Quantum mechanics is a fundamental theory that describes the behavior of nature at and below the scale of atoms.[2]:1.1 It is the foundation of all **quantum physics**, which includes quantum chemistry, quantum field theory, quantum technology, and quantum information science.

Quantum mechanics can describe many systems that classical physics cannot. Classical physics can describe many aspects of nature at an ordinary (macroscopic and (optical) microscopic) scale, but is not sufficient for describing them at very small submicroscopic (atomic and subatomic) scales. Most theories in classical physics can be derived from quantum mechanics as an approximation valid at large (macroscopic/microscopic) scale.[3]

Quantum systems have bound states that are quantized to discrete values of energy, momentum, angular momentum, and other quantities, in contrast to classical systems where these quantities can be measured continuously. Measurements of quantum systems show characteristics of both particles and waves (wave–particle duality), and there are limits to how accurately the value of a physical quantity can be predicted prior to its measurement, given a complete set of initial conditions (the uncertainty principle).

Quantum mechanics arose gradually from theories to explain observations that could not be reconciled with classical physics, such as Max Planck's solution in 1900 to the black-body radiation problem, and the correspondence between energy and frequency in Albert Einstein's 1905 paper, which explained the photoelectric effect. These early attempts to understand microscopic phenomena, now known as the "old quantum theory", led to the full development of quantum mechanics in the mid-1920s by Niels Bohr, Erwin Schrödinger, Werner Heisenberg, Max Born, Paul Dirac and others. The modern theory is formulated in various specially developed mathematical formalisms. In one of them, a mathematical entity called the wave function provides information, in the form of probability amplitudes, about what measurements of a particle's energy, momentum, and other physical properties may yield.

Overview and fundamental concepts

Quantum mechanics allows the calculation of properties and behaviour of physical systems. It is typically applied to microscopic systems: molecules, atoms and sub-atomic particles. It has been demonstrated to hold for complex molecules with thousands of atoms,[4] but its application to human beings raises philosophical problems, such as Wigner's friend, and its application to the universe as a whole remains speculative.[5] Predictions of quantum mechanics have been verified experimentally to an extremely high degree of accuracy. For example, the refinement of quantum mechanics for the interaction of light and matter, known as quantum electrodynamics (QED), has been shown to agree with experiment to within 1 part in 10^{12} when predicting the magnetic properties of an electron.[6]

A fundamental feature of the theory is that it usually cannot predict with certainty what will happen, but only give probabilities. Mathematically, a probability is found by taking the square of the absolute value of a complex number, known as a probability amplitude. This is known as the Born rule, named after physicist Max Born. For example, a quantum particle like an electron can be described by a wave function, which associates to each point in space a probability amplitude. Applying the Born rule to these amplitudes gives a probability density function for the position that the electron will be found to have when an experiment is performed to measure it. This is the best the theory can do; it cannot say for certain where the electron will

be found. The Schrödinger equation relates the collection of probability amplitudes that pertain to one moment of time to the collection of probability amplitudes that pertain to another.[7]:67–87

One consequence of the mathematical rules of quantum mechanics is a tradeoff in predictability between different measurable quantities. The most famous form of this uncertainty principle says that no matter how a quantum particle is prepared or how carefully experiments upon it are arranged, it is impossible to have a precise prediction for a measurement of its position and also at the same time for a measurement of its momentum.[7]:427–435

Another consequence of the mathematical rules of quantum mechanics is the phenomenon of quantum interference, which is often illustrated with the double-slit experiment. In the basic version of this experiment, a coherent light source, such as a laser beam, illuminates a plate pierced by two parallel slits, and the light passing through the slits is observed on a screen behind the plate.[8]:102–111[2]:1.1–1.8 The wave nature of light causes the light waves passing through the two slits to interfere, producing bright and dark bands on the screen – a result that would not be expected if light consisted of classical particles.[8] However, the light is always found to be absorbed at the screen at discrete points, as individual particles rather than waves; the interference pattern appears via the varying density of these particle hits on the screen. Furthermore, versions of the experiment that include detectors at the slits find that each detected photon passes through one slit (as would a classical particle), and not through both slits (as would a wave).[8]:109[9][10] However, such experiments demonstrate that particles do not form the interference pattern if one detects which slit they pass through. This behavior is known as wave–particle duality. In addition to light, electrons, atoms, and molecules are all found to exhibit the same dual behavior when fired towards a double slit.[2]

Another non-classical phenomenon predicted by quantum mechanics is quantum tunnelling: a particle that goes up against a potential barrier can cross it, even if its kinetic energy is smaller than the maximum of the potential.[11] In classical mechanics this particle would be trapped. Quantum tunnelling has several important consequences, enabling radioactive decay, nuclear fusion in stars, and applications such as scanning tunnelling microscopy, tunnel diode and tunnel field-effect transistor.[12][13]

When quantum systems interact, the result can be the creation of quantum entanglement: their properties become so intertwined that a description of the whole solely in terms of the individual parts is no longer possible. Erwin Schrödinger called entanglement "...*the* characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought".[14] Quantum entanglement enables quantum computing and is part of quantum communication protocols, such as quantum key distribution and superdense coding.[15] Contrary to popular misconception, entanglement does not allow sending signals faster than light, as demonstrated by the no-communication theorem.[15]

Another possibility opened by entanglement is testing for "hidden variables", hypothetical properties more fundamental than the quantities addressed in quantum theory itself, knowledge of which would allow more exact predictions than quantum theory can provide. A collection of results, most significantly Bell's theorem, have demonstrated that broad classes of such hidden-variable theories are in fact incompatible with quantum physics. According to Bell's theorem, if nature actually operates in accord with any theory of *local* hidden variables, then the results of a Bell test will be constrained in a particular, quantifiable way. Many Bell tests have been performed and they have shown results incompatible with the constraints imposed by local hidden variables.[16][17]

It is not possible to present these concepts in more than a superficial way without introducing the actual mathematics involved; understanding quantum mechanics requires not only manipulating complex numbers, but also linear algebra, differential equations, group theory, and other more advanced subjects.[18][19] Accordingly, this article will present a mathematical formulation of quantum mechanics and survey its application to some useful and oft-studied examples.

Mathematical formulation

Main article: Mathematical formulation of quantum mechanics

In the mathematically rigorous formulation of quantum mechanics, the state of a quantum

mechanical system is a vector belonging to a (separable) complex Hilbert space . This vector is postulated to be normalized under the Hilbert space inner product, that is, it

obeys , and it is well-defined up to a complex number of modulus 1 (the global phase), that

is, and represent the same physical system. In other words, the possible states are points in the projective space of a Hilbert space, usually called the complex projective space. The exact nature of this Hilbert space is dependent on the system – for example, for describing position and momentum the Hilbert space is the space of complex square-

integrable functions , while the Hilbert space for the spin of a single proton is simply the

space of two-dimensional complex vectors with the usual inner product.

Physical quantities of interest – position, momentum, energy, spin – are represented by observables, which are Hermitian (more precisely, self-adjoint) linear operators acting on the Hilbert space. A quantum state can be an eigenvector of an observable, in which case it is called an eigenstate, and the associated eigenvalue corresponds to the value of the observable in that eigenstate. More generally, a quantum state will be a linear combination of the eigenstates, known as a quantum superposition. When an observable is measured, the result will be one of its eigenvalues with probability given by the Born rule: in the simplest case the

eigenvalue is non-degenerate and the probability is given by , where is its associated eigenvector. More generally, the eigenvalue is degenerate and the probability is

given by , where is the projector onto its associated eigenspace. In the continuous case, these formulas give instead the probability density.

After the measurement, if result was obtained, the quantum state is postulated

to collapse to , in the non-degenerate case, or to , in the general case.
The probabilistic nature of quantum mechanics thus stems from the act of measurement. This is one of the most difficult aspects of quantum systems to understand. It was the central topic in the famous Bohr–Einstein debates, in which the two scientists attempted to clarify these fundamental principles by way of thought experiments. In the decades after the formulation of quantum mechanics, the question of what constitutes a "measurement" has been extensively studied. Newer interpretations of quantum mechanics have been formulated that do away with

the concept of "wave function collapse" (see, for example, the many-worlds interpretation). The basic idea is that when a quantum system interacts with a measuring apparatus, their respective wave functions become entangled so that the original quantum system ceases to exist as an independent entity (see measurement in quantum mechanics[20]).

Time evolution of a quantum state

The time evolution of a quantum state is described by the Schrödinger equation:

Here denotes the Hamiltonian, the observable corresponding to the total energy of the

system, and is the reduced Planck constant. The constant is introduced so that the Hamiltonian is reduced to the classical Hamiltonian in cases where the quantum system can be approximated by a classical system; the ability to make such an approximation in certain limits is called the correspondence principle.

The solution of this differential equation is given by

The operator is known as the time-evolution operator, and has the crucial property that it is unitary. This time evolution is deterministic in the sense that – given an initial

quantum state – it makes a definite prediction of what the quantum state will be at any later time.[21]

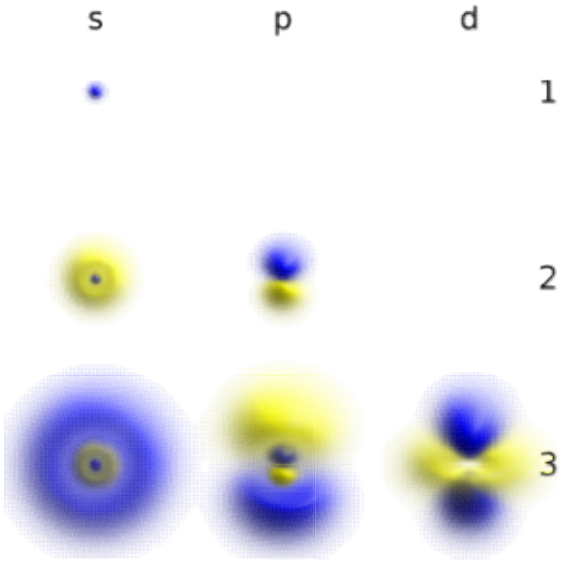


Fig. 1: Probability densities corresponding to the wave functions of an electron in a hydrogen atom possessing definite energy levels (increasing from the top of the image to the bottom: $n = 1, 2, 3, ...$) and angular momenta (increasing across from left to right: s, p, d, ...). Denser areas correspond to higher

probability density in a position measurement. Such wave functions are directly comparable to Chladni's figures of acoustic modes of vibration in classical physics and are modes of oscillation as well, possessing a sharp energy and thus, a definite frequency. The angular momentum and energy are quantized and take **only** discrete values like those shown. (As is the case for resonant frequencies in acoustics.)

Some wave functions produce probability distributions that are independent of time, such as eigenstates of the Hamiltonian.[7]:133–137 Many systems that are treated dynamically in classical mechanics are described by such "static" wave functions. For example, a single electron in an unexcited atom is pictured classically as a particle moving in a circular trajectory around the atomic nucleus, whereas in quantum mechanics, it is described by a static wave function surrounding the nucleus. For example, the electron wave function for an unexcited hydrogen atom is a spherically symmetric function known as an *s* orbital (Fig. 1).

Analytic solutions of the Schrödinger equation are known for very few relatively simple model Hamiltonians including the quantum harmonic oscillator, the particle in a box, the dihydrogen cation, and the hydrogen atom. Even the helium atom – which contains just two electrons – has defied all attempts at a fully analytic treatment, admitting no solution in closed form.[22][23][24]

However, there are techniques for finding approximate solutions. One method, called perturbation theory, uses the analytic result for a simple quantum mechanical model to create a result for a related but more complicated model by (for example) the addition of a weak potential energy.[7]:793 Another approximation method applies to systems for which quantum mechanics produces only small deviations from classical behavior. These deviations can then be computed based on the classical motion.[7]:849

Uncertainty principle

One consequence of the basic quantum formalism is the uncertainty principle. In its most familiar form, this states that no preparation of a quantum particle can imply simultaneously precise predictions both for a measurement of its position and for a measurement of its momentum.[25][26] Both position and momentum are observables,

meaning that they are represented by Hermitian operators. The position operator

and momentum operator do not commute, but rather satisfy the canonical commutation relation:

Given a quantum state, the Born rule lets us compute expectation values for

both and , and moreover for powers of them. Defining the uncertainty for an observable by a standard deviation, we have

and likewise for the momentum:

The uncertainty principle states that

Either standard deviation can in principle be made arbitrarily small, but not both simultaneously.[27] This inequality generalizes to arbitrary pairs

of self-adjoint operators and . The commutator of these two operators is

and this provides the lower bound on the product of standard deviations:

Another consequence of the canonical commutation relation is that the position and momentum operators are Fourier transforms of each other, so that a description of an object according to its momentum is the Fourier transform of its description according to its position. The fact that dependence in momentum is the Fourier transform of the dependence in position means that the momentum operator is equivalent (up to

an factor) to taking the derivative according to the position, since in Fourier analysis differentiation corresponds to multiplication in the dual space. This is why in quantum

equations in position space, the momentum is replaced

by , and in particular in the non-relativistic Schrödinger equation in position space the momentum-squared term is

replaced with a Laplacian times .[25]

Composite systems and entanglement

When two different quantum systems are considered together, the Hilbert space of the combined system is the tensor product of the Hilbert spaces of the two components. For example, let A and B be two quantum systems, with Hilbert

spaces and , respectively. The Hilbert space of the composite system is then

If the state for the first system is the vector and the

state for the second system is , then the state of the composite system is

Not all states in the joint Hilbert space can be written in this form, however, because the superposition principle implies that linear combinations of these "separable" or "product states" are also valid. For

example, if and are both possible states for

system , and likewise and are both

possible states for system , then

is a valid joint state that is not separable. States that are not separable are called entangled.[28][29]

If the state for a composite system is entangled, it is impossible to describe either component system A or system B by a state vector. One can instead define reduced density matrices that describe the statistics that can be obtained by making measurements on either component system alone. This necessarily causes a loss of information, though: knowing the reduced density matrices of the individual systems is not enough to reconstruct the state of the composite system.[28][29] Just as density matrices specify the state of a subsystem of a larger system, analogously, positive operator-valued measures (POVMs) describe the effect on a subsystem of a measurement performed on a larger system. POVMs are extensively used in quantum information theory.[28][30]

As described above, entanglement is a key feature of models of measurement processes in which an apparatus becomes entangled with the system being measured. Systems interacting with the environment in which they reside generally become

entangled with that environment, a phenomenon known as quantum decoherence. This can explain why, in practice, quantum effects are difficult to observe in systems larger than microscopic.[31]

Equivalence between formulations

There are many mathematically equivalent formulations of quantum mechanics. One of the oldest and most common is the "transformation theory" proposed by Paul Dirac, which unifies and generalizes the two earliest formulations of quantum mechanics – matrix mechanics (invented by Werner Heisenberg) and wave mechanics (invented by Erwin Schrödinger).[32] An alternative formulation of quantum mechanics is Feynman's path integral formulation, in which a quantum-mechanical amplitude is considered as a sum over all possible classical and non-classical paths between the initial and final states. This is the quantum-mechanical counterpart of the action principle in classical mechanics.[33]

Symmetries and conservation laws

Main article: Noether's theorem

The Hamiltonian is known as the *generator* of time evolution, since it defines a unitary time-

evolution operator for each value of .

From this relation between and , it follows

that any observable that commutes with will be *conserved*: its expectation value will not change over time.[7]:471 This statement generalizes,

as mathematically, any Hermitian operator can generate a family of unitary operators parameterized

by a variable . Under the evolution generated

by , any observable that commutes

with will be conserved. Moreover, if is

conserved by evolution under , then is

conserved under the evolution generated by .

This implies a quantum version of the result proven by Emmy Noether in classical (Lagrangian) mechanics: for every differentiable symmetry of a Hamiltonian, there exists a corresponding conservation law.

Examples

Free particle

Main article: Free particle

Position space probability density of a Gaussian wave packet moving in one dimension in free space

The simplest example of a quantum system with a position degree of freedom is a free particle in a single spatial dimension. A free particle is one which is not subject to external influences, so that its Hamiltonian consists only of its kinetic energy:

The general solution of the Schrödinger equation is given by

which is a superposition of all possible plane waves , which are eigenstates of the momentum operator with momentum . The coefficients of the superposition

are , which is the Fourier transform of

the initial quantum state .

It is not possible for the solution to be a single momentum eigenstate, or a single position eigenstate, as these are not normalizable quantum states.[note 1] Instead, we can consider a Gaussian wave packet:

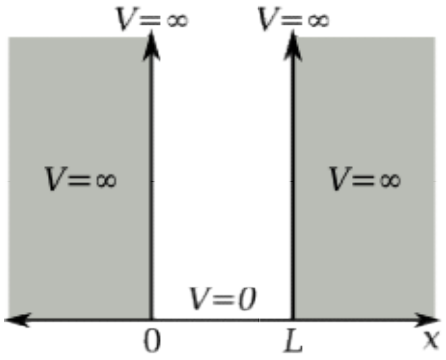
which has Fourier transform, and therefore momentum distribution

We see that as we make smaller the spread in position gets smaller, but the spread in momentum gets larger. Conversely,

by making larger we make the spread in momentum smaller, but the spread in position gets larger. This illustrates the uncertainty principle.

As we let the Gaussian wave packet evolve in time, we see that its center moves through space at a constant velocity (like a classical particle with no forces acting on it). However, the wave packet will also spread out as time progresses, which means that the position becomes more and more uncertain. The uncertainty in momentum, however, stays constant.[34]

Particle in a box



1-dimensional potential energy box (or infinite potential well)

Main article: [Particle in a box]

The particle in a one-dimensional potential energy box is the most mathematically simple example where restraints lead to the quantization of energy levels. The box is defined as having zero potential energy everywhere *inside* a certain region, and therefore infinite potential energy everywhere *outside* that region.[25]:77–78 For the one-dimensional case in

the direction, the time-independent Schrödinger equation may be written

With the differential operator defined by

the previous equation is evocative of the classic kinetic energy analogue,

with state in this case having

energy coincident

with the kinetic energy of the particle.

The general solutions of the Schrödinger equation for the particle in a box are

or, from Euler's formula,

The infinite potential walls of the box determine the

values of

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Thus, at ,

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would conflict with the postulate that has norm 1. Therefore, since , must be an integer multiple of ,

This constraint on implies a constraint on the energy levels, yielding

A [finite potential well](#) i

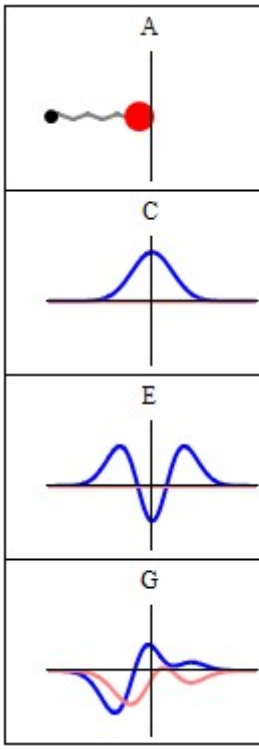
s the generalization of the infinite potential well problem to potential wells having finite depth. The finite potential well problem is mathematically more complicated than the infinite particle-in-a-box problem as the wave function is

not pinned to zero at the walls of the well. Instead, the wave function must satisfy more complicated mathematical boundary conditions as it is nonzero in regions outside the well. Another related problem is that of the recta

ngular potential barrier, which furnishes a model for the quantum tunneling effect that plays an important role in the performance of modern technologies such as flash memory and scanning tunneling microscopy.

Harmonic oscillator

Main article: Quantum harmonic oscillator



Some trajectories of a harmonic oscillator (i.e. a

ball attached to a spring) in classical mechanics (A-B) and quantum mechanics (C-H). In quantum mechanics, the position of the ball is represented by a wave (called the wave function), with the real part s

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y level of the oscillator. This "energy quantization" does not occur in classical physics, where the oscillator can have *any* energy.

As in the classical case, the potential for the quantum harmonic oscillator is given

by[7]:234

This problem can either be treated by directly solving the

Schrödinger equation, which is not trivial, or by using the more

elegant "ladder method" first proposed by Paul Dirac. The eigenvalue

[n s t a t e s](#) are given by

where H_n are the [Hermite polynomials](#)

[ynomials](#)

and the corresponding energy levels a

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