Textbooks for Tomorrow's Scientists

Hairong ZHENG (Editor-in-Chief),
Dan BOYE, Yongzhong XING, Lin ZHANG
and Shaoguang ZHANG

Quantum Mechanics

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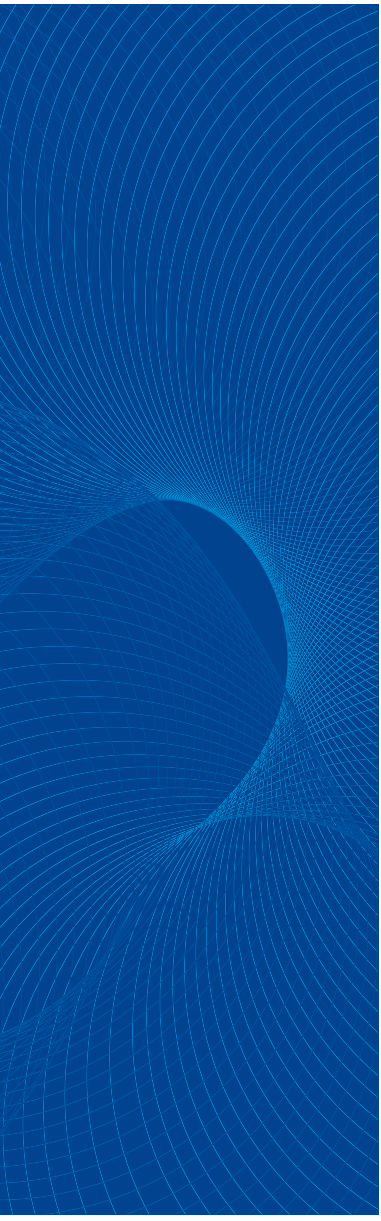

Quantum Mechanics

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This book explores the fundamental principles and theories that foster a practical and intuitive understanding of quantum mechanics. Each chapter is concluded with real-world applications, animations, and discussion questions to help readers better visualize and understand quantum phenomena. It is suitable for undergraduate students in physics and related fields who are looking to learn and strengthen their foundational understanding of quantum mechanics.

Originally designed for bilingual teaching and learning, the book considers differences in cultural background and pedagogical approach, especially their potential influence on scientific reasoning and habitual expression, aiming to bridge those differences from new perspectives.

Hairong ZHENG, the Editor-in-Chief of this book, is a professor at the School of Physics and Information Technology at Shaanxi Normal University, presiding over the national first-class course "Quantum Mechanics" for undergraduates in China. She received her PhD degree from the Department of Physics & Astronomy at the University of Georgia, and has been teaching for over forty years. **Dr. Zheng** has dedicated her career to educating undergraduate and graduate students and also advancing scientific research, publishing well over one hundred scientific research papers in the field of luminescence, laser spectroscopy and nanophotonics.

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Preface

In the historical development of physical science, the laws of classical mechanics have remained virtually unaltered for several centuries. In the late 19th and early 20th centuries, physical science met obstacles at both large velocities and atomic scales. The former was successfully interpreted by Einstein with his special theory of relativity. The problem in small-scale physics, which led to the birth of quantum theory, was examined by the founders of quantum mechanics including Bohr, Heisenberg, Schrödinger, Dirac, Born, and many others. In this book, we concentrate only on non-relativistic quantum mechanics.

Quantum mechanics deals with the small scale of physical objects in the universe; the objects (atoms, nuclei, photons, quarks) are so small that the quantization of physical variables becomes important. It is a radical and revolutionary physical theory for the development of nature science. Quantum mechanics was not developed directly from earlier physical theories. The ideas of it are built from physical concepts that could not be explained in terms of things previously known and that could not be explained adequately with classical ones. In fact it represents a revolutionary departure from classical ideas, creating a totally new way of thinking about the world, which makes quantum theory such an attractive and fascinating subject. As we progress through the course, we will examine the most significant differences from our everyday experience as well as the very basic theories and methods for quantum mechanics. We will find that the motion of objects does not behave according to our (classical) expectations, the particles also have wave-like properties, and the particles could tunnel through a barrier that is not possible in classic physics. Quantum mechanics brings us not only the improved numerical predictions for the microscopic world, but also the conceptual changes that rock the very foundations of classical thought.

Quantum mechanics is the basis for our present understanding of physical phenomena on an atomic scale. Nowadays, quantum mechanics has numerous applications in engineering, including semiconductor transistors, lasers, quantum optics and quantum communication. Engineers would like to make and control electronic, photo-electronic, and optical devices on an atomic scale. In biology there are molecules and cells we wish to understand and modify on an atomic scale. The same is true in chemistry, where an important goal is the synthesis of both organic and

inorganic compounds with precise atomic composition and structure. Quantum mechanics gives the engineer, the biologist, and the chemist the tools with which to study and control such objects.

It is generally believed that no one can discuss what quantum mechanics "means" before he or she gets a firm sense of what quantum mechanics "does". The current book focuses on the basic principles and theory of quantum mechanics in which the general knowledge required for developing a practical and intuitive understanding, is included. As the book is especially designed for bilingual teaching and learning, the characteristics and differences between eastern and western thoughts and presentations are considered, and this book is an attempt to bridge these differences.

The work is supported by the national bilingual teaching project. It is fulfilled with consistent efforts of all the members of the Quantum Mechanics bilingual teaching team in SNNU(Shaanxi Normal University), and many of our graduate and undergraduate students. We would like to thank many people who have given highly valued suggestions, feedbacks and corrections of errors for the book. Our bilingual teaching team members who are not included in the author list of the book, who are Shixian Qu, Guian Li, Hongjun Zhang, Yiping Huo and Hui Sun, have been giving us constant support and help. The authors thank them for many stimulating, constructive discussions and suggestions on the accomplishment of the book and the bilingual teaching of the class. We also would like to thank our teaching assistants and students for very helpful comments and correction of errors and typos.

The specific chapters of the book are fulfilled by Hairong Zheng (SNNU) (Chapters 1&2, also served as the principle author of the book), Yongzhong Xing (SNNU, Tianshui Normal University) (Chapters 3&4), Lin Zhang(SNNU) (Chapter 5), and Shaoguang Zhang (SNNU) (Chapter 6, and animation exercises for all chapters). Every contents of the book have been corrected and edited by Dan Boye from the Davidson College of USA, from both scientific and grammatical aspects.

The book is for undergraduate students majored in physics, and other majors that the basic knowledge of quantum mechanics is required. Though we have made every effort to ensure that our objective can be realized, but we believe that there are still plenty of rooms to improve. Any comments, suggestions and advices are mostly welcomed and highly valued.

Author

The spring of 2014

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Part Ⅰ The Wave Function and Schrödinger Equation

Chapter 1 The wave function and Schrödinger equation

1.1 The wave-particle duality and matter wave

Particles and waves are two distinct entities in classical physics. As we have learned from both text books and daily experiences, a particle is a localized bundle of energy and momentum. At any instant, it can be described by state parameters, such as position q and momentum $\boldsymbol{p}$ (or velocity v if the mass is a constant). The parameters q and p evolve in time according to some equations of motion, such as Newton's law $\boldsymbol{F}=\mathrm{d}\boldsymbol{p}/\mathrm{d}t$. Given the initial values $q(t_i)$ and $p(t_i)$ at time t_i, the position $q(t)$ and momentum $\boldsymbol{p}(t)$ at any time t can be deduced from the equations of motion. In contrast to the particle, a wave is considered as a periodic disturbance spread over space. It usually appears as some kind of periodic movement transferring energy from one point to another. A wave satisfies the superposition rules and presents interference and diffraction phenomena.

1.1.1 The wave-particle duality of light

In the 17th century, two competing theories of light were proposed during the debate about the nature of light: one was offered by Christian Huygens and the other by Isaac Newton. According to the theories, light was thought either to consist of waves (Huygens) or of corpuscles/particles (Newton). Huygens proposed that each point on a light wave front acted as a spherical point source for the progressing wave. Newton's argument satisfactorily and more simply explained geometric optics and did not presume a medium for particle travel.

At the beginning of 19th century (1801～1805), Thomas Young conducted the famous double-slit experiment showing that light from two slits interfere to produce a fringe pattern on a screen, a phenomenon that cannot be described by classical particles. In 1909, Geoffrey Ingram Taylor conducted an experiment that showed the interference phenomena by individual photons. The double-slit experiment has been repeated in many ways over the years and has become a standard demonstration of wave-like motion. But neither Newton nor Young were quite convincing about the nature of light. Light could not be described purely as a wave or as consisting of particles.

In 1900, Max Planck postulated that the energy of oscillators in a black body is an integer multiple of $h\nu$, where h is the Planck constant and ν is the frequency of the oscillator. The problem was that the wave nature of light was widely accepted at that time, the concept have been completely formulated in Maxwell's theory and confirmed by interference and diffraction experiments. After Planck's quanta hypothesis, Albert Einstein postulated the concept of the photon to explain the photoelectric effect in 1905, which also was used later to explain Compton scattering. According to Einstein's assumption, electromagnetic radiation of frequency ν consists of discrete units (quanta) of energy $h\nu$. That is, electromagnetic energy itself is quantized, and a single quantum is called photon. Thus, matter can absorb energy from a monochromatic beam of light of frequency ν only in units of $h\nu$ because the light arrives in the form of discrete quanta, each with energy $h\nu$. Einstein had re-introduced the problem of wave-particle duality for light! The relation between the light wave (ν, λ) and the light photon (ε, p)is presented by the equations

$$\varepsilon = h\nu = \hbar\omega \tag{1.1.1}$$

$$p = \frac{h\nu}{c} = \frac{h}{\lambda} = \hbar k \quad \left(k = \frac{2\pi}{\lambda}\right) \tag{1.1.2}$$

where h is the Planck constant. Eqs.(1.1.1) and (1.1.2) are called the Planck-Einstein relations, which reflect the wave-particle duality of light.

1.1.2 Matter wave and the wave -particle duality of matter

If the light could sometimes behave like particles, then should matter particles also show wave-like behavior? Upon examining Einstein's idea of the parallelism between the light and matter, Louis de Broglie in 1924 proposed that electrons, which generally are believed to be particles, should exhibit wave-like

behavior. The wavelength and frequency of a quantum mechanical particle are associated with its momentum and energy by *de Broglie's hypothesis*

$$\varepsilon = h\nu = \hbar\omega \tag{1.1.3}$$

$$p = \frac{h}{\lambda} = \hbar k \tag{1.1.4}$$

Where ε and p are the energy and momentum of the particle, and ν represents the frequency. The wavelength of the matter wave associated with the particle, λ, is also called *de Broglie wavelength*. In the case of non-relativistic theory, the de Broglie wavelength for a free particle with mass m and energy ε is

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m\varepsilon}} \tag{1.1.5}$$

The wave nature of an electron and de Broglie's hypothesis have been experimentally confirmed by electron diffraction experiments by G. P. Thompson, and C. Davisson & L. Germer. In short, any matter must be considered as having both the particle-like and wave -like properties.

You may want to argue that common sense tells us that billiard balls and ping-pong balls travel along definite trajectories and do not show any wave-like properties! The point is that the wave nature of matter is not apparent for macroscopic phenomena since Planck's constant h is so small. For example, suppose we perform the double-slit experiment with pellets of mass 0.01 kg, moving at 100 m/s. The wavelength associated with these particles is

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m\varepsilon}} \approx 6 \times 10^{-34}\,\mathrm{m} \tag{1.1.6}$$

which is about 10^{-24} times smaller than the radius of the hydrogen atom. The angular spread of the interference pattern would be so small that our instruments would only measure a smooth average, just as what is predicted classically.

Notes:

(1) de Broglie's relationship between wavelength and momentum applies equally well to photons as to particles such as electrons and neutrons. The concept of photon as a particle should be used with caution: not only is it a quantum rather than a classical particle, but a photon cannot be approximated as non-relativistic.

(2) The interference and diffraction phenomena can only be explained on the basis of wave theory, and in a classical wave the energy is spread continuously

through a region of space. How can Einstein's quantum picture of light be reconciled with the wave theory? How do the wave-like properties of particles coexist with their particle-like characteristics (such as a finite size)? You may think that wave and particle characteristics are mutually incompatible, but the ability of microparticles to behave in some circumstances as a wave and in others as a particle is fundamental to quantum physics.

1.1.3 Experimental observations of matter waves

Many experiments have been conducted that examined the matter wave nature of microparticles. In 1927 Clinton Davisson and Lester Germer observed the diffraction of electron beams from a nickel crystal demonstrating the wave-like properties of particles for the first time (*Nature* **119**: 558～560, 1927). The experiment consisted of firing an electron beam from an electron gun toward a nickel crystal at normal incidence. An electron detector was placed at varying angles to measure the number of electrons scattered. The distribution of scattered electrons confirmed the de Broglie hypothesis experimentally. Shortly afterwards, G. P. Thomson did the same with thin films of celluloid and other materials. In 1937, Davisson and Thomson shared the Nobel Prize for the "discovery of the interference phenomena arising when crystals are exposed to electronic beams".

In 1961, Claus Jönsson of Tübingen performed a different type of double-slit experiment with electrons shown in Fig. 1.1(a) (*American Journal of Physics* 42: 4～11, 1974). Pier Giorgio Merli, Giulio Pozzi and Gian Franco Missiroli carried out double-slit interference experiments with single electrons in 1974, in Bologna. Single electron events build to form an interference pattern (Fig. 1.1 (b); *Am. J. Phys.* **44**: 306～307, 1976). In 1989, Akira Tonomura and co-workers performed an experiment at Hitachi, in which there was just one electron in the apparatus at a time when they observed the fringe pattern using a very weak electron source and an electron bi-prism (*American Journal of Physics* 57: 117～120, 1989). The experiment has been performed with photons, electrons, atoms, and even macromolecules C_{60} and C_{70} since then. Each time the same result becomes obvious—something about measuring the position of the particle at the slit reveals its wave nature.

Thus, through the work of Max Planck, Albert Einstein, Louis de Broglie, Arthur Compton, Niels Bohr, and Clinton Davisson, Lester Germer, George Thomson, Claus Jönsson, Pier Giorgio Merli, Akira Tonomura and many

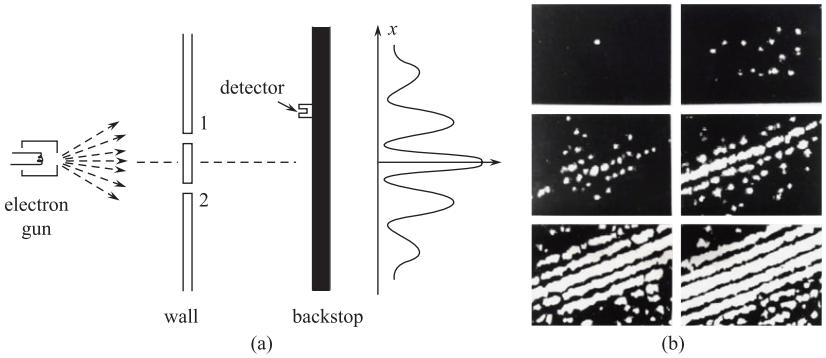


Fig.1.1 (a) Double slit experiment with electrons with both slits open. (Feynman Lectures on Physics, Vol.3, Chapter 1.); (b) Radual accumulation of interference fringes after the diffraction of an increasing number of electrons. The figures show how an interference pattern can be built up from single-electron events (www.lamel.bo.cnr.it/educational/educational.html; P.G.Merli, G.F.Missiroli, and G. Pozzi, Am. J. of Phys. 44;306, 1976)

others, we know that all particles have a wave nature. This phenomenon has been verified not only for elementary particles, but also for compound particles like atoms and molecules. In fact, the wave-particle duality applies to all objects, even macroscopic ones in non-relativistic quantum mechanics. But, because of their small wavelengths, the wave properties of macroscopic objects cannot be detected.

1.2 Wave function and its statistical interpretation

To describe the movement of microparticles, Born suggested that each particle is associated with a wave that is described by the *wave function*, also named the *state function*, $\Psi(\boldsymbol{r},t)$. The dynamics of the particle is then the dynamics of wave function. This claims that *there exists an abstract state function that contains all the information about the state of the dynamic system*.

Since a particle is localized at a point by its nature, while the wave function is a function of $\boldsymbol{r}$ for any given time t, a particle is spread out in space. How can such a function represent the state of a particle? Born's statistical interpretation of the wave function says that *the square of the modulus of the wave function*

$\psi(\boldsymbol{r},t)$, $|\psi(\boldsymbol{r},t)|^2$, *gives the probability density of finding the particle in a unit volume around point* $\boldsymbol{r}$, *at time* t. The probability of finding the particle between a and b, at time t is

$$\int_a^b \mathrm{d}\boldsymbol{r}^3 |\psi(\boldsymbol{r},t)|^2$$

The statistical interpretation points towards an indeterminacy of quantum mechanics. Even if one knows everything about the quantum state of a particle or wave function, one still cannot predict the outcome of a measurement of its position with certainty. All quantum mechanics has to offer is *statistical* information about the *possible* results.

The following conditions should be satisfied by a wave function based on this statistical interpretation:

(1) A wave function is a mathematical tool used to describe a physical system. It is in general a *complex function* of real variables with $|\psi(\boldsymbol{r},t)|^2 = \psi^*\psi$. being real and nonnegative (here ψ^* is the complex conjugate of ψ).

(2) The wave function and its first derivative are required *to be continuous and single-valued at any position* for finite or analytical potentials. If there was a discontinuity at any point, there would exist two values of $\psi(\boldsymbol{r},t)$ at that point, leading to the result of there being no unique value for the probability for that point.

(3) Any state of a particle can be represented by a wave function $\psi(\boldsymbol{r},t)$. The *probability density* for the spatial distribution of the particle at the instant t is determined by $|\psi(\boldsymbol{r},t)|^2$.

(4) *A wave function is non-singular*. Since the probability density for the spatial distribution of the particle at instant t is determined by $|\psi(\boldsymbol{r},t)|^2$, the equation of

$$\int_{\text{all space}} \mathrm{d}\boldsymbol{r}^3 |\psi(\boldsymbol{r},t)|^2 = \text{finite number} \tag{1.2.1}$$

must be satisfied for the wave function to be normalized. A non-singular wave function that remains finite everywhere is essential for ensuring the validity of the above equation.

(5) The probability of finding the particle in volume V at time t is

$$P_V = \int_V \mathrm{d}\boldsymbol{r}^3 |\psi(\boldsymbol{r},t)|^2 = \int_V \mathrm{d}\boldsymbol{r}^3 \psi(r,t)^* \psi(\boldsymbol{r},t) \tag{1.2.2}$$

which can only take values from 0 to 1 for a normalized $\psi(\boldsymbol{r},t)$. The probability

of finding the particle in all space should be 1 for each value of t

$$\int_{\text{all space}} \mathrm{d}\boldsymbol{r}^3 \,|\psi(\boldsymbol{r},t)|^2 = 1 \tag{1.2.3}$$

This is called the *normalization condition for the wave function* $\psi(\boldsymbol{r},t)$. The wave function satisfying the above equation is called a normalized wave function. Thus $|\psi(\boldsymbol{r},t)|^2$ should be finite and integrable.

(6) If the wave function ψ describes a state of the system, then $\alpha\psi$, where α is an arbitrary complex constant, describes the same state of the system. There exists an arbitrary phase factor for a wave function describing a given state, even if it is a normalized one.

(7) The total probability of finding the particle in a finite volume V can only change with time if there is a flow of probability across the surface of V. Therefore, probability should satisfy the continuity equation. It is conserved in all space.

(8) The time evolution of a wave function is described by the laws of quantum mechanics (i.e. the Schrödinger equation) that we will study in the coming sections.

Summarizing the above discussion, one has the following postulate:

The state of a non-relativistic quantum particle at time t is described by a continuous, non-singular, complex wave function $\psi(\boldsymbol{r},t)$, *which can be normalized so that the square of its modulus is equal to the probability density*

The Heisenberg uncertainty principle, also called the Heisenberg indeterminacy relation, says that

$$\Delta k \Delta x \geqslant 1/2 \quad \text{or} \quad \Delta x \Delta p \geqslant \hbar/2 \tag{1.2.4}$$

The relation states that there is a quantitative limitation on the accuracy with which we can describe a system using our familiar, classical notions of position and momentum. Position and momentum are said to be complementary or canonically-conjugate variables. The wave function cannot describe a particle that is both well-localized in space and has a well-defined momentum. This is in contrast to classical mechanics.

In classical mechanics, the state of dynamic system is completely specified by the position and momentum (or velocity if we assume the mass of the system does not change during the movement) of each particle of the system. This presumes that, at least in principle, the position and momentum of a particle can be measured precisely at each instant of time. The position and momentum of the

particle at any instant of time are completely determined by those of the particle at a previous instant. The system is deterministic. It is intuitively obvious that it is possible to measure the particle's position and momentum simultaneously. Yet in the micro world, we cannot see or touch any particle with complete objectivity. Quantum mechanics tells us that the state of the system is described by a wave function rather than the position and momentum. If the particle is in a certain state $\psi(\boldsymbol{r},t)$, the most specific information about the position of the particle is the probability and the ratio of the probability at $\boldsymbol{r}_1$ relative to that at $\boldsymbol{r}_2$ (that is $|\psi(\boldsymbol{r}_1,t)|^2:|\psi(\boldsymbol{r}_2,t)|^2$). These are all one can get by any possible means of measurement.

Since quantum mechanical predications are expressed in terms of probabilities, it can only be tested experimentally by carrying out a large number of identical measurements . Although quantum mechanics **cannot**, in general, predict the precise result of any individual measurement, it **can** predict its statistical distribution and the expectation values of any physical observables and their deviations.

As we shall see very soon, the time evolution of the state function itself is determined uniquely by its initial condition according to the Schrödinger equation. But the state function of the system is probabilistic to begin with. We will learn that the prediction of the dynamics of the system in terms of physically measurable properties is probabilistic, not deterministic, as well.

1.3 The principle of superposition

The statistical interpretation of a wave function also implies that the linear combination of two state functions is another possible state function, i.e., the state function satisfies the "principle of superposition" by

$$\psi = a_1\psi_1 + a_2\psi_2 \tag{1.3.1}$$

where a_1 and a_2 are complex numbers.

More generally, if $\psi_1,\psi_2,\cdots,\psi_n$ are states of the system, then their linear combination $\psi = a_1\psi_1 + a_2\psi_2 + \cdots + a_n\psi_n = \sum_{i=1}^{n} a_i\psi_i$ is another possible state of the system. This property looks simple but has profound mathematical and physical implications.

Taking Young's double-slit experiment as an example, we suppose a particle in the state ψ can evolve from two different possible paths with the relative probability of $|a_1|^2:|a_2|^2$. The particle in the final ensemble is in a "mixed state" of $\psi=a_1\psi_1+a_2\psi_2$, which is a superposition of two states ψ_1 and ψ_2. The probability distribution function of the particle in the final state is proportional to $|\psi|^2$ containing not only the terms of $|a_1|^2|\psi_1|^2+|a_2|^2|\psi_2|^2$ but also the cross terms (or "interference terms") of $a_1^* a_2\psi_1^*\psi_2+a_1 a_2^*\psi_1\psi_2^*$. Thus, $|\psi|^2$ depends on the relative phase. Since the probability distribution is proportional to $|\psi|^2$, whenever the final state function is a superposition of two or more state functions, the probability distribution function corresponding to the final state depends on the relative phases of the constituent state functions. This can lead to the constructive and destructive interference phenomena that was observed in Young's double-slit experiment.

1.4 The Schrödinger equation

The wave function is introduced for describing a physical system in quantum mechanics. But how does the wave function evolve over time? The answer is determined by the Schrödinger equation. This equation of motion is stated in the following postulate of quantum mechanics:

All state functions satisfy the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r},t)=\hat{H}\Psi(\boldsymbol{r},t) \tag{1.4.1}$$

where $\hat{H}$, the Hamiltonian of the system, is an operator corresponding to the total energy of the system. The specific form of an operator can be obtained from its analog in classical theory (please refer to the corresponding postulates in Chapter 3). It is a linear operator acting on the wave function Ψ. $\hbar=\dfrac{h}{2\pi}$ is the reduced Planck constant, and i is the imaginary unit.

Since the state of any system is completely specified by its wave function, the solution of the Schrödinger equation for $\Psi(\boldsymbol{r},t)$ completely describes the state of the dynamic system at all times once the initial condition $\Psi(\boldsymbol{r},t=0)$ and the Hamiltonian are known.

For the case of a single particle moving in three dimensions, if the potential is described with function $V(\boldsymbol{r})$, then the Hamiltonian of the system is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) \tag{1.4.2}$$

and the Schrödinger equation reads

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r},t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\boldsymbol{r},t) + V(\boldsymbol{r})\Psi(\boldsymbol{r},t) \tag{1.4.3}$$

Here $\boldsymbol{r}=(x,y,z)$is the position of the particle in three-dimensional space; $\Psi(\boldsymbol{r},t)$ is the wave function that is the probability amplitude for the particle with position $\boldsymbol{r}$ at time t; m is the mass of the particle; ∇^2 is the Laplace operator.

The Schrödinger equation for a N-particle system can be presented as

$$\begin{aligned}\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\cdots,\boldsymbol{r}_N,t) = &-\hbar^2\left(\frac{\nabla_1^2}{2m_1}+\frac{\nabla_2^2}{2m_2}+\cdots+\frac{\nabla_N^2}{2m_N}\right)\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\cdots,\boldsymbol{r}_N,t)\\ &+V(\boldsymbol{r}_1,\boldsymbol{r}_2,\cdots,\boldsymbol{r}_N)\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\cdots,\boldsymbol{r}_N,t)\end{aligned} \tag{1.4.4}$$

Notes:

1. Type of differential equation

The Schrödinger equation is a complex, first-order partial differential equation in time and second-order in space.

2. Linear characteristics

The wave functions describing the particles obey the superposition principle. They must satisfy a linear equation and are complex in general. If $\Psi_A(\boldsymbol{x},t)$ and $\Psi_B(\boldsymbol{x},t)$ are solutions to the Schrödinger equation, then $a\Psi_A+b\Psi_B$, where a and b are any complex numbers, must be a solution of the equation.

3. Local conservation of probability

The probability flux satisfies the continuity equation, which is the mathematical equivalent of the probability conservation law

$$\frac{\partial}{\partial t}P(\boldsymbol{r},t) + \nabla\cdot\boldsymbol{j} = 0 \tag{1.4.5}$$

where $P(\boldsymbol{r},t)=\Psi^*(\boldsymbol{r},t)\Psi(\boldsymbol{r},t)$is the probability density of the particle.

$$\boldsymbol{j} = \frac{\hbar}{m}\cdot\frac{1}{2\mathrm{i}}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) = \frac{\hbar}{m}\mathrm{Im}(\Psi^*\nabla\Psi) \tag{1.4.6}$$

is the probability flux. For example, the wave function and probability flux of a plane wave have the forms

$$\Psi(\boldsymbol{r},t)=A\mathrm{e}^{\mathrm{i}(kr-\omega t)} \tag{1.4.7}$$

and

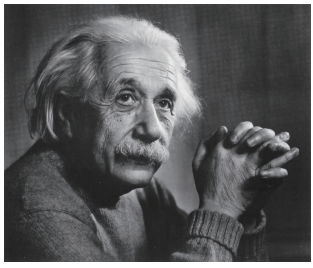
$$\boldsymbol{j}(\boldsymbol{r},t)=|A|^2\frac{\hbar k}{m} \tag{1.4.8}$$

It can be seen that not only is the probability of finding the particle the same everywhere, but also the probability flux describes an object moving at the classical velocity p/m as is expected.

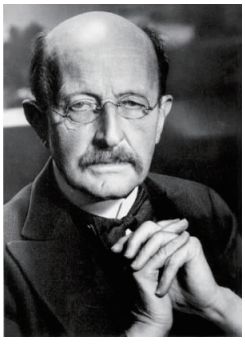
4. It is a postulate

The Schrödinger equation is one of the postulates in the quantum theory. It cannot be established or derived from any other theories or laws. The only way to examine it is to see if any result from the Schrödinger equation is reflected by experiments.

Biography



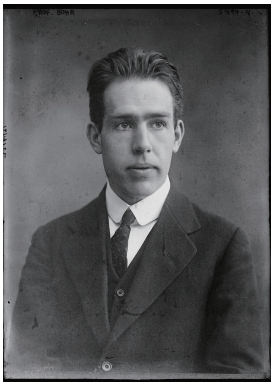
Albert Einstein (14 March, 1879～18 April, 1955) was a German-born theoretical physicist who is widely regarded as one of the most influential scientists of all time. He made tremendous contributions to physics and is best known for his theories of special relativity and general relativity. Einstein received the 1921 Nobel Prize in Physics "for his services to Theoretical Physics, and especially for his discovery of the law of the photoelectric effect."



Max Planck (23 April, 1858～4 October, 1947) was a German physicist. He is considered a founder of the quantum theory, and one of the most important physicists of the 20 th century. His radiation theory is the most significant lodestar for modern physical research. Planck was awarded the Nobel Prize in Physics in 1918 "for his work on the establishment and development of the theory of elementary quanta."



Werner Heisenberg (5 December, 1901 ~ 1 February, 1976) was a German theoretical physicist. He made foundational contributions to quantum mechanics and is best known for asserting the uncertainty principle of quantum theory. His quantum mechanics has created new concepts, and has led physics into fresh trains of thought. Heisenberg was awarded the 1932 Nobel Prize in Physics "for the creation of quantum mechanics, the application of which has led to the discovery of the allotropic forms of hydrogen."



Niels Henrik David Bohr (7 October, 1885~18 November, 1962) was a Danish physicist. He has been described as one of the most influential physicists of the 20 th century. Bohr received the Nobel Prize for Physics in 1922 "for his contributions which were essential to modern understandings of atomic structure and quantum mechanics."



Paul Adrien Maurice Dirac (8 August,1902~20 October, 1984) was a British theoretical physicist. He made fundamental contributions to the early development of both quantum mechanics and quantum electrodynamics. Dirac shared the Nobel Prize in physics for 1933 with Erwin Schrödinger and Heisenberg "for the discovery of new fruitful forms of the theory of atoms and for its applications."



Max Born (11 December, 1882～5 January, 1970) was a German born physicist and mathematician. He made great contributions to the development of quantum mechanics, so solid-state physics and optics. Born won the 1954 Nobel Prize in Physics "for his fundamental research in quantum mechanics, especially for his statistical interpretation of the wave function."



Clinton Joseph Davisson (22 October, 1881～1 February, 1958), was an American physicist who won the 1937 Nobel Prize in Physics "for his discovery of electron diffraction by crystals." Davisson shared the Nobel Prize with George Paget Thomson, who independently discovered electron diffraction at about the same time.

Lester Halbert Germer (10 October, 1896～3 October, 1971) was an American physicist. With Clinton Davisson, he proved the wave-particle duality of matter in the Davisson-Germer experiment, which was important to the development of the electron microscope.



Thomas Young (13 June, 1773～10 May, 1829) was an English genius and polymath, born in England. His research fields include Physics, Physiology, Egyptology. He is famous with the public for having partly deciphered Egyptian hieroglyphs before Champollion did. Young made notable scientific contributions to the fields of vision, light, solid mechanics, energy, physiology, language, musical harmony and Egyptology.

Essay:Schrödinger cat and EPR paradox

1. Schrödinger cat paradox

Schrödinger's cat is a thought experiment devised by Erwin Schrödinger in 1935, and is often described as a paradox, It illustrates what Schrödinger saw as the problem of the Copenhagen interpretation of quantum mechanics applied to everyday objects. The Copenhagen interpretation is an interpretation of quantum mechanics, in which the state of every particle is described by a wave function. According to this interpretation, the act of any measurement causes the calculated set of probabilities to "collapse" to the value defined by the measurement. The experiment presents a cat that might be alive or dead, depending on an earlier random event. In the course of developing this experiment, he created the term entanglement.

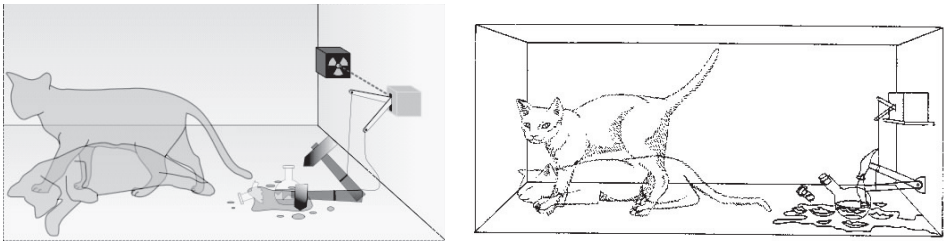


Fig.1.2 Illustrations of Schrodinger's cat paradox
(from en.wikipedia.org/wiki/)

Schrödinger's thought experiment (Fig. 1. 2) can be briefly described as follows: A cat, along with a flask containing some poison, is placed in an isolated, sealed box. If an internal Geiger counter detects radiation, the flask is shattered, releasing the poison that kills the cat. The Copenhagen interpretation of quantum mechanics implies that after a while, the cat is simultaneously alive and dead. Yet, when we look in the box, we see the cat either alive or dead, not both alive *and* dead.

The experiment was intended as a discussion of the article that had highlighted the strange nature of quantum superposition. The Copenhagen interpretation implies that the superposition undergoes collapse into a definite state only at the exact moment of quantum measurement.

Schrödinger's cat poses the question, when does a quantum system stop existing as a mixture of states and become one or the other? If the cat survives, it remembers only being alive. But explanations of the Schrödinger's cat experiments require that macroscopic objects (the cat) do not always have unique classical descriptions. The purpose of the experiment is to illustrate this apparent paradox.

2. EPR paradox

The EPR paradox is a thought experiment which challenged a long-held idea about the relation between the observed values of physical quantities and the values that can be accounted for by a physical theory. Albert Einstein, Boris Podolsky, and Nathan Rosen introduced the thought experiment in 1935 to argue that quantum mechanics is not a complete physical theory ("Can Quantum-mechanical Descriptions of Physical Reality be Considered Complete?" *Physical Review*, volume 47, pp. 777 ~ 780, 1935). The EPR paradox draws on a phenomenon of quantum entanglement that is predicted by quantum mechanics. It shows that measurements performed on spatially separated parts of a quantum system can apparently have an instantaneous influence on one another.

Suppose there is a source (e.g. pi meson (π) decay) that emits electron-positron pairs, and their spins are opposite. The electron is sent to destination A, and the positron is sent to destination B. According to quantum mechanics, one can arrange the source so that each emitted pair occupies a spin singlet quantum state, which can be viewed as a superposition of state I and state Ⅱ. In state I, the electron has spin pointing upward along the z-axis ($+z$) and the positron has spin pointing downward along the z-axis ($-z$). Vice versa, the electron may have spin in the $-z$ direction and the positron has spin at $+z$ direction in state Ⅱ. Therefore, it is impossible to associate either particle in the spin singlet with a state of definite spin. The particles are thus said to be entangled.

Following the above description, if we measure the electron's spin about the x-axis, it automatically tells us the positron's spin about the x-axis. Since we have done the measurement without disturbing the positron in any way, it cannot be that the positron "only came to have that state when you measured it", because we didn't measure it! It must have had that spin *all along*. Also you can now measure the positron's spin about the y-axis. So it follows that the positron has had a definite spin about two axes—much more information than the positron is capable of holding, implying a "hidden variable" as indicated by EPR.

According to its authors, the EPR experiment yields a dichotomy:

Either the result of a measurement performed on the part **A** of a quantum system has a non-local effect on the physical reality of another distant part **B**, in the sense that quantum mechanics can predict outcomes of measurements carried out at **B**;

or

Quantum mechanics is incomplete in the sense that some element of physical reality corresponding to **B** cannot be accounted for by quantum mechanics implying that an extra variable is needed to account for it.

The EPR paradox is a paradox in the following sense: if one adds to quantum mechanics some seemingly reasonable (but actually wrong, or questionable as a whole) conditions like local realism, counterfactual definiteness, incompleteness, then one obtains a contradiction. However, quantum mechanics by itself does not appear to be internally inconsistent, nor does it contradict relativity. As a result of further theoretical and experimental developments since the original EPR paper, most physicists today regard the EPR paradox as an illustration of how quantum mechanics violates classical intuitions.

Associated application :TEM and SEM

TEM (transmission electron microscope) and SEM (scanning electron microscope)

The wavelength of electrons can be much shorter than that of visible light so that electron microscopes have much greater resolving power than light microscopes.

The idea of such a device was tossed about in the café's and bars of Paris and Berlin as early as 1928. The development of electron tubes and circuits, vacuum technology and electron beam control led to the construction of the first transmission electron microscope (TEM) with magnetic lenses by electrical engineers Max Knoll and Ernst Ruska in Berlin in 1931(see Fig.1.3). The TEM was the first type of Electron Microscope to be developed and is modeled on the light transmission microscope except that a focused beam of electrons is used instead of light to "see through" the specimen. Although the overall performance of the TEM has been improved thousands of time since its invention, it is basically the same in principle as that first designed by Knoll and Ruska: a device that focuses electron beams with magnetic lenses and creates a flat-looking two-

dimensional shadow pattern on its screen, the result of varying degrees of electron transmission through the object.

For the TEM, a "light source" at the top of the microscope emits electrons that travel through vacuum in the column of the microscope. As glass lenses focus light in the light microscope, the TEM uses electromagnetic lenses to focus electrons into a very narrow beam. The electron beam then travels through the specimen of study. At the bottom of the microscope the unscattered electrons hit a fluorescent screen, which gives rise to a "shadow image" of the specimen with its different parts displayed in varied darkness according to their density (Fig.1.4).

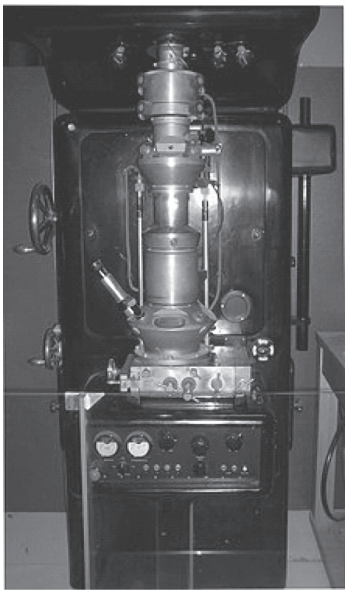


Fig.1.3 The electron microscope constructed by Ernst Ruska in 1931 (from en. wikipedia. org/wiki)

With a TEM, we can see objects to the order of a few angstrom (10^{-10} m). The possibility for high magnifications has made the TEM a valuable tool in both medical, biological and materials research. The best optical microscopes using UV light have a magnification of about 2000 and can resolve two objects separated by 100 nm. The magnification of a TEM is 10,000 to 100,000 in practice, with a maximum resolution about 0.2 nm.

Another type of electron microscope with less resolution and magnification than the TEM, but capable of producing striking three-dimensional images, is the scanning electron microscope (SEM). The SEM was the brainchild of the same Max Knoll who helped invent the TEM. The first operating scanning microscope was built by M. Von Ardenne in 1937, and it was extensively developed and perfected in the early 1940s. (The resolution is about 10 nm). The SEM operates in a very similar way as TEM does. The only difference is that the signals collected from the sample are reflected electrons in SEM, while the signals are given by transmitted electrons in TEM.