

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.

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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).

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.

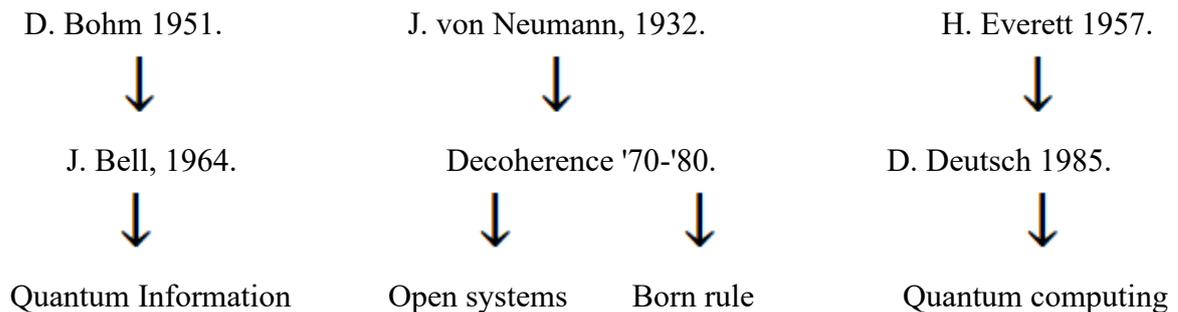


Figure 1. The course of development of some quantum sciences.

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, $e+p = \text{atom} = \text{CM} + \text{R}$. 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:

$$\mathcal{H}_e \otimes \mathcal{H}_p = \mathcal{H}_{\text{atom}} = \mathcal{H}_{\text{CM}} \otimes \mathcal{H}_R. \quad (3)$$

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

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

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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