined at every point in spacetime. Particles then emerge as excitations of these fields. From this perspective, there are fields corresponding to all types of particles, whether massive or massless, charged or neutral, and with spin (in unit of $\hbar$) zero, one half, one, one and a half, two, and so on. The framework for QFT is four-dimensional Minkowski spacetime, where all calculations are done.

A natural next step in the development of the quantum program is the formulation of QFT on curved spacetime.

QFT ON EXPANDING SPACETIME

Modern Cosmology is based on Einstein's Theory of General Relativity (CARROLL, 2019) and deals with phenomena in expanding spacetime. In expanding spacetime, such as spatially flat Friedmann-Lemaitre-Robertson-Walker (FLRW) spacetime (probably the most used spacetime by cosmologists), fields behave differently from what we know in the Minkowski spacetime of particle physics.

Spatially flat FLRW spacetime metric is of the form

$$ds^2 = -dt^2 + a(t)^2 d\vec{x}^2, \tag{13}$$

where t is cosmological time, $\vec{x}$ are comoving spatial coordinates and $a(t)$ is the scale factor of the Universe. We also use another time coordinate, the conformal time η defined as

$$dt = a(\eta) d\eta, \tag{14}$$

and the metric is now

$$ds^2 = a(\eta)^2 \left(-d\eta^2 + d\vec{x}^2\right). \tag{15}$$

For example, the action functional for real scalar field $\phi(\eta, \vec{x})$ (in FLRW spacetime) is (MUKHANOV AND WINITZKI, 2007)

$$S[\phi] = \frac{1}{2}\int d\eta d^3\vec{x} a^2 \left[\phi'^2 - (\nabla\phi)^2 - m^2 a^2 \phi^2\right], \tag{16}$$

where prime denotes derivative with respect to conformal time. Redefining scalar field

$$\chi(\eta, \vec{x}) = a(\eta)\phi(\eta, \vec{x}), \tag{17}$$

the action will look almost the same as the action for Minkowski spacetime

$$S[\chi] = \frac{1}{2}\int d\eta d^3\vec{x} \left[\chi'^2 - (\nabla\chi)^2 - m_{eff}^2 \chi^2\right], \tag{18}$$

where, now, we have time dependent effective mass squared

$$m_{eff}^2(\eta) = m^2 a^2(\eta) - \frac{a''(\eta)}{a(\eta)}. \tag{19}$$

This time dependence of effective mass accounts for the interaction of the field with the gravitational background. Dynamical equation for the field $\chi(\eta, \vec{x})$ is, without surprise, again of Klein-Gordon type

$$\ddot{\chi}(\eta, \vec{x}) - \nabla^2\chi(\eta, \vec{x}) + m_{eff}^2(\eta)\chi(\eta, \vec{x}) = 0. \tag{20}$$

Solving this equation, and after canonical quantization procedure, we end up with quantum field $\hat{\chi}(\eta, \vec{x})$, whose mode expansion is

$$\hat{\chi}(\eta, \vec{x}) = \frac{1}{\sqrt{2}} \frac{1}{(2\pi)^{3/2}} \int d^3\vec{k} \left[\hat{a}_{\vec{k}} v_{\vec{k}}^*(\eta) e^{i\vec{k}\cdot\vec{x}} + \hat{a}_{\vec{k}}^\dagger v_{\vec{k}}(\eta) e^{-i\vec{k}\cdot\vec{x}}\right]. \tag{21}$$

The mode functions satisfy the equation

$$v''_{\vec{k}}(\eta) + \Omega_{\vec{k}}^2(\eta) v_{\vec{k}}(\eta) = 0, \tag{22}$$

where $\Omega_{\vec{k}}$ is now

$$\Omega_{\vec{k}}(\eta) = +\sqrt{\vec{k}^2 + m_{eff}^2(\eta)}. \tag{23}$$

Mode functions satisfy the same normalization conditions as in Minkowski spacetime

$$W(v_{\vec{k}}, v_{\vec{k}}^*) \equiv v'_{\vec{k}}(\eta) v_{\vec{k}}^*(\eta) - v_{\vec{k}}(\eta) v'^*_{\vec{k}}(\eta) = 2i, \tag{24}$$

and non-vanishing commutation relation for time-independent operators $\hat{a}_{\vec{k}}$ and $\hat{a}_{\vec{q}}^\dagger$ is again

$$\left[\hat{a}_{\vec{k}}, \hat{a}_{\vec{q}}^\dagger\right] = \delta^{(3)}(\vec{k} - \vec{q}). \tag{25}$$

This means that $\hat{a}_{\vec{k}}$ and $\hat{a}_{\vec{q}}^\dagger$ can be again interpreted as the annihilation and creation operators.

Now that we know how to quantize scalar fields in expanding spacetime and interpret results, we can use it to study cosmological perturbations.

COSMOLOGICAL PERTURBATIONS

Real scalar fields are used most of the time in cosmology. We know how to mimic various cosmological fluids using scalar fields (MUKHANOV, 2005). We also know how to use scalar fields to study cosmological inflation (STAROBINSKY, 1980; GUTH, 1981; LINDE, 1982,) and to interpret the Cosmic Microwave Background Radiation (CMBR) spectrum (LYTH AND LIDDLE, 2009). We are also able to address the problem of primordial black hole formation as a dark matter candidate (BILIĆ *et al.*, 2025). All of this is done using cosmological perturbation theory.

Cosmological perturbations of spacetime are introduced through the metric

$$g_{\mu\nu}(\eta,\vec{x}) = \overline{g}_{\mu\nu}(\eta) + \delta g_{\mu\nu}(\eta,\vec{x}), \tag{26}$$

where $\overline{g}_{\mu\nu}(\eta)$ are components of non-perturbed spatially homogenous and flat background FLRW metric tensor, while $\delta g_{\mu\nu}(\eta,\vec{x})$ are metric perturbations. Explicitly,

$$\begin{aligned} ds^2 = {} & a^2\left[-(1+2A)d\eta^2 + 2(\partial_i B)d\eta dx^i\right] + \\ & a^2\left[\left(1-2(D+\frac{1}{3}(\partial_k\partial_k E))\right)\delta_{ij} + 2(\partial_i\partial_j E)\right]dx^i dx^j, \end{aligned} \tag{27}$$

where $A(\eta,\vec{x})$, $B(\eta,\vec{x})$, $D(\eta,\vec{x})$ and $E(\eta,\vec{x})$ are the scalar type metric perturbations. Perturbations of vector and tensor type are also present but are not explicitly written here. Perturbations $\delta\phi(\eta,\vec{x})$ of the scalar field are introduced in the same way

$$\phi(\eta,\vec{x}) = \phi_0(\eta) + \delta\phi(\eta,\vec{x}), \tag{28}$$

where $\phi_0(\eta)$ is non-perturbed solution of Klein-Gordon equation for spatially homogenous and flat background FLRW spacetime. The next step is to engage in the perturbation theory.

Before we enter into the perturbation theory, it is important to stress that neither $\delta\phi(\eta,\vec{x})$ nor $\delta g_{\mu\nu}(\eta,\vec{x})$ would be physical variables. They depend on choice of what coordinates are in use. The change of the coordinate system will change their values. A gauge-invariant definition of cosmological perturbations is unavoidable in order to make connection with physical observables, which are gauge-invariant. We need to define gauge-invariant perturbations by constructing quantities that remain invariant under coordinate transformations.

One such quantity (of scalar type) is Burdeen gauge invariant potential (BURDEEN, 1982)

$$\psi(\eta,\vec{x}) \equiv D + \frac{1}{3}(\partial_k\partial_k E) - H(B - \frac{\partial E}{\partial\eta}), \tag{29}$$

where $H(\eta) = a'/a$ is the Hubble parameter. We can also mention a very useful Mukhanov-Sasaki gauge invariant variable (MUKHANOV *et al.*, 1992) using Burdeen potential

$$v(\eta,\vec{x}) \equiv a(\eta)\delta\phi(\eta,\vec{x}) + \frac{a(\eta)\phi_0'(\eta)}{H(\eta)}\psi(\eta,\vec{x}), \tag{30}$$

Mukhanov-Sasaki variable will be our real scalar field to be quantized.

The action functional for this real scalar field is

$$S = \frac{1}{2}\int d\eta d^3\vec{x}\left((v')^2 - (\nabla v)^2 + \frac{z''}{z}v^2 \right), \tag{31}$$

where the so-called pump field $z(\eta)$ depends only on the background quantities

$$z(\eta) = \frac{a(\eta)\phi_0'(\eta)}{H(\eta)}. \tag{32}$$

Using the quantization procedure outlined in the previous section, we are able to quantize cosmological perturbations, compute the relevant quantities, and connect the resulting theoretical predictions with concrete observational data (MUKHANOV, 2005).

Let us mention and emphasize here a few very important applications of Quantum Theory in Cosmology, as well as an alternative, intuitive, and very useful formulation of Quantum Mechanics and QFT – the path-integral formulation (FEYNMAN AND HIBBS, 1965). It contributes to the introduction of the wave function of the universe (HARTLE AND HAWKING, 1983), one of the most widely studied approaches to Quantum Cosmology and, more broadly, Quantum Gravity.

There is no doubt that on the horizon of recent, modern, and, in particular, forthcoming applications of Quantum Mechanics, we find physics at the Planck scale. This line of research continues to challenge our fundamental understanding of spacetime at extremely small distances. Non-Archimedean spacetime (DRAGOVICH *et al.*, 2017) and the path-integral formulation of quantum dynamics on ultrametric spaces (DJORDJEVIC AND DRAGOVICH, 1997), together with Quantum Theory on non-commutative spacetime (SZABO, 2003), represent new and intriguing directions for Quantum Theory in its second century.

FINAL TOUGHTS

It is logical, and history of science shows it, that scientific development is very important, at least for later practical purposes, such as "making life easier." This article represents an attempt to connect various phases in the development of the quantum paradigm, following only one of the many branches that scientists carefully developed, starting from the micro-world and extending to the entire Universe.

Finally, we can proudly state that Quantum Theory is a highly successful and fruitful physical theory. According to Görnitz (GÖRNITZ, 2010), "About one third of the gross national product in the developed countries results from its applications. The applications of this theory range from nuclear power to all tools for computing, lasers, solar cells, and so on."

If the Universe is the Answer, what is the Question? (LEDERMAN, 2006).

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THREE QUESTIONS ON THE FUTURE OF QUANTUM SCIENCE AND TECHNOLOGY

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ABSTRACT. The answers on the current status and future development of Quantum Science and Technology are presented.

Keywords : quantum science, quantum technology.

INTRODUCTION

The Editorial Board of the Kragujevac Journal of Science decided to ask the prominent researchers and scholars to take part in the poll on the status and the future of Quantum Science and Technology. The Poll is stated (but not limited) by the following questions:

- Do you find the Quantum Measurement Problem worth striving?
- Which research directions do you find prominent in the quantum (a) theory and (b) application (including quantum technology)?
- What would you expect of the future post-quantum theory?

Here we thank for all answers received and Ralph Puchta for his initiative and commitment.

DO YOU FIND THE QUANTUM MEASUREMENT PROBLEM WORTH STRIVING?

Francesco Buscemi.[1] I really have no idea if or how the quantum measurement problem may be solved. Quantum theory itself has nothing to say about a putative solution, so, if I must pick one, I would say that any genuine resolution of the measurement problem, if it exists at all, would have to come from new physics for which we currently have neither hints nor any operational need, in a sense. For the moment, the problem seems to tell us more about the limits of our preferred narratives than about the limits of formalism itself.

David Deutsch.[2] It was solved by Hugh Everett in 1957. (And, according to Bitbol (BITBOL, 1996), by Schrödinger a little earlier but not published.)

Ruth E. Kastner:[4] Absolutely. The measurement problem is the inability of the theory to specify in physical terms what counts as a "measurement" meriting the assignment of an eigenstate of the measured observable to the system. I have argued that the measurement problem is a serious theoretical anomaly afflicting the conventional formulation of quantum theory, which presupposes that the only actual physical evolution taking place is always unitary, governed by the Schrodinger equation. For example, Everettian approaches remain afflicted by

the measurement problem since they cannot differentiate a correlating (entangling) interaction from an interaction yielding a definite outcome, leading to in-principle inconsistency. The latter is revealed in the possibility of empirically detectable discrepancies in Wigner's Friend-type scenarios. (See, e.g., KASTNER, 2020; KASTNER, 2024.)

The conventional adherence to the assumption of unbroken unitary evolution is what produces the measurement problem. It is resolved by adopting a historically present but neglected theory of field behavior, the 'direct action theory' or 'absorber theory of radiation'. My publications, in particular (KASTNER, 2022), present the solution, applicable to the fully relativistic domain, in terms of this theory.

Olimpia Lombardi.[5] During the early years after the formulation of quantum mechanics, the orthodox interpretational framework was tied to an instrumentalist reading: quantum features were discussed only in terms of possible measurements results, under the assumption that the concept of quantum measurement should be taken as a primitive concept of the theory. However, in the last decades, the traditional instrumentalist perspective has begun to lose its original strength. On the one hand, from a cosmological viewpoint, a quantum account of the universe cannot be based on measurement understood as an interaction between a system and a measuring apparatus. On the other hand, several realist interpretations of quantum mechanics have been proposed, with the purpose of understanding how reality would be if the theory were true.

From a more general viewpoint, the question is: Why is it worth insisting on the interpretation of quantum physics, not only quantum mechanics but also quantum field theory? If most interpretations are empirically equivalent, what is the point of carrying on the interpretive debates? I am certain that it is worth insisting on the interpretation of quantum physics because only at the interpretative level is a proper understanding of the subject achieved. Of course, the problem now consists in elucidating what is meant by *understanding*.

Understanding is an epistemic state that entails more than mere knowing: I may know that the fall of the Western Roman Empire occurred, but, at the same time, I may not understand that historical process. I consider that this plus of understanding over knowledge involves two features: *projectability* and *transferability*. On the one hand, subjects understand a certain knowledge better to the extent that they can project it further. For example, they can use it successfully to obtain new knowledge, they can infer causal connections from it, they can draw conclusions on its basis, they can transfer it to cases not originally considered and even strongly novel, they can even imagine counterfactual situations that fit it. On the other hand, subjects understand a certain knowledge better to the extent that they can transmit it to other subjects, even those who are not familiar with it. For example, the fact that a scientist can "explain" their topic of study to a layman is a symptom of their understanding, without requiring that the layman achieves a high level of comprehension. Of course, if the topic is very technical, in this process the "explainer" has to appeal to multiple resources, such as the use of images, metaphors, analogies, etc.; but it is precisely their capacity to generate such resources that shows their degree of understanding.

On the basis of these notes of what I conceive as understanding, it is easy to see why I consider that an interpretation of quantum physics provides understanding. If we only possess a formalism with the minimal interpretation that allows theory to be applied, we do not reach an understanding of the matter since we hardly have the necessary tools to project and transfer our knowledge. The full interpretation of formalism is what allows us to extend the quantum knowledge to new situations, to make inferences about which facts are in accordance with the picture provided by the theory, and to evaluate how well the world described by the theory fits into the categories that are at the basis of our traditional conception of reality. And it is only in terms of an interpretation that we can attempt to convey an image of quantum reality through ordinary language.

But even accepting what has been said so far about the notion of understanding, someone of instrumentalist temperament might insist: if the "operational core" of quantum physics has been so overwhelmingly successful in empirical terms, why do we need to understand it through interpretation? My answer is that understanding in the field of quantum physics has consequences for scientific practice itself. Certain interpretations lead to theories that may be more akin to other theoretical domains of physics, such as the conceptual link between quantum mechanics and quantum field theory, or to other scientific disciplines, such as chemistry. Furthermore, the instrumentalist spirit is perhaps one of the factors that discourage young people who seek to understand how the world works and that drive them away from physics. But I believe that the answer to the instrumentalist challenge depends primarily on how each of us conceives of the scientific enterprise. If science is understood exclusively as a means to produce technology in the form of concrete or abstract objects to be injected into consumer society and/or to improve the material lives of human beings, then the discussions about the interpretation of quantum theory make no sense. But those of us who believe that science is an end in itself, because it is essential to the intellectual development of human beings, will continue to think that the understanding provided by the interpretations of quantum physics has intrinsic value.

Tim Maudlin.[6] No serious physical theory with pretensions to being exact and fundamental should mention the term "measurement" in its fundamental principles, because that concept is not sufficiently sharp in meaning. "Measurements" are just some vaguely defined class of physical interactions between systems, with no special significance for the basic dynamics. Since some approaches (e.g. the "Copenhagen Interpretation") do employ the concept of measurement, these approaches should be replaced with theories that don't, for example pilot-wave theories or spontaneous collapse theories.

Philip Pearle.[7] The short answer is yes! When I took my first course in quantum theory, in my undergraduate Junior year, I saw that there was a problem. The indifference to it of the physics community then (which has been much improved in the 70 years since then) made me think this problem was worth making my life's work. I give a detailed account of my first encounter with quantum theory and my subsequent engagement with the Measurement Problem in the Preface of my recent book (PEARLE, 2024).

Briefly, the Measurement Problem is that, when describing an experiment, the wave function (evolving under Schrodinger's equation) does not correspond to reality, to the single actual outcome seen in the laboratory. Instead, the wave function is the sum of such outcomes, which is pretty weird. But we need to have the wave function describe reality, so the rules of quantum theory invoke an ill-defined "collapse postulate": the wave function somehow "jumps" to one or another outcome. As I detail in the first chapter of my book, Schrodinger thought this abandonment of his equation was very wrong, and he called it "the most interesting point of the entire theory."

There have been quite a few suggestions for resolving the Measurement Problem, prominent among them being adoption of the deBroglie-Bohm Pilot Wave alternative theory, or choosing some variant of the Many-Worlds theory. My own approach has been one I like to believe Schrodinger would have liked.

I add a term to Schrodinger's equation, so that the wave function smoothly evolves to describe a single outcome of an experiment. The extra term depends on a randomly fluctuating field, and each possible field leads to a definite outcome.

My first paper proposing this resolution was published in 1976, but it wasn't until 1989 that I introduced what I regard as a satisfactory embodiment of this idea, the Continuous Spontaneous Localization (CSL) theory. In the ensuing 36 years, there have been hundreds of theoretical and experimental papers on CSL. The experiments have neither proved CSL is correct nor ruled it out. If it is verified, it means that experiments will show that standard quantum theory is wrong in certain circumstances, and that would be tremendously exciting!

Lev Vaidman.[9] Yes.

Vlatko Vedral.[10] I think that there is no such thing as the measurement problem in quantum physics. Most of our lack of progress in finding a new theory has to do with the mistaken belief in the existence of the measurement problem. The key to understanding why there is no measurement problem is treating everything quantum mechanically, both the system and the apparatus (or anything else that is relevant for the analysis). I've written extensively about this and the related topics in my upcoming book "Portals to a New Reality" (VEDRAL, 2025).

Karol Życzkowski.[11] The "problem of quantum measurement" is an intriguing topic from a philosophical perspective, as ongoing research can deepen our understanding of the foundations of quantum theory. From a physicist's standpoint, I do not expect our current methods for estimating the probability of a particular measurement outcome to change significantly. These calculations, which are essential for experimental work at the microscopic scale, largely remain unaffected by the choice of interpretation of quantum theory. In fact, it is possible to perform complex quantum mechanical calculations and carry out sophisticated experiments without committing to any specific interpretation of quantum theory.

WHICH RESEARCH DIRECTIONS DO YOU FIND PROMINENT IN (a) THEORY AND (b) APPLICATION (INCLUDING QUANTUM TECHNOLOGY)?

Francesco Buscemi. I believe we should more decisively push toward an observer-dependent perspective, not only in quantum theory but in science as a whole, including cosmology. This idea is not new; it is as old as science itself. From time to time it resurfaces, and when it does it sheds new light on physics, yet it is quickly overshadowed again by the powerful illusion that we call "objective reality". In this spirit, I expect research directions that put center stage what an observer can infer and learn, and how such inferences are constrained or enabled by physical theory, to become increasingly prominent. Such an approach may guide both theoretical developments and quantum technologies.

David Deutsch. (a) Put quantum field theory on a sound ontological (not just predictive) footing; (b) Not my field.

Ruth E. Kastner: There are several prominent directions currently, but the fact of their prominence is not a reflection of their fruitfulness. A general approach of increasing prominence (deservedly so) is exploring the idea that spacetime is not a fundamental background for physical systems but instead is an emergent manifold. One version of this approach, based on the transactional formulation, yields Einstein's equations of the general theory of relativity together with the cosmological constant (replacing the need for 'dark energy') and MOND correction (replacing the need for 'dark matter'); (SCHLATTER, AND KASTNER 2023).

Olimpia Lombardi: Nobody can deny the great relevance of quantum technology. Although I am not specialist in technological matters, I think that the most striking practical consequences of quantum theory are quantum information and quantum computing, as well as the production of novel quantum states of matter.

From a theoretical point of view, in addition to specific developments—such as protection against environmental noise or applications of entanglement and non-locality, just to mention a few examples, I believe that the interpretative work should not be overlooked, for the reasons I mentioned in my answer to the previous question. In particular, the research on quantum information and quantum computing has renewed the interest in questions about the foundations of the theory.

Tim Maudlin. As far as pure theory, both the pilot wave and spontaneous collapse approaches are worthy of pursuit. Perhaps the Many Worlds theory is, but it still faces basic

conceptual issues that have not been resolved. As far as technological design, I have no idea. I am not trained in engineering. There, all one really wants is some easily usable formalism that makes accurate predictions for the sorts of procedures you are interested in as an engineer (e.g. calculation, data processing, information transmission). It is perfectly possible that approaches not sharp enough for foundational theories can serve these purposes.

Philip Pearle. Unified with the answer to the third question, please see below.

Lev Vaidman: We have to come to agreement about interpretation and continue to look for new quantum devices.

Vlatko Vedral. The next two decades of science (and not just physics) will be defined by quantum physics going further and further into the macro domain. Chemistry, Biology, Neuroscience, and so on will ultimately be understood in terms of quantum physics. This will be enabled by the rapid development of quantum technologies, and we will also be witnessing the birth of a large-scale, universal quantum computer.

Karol Życzkowski: While it is hardly possible to demonstrate rigorously that quantum theory is the ultimate description of the microscopic world, all experimental data collected so far are consistent with its predictions. As a result, it is likely that quantum theory will continue to be used successfully in describing experiments and predicting new effects throughout the 21st century. Instead of questioning whether quantum mechanics accurately describes micro-scale phenomena, we often focus on identifying which quantum effects can be harnessed for technological purposes.

Recent advances in quantum physics have already led to the development of lasers, diodes, transistors, electron microscopes, and integrated circuits. Furthermore, ongoing experimental progress has rapidly expanded applications such as quantum information processing. Devices for quantum cryptography and quantum communication, which provide theoretically unbreakable security, are already commercially available. However, quantum computing remains in its early stages, with the key challenge being how to achieve a true quantum computational advantage: to solve a concrete and useful computational problem which cannot be solved by the classical computers.

It is expected that this area will continue to evolve rapidly, integrating insights from experimental physics, theoretical physics, mathematics, and information science. Over the next decade, research will likely focus on identifying which quantum states, quantum operations, and quantum protocols will be most useful for quantum information processing.

WHAT WOULD YOU EXCPECT OF THE FUTURE POST-QUANTUM THEORY?

Francesco Buscemi. If a future post-quantum theory ever emerges, to deserve that name, it would have to depart from quantum theory at least as radically as quantum theory departed from classical physics. It is worth recalling that the inadequacy of classical theory was made evident by relatively simple, low-energy experiments at the end of the nineteenth and the beginning of the twentieth century. By contrast, and this is an important methodological point, we currently have no experimentally demonstrated situations in which quantum theory is inadequate. The open issues we do have are conceptual or theoretical rather than empirical. The regimes where quantum theory might conceivably fail lie at extreme scales not yet accessible to experiment. Without concrete empirical hints, imagining a genuinely new framework becomes exceedingly difficult. In this sense, talk of a post-quantum theory today feels uncomfortably close to "armchair philosophizing", carried out without the observational footholds that historically guided genuine theoretical revolutions.

David Deutsch. Can't prophesy of course, but I wouldn't be at all surprised if explaining dark energy and/or the inflation field or even dark matter turned out to require post-quantum theories. See also Marletto's constructor-theoretic formulation of thermodynamics (MARLETTO,

2016), which I consider to be the deepest to date. Not exactly post-quantum yet but certainly complementary to quantum.

Ruth E. Kastner: I am not quite sure what is meant by 'post-quantum theory'. Basic quantum theory could well be sufficient once it is reformulated in the direct-action picture, to take into account real physical non-unitary processes, and thus to be able to explain what counts as a "measurement". (See, in particular, KASTNER 2022, Chapter 5). And indeed that also gets us a unification of quantum theory and general relativity, as shown in the above publication.

Olimpia Lombardi: Of course, we are all waiting for the unification of quantum theory and general relativity. However, regrettably, there is still no far-reaching quantum gravity theory that is both fully articulated and experimentally confirmed, and I have doubts that such a theory will be achieved in the near future.

Tim Maudlin. I am not sure what "post-quantum" means here, exactly because there is no agreed-upon understanding of quantum theory. Of course, any future theory must account for the same iconic quantum-mechanical effects—such as two-slit interference, the disappearance of interference when the apparatus includes a monitor, and violations of Bell's Inequality. Regarding the latter, I rather suspect that we may enter a "post-Relativistic regime" rather than a "post-quantum" one. Special and General Relativity are clearly enough defined theories that it will be obvious if a fundamental principle of them is given up. For example, if superluminal signaling can be demonstrated in the lab.

Philip Pearle. There is general agreement that the most fundamental problem is to obtain a sound theory that combines General Relativity with Quantum theory. It is my hope that the ideas behind CSL will somehow find a home in this new theory. It may be that this new theory will be quite different from either General Relativity or Quantum Theory but, since both theories are so successful in their respective realms, one would expect that approximations applied to the new theory would yield GR or QT in suitable circumstances.

Lev Vaidman: I see no "clouds". There is no reason to look for another theory; quantum predictions and observations fully agree. There will be no post-quantum theory.

Vlatko Vedral. I expect the same scientific paradigm to be followed. Our next theory of physics will be a unification and generalisation of quantum physics and general relativity, and it (the next theory) will reduce to quantum physics and general relativity in some special limits. It is impossible to know what this theory will be like, but one thing I can bet on is that it won't be a return to classical physics. Q-numbers are here to stay and, if anything, the fundamental elements of reality in the new theory will only be even weirder.

Karol Życzkowski: Post-quantum theories and other *generalized probabilistic theories* (GPT) models will continue to be an active area of research in theoretical physics. Personally, I am interested in this topic and have worked on generalized quantum theories, but I do not believe such theories will have practical significance within my lifetime. It is conceivable that generalized quantum theories could make predictions beyond those of standard quantum mechanics, but these effects are likely limited to extreme conditions—such as very high energy, temperature, density, or acceleration—that are not relevant for the typical experiments of the coming decades.

GENERAL OPINIONS

Ivan Gutman:[3] Since its appearance a little more than a century ago, quantum theory found outstanding, marvelous and magnificent applications, mainly in material science and chemistry, and became by now a standard method of research. Quantum theory yielded results and methods of significant technological importance. Yet, if we would dig a bit deeper, we would see that today Schrödinger's cat is alive as much as it was in 1935. The conundrum

envisaged by Einstein Podolsky and Rosen is today as obscure as then, except that we now know that it was not a figment.

Milena Petković.[8] The formulation of new chemical concepts and methodologies is expected to enhance our understanding of reaction mechanisms. Significant steps in this direction were taken during the first two decades of the 21st century. For example, analysis of the extreme values of the reaction force enabled a conceptual shift from viewing the transition state as a single structure to recognizing a transition state region, where the key electronic rearrangements associated with bond cleavage and bond formation take place (TORO- LABBÉ, 2009). Further, on the basis of Bader's Atoms in Molecules theory (BADER, 1990), the energy decomposition method known as the Interacting Quantum Atoms approach (BLANCO *et al*., 2005) was developed; when coupled with the Relative Energy Gradient method, it enables the identification of the driving forces behind chemical transformations (THACKER, *et al*., 2017). These advances indicate that novel chemical concepts and approaches will continue to emerge, providing even deeper insights into reaction mechanisms.

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