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Entry

Foundations of Quantum Mechanics

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Definition: Quantum mechanics is a mathematical formalism that models the dynamics of physical objects. It deals with the elementary constituents of matter (atoms, subatomic and elementary particles) and of radiation. It is very accurate in predicting observable physical phenomena, but has many puzzling properties. The foundations of quantum mechanics are a domain in which physics and philosophy concur in attempting to find a fundamental physical theory that explains the puzzling features of quantum mechanics, while remaining consistent with its mathematical formalism. Several theories have been proposed for different interpretations of quantum mechanics. However, there is no consensus regarding any of these theories.

Keywords: wavefunction; superposition; measurement; ontology; non-locality; simultaneity; entanglement

Citation: Yasmineh, S. Foundations of Quantum Mechanics. *Encyclopedia* **2022**, *2*, 1082–1090. https://doi.org/10.3390/encyclopedia2020071

Academic Editors: David Carfi, Raffaele Barretta and Marek Szopa

Received: 10 April 2022
Accepted: 24 May 2022
Published: 26 May 2022

1. Introduction

Quantum mechanics began in 1900, when Max Planck found a formula that fit the experimental data of the radiation emitted by a black body. Contrary to classical physics, Planck's formula suggests that radiation is emitted in definite packets of energy called 'quanta'. Whether discontinuity of radiation is clearly implied by black-body radiation is still debated; see Passon and Grebe-Ellis [1] and the references therein for this debate. What is relevant here is that the energy, E, of each packet is proportional to the frequency, ν, of the radiation, and the constant of proportionality is a fundamental constant, called Planck's constant, h [2]. Planck's formula is defined as follows:

$$E = h\nu \quad (1)$$

Quantum mechanics clarifies many startling features usually encountered in the microcosmic realm. These astonishing features were best illustrated by the double-slit experiment. It involves the firing of particles, such as electrons, one by one on a plate in which there are two slits, A and B. The particles arrive one by one, such that single random impacts are registered on a detecting screen beyond the plate. However, the collective outcome of a large number of impacts on the detecting screen reveals an interference pattern of alternating dark and light bands. Such a collective pattern is characteristic of particles behaving as incoming waves from both slits. Meanwhile, the interference pattern has been built up out of a succession of separate and independent individual impacts.

Once detectors are placed at slits A and B to determine the slit through which each particle goes, the interference pattern ceases to exist. This strange feature seems to unintuitively suggest that each particle passes through both slits when there are no detectors and through only one slit when detectors are present [3,4].

Thus, it seems impossible to observe interference and simultaneously determine which slit the particle has passed through.

The formal explanation of such phenomena, as well as many others, started in 1925 with the advent of matrix mechanics developed by Werner Heisenberg, and several months later, with that of wave mechanics developed by Erwin Schrödinger. Matrix mechanics and wave mechanics are mathematically equivalent, although the mathematical formalism of the latter was more familiar to physicists at that time. Matrix mechanics interprets the states

of a physical system by matrices that evolve in time, whereas wave mechanics interprets these states by wavefunctions governed by a linear differential equation.

2. Standard Quantum Mechanics

Quantities that can be measured, such as the position, momentum, or energy of a particle, are usually called observables. Every observable is represented by a Hermitian operator and the eigenvectors of a Hermitian operator form an orthonormal coordinate system. Thus, every observable can be considered as corresponding to an orthonormal coordinate system. For a given observable, a complex number called 'quantum amplitude' is assigned to each point of the coordinate system. The square of the quantum amplitude is the probability of finding the associated point of the coordinate system if the relevant measurement is performed.

Wave mechanics defines a vector space V, whose elements are called state vectors, each of which is usually denoted by the symbol $|\psi\rangle$ called "ket-vector ψ" (or simply ket ψ) according to Dirac's notation. Any physical system (for example, a particle or collection of particles) has a quantum state generically represented by a state vector $|\psi\rangle$ formed by a linear combination of the coordinate system's basis vectors $|e_i\rangle$ associated with a given observable.

In a discrete coordinate system, the quantum state $|\psi\rangle$ is defined as follows:

$$|\psi\rangle = \sum_i a_i |e_i\rangle \tag{2}$$

The coordinates a_i ; $i = 1, 2, 3 \ldots$ are the quantum amplitudes, each of which a_i is the inner product of its corresponding basis vector $|e_i\rangle$ on the state vector $|\psi\rangle$, defined as follows:

$$a_i = \langle e_i|\psi\rangle \tag{3}$$

Here $\langle e_i|$ is a "bra-vector e_i" (or simply bra e_i) which is the complex conjugate of $|e_i\rangle$. The bra $\langle e_i|$ acts on the state vector $|\psi\rangle$ to extract the corresponding quantum amplitude a_i. The bras $\langle e_i|$; $i = 1, 2, 3 \ldots$ form a vector space called the dual space of V. The complex-valued linear function formed from the inner products $\langle e_i|\psi\rangle$ is also called the wavefunction and is denoted $\psi(e_i)$.

For example, if the system consists of a particle in a one-dimensional continuous coordinate system (O, x), the wavefunction $\langle x|\psi\rangle \equiv \psi(x)$ represents the quantum amplitudes of the positions of the particles. The complex-valued wavefunction $\psi(x)$ can be expressed in polar form as follows:

$$\psi(x,\ t) = R(x,t)e^{iS(x,t)} \tag{4}$$

where $R(x,t)$ is the modulus of the quantum amplitude and $S(x,t)$ is its phase.

The state vector $|\psi\rangle$ and wavefunction $\psi(x)$ are equivalent. They are different mathematical representations of the same physical system, and can thus be used interchangeably to describe the system. The state vector represents the quantum state as a vector in a complex-valued linear vector space V called "Hilbert space". Wavefunction $\psi(x)$ represents the quantum state as a mathematical function in an abstract space called the configuration space. For a single particle, the configuration space is equivalent to a real, three-dimensional physical space. For n particles, the configuration space is a 3n-dimensional abstract space.

For example, to represent the location of a particle (or set of particles), the wavefunction or state vector is a superposition of all possible locations of the particle (or set of particles), such that a quantum amplitude is assigned to each position (or set of positions). The square of each quantum amplitude is the probability of finding a particle (or set of particles) at the corresponding location (or locations).

The rate of change of the wavefunction or state vector is proportional to its energy, as defined by the Schrödinger equation:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = H\psi(x,t) \tag{5}$$

This equation states that the partial derivative of the wavefunction with respect to time is proportional to the Hamiltonian H acting on the wavefunction. The Hamiltonian defines the energy of a physical system, and captures its dynamics.

Suppose the wavefunction (or state vector) describing a microscopic system is a superposition of different states. Then, the Schrödinger equation's evolution ought to imply that the measuring instrument should also be in a macroscopic superposition of a plurality of distinct states. However, this does not correspond to the observed behaviour of the measuring instrument, which attributes a definite outcome to the measured microscopic system. The fact that a measurement has a definite outcome, while Schrodinger's equation predicts a chain of superpositions, is called the measurement problem. To solve this problem, standard quantum mechanics considers that a wavefunction (or state vector) is governed by two dynamical rules. The first rule stipulates that when no measurement is made, the system evolves in a deterministic manner in accordance with Schrödinger's equation. In contrast, the second rule postulates that when a measurement is conducted, the wavefunction instantaneously and randomly collapses to one particular state. For example, the impact of measuring a system represented by the state vector of Equation (2) collapses the state vector $|\psi\rangle$ into a unique state $|e_i\rangle$, as follows:

$$|\psi\rangle = |e_i\rangle \tag{6}$$

The standard approach to quantum mechanics, often called the Copenhagen interpretation, considers that the measuring instruments belong to the classical realm while microscopic objects belong to an unknowable quantum realm. The Copenhagen interpretation considers standard quantum mechanics as an instrument which allows us to determine the effects of microscopic objects on macroscopic instruments.

3. Conflicts in the Standard Formulation of Quantum Mechanics

In the double-slit experiment, an electron passing through slit A can be represented by state vector $|A\rangle$. Similarly, an electron passing through slit B can be represented by state vector $|B\rangle$. An electron passing simultaneously through both slits A and B is in a superposition state. Its state vector is:

$$|\psi\rangle = a|\,A\rangle + b|B\rangle \tag{7}$$

where a and b are quantum amplitudes whose squares $|a|^2$ and $|b|^2$ represent the probabilities of the particle to be measured by detectors D_A and D_B at slits A and B, respectively.

When there are no detectors, the state vector $|\psi\rangle = a|\,A\rangle + b|B\rangle$ of the electron passes through both slits and evolves according to the continuous and deterministic Schrödinger equation.

When a detector measures from which slit the electron passes, the wavefunction collapses to one particular state; thus, the electron passes through only one slit. For example, if detector D_A indicates that the electron passes through slit A, then the state vector of Equation (7) becomes

$$|\psi\rangle = |A\rangle \tag{8}$$

The transformation from a deterministic and continuous evolution of the physical state into a probabilistic, discontinuous and nonlinear state seems to solve the measurement problem, but creates conflict in the formalism of quantum mechanics.

As explained by Norsen [5], in addition to the above conflict in the formalism of quantum mechanics, there are at least two others concerning relativity and the ontology of the wavefunction.

The relativity problem comprises two subproblems. The first concerns the 'relativity of simultaneity', while the second concerns 'locality'. In contrast, a wavefunction representing a spatially spread-out electron is defined at a single instant, thus contradicting the notion of 'relativity of simultaneity'. For example, and as will be explained in relation to Equation (9),

the state of one particle of a system composed of two entangled particles cannot be described independently of the state of the other. Neither one of the particles has a determinate state before it is measured, and when it is measured, the other particle should 'simultaneously' acquire a determinate state. However, according to special relativity, 'simultaneity' has no sense independently of any frame of reference, and there should be no preferred frame of reference [6,7].

The nonlocality problem arises from the fact that a dynamical collapse of the wave function conflicts with relativistic locality as highlighted by a thought experiment in the EPR paper [8]. In its simplified version by Bohm [9], this thought experiment considers two particles, A and B, characterised by two spins travelling in opposite directions and coming out from a source equidistant between two experimenters, Alice and Bob. Let particles A and B be heading towards Alice and Bob, respectively. For example, the source is a nucleus that decays from a state that has no spin by emitting particles A and B in opposite directions at equal speeds. Spin is an intrinsic property of a system that, when measured along an arbitrary axis, can only point in two opposing directions of the axis denoted $|+\rangle$ and $|-\rangle$. As the spin of the nucleus is zero, particles A and B have opposite spins. The two-spin system formed by particles A and B has no net spin and is said to be in an entangled state, which can be expressed as follows:

$$|\psi\rangle = c_1|+-\rangle + c_2|-+\rangle \tag{9}$$

The first and second labels in each ket refer to Alice and Bob, respectively. In other words, $|+-\rangle$ is a state in which particle A (heading toward Alice) has a positive component along the z-axis and particle B (heading toward Bob) has a negative component along the z-axis. In contrast, $|-+\rangle$ is a state in which particle A has a negative component along the z-axis, and particle B has a positive component along the z-axis. The entangled state $|\psi\rangle$ is a superposition of two states, $|+-\rangle$ and $|-+\rangle$ affected by quantum amplitudes c_1 and c_2, respectively.

Equation (9) indicates that the measurement outcomes for both particles are correlated. However, neither particle A nor particle B had a definite spin along any axis until a measurement was made. Suppose that Alice obtains $|+\rangle$ by measuring the particle spin along the z-axis. This means that the entangled state $|\psi\rangle$ has collapsed into a single state $|+-\rangle$, as follows:

$$|\psi\rangle = |+-\rangle \tag{10}$$

Alice can then confirm that if Bob also measures the particle spin along the z-axis, he must find $|-\rangle$. This implies that the measurement of particle A has an instantaneous effect on particle B. As this is forbidden by relativity, EPR argued that the correlation of measurement outcomes must have been the result of a hidden variable that travelled with both particles.

It was later discovered that the EPR phenomenon could be experimentally tested using Bell's inequality [10]. Bell's inequality shows that if particles A and B are considered as separate systems with properties that depend only on their local environments, then the measurement correlations would be weaker than those predicted by quantum mechanics.

The validity of quantum entanglement implying a non-local connection has been proven by many experiments, such as Aspect's experiment [11]. It follows that quantum mechanics infers the notions of nonlocality and simultaneity which are banned by the postulates of relativity.

Finally, the ontological problem concerns the physical definition of a wavefunction. For more than one particle, the wavefunction is defined in a high-dimensional space different from real physical space.

4. Different Interpretations of Quantum Mechanics

Various ontologies have been proposed to explain these problems. These ontologies can be divided into two main groups. The first is Psi-ontic which considers the quantum

state to be an element of reality. The second is the Psi-epistemic which considers the quantum state to be a probabilistic representation of the observer's knowledge [12,13].

One of the most prominent Psi-epistemic views is QBism (Quantum Bayesianism), suggesting that the wavefunction is not a real physical entity, but simply a representation of an experimenter's knowledge about a quantum system. Wavefunction evolution is considered to be the evolution of our probabilities for the outcomes of potential measurements and not the evolution of the physical system [14]. The probabilities are determined according to a Bayesian updating. Consequently, wavefunction collapse is not a real physical process and should be regarded as an update of the experimenter's knowledge [15]. This epistemic view seems to solve measurement and relativity problems. Spekkens [16] presented Psi-epistemic models that can explain some of the perplexing features of quantum mechanics.

We note that the Copenhagen interpretation can also in some sense be regarded as epistemic due to the fact that the collapse of the wavefunction is not considered to be ontological.

On the other hand, the proponents of the Psi-ontic view, as explained by Maudlin [17], consider that some phenomena, such as the interference pattern in a two-slit experiment, imply that the wavefunction should represent some real physical features of a physical system. Interference demands that some parts of the wavefunction cancel one another while other parts add to each other, irrespective of what an observer believes about the experiment According to the Psi-ontic view, the properties of the wavefunction should reflect those of the physical system.

Several candidate Psi-ontic models propose some solutions to the above problems. Drummond [18] provides an outline of these theories. The main current theories are the many-world theory [19], the pilot-wave theory [20,21], and the spontaneous collapse theory [22].

4.1. Everett's Many-World Theory

The many-world theory [19] postulates that all measurement results exist but in different worlds and thus, there is no collapse of the wavefunction. Whenever a quantum measurement is made, the world splits into multiple worlds, depending on the number of superposed macroscopic states. For one observer, it seems that only one outcome occurred.

A deterministic branching takes place at each measurement [23]. On one branch, a first measuring instrument in one world detects the particle while a second measuring instrument in another world does not. At the same time, but on the other branch, the first measuring instrument does not detect the particle, while the second measuring instrument does. The proponents of this theory argue that the many-world theory takes quantum mechanics literally: there is only the wavefunction that evolves according to Schrödinger's equation. However, it is ontologically difficult to reconcile this interpretation with common sense. Moreover, the axioms of quantum mechanics say nothing about the existence of multiple physical worlds [24]. It also pauses some probabilistic problems that some authors such as Greaves [25] have tried to answer.

4.2. De Broglie–Bohm Theory

This theory has been introduced by Louis de Broglie [26] and independently rediscovered by David Bohm [21]. The de Broglie–Bohm theory is discussed by many authors, including Bricmont [27], Dürr and Lazarovici [28], Holland [29], Friebe et al. [30], and in the introduction to the Symposium Louis de Broglie [31]. This theory stipulates that a particle always has a definite position on a well-determined trajectory in real space. The movement of the particle is influenced by a corresponding wavefunction, that gives rise to wave-like properties. The dynamical law governing the wave is simply the Schrödinger equation; Equation (5). The dynamical law governing the evolution of the particle's position, $X(t)$ is:

$$\frac{dX}{dt} = \frac{\hbar}{m}\frac{\partial S(X,t)}{\partial t} \tag{11}$$

where $\partial S(X,t)/\partial t$ is the gradient of the phase of the wavefunction evaluated at actual position $X(t)$ of the particle. The above formula indicates that the evolution of the particle is guided by the wavefunction.

For an n-particle wavefunction $\psi(x_1, \ldots, x_i, \ldots x_n, t)$ where x_i represents the position of the ith particle, the expression above can be generalised as follows:

$$\frac{dX_i}{dt} = \frac{\hbar}{m} \frac{\partial S(X_1, \ldots, X_i, \ldots, X_n, t)}{\partial t} \tag{12}$$

Equation (12) implies that the motion of the ith particle at a given time, t, depends on the positions of all other particles at the same time, t, thus accounting for the nonlocality of entangled particles. However, Equation (12) seems also to imply a notion of absolute simultaneity.

Moreover, the de Broglie–Bohm theory satisfies a 'quantum equilibrium hypothesis' stipulating that the positions of the particles are distributed in accord with the probability density ρ, as follows:

$$\rho = |\psi|^2 \tag{13}$$

when the position of a particle is measured at a given instant, t, the outcome is the actual position of the particle at that instant, thus solving the measurement problem.

However, the definition of the wavefunction in the configuration space remains unclear. De Broglie has attempted to modify the theory in such a manner that the interactions between quantum systems take place in the real, three-dimensional space and not in configuration space [32]. More recent works are discussed in [27–30].

4.3. GRW Spontaneous Collapse Theory

The GRW spontaneous collapse theory [22] stipulates that the wavefunction $\psi(x,t)$ of a physical system evolves according to the deterministic Schrödinger's equation almost all the time, except for on very rare and random occasions when it experiences a spontaneous collapse and becomes localised in real space. A spontaneous collapse is defined by multiplying the wavefunction by a Gaussian localising function, $g(x)$. Suppose the localisation occurs at an instant, t; then, the wavefunction $\psi(x,t^+)$ immediately after instant t is defined by the action of a normalised localising function $g(x)$ on the wavefunction $\psi(x,t^-)$ just before instant t:

$$\psi(x,t^+) = g(x)\psi(x,t^-) \tag{14}$$

The localisations occur at an exceedingly small frequency, such that they have almost no effect on microscopic systems. In contrast, the effects of spontaneous localisation on macroscopic objects are amplified by entanglement. A macroscopic object comprises an immensely large number of entangled particles, and when the wavefunction of one particle collapses, the wavefunctions of all other entangled particles also collapse. Actually, all entangled particles are represented by a single wavefunction that collapses globally for all particles at once. This model suggests that it is sufficient for a microscopic object to collapse at an average rate of 100 million years, to guarantee a definite state for a macroscopic object.

GRW provides a physical explanation of the wavefunction and accounts for nonlocality. Nevertheless, the problem of simultaneity remains unsolved and it appears to be ad hoc.

It has been shown [33] that the instantaneous collapse of a wavefunction remains inconsistent with the requirements of special relativity. An instantaneous collapse in one Lorentz frame may not be instantaneous in another.

5. Other Viewpoints

There are many other interpretive models and theories for quantum mechanics. However, there is no consensus in the physics or philosophy of physics communities regarding a single model. The basic problem that remains is the inconsistency of almost all of the above models with relativity, and in particular, non-locality and simultaneity. Even in Everett's interpretation, the instant of subdivision between different worlds is implicitly assumed to

be simultaneous in these worlds. It seems hard to understand what a simultaneous action between a multitude of disconnected worlds means, if it even makes any sense.

The main problem with simultaneity is that in a quantum system composed of a pair of entangled particles, it is necessary that when the state of one particle is measured, the other particle should at the 'same instant' acquire a determinate state. However, there is no meaning of a 'same instant' for spatially separated positions.

Other approaches, such as superdeterminism, temporal nonlocality and retrocausality, attempt to solve the conflict between quantum mechanics and relativity. Superdeterminism argues that there should be a theory underlying quantum mechanics that is both local and deterministic [34].

Retrocausality explains the violation of Bell's inequality by the backward-in-time propagation of measurement results in an entangled system in a completely local manner [35,36].

Temporal nonlocality proposes to resolve the inadequacy between quantum mechanics and relativity by treating space and time in similar ways. It proposes that the influence of the measurement of one particle on the state of another entangled particle is not only non-local in space, but also non-local in time [37].

The author proposes to consider the evolution of a wavefunction from the perspective of proper time [38] such that the wavefunction becomes relativistically invariant for all inertial observers.

6. Quantum Computing

Quantum computing is an immediate application of the foundations of quantum mechanics. In classical computing, information is represented by bits, where each bit can have one of two mutually exclusive values: 0 or 1. In quantum computing, we use the wavefunction or state-vector of a physical system to construct a quantum bit or 'qubit' for short [39]. For example, in the double-slit experiment, let slit A be represented by 0 and slit B be represented by 1. Then, according to Equation (7), the state vector of a particle passing through the double slit can be expressed by a qubit $|\psi\rangle$ which is defined as a linear superposition of states, as follows:

$$|\psi\rangle = a|0\rangle + b|1\rangle \tag{15}$$

where quantum amplitudes a and b are complex numbers that can take any value as long as the sum of their mod squares is equal to 1, and kets $|0\rangle$ and $|1\rangle$ are the computational basis states. The probability of detecting a particle through slit A is $|a|^2$ and the probability of detecting a particle through slit B is $|b|^2$. A qubit can be in an infinite number of states between $|0\rangle$ and $|1\rangle$ and can thus have an infinite number of possible values.

However, we cannot conduct an experiment to determine the quantum state (i.e., the values of a and b) of a qubit. As seen in the double-slit experiment, we have always found electrons passing through only one slit. In other words, when a measurement is made, the outcome is either 0 with probability $|a|^2$ or 1 with probability $|b|^2$. If that is the case, then the qubit would be less useful than the classical bit. However, qubits evolve deterministically according to Schrödinger's equation. They can also be transformed or can interfere with each other, leading to measurement outcomes that depend on the different properties and original states of these qubits. These different manipulations and transformations of qubits can be represented by quantum gates defined in tables. Quantum gates can be connected to form quantum circuits, which can be used to perform quantum computations and quantum algorithms.

We note that the classical bit is only a specific type of qubit, where one of the quantum amplitudes is equal to 1, and all others are equal to zero. Thus, all classical computations can be performed using more general quantum computations, with the qubit as its basic unit of computation.

In principle, a qubit can be materialised by any real physical system with two states. We considered a qubit to represent the passage of a particle through a double slit. More

concrete examples take advantage of the spin or energy levels of a system or the polarisation of photons. The polarisation of a photon can be vertical or horizontal, or a superposition of both. Photons are used for communication; however, they cannot be used to build quantum circuits. Energy levels can be used by trapping ions in an electric or magnetic field at a temperature near absolute zero. The spin of an electron can be used by bounding it to a small semiconductor called a quantum dot. Spins can also be used to trap electrons or ions in synthetic diamonds.

Quantum computing is in progress, and is likely to offer many new capabilities that cannot be achieved by classical computing.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

Conflicts of Interest: The authors declare no conflict of interest.

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