

## QUANTUM SYSTEMS

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### Summary

Quantum physics is mainly concerned with the microscopic world, but all of physics is quantum physics. This means that the laws of classical physics follow from the laws of quantum physics. The particle nature of light was established through study of photoelectric effects, spectra of blackbody radiations, and many other phenomena. Thus, the light has the dual nature of being wave and particle. Likewise, it was established through experiments such as diffraction phenomenon that the electron as well as other particles has the wavelike property. As the results, all material particles and fields have the dual nature. The wave and particle properties are related by de Broglie relations:  $E = h\nu$  and  $p = h/\lambda$ , where  $E$  and  $p$  are the energy and momentum of the particle and  $\nu$  and  $\lambda$  are the frequency and wavelength of the wave.

The universal constant  $h$  called the Planck constant is a key to relate the particle nature to the wave nature. The value of  $h$  is exceedingly small in the macroscopic scales:  $h \sim 6.6 \times 10^{-34}$  joule·sec. As the result, the quantum effect is only important for microscopic phenomena under usual circumstances.

The only way to reconcile the particle nature and the wave nature to each other is to identify the wave as a wave which expresses the probability distribution for finding the particle at various positions in space. The wave is called the wave function usually denoted by  $\Psi$ , which is a function of space and time. The fundamental equation to describe its time evolution is the Schrödinger equation and the interpretation of  $\Psi$  is that the absolute square of  $\Psi$  gives the probability for finding the particle at the spacetime point.

The characteristic features of quantum systems are the uncertainty and discreteness of physical quantities contrary to classical systems. The uncertainty nature originates from the probabilistic nature of the wave function and a pair of physical quantities such as position and momentum cannot take definite values at the same time. The discrete nature is also an outcome of the wave nature of quantum system. In particular, the energy of the electron in an atom can take only one of the discrete values allowed, and thus the state of the electron can change discontinuously thereby emitting light with definite energy.

Particles of the same kind are perfectly identical and indistinguishable with each other. In quantum physics, this leads to the wave function of a multi-particle system being either symmetric or antisymmetric under exchange of any pair of identical particles. It is antisymmetric for electrons, and this leads to Pauli's exclusion principle which states that no two electrons can occupy the same state.

The structures of atoms, molecules, and solids are well understood based upon the discrete nature of allowed energies for electrons and the exclusion principle for electrons. Electric conductivity of solids is a good example to show how quantum physics can well explain the characteristic properties of solids.

The electromagnetic interaction between charged particles and the electromagnetic field is derived from the gauge invariance of the interaction and the minimal coupling based on the invariance leads to the correct interaction. Quantum mechanical calculation of the radiative transition of atoms is presented and the results fit well with the observation.

Quantum mechanics is a self-contained fundamental theory of the microscopic world and able to describe even quantitatively all kinds of microscopic phenomena.

Under extreme condition such as very low temperature, quantum effect can appear in macroscopic scales. Superconductivity and superfluidity are remarkable quantum phenomena of macroscopic scales.

## Introduction

Quanta and relativity are the two phenomena of physics which are quite outside our daily experiences. We shall look into the origins of the concept of quanta and the laws of quantum physics in this chapter. It is really remarkable that physicist's view of nature changed totally and new perspectives were opened up within about 25 years in the early 20th century.

One of the great intellectual upheavals of the 20th century physics came out of the gradual realization that classical physics, i.e. the Newtonian mechanics and Maxwell's theory of electromagnetism, was not appropriate in the domain of the atomistic physical world. Classical physics had worked so well on the large scale but failed on the small scale of the atomic dimension. Physics in the realm of atoms, nuclei, and elementary particles can be well described only in terms of the quantum nature of matter and radiation, and these aspects of nature referred to as quantum phenomena. The basic theory of quantum phenomena is known as quantum mechanics.

Although quantum physics is mainly concerned with the microscopic world, all of physics is quantum physics. If we know the basic laws governing the microscopic world, at least in principle we can predict the behavior of macroscopic systems composed of a huge number of atoms. This means that the laws of classical physics follow from the laws of quantum physics. Therefore, the laws of quantum physics are the most general and basic laws of nature.

First we shall describe the quantum nature of the electromagnetic wave. The photoelectric effect and the blackbody radiation offered us the first evidence for the quantum nature of light (see *Particles and Fields*). The photoelectric effect is the phenomenon in which electrons are emitted from a metal surface when the metal is irradiated by a beam of light. The energy spectrum of the electrons emitted depends on the wavelength but not on the intensity of light. Furthermore, electrons are emitted only when the wavelength of light is less than a certain critical value, which depends on the material used. In Fig.1 we show the current due to the emitted electrons as a function of the wavelength  $\lambda$  of light.

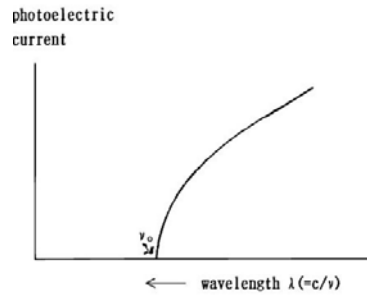


Figure 1. Photoelectric current as a function of wavelength of light

The above characteristics of the photoelectric effect can be understood only if the process is absorption of one quantum of light, a photon, by an electron in a metal. Then, the energy balance of the photoelectric effect is given by

$$h\nu = K_{\max} + h\nu_0 \quad (1)$$

where  $\nu$  is the frequency of light ( $\nu = c/\lambda$ ),  $h\nu$  the energy of the photon,  $K_{\max}$  the maximum energy of the emitted electrons, and  $h\nu_0$  the minimum energy needed for an electron to get out from the metal surface. From Eq.(1), photoelectrons can be emitted only when  $\nu > \nu_0$ , thus confirming the experimental results shown in Fig.1. Photoelectric effects show that a beam of light consists of a stream of photons traveling along the beam with the speed of light and that each photon carries an energy  $h\nu$ , where  $h$  is the Planck constant.

The photon concept was also supported by an experiment first carried out by Compton in 1923. He studied the behavior of X-rays scattered from a target material made of graphite. The wavelengths of the scattered X-rays varied with scattering angles. Compton realized that the scattering is an elastic collision of a photon with an electron in the material. In Fig.2 we show the kinematics of the Compton scattering, where  $\lambda$  and  $\lambda'$  are the wavelengths of the incident and scattered lights,  $\varphi$  is the scattering angle and  $\theta$  the recoil angle of the electron.

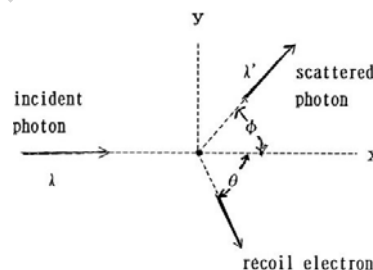


Figure 2. Kinematics of the Compton scattering

If a photon with wavelength  $\lambda$  carries a momentum  $p = h/\lambda$  and an energy  $E = h\nu = ch/\lambda$ , the momentum and energy conservations of the Compton scattering are

$$\begin{aligned}
 h/\lambda &= (h/\lambda') \cos \varphi + mv_x \\
 0 &= (h/\lambda') \sin \varphi - mv_y \\
 hc/\lambda &= hc/\lambda' + m(v_x^2 + v_y^2)/2
 \end{aligned} \tag{2}$$

The first two equations are the momentum conservation laws and the last one is the energy conservation law, where  $m$  is the rest mass of the electron. We have chosen the  $x$ -axis as one along the direction of motion of the incident photon and the  $y$ -axis as one perpendicular to the  $x$ -axis and in the scattering plane.

From these equations we can find, after neglecting  $v^2/c^2$  in comparison with unity,

$$\lambda' = \lambda + (h/mc)(1 - \cos \varphi) \tag{3}$$

The scattered light has a longer wavelength ( $\lambda > \lambda'$ ) than the incident light except at  $\varphi = 0$ . This equation fits nicely the observed relation between the wavelength  $\lambda'$  and the scattering angle  $\varphi$  of the photon, thus confirming the particle nature of light. The quantity  $h/mc$  is called the Compton wavelength of the electron, which is  $2.426 \times 10^{-12}$  m.

The dual nature of light being wave and particle was well established through many experiments such as photoelectric effects, blackbody radiations and Compton scatterings. The particle and wave properties of light are related by

$$E = h\nu, \quad p = h/\lambda \tag{4}$$

where  $\nu\lambda = c$ .

The value of the Planck constant  $h$  is

$$h = 6.626 \times 10^{-27} \text{ erg} \times \text{sec} = 6.626 \times 10^{-34} \text{ joule} \times \text{sec} \tag{5}$$

The Planck constant characterizing the quantum nature of radiation and matter is numerically extremely small when measured in units which are appropriate for description of macroscopic phenomena. The physical dimension of  $h$  is

$$\begin{aligned}
 [h] &= [\text{time}] \times [\text{energy}] = [\text{length}] \times [\text{momentum}] \\
 &= [\text{angular momentum}]
 \end{aligned} \tag{6}$$

A physical quantity of this dimension is known as action, and accordingly the Planck constant is called the quantum of action.

In the theory of relativity, the energy  $E$  and momentum  $p$  of a body are related by  $E^2 = c^2 p^2 + m^2 c^4$ , where  $m$  is the rest mass of the body. The relation  $E = cp$  which we can obtain from Eq.(4) expresses that the photon is a massless particle ( $m = 0$ ). The experimental results of the Compton scatterings clearly show that a beam of light consists of a stream of massless photons traveling with the speed of light.

In order to further elucidate the relation between the wave and quantum natures of light, we shall consider the double-slit experiment of Young (see *Development of Fundamentals in Physics*). The essential geometry of the double-slits experiment is shown in Fig.3.

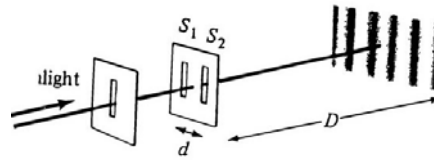


Figure 3. The double slit-experiment

A monochromatic light from a single source passes first through a thin slit and next through two very narrow parallel slits separated by a short distance, and finally impinges upon a screen. Then we find interference fringes on the screen as shown in the figure. This interference pattern can be well understood in terms of the wave nature of light. In Fig.4 we show how the waves with a definite wavelength propagate from each of the double-slits towards the screen and interfere with each other, when we look at the waves in a horizontal plane.

The quantum nature of the light appears when we use an extremely weak light in intensity. A very weak light beam would be a train of photons separated by a large distance from each other. When the beam hits the screen, only a single spot on the screen is illuminated at a time, which shows clearly that photons behave as localized objects or particles. When we keep observing bright spots on the screen, the positions of the spots change from one place to another more or less randomly. If we keep registering bright spots on the screen during a certain time interval, there gradually appears an interference pattern with increasing number of spots as shown in Fig.5. For large enough number of spots, the pattern becomes identical with the interference fringes observed on the screen when we used an intense light beam.

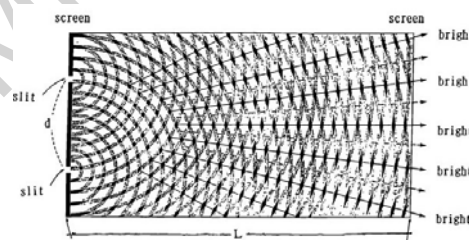


Figure 4. Interference of two waves in the double-slit experiment

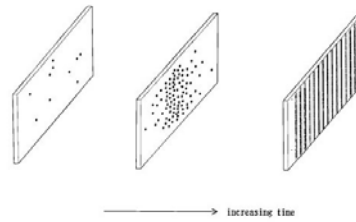


Figure 5. Interference pattern of the double-slit experiment with very weak light

Since photons in a weak light beam are separated by a large distance from each other, they should behave independently with no correlation between them. Yet, they behave statistically to form the typical interference pattern as a whole. A plausible reason for the formation of the pattern is that the pattern is the property of the wave of a single photon and that the wave represents probability distribution of the position of the photon. This probability wave is called a wavefunction of the photon.

A photon has a finite probability to pass through either one of the two slits and the two probability waves passed through the two slits interfere to each other. Bright lines on the screen are lines connecting positions where photons hit with large likelihood and dark lines are those where photons hit with small likelihood. Each photon can hit only one spot on the screen. But, if many photons with the same wave function impinge upon the screen, statistically they hit the screen according to the probability distribution specified by the interference pattern. This is similar to throwing a dice repeatedly. In each trial, we will get a definite number out of 1 to 6. If we repeat throwing the dice many times, each of the numbers from 1 to 6 will be obtained with an equal probability of  $1/6$ . Namely, the result of each trial is not deterministic, but the averaged results over many trials are well predicted through the predetermined probability distribution.

The results of the double-slits experiments with a weak light beam clearly show that the wave of light is a wave of the probability distribution of a single photon in space and time. Therefore, contrary to classical physics, motion of photons is not deterministic but probabilistic in nature. The electromagnetic wave has a dual nature. It has a wavelike property which causes it to show interference and diffraction patterns, and a particle like property as shown by the quantum nature of photons. Then it might be natural to ask whether particles such as electrons might also have wave properties similar to the light.

The photon has a momentum  $p$  and an energy  $E$  given by  $p = h/\lambda$  and  $E = h\nu$ , where  $\lambda$  is the wavelength and  $\nu$  is the frequency of the photon. By analogy, De Broglie speculated in 1924 that particles might have wave properties and that their wavelengths and frequencies and their momenta and energies are related by the following relations:

$$E = h\nu, \quad p = h/\lambda \quad (7)$$

The waves associated with matter are called the de Broglie waves.

In 1927, Davisson and Germer confirmed that electrons indeed have wave properties. In their experiments a beam of electrons with a given energy and a given momentum was

scattered by a nickel crystal upon which the beam was incident. They found that the electrons were reflected very strongly at certain special angles, which is similar to the Bragg reflection of X-rays from crystals.

Suppose a beam of electrons with a fixed energy is directed perpendicularly at a target crystal which consists of periodic arrays of identical atoms. To illustrate the principle, we consider a one-dimensional array of identical atoms as shown in Fig.6. The same principle applies to a two or three-dimensional array of identical atoms.

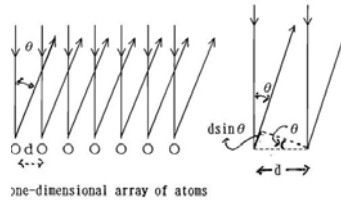


Figure 6. The Wave property of electrons

The incident electron wave is reflected by each atom in the row. In certain directions the reflected waves from all the atoms will reinforce each other, while in other directions they will tend to cancel. The condition for constructive interference is that the differences in the distances from different atoms to the point of observation are integral multiples of the wavelength. If the point of observation is very far away from the target crystal, the condition for constructive interference is

$$d \sin \theta = n\lambda \quad (8)$$

where  $n$  is an integer,  $d$  the lattice spacing and  $\theta$  the diffraction angle. The observed diffraction maxima occurred at angles expected from Eq.(8).

Similar experiments for other particles such as protons, neutrons, and atoms were carried out later and revealed that they all share the same wave property with electrons. Therefore, we can safely conclude that all matter has the dual property of being waves and particles. The wave nature of a macroscopic body is not apparent in ordinary circumstances, because its wavelength  $\lambda (= h/p = h/mv)$  is too small for any interference effect to be observed. Thus, macroscopic bodies can be safely treated as particles totally disregarding their wave properties.

### Structure of Atoms

The study of the structure of the hydrogen atom as well as those of other atoms played indispensable roles in establishing the quantum nature of microscopic objects and the laws of quantum physics. Through Rutherford's experiments it was found that an atom consists of electrons orbiting about a nucleus. But according to classical electromagnetic theory, an accelerating charged particle must emit radiant energy and thus a circulating electron must continuously radiate and lose energy. This means that atomic electrons are unstable and soon or later fall into the nucleus by losing its energy. Thus, the atoms in the universe should have collapsed long time ago. In 1913 Bohr proposed a



revolutionary model of the atomic structure in which he gave a prescription to solve the stability problem of atomic orbits of electrons in an atom.

The hydrogen atom consists of a proton and an electron. When the electron orbits the massive proton in a circular orbit of radius  $r$ , the balance between the centrifugal and electrostatic coulomb forces is given by

$$mv^2/r = e^2/r^2 \quad (9)$$

where  $v$  is the velocity of the electron along the circular orbit.

Bohr's first postulate is that only those atomic orbits occur for which the angular momentum of the orbiting electron is an integral multiple of  $h/2\pi$ . Mathematically this postulate is

$$mvr = n(h/2\pi) \quad (n = 1, 2, 3, \dots) \quad (10)$$

Bohr's second postulate is that no electron radiates energy as long as it remains in one of the orbital energy states specified by the first postulate and that radiation occurs only when an electron goes from a higher energy state to a lower one, the energy of the quantum of radiation being equal to the energy difference of the states.

The Bohr model based on the two postulates explained rather well the atomic spectra of hydrogen. We shall here describe the Bohr model in a somewhat different way from his original one, thereby employing explicitly the wave nature of the electron due to de Broglie. From Eq.(9) the momentum of the electron moving along an atomic orbit is given by

$$p = mv = (e^2 m/r)^{1/2} \quad (11)$$

The hydrogen atom has a radius of about  $10^{-10}$  m. Using this value for  $r$ , we can estimate the de Broglie wavelength of the electron and it is given by

$$\lambda = h/p = (h/e)(r/m)^{1/2} \sim 4 \times 10^{-10} \text{ m}$$

Since the wavelength is comparable to the radius of the atom, the wave nature of the electron must be taken into account in describing atomic orbits of the electron. If an electron wave circles along its orbit as shown in Fig.7, the wave can only be stable when the orbit length is an integral multiple of wavelength. Otherwise, the wave will be diminished to zero through interferences of waves repeatedly circulating about the nucleus.

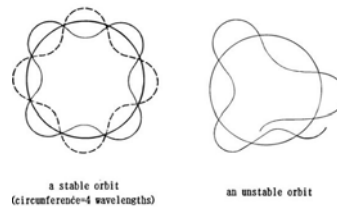


Figure 7. Waveproperty of an electron in an electronic orbit

This condition is given by

$$n\lambda_n = 2\pi r_n \quad (n = 1, 2, 3, \dots), \quad (12)$$

where  $n$  is any positive integer,  $r_n$  the radius of the orbit, and  $\lambda_n$  the wavelength of the electron in the orbit. This condition is identical with Eq.(10) because of the relation  $\lambda = h/p = h/mv$  for the de Broglie wave. Thus, the wave nature of an electron gives a basis for Bohr's first postulate and leads to the discreteness of atomic orbits allowed for the electron. These orbits are called Bohr orbits.

The radius of the smallest orbit  $r_1$  is called the Bohr radius  $r_B$ , which in view of Eqs.(9) and (12) is given by

$$r_B = \hbar^2 / e^2 m = 0.53 \times 10^{10} \text{ m} \quad (13)$$

and the radii of other orbits are given by  $r_n = n^2 r_B$ . Here,  $\hbar$  is defined by  $\hbar = h/2\pi$ .

The energy of the atom consists of the kinetic and potential energies of the electron. The energy of the electron in the  $n$ -th orbit is  $E_n = mv_n^2/2 - e^2/r_n$ , where  $v_n$  is the velocity of the electron in the  $n$ -th orbit. Using Eqs.(10) and (11), we obtain

$$E_n = -\left(1/2n^2\right)mc^2\left(e^2/\hbar c\right)^2 = -\left(13.6/n^2\right)\text{eV} \quad (14)$$

By the definition of energy, the zero point of energy is taken for  $r = \infty$  and  $v = 0$ . As the electron comes closer to the proton, it loses energy by emitting radiations and falls into a stationary state of the hydrogen atom, whose energy is negative. The lowest energy state ( $n = 1$ ) is the ground state and other states of higher energies are excited states of the hydrogen atom.

In Fig.8 we show the energy level diagram for a hydrogen atom. There exist an infinite number of discrete levels between the  $n = 1$  ground state and the state of  $n = \infty$ . At the level where  $n = \infty$ , the electron is free from the atom but it is at rest ( $v = 0$ ). States of positive energies represent states of a free electron and their energies are the kinetic energy of the free electron, which can take any value from zero to plus infinity.

In 1926, Schrödinger incorporated de Broglie's postulate on the wave nature of a particle into a mathematical formulation from which all wave aspects of the particle can be derived. The Schrödinger equation is an equation of motion of de Broglie waves. The solution of the equation is a function of space and time denoted as  $\Psi$  and referred to as the wave function.

The correct meaning of the wave function  $\Psi$  was proposed in 1926 by Born which is now become known as the orthodox interpretation of  $\Psi$ . Born proposed that the electron is truly a particle and that the  $\Psi$  wave associated with it is a probability function that would tell us where the electron is most likely to be. If we calculate the likelihood of finding an electron somewhere in a hydrogen atom by using the wave function  $\Psi$ , we get whole range of potential locations of the electron in the atom. Thus the electron is associated with a cloud of possibilities and the densest part of the cloud is the most likely place to find the electron.

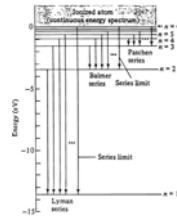


Figure 8. The energy level diagram for a hydrogen atom

It turned out that the Schrödinger equation for hydrogen has solutions only for specific values of energy which are exactly equal to those of the Bohr orbits. According to Born's interpretation of the wave function, the atomic electron is not really whirling about the nucleus like the motion of the planets about the sun, but instead it was smeared out in space as predicted by the wave function. The Schrödinger equation for the electron in a hydrogen atom is

$$-\left(\hbar^2/2m\right)\nabla^2\Psi + V\Psi = i\hbar\partial\Psi/\partial t \quad (15)$$

where  $\hbar = h/2\pi$  and  $V$  is the coulomb potential between the electron and the proton:

$$V = -e^2/r \quad (16)$$

The Schrödinger equation cannot be derived from previous classical ideas. It is a postulate which can be only justified by its ability to predict various physical phenomena and by comparison of the predicted results with the results of experiments. We find from Eq.(15) that the wave function  $\Psi$  is a complex quantity contrary to waves in classical physics. Even if  $\Psi$  is everywhere real at an instantaneous time, it will develop its imaginary part because of the presence of the factor  $i$  in the right-hand side of the Schrödinger equation. Also the Planck constant appears in the equation meaning that the quantum nature of the wave is taken into account.

According to Born's interpretation of the wave function, the probability for finding a particle in an infinitesimal volume element  $dV$  at a position  $r$  is given by

$$\Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t)dV \quad (17)$$

Since  $\Psi^* \Psi$  is real and positive, there is no problem in interpreting this quantity as the probability. Since the particle must be somewhere in the entire space, the integral of the probability over the entire space must be one:

$$\int \Psi^*(\mathbf{r}, t) \Psi(\mathbf{r}, t) dV = 1 \quad (18)$$

Measured values of any physical quantity  $A$  which is a function of the position and momentum of a particle follow a statistical distribution specified by the wave function just like the position of the particle. And its average value over many measurements is given by

$$\langle A \rangle = \int \Psi^*(\mathbf{r}, t) A(\mathbf{r}, \mathbf{p}) \Psi(\mathbf{r}, t) dV \quad (19)$$

The probabilistic or statistical interpretation of the wave function  $\Psi$  suggests that we can compute only the likelihood of events. In 1927, Heisenberg proposed the uncertainty principle which gives reason to the indeterminacy of physical quantities. It states that in a simultaneous measurement the uncertainty  $\Delta x$  in the position multiplied by the uncertainty  $\Delta p$  in momentum is at best about equal to the Planck constant  $h$ :

$$\Delta x \Delta p \geq h \quad (\text{for one - dimensional space})$$

(A rigorous uncertainty relation will be given later after defining  $\Delta x$  and  $\Delta p$ .)

Suppose we try to measure the position and momentum of a moving body. If the body is of a macroscopic size, we can, for example, use sunlight bouncing off the body to find out its position and momentum (velocity). Similarly, suppose we use a beam of photons to observe the position and momentum of a microscopic object such as an electron. A photon with a given momentum will have a corresponding wavelength  $\lambda$ . A photon wave will bend around an electron yielding only a coarse determination of the electron position. Its precision  $\Delta x$  is of the order of the photon wavelength  $\lambda$  ( $\Delta x \sim \lambda$ ). When a photon interacts with an electron, it will disturb the motion of the electron. The momentum change of the electron during the interaction is equal to the momentum of the photon either emitted or absorbed by the electron. This imposes the limit to the precision in the momentum measurement of the electron;  $\Delta p \sim (\text{photon momentum}) \sim h/\lambda$ . Then, the product  $\Delta x \Delta p$  is about equal to the Planck constant  $h$ .

The way to sharpen the position measurement of the electron is to use the small photon wavelength comparable or less than the size of the electron. But, then the motion of the electron will be strongly disturbed by the large photon momentum and the uncertainty in the momentum measurement will increase. Conversely, the way to sharpen the momentum measurement is to use the large photon wavelength so that the momentum

uncertainty becomes small. However, the position uncertainty will increase in proportion to the wavelength used. Heisenberg's uncertainty relation does not exclude the possibility of measuring either the position or the momentum of a particle with an infinite precision, but it excludes the possibility for measuring both the position and momentum with an infinite accuracy at the same time.

Planck's constant  $h$  is an extremely small number ( $\sim 6.6 \times 10^{-34}$  joule-sec). For an ordinary macroscopic body with mass  $m$ ,  $\Delta x \Delta v \sim h/m$ , so that the product of the uncertainties in the position and velocity of the body is negligibly small because of the small  $h/m$ . The uncertainties become important only for objects with an extremely small mass such as an electron or an atom.

For example, the product of  $\Delta x \Delta v$  due to the uncertainty relation for a body with mass of 1kg is  $\Delta x \Delta v \sim 6.6 \times 10^{-34} \text{ m}^2/\text{s}$ . If we take, for example,  $\Delta x \sim 10^{-17} \text{ m}$ , we obtain  $\Delta v \sim 6.6 \times 10^{-17} \text{ m/s}$ . These values are very much smaller than the magnitudes of experimental errors in measurements of the position and velocity of any macroscopic body. On the contrary,  $\Delta x \Delta v$  for an electron with mass  $9.1 \times 10^{-31} \text{ kg}$  is about  $0.7 \times 10^{-3} \text{ m}^2/\text{s}$ . If we take  $\Delta x \sim 10^{-10} \text{ m}$  which is of an order of the atomic radii, we obtain  $\Delta v \sim 0.7 \times 10^7 \text{ m/s}$  which is quite a large uncertainty in the electron velocity.

Although the Schrödinger equation cannot be derived from any of classical equations, it must represent classical motion of a particle under conditions where the wave nature of the particle can be neglected. The Schrödinger equation for the electron in a hydrogen atom is given by Eq.(15) supplemented by Eq.(16). If we multiply  $\Psi^*$  upon the equation (15) from the left and integrate over the entire space, we have

$$\int \Psi^*(\mathbf{r}, t) (\mathbf{p}^2 / 2m) \Psi(\mathbf{r}, t) d\mathbf{r} + \int \Psi^*(\mathbf{r}, t) V(\mathbf{r}) \Psi(\mathbf{r}, t) d\mathbf{r} = \int \Psi^*(\mathbf{r}, t) E \Psi(\mathbf{r}, t) d\mathbf{r} \quad (20)$$

Here we substituted  $E$  for  $i\hbar\partial/\partial t$  and  $\mathbf{p}$  for  $-i\hbar\nabla$ .

This relation means that the sum of the average values of kinetic and potential energies is equal to the average value of the total energy  $E$  of the electron in the hydrogen atom, which corresponds to the relation  $E = \mathbf{p}^2/2m + V$  in classical physics. Thus the Schrödinger equation can be interpreted as the relation  $E = \mathbf{p}^2/2m + V$  applied to the wave function  $\Psi$ , where  $E$  and  $\mathbf{p}$  are the differential operators acting upon  $\Psi$ . When the probability distribution specified by  $\Psi$  is such that the deviations of the position and momentum from their average values are small in macroscopic scales, then the Schrödinger equation can describe well the classical motion of the electron.

In order to see why we substituted  $E$  by  $i\hbar\partial_t$ , and  $\mathbf{p}$  by  $-i\hbar\nabla$ , let us consider the Schrödinger equation for a free particle moving in one dimensional space:

$$-\left(\hbar^2/2m\right)d^2\Psi/dx^2 = i\hbar\partial\Psi/\partial t \quad (21)$$

A solution of the equation with a definite wavelength  $\lambda$  and a definite frequency  $\nu$  can be written as

$$\Psi(x, t) = A \exp\left[i2\pi\left(x/\lambda - \nu t\right)\right] \quad (22)$$

where  $A$  is the normalization constant of the wave function. Since we allow wave functions to be complex, we took the wave function of an exponential form. Since  $\Psi^* \Psi$  is constant everywhere, the wave function  $\Psi$  represents a state of uniform density of the electron in space.

Operating  $i\hbar\partial_t$  and  $-i\hbar\nabla$  on  $\Psi$  are equal to multiplying  $2\pi\hbar\nu$  ( $= h\nu = E$ ) and  $2\pi\hbar/\lambda$  ( $= h/\lambda = p$ ) on  $\Psi$  respectively, if we use the de Broglie relations between the wave nature and the particle nature of the electron. Thus, the substitutions  $i\hbar\partial_t$  for  $E$  and  $-i\hbar\nabla$  for  $\mathbf{p}$  are justified.

Any wave function which satisfies the equation  $i\hbar\partial\Psi/\partial t = E\Psi$  with a constant  $E$  represents a stationary state with the given energy  $E$ . The time-dependence of a stationary state  $\Psi$  is given by  $\Psi = \exp(-Et/\hbar)\Phi(\mathbf{r})$  where  $\Phi(\mathbf{r})$  depends only upon the spatial coordinates of the particle. The Schrödinger equation for the time-independent wave function  $\Phi$  is given by

$$-\left(\hbar^2/2m\right)\nabla^2\Phi + V\Phi = E\Phi \quad (23)$$

which is called the time-independent Schrödinger equation.

The Schrödinger equation (15) is linear in  $\Psi$ . If  $\Psi$  is a solution of the equation, any multiple of  $\Psi$  is also a solution. Thus, if we find a solution, we can always multiply it by an appropriate constant so that the wave function satisfies the normalization condition (18). Furthermore, if we find two or more than two solutions, any linear combination of the solutions is also a solution. Thus we can superpose any number of solutions to obtain a solution. This is an important property of wave functions of quantum systems and called the superposition principle of quantum mechanics.

In classical physics, a particle moving in a potential can take any value of energy from the minimum value which corresponds to the particle at rest at the position of the potential minimum to plus infinity which corresponds to the particle moving with an infinite kinetic energy. On the contrary, values of energy allowed for a quantum system are not continuous in general. In particular, when a system is confined in a finite region of space, the energy of the system can only take discrete values instead of continuous ones. Thus the energy of the quantum system is quantized.

As a simple example to show how the discrete nature of energy appears, we shall consider a particle moving in an infinitely high square potential well in one-dimensional space. The potential is given by  $V(x) = 0$  for  $0 \leq x \leq a$  and  $V(x) = +\infty$  for  $x < 0$  and  $x > a$ . The time-independent Schrödinger equation for the particle moving in this potential is

$$-\left(\hbar^2/2m\right) d^2\Phi/dx^2 = E\Phi \quad (0 \leq x \leq a) \quad (24)$$

Since the particle cannot have an infinite amount of potential energy,  $\Phi$  must vanish in the regions where  $V = +\infty$ . Thus,  $\Phi$  is confined in the finite region ( $0 \leq x \leq a$ ) and  $\Phi = 0$  at the boundaries of the potential because of the continuity of the wave function;  $\Phi(0) = \Phi(a) = 0$ . The wave function in the region  $0 \leq x \leq a$  is given by

$$\Phi(x) = A \sin \left\{ (2mE)^{1/2} x / \hbar \right\} \quad (25)$$

where  $A$  is the normalization constant.

The wave function  $\Phi$  was chosen to satisfy the boundary condition  $\Phi(0) = 0$ . The other boundary condition  $\Phi(a) = 0$  requires that  $(2mE)^{1/2} a / \hbar = n\pi$ , where  $n$  is a positive integer ( $n = 1, 2, \dots$ ). From this we obtain the values of energy allowed for the particle:

$$E_n = n^2 \pi^2 \hbar^2 / 2ma^2 \quad (n = 1, 2, \dots) \quad (26)$$

The wave functions for lower values of  $n$  are shown in Fig.9.

The amount of the discreteness in energy is proportional to  $1/a^2$  and it vanishes for large enough values of  $a$ . Thus, the discrete nature of energy is due to the finiteness of  $a$ , i.e. due to the system being confined in a finite region of space.

The lowest energy  $E_1$  for this system is not zero but finite. Since the particle cannot be at rest at a fixed position due to the uncertainty principle, the non-vanishing lowest energy comes from the minimum motion of the particle in accordance with the uncertainty principle. This energy is called the energy of the zero point oscillation of the particle.

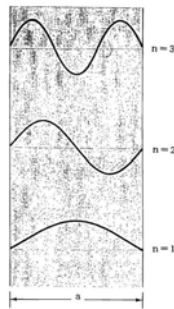


Figure 9. The wave functions of a particle moving in an infinitely high square potential

Likewise, the Schrödinger equation for the electron in a hydrogen atom has a solution only for the discrete values of energy given by Eq.(14). The positive integer  $n$  which specifies the state of the electron is called the principal quantum number. The discreteness of the energy is due to the condition that the wave function should

approach zero for large distances from the nucleus, so that the electron is confined in a finite region of space.

If the electron can be at rest at the position of the nucleus, the energy would be infinitely negative due to the infinite negative coulomb potential energy. Since this is not possible due to the uncertainty principle and the electron has to move about the position of the nucleus even in its state of minimum motion, the lowest energy  $E_1$  of the electron in a hydrogen atom is finite instead of minus infinity.

The energy alone is not enough to completely specify the state of motion of an electron in an atom. In classical physics not only energy but also angular momentum is conserved for an isolated system, and a definite value of angular momentum and its direction can be assigned to the state of motion. Furthermore, electrons are spinning about their own axes so that the direction of spin can be assigned to each of the electrons.

In quantum physics the values of angular momentum of an electron or any particle can take only discrete values just like energy. They are integral multiples of the unit angular momentum  $\hbar$  ( $= h/2\pi$ ) (see *Development of Fundamentals in Physics*). If we denote the magnitude of angular momentum by  $lh/2\pi$ , we call  $l$  ( $= 0, 1, 2, \dots$ ) the orbital quantum number of the electron orbit.

Because of the uncertainty principle, different components of the angular momentum cannot take definite values at the same time. Let us denote the angular momentum by  $\mathbf{L}$  which is a vector quantity. If  $\mathbf{L}$  is fixed in space so that all the components of  $\mathbf{L}$  have definite values, the electron would be confined in a plane perpendicular to the direction of  $\mathbf{L}$ . If  $\mathbf{L}$  were in the  $z$ -direction, the electron has to be in the  $xy$ -plane at all times. Then the uncertainty in the  $z$ -component of the position of the electron is zero, which contradicts the uncertainty principle unless the  $z$ -component of the electron momentum is infinitely uncertain.

Therefore, we can only assign definite values to the magnitude of the angular momentum and its one of the components, e.g.  $L_z$ , at the same time. Values of the other components,  $L_x$  and  $L_y$ , cannot have definite values (see *Development of Fundamentals in Physics*). Since only one component  $L_z$  of  $\mathbf{L}$  and the magnitude  $L$  have definite values, the direction of  $\mathbf{L}$  is constantly changing as shown in Fig.10. Thus the average values of  $L_x$  and  $L_y$  are zero, while  $L_z$  always has a definite value which is an integral multiple of the unit angular momentum:  $L_z = m\hbar$  ( $m = 0, \pm 1, \pm 2, \dots$ ). The number  $m$  is called the magnetic quantum number of the electron orbit.

For a given value of the orbital quantum number  $l$ , there exist  $2l+1$  different values of the magnetic quantum number  $m$  ( $m = 0, \pm 1, \pm 2, \dots, \pm l$ ), because the magnitude of  $L_z$  cannot exceed the magnitude of the angular momentum  $L$ . The different values of  $m$  correspond to different orientations of the angular momentum vector  $\mathbf{L}$ .

In addition to the orbital angular momentum, the electron has its spin angular momentum. Since only two different spin states were observed for the electron in the



Stern-Gerlach experiment (see *Particles and Fields*), the spin  $s$  of the electron is  $1/2$  in the unit of  $\hbar$  because of the relation  $2s+1 = 2$ . The spin state of an electron is specified by the value of  $s_z$  which can take either  $+1/2$  or  $-1/2$  in units of  $\hbar$ . The value of  $s_z$  is called the spin quantum number. Spin is similar to orbital angular momentum, but it is not quite right to imagine that something is rotating in space inside the electron. The real meaning of spin can be only clarified by Dirac's relativistic theory of electrons.

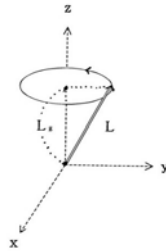


Figure 10. Motion of an angular momentum vector with a definite magnitude

In order to illustrate how the angular momentum is quantized in units of  $\hbar$ , we shall consider the motion of a particle in a two-dimensional plane. In classical physics the orbital angular momentum  $\mathbf{L}$  of a particle moving about the origin of the coordinates is given by  $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ . The orbital angular momentum in quantum physics is obtained by substituting  $\mathbf{p}$  by  $-i\hbar\nabla$ :

$$\mathbf{L} = \mathbf{r} \times (-i\hbar\nabla) = -i\hbar\mathbf{r} \times \nabla \quad (27)$$

If a particle moves in a plane as shown in Fig.11, the angular momentum  $\mathbf{L}$  is given by

$$L = -i\hbar(x\partial_y - y\partial_x) = -i\hbar\partial_\theta \quad (28)$$

where the plane of motion is taken to be the  $xy$ -plane and  $\theta$  is the polar angle shown in the figure.



Figure 11. The angular momentum of a particle moving in the  $x$ - $y$ -plane

The wave function  $\Phi$  for the stationary rotational motion of a particle satisfies the following equation:

$$L\Phi = -i\hbar\partial\Phi/\partial\theta = m\hbar\Phi \quad (29)$$

Here  $m\hbar$  is the value of the angular momentum of the stationary motion.

Solutions of Eq.(29) are of an exponential form in  $\theta$  and given by

$$\Phi = (2\pi)^{-1/2} \exp(im\theta) \quad (30)$$

Here the normalization constant was chosen to satisfy  $\int \Phi^* \Phi d\theta = 1$ , where the integration over  $\theta$  is from 0 to  $2\pi$ .

Since the range of the variable  $\theta$  is  $0 \leq \theta \leq 2\pi$  and the two angles  $\theta = 0$  and  $\theta = 2\pi$  represent the same angle, the periodic condition  $\Phi(0) = \Phi(2\pi)$  must be satisfied. From this we obtain  $m = \text{integer}$ . Thus,  $L$  can take only discrete values given by  $m\hbar$ , where  $m$  is an integer ( $0, \pm 1, \pm 2, \dots$ ). It is clear that the discreteness in values of  $L$  came from the space of motion being finite ( $0 \leq \theta \leq 2\pi$ ) just like the discreteness in energy came from the finite extension of the wave function in space.

A stationary state of a quantum system with a definite energy is characterized by a set of quantum numbers. Such a state is called a quantum state. In case of a hydrogen atom, the quantum numbers are the principal quantum number  $n$ , the orbital quantum number  $l$  denoting the magnitude of angular momentum, the magnetic quantum number  $m$  denoting the magnitude of  $L_z$ , and the spin quantum number  $s_z$ .

The energy diagram of the hydrogen atom was shown in Fig.8. The energy of a quantum state is determined only by the principal quantum number  $n$  and does not depend on the other quantum numbers. Therefore, for each quantum state specified by  $n$ , there exist several different states with different values of the other quantum numbers. States with the same energy are called degenerate in energy. It has been shown that for a given value of the principal quantum number  $n$  the values of the orbital quantum number  $l$  can take any integer value from 0 to  $n - 1$  (see *Physical Systems and Laws*). Then, for a given value of  $n$  there exist  $2n^2$  degenerate states different in  $l$ ,  $m$ , or  $s_z$ ;  $\sum 2(2l + 1) = 2n^2$ , where the summation  $\Sigma$  is over  $l$  from 0 to  $n - 1$ .

For multi-electron atoms the quantum state with the same  $n$  but different  $l$  differ in energy and the degeneracy in states is somewhat removed compared to the hydrogen atom. The Coulomb force acting on an electron in a multi-electron atom is not exactly proportional to the inverse square of the distance from the nucleus because of charge screening effects due to the presence of other electrons inside the orbit of the electron. The degeneracy of states with different values of  $l$  is only perfect in the case of a pure coulomb force inversely proportional to the inverse square of the distance. We shall discuss electronic configurations of multi-electron atoms in a later chapter (see *Particles and Fields*).

One of the utmost important concepts in modern physics is that fundamental particles of the same kind are perfectly identical and indistinguishable with each other. If there exist more than one electron in a system, they follow the same Schrödinger equation and there is no way to differentiate them from one another. In 1925 Pauli discovered a

fundamental principle called the exclusion principle which governs the electronic configurations of atoms having more than one electron. The principle states that no two electrons can exist in the same quantum state.

The quantum states of the electron in a complex atom having more than one electron are labeled by a set of quantum numbers just like those of the electron in the hydrogen atom. These quantum numbers are the principal quantum number, the orbital quantum number, the magnetic quantum number and the spin quantum number. For every electron in the atom, there is a unique set of the four quantum numbers which completely specifies the state of the electron.

Because of Pauli's exclusion principle, one and only one electron can have a given set of the quantum numbers. In the normal configuration of an atom the electrons occupy quantum states of lower energies so that the total energy of the multi-electron atom becomes minimum, thereby only one electron occupies each of the quantum states. This way of arranging the electronic configurations in an atom fits well the configurations of multi-electron atoms and can explain the chemical activity of the elements, thus providing the underlying basis for the concept of valence bond for molecular bindings.

Not only electrons but also protons and neutrons follow the exclusion principle. In general, it is known that any fermion with a half-odd integer spin ( $s = 1/2, 3/2, \dots$ ) including quarks and leptons follow the exclusion principle. On the contrary, any number of photons can exist in the same quantum state. In general, any number of bosons of the same kind with an integer spin ( $s = 0, 1, 2, \dots$ ) can exist in the same quantum state.

The indistinguishability of identical particles from one another imposes an important condition on wave functions of a multi-particle system. The wave function of a stationary state of a system composed of two identical particles can be written as  $\Phi(1, 2)$ , where 1 and 2 denote all the necessary variables to specify the states of the particles 1 and 2 respectively. Since the particles are indistinguishable from each other, there should be no change in the probability density  $\Phi^* \Phi$  if we exchange the two particles;

$$\Phi^*(1, 2) \Phi(1, 2) = \Phi^*(2, 1) \Phi(2, 1)$$

This condition leads to either one of the two possibilities:

$$\Phi(1, 2) = \pm \Phi(2, 1) \quad (31)$$

That is, the two-particle wave function is either symmetric or antisymmetric under the exchange of the two particles. The wave function  $\Phi$  itself is not an observable quantity and it can change sign under the exchange of the two particles without changing value of any physically observable quantity (see *Development of Fundamentals in Physics* for more detailed discussion).

Electrons or spin half-integer fermions obey the minus sign rule and photons or spin integer bosons obey the plus sign rule under the exchange of two identical particles. The

exclusion principle is a direct consequence of the antisymmetric property of two electron wave functions. If  $l = 2$ , the wave function must vanish because of its antisymmetric property ( $\Phi(1, 1) = -\Phi(1, 1) = 0$ ). From this we can prove that no two electrons can exist in the same state.

Unlike fermions, bosons can occupy the same state without any limit on their number. Thus, under appropriate circumstances quite a large number of identical bosons can occupy the same lowest energy state so that it causes a macroscopic quantum effect. This kind of phenomenon is called the Bose–Einstein condensation. We will discuss some of the condensation phenomena in a later chapter.

The symmetry property of multi-particle wave functions under exchange of any pair of the particles has important effects on the statistical property of many particle systems. For example, in thermal equilibrium with a definite temperature the energy distribution of a particle depends upon whether the particle is a fermion or boson.

In classical physics the probability  $P(\varepsilon)d\varepsilon$  for finding a particle whose energy lies between  $\varepsilon$  and  $\varepsilon + d\varepsilon$  is given by the Maxwell-Boltzmann distribution  $P(\varepsilon) = e^{-\alpha} e^{-\varepsilon/kT}$  (see *Physical Systems and Laws*). In quantum physics the probability for finding a fermion in a quantum state with energy  $\varepsilon$  is

$$P(\varepsilon) = \left[ e^{\alpha} e^{\varepsilon/kT} + 1 \right]^{-1} \quad (\text{for fermions}) \quad (32)$$

and that for a boson is

$$P(\varepsilon) = \left[ e^{\alpha} e^{\varepsilon/kT} - 1 \right]^{-1} \quad (\text{for bosons}) \quad (33)$$

Here the constant  $\alpha$  depends on the properties of the particular system. The +1 term in Eq.(32) assures that  $P(\varepsilon)$  will never exceed 1 irrespective of values of  $a$  and  $\varepsilon$  in accordance with the exclusion principle. The –1 term in Eq.(34) expresses that bosons can occupy the same state, so that  $P(\varepsilon)$  could become larger than 1. Both these distributions approach the classical Maxwell-Boltzmann distribution for  $\varepsilon \gg kT$ , but they are significantly different from the Maxwell-Boltzmann distribution at low values of  $\varepsilon/kT$ . In Fig.12 we show three distribution functions as a function of  $\varepsilon/kT$ .

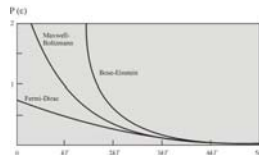


Figure 12. Three statistical distribution functions as a function of  $\varepsilon(\alpha = -1)$ .

It should be mentioned that to find the actual number of particles with an energy  $\varepsilon$ , the function  $P(\varepsilon)$  must be multiplied by the number of different states with this energy  $\varepsilon$ .

We will describe short derivations of the distribution functions (32) and (33). Suppose that the probability for finding a particle with energy  $\varepsilon$  relative to the probability for finding no particle with energy  $\varepsilon$  is  $p = e^{-\alpha} \exp(-\varepsilon/kT)$ . The average number of the fermions with energy  $\varepsilon$  is  $P(\varepsilon) = p/(1+p) = [(1/p) + 1]^{-1}$  and that of the bosons is  $P(\varepsilon) = (\Sigma np^n)/(\Sigma p^n) = p/(1-p) = [(1/p) - 1]^{-1}$ . These give the correct distributions (32) and (33) (see *Development of Fundamentals in Physics*) for more detailed derivations).

Finally we shall mention a little about the relativistic extension of the Schrödinger equation for electrons. In 1928, Dirac revised the Schrödinger equation to include spin and relativity and his theory revealed for the first time the existence of positrons (anti-matter) associated with electrons (matter).

The Schrödinger equation is linear in the time derivative of  $\Psi$  but quadratic in the space derivatives of  $\Psi$ . Thus, the time and space coordinates are not treated on equal footing contrary to the relativistic requirement for the basic equations of elementary particles. Furthermore, spin of the electron has to be introduced in an *ad hoc* manner as an additional dynamical variable of the electron.

Dirac's relativistic equation for free electrons is linear in both the time and space derivatives and given by

$$(E - c\boldsymbol{\alpha} \cdot \mathbf{p} - mc^2\beta)\Psi = 0 \quad (34)$$

where  $\mathbf{p} = -i\hbar\nabla$  and  $E = i\hbar\partial t$ .

Multiplying  $(E + c\boldsymbol{\alpha} \cdot \mathbf{p} + mc^2\beta)$  from the left, we can obtain the relativistic energy-momentum-mass; relation applied on  $\Psi$ :

$$\begin{aligned} (E + c\vec{\alpha} \cdot \mathbf{p} + mc^2\beta)(E - c\vec{\alpha} \cdot \mathbf{p} - mc^2\beta)\Psi \\ = [E^2 - (c^2 p^2 + m^2 c^4)]\Psi = 0 \end{aligned} \quad (35)$$

provided  $(c\boldsymbol{\alpha} \cdot \mathbf{p} + mc^2\beta)^2 = c^2 p^2 + m^2 c^4$ . This leads to the following relation which must be satisfied by  $\alpha_i$ s and  $\beta$ :

$$\begin{aligned} \alpha_i^2 = 1 \quad (i = x, y, z), \quad \alpha_i \alpha_j + \alpha_j \alpha_i = 0 \quad (\text{for } i \neq j) \\ \beta^2 = 1, \quad \beta \alpha_i + \alpha_i \beta = 0 \end{aligned} \quad (36)$$

Obviously these cannot be satisfied if  $\alpha_i$ s and  $\beta$  are ordinary numbers. Dirac assumed that they are  $4 \times 4$  matrices instead of pure numbers and  $\Psi$  has four components instead of one. The product of two matrices  $A$  and  $B$  is not commutable and  $AB$  differs

from  $BA$  in general. If we denote elements of  $A$  by  $a_{ij}$  and that of  $B$  by  $b_{ij}$  ( $i = 1,2,3,4; j = 1,2,3,4$ ), the element  $c_{ij}$  of the product matrix  $C(= AB)$  is given by  $c_{ij} = \sum_k a_{ik} b_{kj}$  where  $\sum_k$  is sum over  $k = 1, 2, 3, 4$ .

An explicit example of the matrices  $\alpha_i$ s and  $\beta$  is

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (37)$$

Here  $\sigma_i$ s are  $2 \times 2$  matrices called the Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (38)$$

The  $4 \times 4$  matrices  $\alpha_i$ s and  $\beta$  operate upon the four component wave function  $\Psi$ . If we express the wave function by

$$\begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \end{bmatrix} \quad (39)$$

the result of operating a matrix  $A$  on  $\Psi$  is  $(A\Psi)_i = \sum_j A_{ij} \Psi_j$ .

There exist four solutions of Eq.(34) for a given value of momentum  $\mathbf{p}$ . They are classified by the sign of energy and the direction of spin of the electron. For example, if we consider the electron at rest ( $\mathbf{p} = 0$ ), the Dirac equation becomes  $E\Psi = mc^2\beta\Psi$ , or  $E\Psi_1 = mc^2\Psi_1$ ,  $E\Psi_2 = mc^2\Psi_2$ ,  $E\Psi_3 = -mc^2\Psi_3$ ,  $E\Psi_4 = -mc^2\Psi_4$ . Thus, there exist two positive energy solutions with energy  $mc^2$  and two negative energy solutions with energy  $-mc^2$ . They are

$$\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \quad E = mc^2$$

and

$$\begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} E = -mc^2$$

If we define the spin angular momentum of the electron by  $\mathbf{s} = (\hbar/2)\Sigma$ , where  $\Sigma$  is the  $4 \times 4$  matrix

$$\Sigma = \begin{pmatrix} \boldsymbol{\alpha} & 0 \\ 0 & \boldsymbol{\alpha} \end{pmatrix} \quad (40)$$

then the four solutions can be classified by the sign of energy and the direction of spin:

$$\begin{array}{cccc} E & +mc^2 & +mc^2 & -mc^2 & -mc^2 \\ s_z & +\hbar/2 & -\hbar/2 & +\hbar/2 & -\hbar/2 \\ \Psi & \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \end{array} \quad (41)$$

Dirac's relativistic theory of the electron introduces the four-component wave function and incorporates in a natural way the spin and antimatter degree of freedom of the electron. The negative energy solutions are interpreted as the positive energy states of the antielectrons (positrons) as was proposed in the hole theory of electrons (see *Particles and Fields*). According to this theory vacuum is the state in which all the negative energy states are occupied by electrons in accordance with the Pauli principle and all the positive energy states are empty. When an electron in a negative energy state moves into a positive energy state, we obtain an electron in that positive energy state and a hole in the negative energy state. This hole behaves as a particle with charge opposite to electrons and energy opposite to the negative energy of the state, thus can be identified as the positron or the antimatter of electrons.

### 1. Quantum Mechanical Laws

As we discussed in the introduction, any material particle has the wavelike property just like the wave of light. The wave nature of matter requires that a wave equation be used to find the displacement of the matter wave, which is a function of position and time. The theory of the material wave was formulated by Schrödinger in 1926.

The wave of a material particle is usually denoted by  $\Psi(x, y, z, t)$  or  $\Psi(r, t)$ , which is called the wave function of the particle. Let us consider a simple wave with wavelength  $\lambda$  and frequency  $\nu$  moving in one-dimensional space. Such a wave is expressed as

$$\sin[2\pi(x/\lambda - \nu t)] \quad \text{or} \quad \cos[2\pi(x/\lambda - \nu t)]$$

In 1925 de Broglie introduced a hypothesis that the wave nature and particle nature of matter are related by

$$h\nu = E \quad \text{and} \quad h/\lambda = p \quad (42)$$

where  $E$  and  $p$  are the energy and momentum of the particle.

If we use the de Broglie hypothesis, waves with definite frequency and wavelength can be expressed in terms of the energy and momentum of the material particle:

$$\sin\left[(1/\hbar)(px - Et)\right] \quad \text{or} \quad \cos\left[(1/\hbar)(px - Et)\right]$$

Any combination of the sine and cosine waves represents a wave propagating along the  $x$ -direction with wavelength  $\lambda$  and frequency  $\nu$ . Since the concept of matter waves cannot be derived from any previous classical concepts, we allow a wave function to take a complex value in general. This is contrary to waves in classical physics which always take real values. By taking a certain combination of sine and cosine waves, we obtain a wave of exponential form:

$$\Psi = \exp [i(px - Et)/\hbar] \quad (43)$$

This form of wave is called the plane wave of a material particle.

The plane wave has a simple property that its derivatives are equal to multiplications by constant factors upon the wave function:

$$-i\hbar\partial\Psi/\partial x = p\Psi, \quad i\hbar\partial\Psi/\partial t = E\Psi \quad (44)$$

These relations are interpreted as meaning that the momentum and energy of the particle may be replaced by the differential operators  $-i\hbar\partial/\partial x$  and  $i\hbar\partial/\partial t$  respectively, which operate on the wave function  $\Psi$ .

The classical expression for the Hamiltonian of a particle with mass  $m$  is  $H = p^2/2m + V(x)$ , which is the energy  $E$  of the particle expressed in terms of the momentum and position of the particle. The wave equation for  $\Psi$  is obtained as the equality  $H = E$  applied on the wave function,  $H\Psi = E\Psi$ , whereby the differential operators are substituted for  $p$  and  $E$ . The result is

$$H\Psi = -\left(\hbar^2/2m\right)\partial^2\Psi/\partial x^2 + V\Psi = i\hbar\partial\Psi/\partial t \quad (45)$$

This is the Schrödinger equation for one-dimensional matter waves.

In three-dimensional space, the momentum and energy of a particle are expressed by the following differential operators acting on wave functions:



$$\mathbf{p} = -i\hbar\nabla, \quad E = i\hbar\partial t \quad (46)$$

The Schrödinger equation for three-dimensional matter waves is

$$H\Psi = -\left(\hbar^2/2m\right)\nabla^2\Psi + V\Psi = i\hbar\partial\Psi/\partial t \quad (47)$$

$$\text{where } \nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2.$$

The Schrödinger equation must be supplemented by additional conditions in order that its solutions have physical significance. The conditions are that  $\Psi$  and its derivatives  $\nabla\Psi$  and  $\partial_t\Psi$  must be single-valued, finite and continuous everywhere in space and time. These correspond to conditions in classical physics that the position, momentum, and energy of a particle are finite and change continuously in time.

Now we have to decide how to interpret the wave function of a particle. As inferred from the results of the double-slit experiments (see *section 1*), the intensity of the wave should provide a prediction of probable locations of the particle. We postulate that the probability that a particle is located within a small volume element  $dV$  at a position  $\mathbf{r}$  is given by

$$P(\mathbf{r}, t)dV = \Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t)dV \quad (48)$$

where  $\Psi^*$  is the complex conjugate of  $\Psi$ . Since  $\Psi^*\Psi$  is positive,  $P$  is positive too.

The particle must be somewhere in the entire region of space, which requires that the probability  $P$  integrated over the entire space must be equal to 1:

$$\int \Psi^*\Psi dV = 1 \quad (49)$$

When this condition is satisfied, the wave function is said to be normalized. An important consequence of the wave nature of matter and its probability interpretation is that any physical quantity associated with the particle cannot take a definite value in general, but instead its probability distribution is specified by the wave function.

For example, the position of a particle described by a wave function  $\Psi$  spreads over the region where  $\Psi \neq 0$  and the average or expectation value of  $x$  component of  $\mathbf{r}$  is given by

$$\langle x \rangle = \int xP(\mathbf{r}, t) dV = \int \Psi^*(\mathbf{r}, t)x\Psi(\mathbf{r}, t) dV \quad (50)$$

Similar expressions are valid for the other components of  $\mathbf{r}$ .

The knowledge of  $P(\mathbf{r}, t)$  allows us to calculate the expectation value of any function of  $\mathbf{r}$ . For example, the average value of  $x^2$  is given by

$$\langle x^2 \rangle = \int \Psi^*(\mathbf{r}, t) x^2 \Psi(\mathbf{r}, t) dV \quad (51)$$

In general,  $\langle x^2 \rangle \neq \langle x \rangle^2$  unless  $P(\mathbf{r}, t)$  has no spread in  $x$ . The value of  $\Delta x$  ( $\geq 0$ ) defined by

$$(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 \quad (52)$$

indicates the shape of the probability distribution function  $P$  in  $x$ .

Low values of  $\Delta x$ ,  $\Delta y$ , and  $\Delta z$  indicate a sharp distribution and high values of them indicate a broad distribution in the position of the particle. A distribution that has no spread ( $\Delta x = \Delta y = \Delta z = 0$ ) is one for which the probability of the particle being at a certain position is one and the probabilities of being at other positions are 0. A wave function with  $\Delta x = \Delta y = \Delta z = 0$  corresponds to the particle locating at a definite position in space.

Like  $\langle x \rangle$ , the expectation values of the momentum and energy of the particle are given by

$$\begin{aligned} \langle \mathbf{p} \rangle &= \int \Psi^*(\mathbf{r}, t) (-i\hbar \nabla) \Psi(\mathbf{r}, t) dV, \\ \langle E \rangle &= \int \Psi^*(\mathbf{r}, t) (i\hbar \partial_t) \Psi(\mathbf{r}, t) dV \end{aligned} \quad (53)$$

As we will find later,  $\langle \mathbf{p} \rangle$  and  $\langle E \rangle$  are real in spite of the presence of the factor  $i$  in the right-hand sides of Eq.(51). We can also define the spreads of  $\mathbf{p}$  and  $E$  similar to the spread of the position.

It was realized by Heisenberg in 1927 that there is a fundamental limit to the accuracy to which position and momentum can be defined at the same time, although either the position or the momentum alone can be defined without any limit to the accuracy.

In Fig.13 we show three typical forms of wave function in one-dimensional space. The function  $A$  has many well-developed sinusoidal waves with a definite wavelength, but the wave is not a pure sine wave because it is cut off at both ends. Therefore, the wavelength is not precisely defined and there is a small spread in its wavelength and thus in its momentum. Since the function  $A$  extends over a large distance, it represents a particle which has a well-defined momentum but a poorly-defined position. On the contrary, the function  $C$  represents a particle which has a well-defined position but a poorly-defined momentum. The function  $B$  represents an intermediate situation in which the position and momentum of a particle are defined with intermediate accuracies.

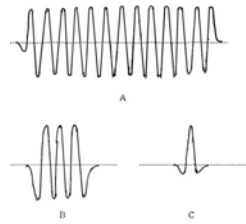


Figure 13. Three typical forms of wave function in one-dimensional space

We can roughly estimate the relation between the spreads in position and momentum. For the wave function *A* we can take the length of the wave train as a measure of the uncertainty in position. If the wave train consists of  $n$  full waves, we obtain  $\Delta x \sim n\lambda \sim nh/p$ , where  $\lambda$  is the wavelength and  $p$  is the momentum. The uncertainty in wavelength would be roughly given by  $\Delta\lambda/\lambda \sim \Delta p/p \sim 1/n$ . From these rough estimates we obtain  $\Delta x \Delta p \sim h$ . Similarly if we plot waves as a function of time at a fixed position, we can find that the product of the uncertainties in energy and time is roughly given by  $\Delta E \Delta t \sim h$ .

We can prove that the exact lower limit of  $\Delta x \Delta p$  is equal to  $\hbar/2$ , which is obtained for waves of a Gaussian form. From these results, it is clear that position and momentum cannot take definite values at the same time. Also we can prove that the lower limit of  $\Delta E \Delta t$  is equal to  $\hbar/2$ . For particles in three-dimensional space the exact uncertainty relations are

$$\Delta x \Delta p_x \geq \hbar/2, \quad \Delta y \Delta p_y \geq \hbar/2, \quad \Delta z \Delta p_z \geq \hbar/2 \quad (54)$$

and

$$\Delta E \Delta t \geq \hbar/2 \quad (55)$$

Notice that the uncertainty relations should be applied for a pair of the same components of the position and momentum vectors.

For most quantum systems the product of uncertainties in position and momentum or in time and energy is

$$\Delta x \Delta p_x \sim \Delta y \Delta p_y \sim \Delta z \Delta p_z \sim \Delta E \Delta t \sim h \quad (56)$$

as indicated by the rough estimates of the uncertainty relations based on Fig.13. In classical physics a state of a particle can be specified by assigning a point in the six-dimensional phase space ( $r$ - $p$  space) to the state, while in quantum physics we can specify a point in the phase space only within the uncertainties given by Eq.(56).

Therefore, we divide the whole phase space into small cells with constant volume  $h^3$  and assign one of the cells to denote a state of the particle, The volume of the unit cell is

determined by the uncertainty relations and cannot be taken smaller than  $h^3$ . Likewise, if a system is composed by  $N$  particles, we divide the phase space into small cells of constant volume  $h^{3N}$ , each of which denotes a different state of the multi-particle system.

In statistical physics it is important to know what microstates are and how we enumerate the number of microstates for a given macrostate (see *Physical Systems and Laws*). The uncertainty relations (56) lead to a natural choice of microstates that each small cell with volume  $h^{3N}$  in phase space corresponds to a microstate of a  $N$ -particle system. This is contrary to the situation in classical physics where any two neighboring points in phase space can be differentiated in principle and thus corresponds to different microstates of the system.

Quantum systems are characterized by their probabilistic nature and consequently most of the physical quantities of a quantum system usually do not take definite values. However, states of a quantum system with a definite energy play important roles because any isolated quantum system has a constant energy due to the energy conservation law. These states are called the stationary states of the quantum system. Wave functions for stationary states satisfy the following equation:

$$i\hbar\partial\Psi/\partial t = E\Psi \quad (57)$$

where  $E$  is the energy of the stationary state. The solution of Eq.(57) is

$$\Psi = \exp(-iEt/\hbar) \Phi(\mathbf{r}) \quad (58)$$

where  $\Phi$  is independent of time. The time-independent wave function  $\Phi$  satisfies the following time-independent Schrödinger equation:

$$H\Phi = \left[ -\left(\hbar^2/2m\right)\nabla^2 + V(\mathbf{r}) \right] \Phi = E\Phi \quad (59)$$

A stationary state of a quantum system is characterized not only by its energy but also by other quantities with definite values. For example, a free electron moving at a constant velocity has a definite linear momentum and an electron orbiting the nucleus of an atom has a definite angular momentum. Also an electron has its spin angular momentum.

In classical physics various physical quantities of a system can have definite values at the same time within experimental accuracies. Contrary to this, in quantum physics we have to ask under what conditions a physical quantity can have a definite value and what physical quantities can have definite values together with energy at the same time.

Let us consider a physical quantity  $A$  which is an operator acting upon wave functions. If a wave function  $\Psi$  satisfies the following equation

$$A\Psi = a\Psi \quad (60)$$

with constant  $a$ , the wave function  $\Psi$  is called the eigenstate of  $A$  with the eigenvalue  $a$ . Thus, a stationary state is an eigenstate of the Hamiltonian with eigenvalue  $E$  which is equal to the energy of the state.

Since  $\langle A \rangle = \int \Psi^* A \Psi dV = a \int \Psi^* \Psi dV = a$ ,  $a$  is equal to the average or expectation value of  $A$  for the state  $\Psi$ . Furthermore,  $\Delta A$  is zero for  $\Psi$ ;  $(\Delta A)^2 = \int \Psi^* (A - \langle A \rangle)^2 \Psi dV = \int \Psi^* (a - a)^2 \Psi dV = 0$ . Therefore, an eigenstate  $\Psi$  is a state with a definite value of  $A$  given by  $a$ . Any eigenvalue of a physical quantity must be real, because measured values of the quantity are real. An operator whose eigenvalues are real is called a hermitian operator, and in quantum mechanics any physical quantity must be represented by a hermitian operator acting upon wave functions.

Mathematically a hermitian operator  $A$  is defined by the condition that

$$\int \varphi^* A \psi dV = \int (A \varphi)^* \psi dV \quad (61)$$

for any pair of wave functions  $\psi$  and  $\varphi$ . If  $\psi = \varphi$  and  $\psi$  is an eigenstate of  $A$  with eigenvalue  $a$ , the hermitian condition (61) becomes  $a = a^*$ , i.e.  $a$  is real. As an example, we can find that the momentum  $\mathbf{p}$  ( $= -i\hbar\nabla$ ) is hermitian in spite of the presence of the factor  $i$  in it;  $\int \varphi^* \mathbf{p} \psi dV = \int \varphi^* (-i\hbar\nabla \psi) dV = \int (i\hbar\nabla \varphi^*) \psi dV = \int (-i\hbar\nabla \varphi)^* \psi dV = \int (\mathbf{p} \varphi)^* \psi dV$ , where we used integration by parts in deriving the expression in the middle.

Eigenvalues of a physical quantity are either continuous or discrete in a certain range of values allowed. In particular, when a system is confined in a finite region of space, eigenvalues of physical quantities take only discrete values contrary to the situation in classical physics where values of any physical quantity can be varied continuously. For example, energy levels of a hydrogen atom are discrete and angular momentum of any quantum system can take only discrete values quantized in unit of  $\hbar$ . This discrete nature of physical quantities plays important roles in describing various quantum mechanical phenomena as we will find in a later chapter (see *Particles and Fields*).

Two eigenstates of a physical quantity  $A$  with different eigenvalues are orthogonal to each other. Consider two eigenstates  $\psi_a$  and  $\psi_{a'}$ , with eigenvalues  $a$  and  $a'$ . Because of the hermiticity of  $A$ , we obtain  $\int \psi_{a'}^* A \psi_a dV = \int (A \psi_{a'})^* \psi_a dV$ . This leads to  $(a - a') \int \psi_{a'}^* \psi_a dV = 0$ . If  $a \neq a'$ , then we obtain the orthogonality relation  $\int \psi_{a'}^* \psi_a dV = 0$ :

$$\int \psi_{a'}^* \psi_a dV = \begin{cases} 0 & \text{for } a \neq a' \\ 1 & \text{for } a = a' \end{cases} \quad (62)$$

In general, we can express any state  $\psi$  as a linear superposition of the eigenstates of  $A$ ;  $\psi = \sum_a c_a \psi_a$  with constant coefficients  $c_a$ . Then the average value of  $A$  is given by  $\langle A \rangle = \int \psi^* A \psi dV = \sum_a a |c_a|^2$ , and the probability for observing value  $a$  of  $A$  is  $|c_a|^2$ . The normalization condition of  $\psi$  is  $\sum_a |c_a|^2 = 1$ . Because of the orthogonality conditions (62), the coefficients  $c_a$  are given by  $c_a = \int \psi_{a'}^* \psi dV$ .

If we make observation of a quantity  $A$  for a state  $\psi$  and obtain value  $a$ , then the state would change from  $\psi$  to the eigenstate  $\psi_a$  because the new state has the definite value  $a$  of  $A$ . This sudden change of state due to the observation is due to the probabilistic nature of wave functions. The information obtained through measurements changes the probability distribution of the system and thus the wave function.

Next, we shall consider conditions for two quantities  $A$  and  $B$  can take definite values at the same time. We define the commutator of  $A$  and  $B$  by

$$[A, B] = AB - BA \quad (63)$$

When  $[A, B] = 0$ , we say that  $A$  and  $B$  commute with each other.

When two quantities  $A$  and  $B$  commute, we can find wave functions which are eigenstates of both  $A$  and  $B$  at the same time. Let  $\Psi_{a,b}$  is such an eigenstate with eigenvalue  $a$  for  $A$  and  $b$  for  $B$ :

$$A\Psi_{a,b} = a\Psi_{a,b}, \quad B\Psi_{a,b} = b\Psi_{a,b} \quad (64)$$

Since  $[A, B] \Psi_{a,b} = (ab - ba) \Psi_{a,b} = 0$ , there is no inconsistency between  $[A, B] = 0$  and  $\Psi_{a,b}$  being an eigenstate of both  $A$  and  $B$ . In general, if two quantities commute, the both quantities can have definite values at the same time. On the contrary, if  $[A, B] = C$  ( $\neq 0$ ), we obtain  $C \Psi_{a,b} = 0$ , which means that  $\Psi_{a,b} = 0$  unless  $C = 0$ . Thus, two physical quantities which do not commute to each other cannot have definite values at the same time in general.

If a quantity  $A$  commutes with the Hamiltonian  $H$ , i.e.  $[A, H] = 0$ ,  $A$  can take definite values together with energy. Furthermore,  $A$  is conserved and the value of  $A$  does not change in time. Change of  $\langle A \rangle$  in time is given by

$$\begin{aligned} d\langle A \rangle/dt &= d\left(\int \Psi^* A \Psi dV\right)/dt \\ &= \int \left(d\Psi^*/dt\right) A \Psi dV + \Psi^* A (d\Psi/dt) dV = \\ &= (i/\hbar) \int (H\Psi)^* A \Psi dV - (i/\hbar) \int \Psi^* A (H\Psi) dV \\ &= (i/\hbar) \int \Psi^* [H, A] \Psi dV \end{aligned} \quad (65)$$

Here we used the Schrödinger equation  $i\hbar\partial\Psi/\partial t = H\Psi$  and its complex conjugated equation  $-i\hbar\partial\Psi^*/\partial t = (H\Psi)^*$ . Also we used the relation  $\int (H\Psi)^* \Psi dV = \int \Psi^* H(A\Psi) dV$  due to the hermiticity of  $H$ . From the result, it is clear that  $A$  is conserved provided  $[H, A] = 0$ .

Classically the state of a particle is given by specifying its position and momentum and thus they are the most fundamental dynamical variables to describe motion of the particle. Commutation relations among these fundamental variables are

$$[x, p_x] = [y, p_y] = [z, p_z] = i\hbar \quad (66)$$

and all other commutators such as  $[x, y]$ ,  $[x, p_y]$ ,  $[p_x, p_y]$  are zero. These relations can be derived by substituting  $\mathbf{p}$  by  $-i\hbar\nabla$ . For example,  $[x, p_x] = x(-i\hbar\partial_x) - (-i\hbar\partial_x)x = i\hbar$ .

From the commutation relations we can derive the uncertainty relations (54). Thus the position and momentum of a particle cannot take definite values at the same time and we can only specify the position but not the momentum, or the momentum but not the position in quantum mechanics.

[Proof of  $\Delta x \Delta p_x \geq \hbar/2$ : Let us introduce  $f = (x - \langle x \rangle)\psi$  and  $g = (p_x - \langle p_x \rangle)\psi$  for an arbitrary wave function  $\psi$ . Since  $\int f^* f dV \cdot \int g^* g dV \geq |\int f^* \cdot g dV|^2$  in general, we obtain  $(\Delta x)^2 (\Delta p_x)^2 \geq |\int \psi^* (x - \langle x \rangle) (p_x - \langle p_x \rangle) \psi dV|^2$ . Now introducing  $\alpha = x - \langle x \rangle$  and  $\beta = p_x - \langle p_x \rangle$ ,  $\alpha\beta = (\alpha\beta + \beta\alpha)/2 + (\alpha\beta - \beta\alpha)/2 = (\alpha\beta + \beta\alpha)/2 + i\hbar/2$ . The operator  $\alpha\beta + \beta\alpha$  is hermitian and the value of  $\int \psi^* [(\alpha\beta + \beta\alpha)/2] \psi dV$  is real. Then putting this real value equal to  $c$ , we obtain  $|\int \psi^* \alpha\beta \psi dV|^2 = |c + i\hbar/2|^2 \geq |c|^2 + (\hbar/2)^2 \geq (\hbar/2)^2$ . This leads to  $\Delta x \Delta p_x \geq \hbar/2$ .]

In classical mechanics the angular momentum of a particle with respect to a given point in space is conserved, when the potential energy of the particle depends only on the distance from the particle to the given point. That is, the angular momentum is conserved when the Hamiltonian of the system is rotational invariant.

The angular momentum  $\mathbf{L}$  of a quantum system is defined by

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} = -i\hbar \mathbf{r} \times \nabla \quad (67)$$

and  $\mathbf{L}$  is conserved when  $\mathbf{L}$  commutes with the Hamiltonian of the system. The angular momentum defined by Eq.(67) is called the orbital angular momentum.

The commutation relations for the components of the angular momentum can be easily calculated by using Eq.(67) and they are

$$[L_x, L_y] = i\hbar L_z, \quad [L_y, L_z] = i\hbar L_x, \quad [L_z, L_x] = i\hbar L_y \quad (68)$$

By using Eq.(68) we can find that any component of  $\mathbf{L}$  commutes with the square of the angular momentum:

$$[\mathbf{L}^2, L_x] = [\mathbf{L}^2, L_y] = [\mathbf{L}^2, L_z] = 0 \quad (69)$$

From Eqs.(68) and (69) only one of the three components of  $\mathbf{L}$  and  $\mathbf{L}^2$  can have definite values at the same time.

Let us consider states with definite values of  $\mathbf{L}^2$  and  $L_z$ . If we denote the eigenstates of both  $\mathbf{L}^2$  and  $L_z$  by  $\psi_{\lambda,\mu}$  with eigenvalues  $\lambda\hbar^2$  and  $\mu\hbar$  respectively, we have

$$\mathbf{L}^2\psi_{\lambda,\mu} = \lambda\hbar^2\psi_{\lambda,\mu} \quad \text{and} \quad L_z\psi_{\lambda,\mu} = \mu\hbar\psi_{\lambda,\mu}$$

We introduce operators  $L_{\pm} = L_x \pm iL_y$ , whose commutation relations with  $L_z$  and  $\mathbf{L}^2$  are

$$[L_{\pm}, \mathbf{L}^2] = 0, \quad [L_z, L_{\pm}] = \pm\hbar L_{\pm}, \quad [L_+, L_-] = 2\hbar L_z \quad (70)$$

Applying  $[L_{\pm}, \mathbf{L}^2] = 0$  upon  $\psi_{\lambda,\mu}$ , we obtain

$$\mathbf{L}^2 L_{\pm}\psi_{\lambda,\mu} = L_{\pm}\mathbf{L}^2\psi_{\lambda,\mu} = \lambda\hbar^2 L_{\pm}\psi_{\lambda,\mu}$$

This means that  $L_{\pm}\psi_{\lambda,\mu}$  is the eigenstate of  $\mathbf{L}^2$  with the eigenvalue  $\lambda\hbar^2$ . Applying  $[L_z, L_{\pm}] = \pm\hbar L_{\pm}$  upon  $\psi_{\lambda,\mu}$ , we obtain

$$L_z L_{\pm}\psi_{\lambda,\mu} = L_{\pm}(L_z \pm \hbar)\psi_{\lambda,\mu} = \hbar(\mu \pm 1)L_{\pm}\psi_{\lambda,\mu}$$

This means that  $L_{\pm}\psi_{\lambda,\mu}$  is the eigenstate of  $L_z$  with eigenvalue  $(\mu \pm 1)\hbar$ . Therefore,  $L_+$  increases the eigenvalue of  $L_z$  by 1 and  $L_-$  decreases it by 1 in unit of  $\hbar$ . If we apply  $L_+$  repeatedly  $n$  times on  $\psi_{\lambda,\mu}$  we obtain an eigenstate with the eigenvalue of  $L_z$  equal to  $(\mu + n)\hbar$ . For a given value of  $\mathbf{L}^2 (= \lambda\hbar^2)$  the eigenvalues of  $L_z$  must be limited by  $(\mu + n)^2 \leq \lambda$ . Therefore, for a certain value of  $n$ ,  $(L_+)^{n+1}\psi_{\lambda,\mu} = 0$  so that no eigenstate with an eigenvalue more than  $(\mu + n)\hbar$  exists. Putting  $\mu + n = l$ , this means that  $L_+\psi_{\lambda,l} = 0$  and  $L_z\psi_{\lambda,l} = l\hbar\psi_{\lambda,l}$ . Applying the identities  $L_- L_+ = \mathbf{L}^2 - L_z(L_z + \hbar)$  upon the eigenstate  $\psi_{\lambda,l}$  we obtain

$$0 = L_- L_+ \psi_{\lambda,l} = [\mathbf{L}^2 - L_z(L_z + \hbar)] \psi_{\lambda,l} = [\lambda - l(l+1)]\hbar^2 \psi_{\lambda,l}$$

From this we obtain  $\lambda = l(l+1)$ , where  $l$  is the largest eigenvalue of  $L_z$  in unit of  $\hbar$ .

Applying  $L_-$  repeatedly upon  $\psi_{\lambda,l}$ , we can obtain eigenstates of  $L_z$  with eigenvalues  $(l-1)\hbar$ ,  $(l-2)\hbar$ , etc. Again there must exist the lower limit of the eigenvalues of  $L_z$  so that  $(L_-)^{n+1}\psi_{\lambda,l} = 0$  for a certain value of  $n$ . Then the lowest eigenvalue is given by  $\mu = l - n$ . Applying the equality  $L_+ L_- = \mathbf{L}^2 - L_z(L_z - \hbar)$  upon  $\psi_{\lambda,l-n}$  we obtain



$$0 = L_+ L_- \psi_{\lambda, l-n} = [\lambda - (l-n)(l-n-1)] \hbar^2 \psi_{\lambda, l-n}$$

This leads to the condition  $\lambda = l(l+1) = (l-n)(l-n-1)$  or  $2l = n$ . Thus the value of  $l$  must be either an integer or a half-integer.

Summarizing, the eigenvalues of  $\mathbf{L}^2$  and  $L_z$  are given by

$$\mathbf{L}^2 : l(l+1)\hbar^2; l = 0, 1/2, 3/2, \dots \quad (71)$$

$$L_z : m\hbar; m = l, l-1, l-2, \dots, -l+1, -l \quad (72)$$

For a given value of  $l$  the eigenvalue of  $L_z$  can take  $(2l+1)$  different values given by Eq.(72). We will call  $l$  as the orbital quantum number and  $m$  as the magnetic quantum number of the state.

The possible eigenvalues of  $\mathbf{L}^2$  and  $L_z$  were derived solely by use of the commutation relations (68) among the components of the angular momentum. When the angular momentum is the orbital angular momentum defined by Eq.(67),  $L_z$  expressed in terms of the spherical polar coordinates  $(r, \theta, \varphi)$  becomes  $L_z = -i\hbar\partial_\varphi$ . The spherical polar coordinates are shown in Fig.14.

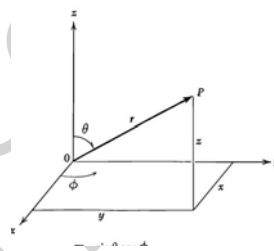


Figure 14. The Spherical polar coordinates

The eigenstates of  $L_z$  satisfy  $L_z \psi = -i\hbar\partial_\varphi \psi = \mu\hbar\psi$  and their  $\varphi$  dependences are given by  $\psi \sim \exp(i\mu\varphi)$ . Since  $\varphi \Rightarrow \varphi + 2\pi$  means no rotation and  $\varphi$  must be single valued, we obtain that  $\exp(i2\pi\mu) = 1$ . From this  $\mu$  must be an integer and thus  $l$  also must be an integer too.

The commutation relations (68) allow the possibility that the magnitudes of an angular momentum assume half-integer values such as  $l = 1/2$  and  $l = 3/2$  as shown by Eq.(71). According to Stern-Gerlach experiments or electronic configurations of multi-electron atoms the electron has an additional degree of motion besides its orbital motion in space. The angular momentum of this additional degree of freedom is called spin. There exist two spin states for the electron which means that the magnitude of the electron spin is  $1/2$  in unit of  $\hbar(2l+1 = 2, l = 1/2)$ .

The spin degree of freedom is incorporated into wave functions by assuming that wave functions of the electron have two components instead of one. Then the spin angular

momentum  $\mathbf{S}$  is expressed as the matrix operator acting upon the two component wave functions:

$$\mathbf{S} = (\hbar/2)\boldsymbol{\sigma} \quad (73)$$

where  $\boldsymbol{\sigma}$  is the Pauli matrix whose components are given by the following  $2 \times 2$  matrices (see Eq.(38)):

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (74)$$

The components of the spin satisfy the commutation relations (68) as we can easily check, and thus spin  $\mathbf{S}$  is qualified as an angular momentum. If we denote a two component wave function by

$$\Psi(\mathbf{r}, t) = \begin{bmatrix} \Psi_1(\mathbf{r}, t) \\ \Psi_2(\mathbf{r}, t) \end{bmatrix} \quad (75)$$

the spin acts upon  $\Psi$  according to the multiplication rule of matrices upon two component vectors. If  $A$  is a  $2 \times 2$  matrix whose elements are  $A_{ij}$  ( $i = 1, 2, j = 1, 2$ ), then  $(A\Psi)_i = \sum_j A_{ij} \Psi_j$ .

The eigenstates of  $S_z$  satisfy

$$S_z \begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix} = (\hbar/2) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix} = (\hbar/2) \begin{bmatrix} \Psi_1 \\ -\Psi_2 \end{bmatrix} = m_s \hbar \begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix}$$

Then we obtain two eigenstates with eigenvalues  $m_s \hbar = \pm(1/2)\hbar$  ( $m_s = \pm 1/2$ ):

$$\Psi_{\uparrow} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} (m_s = 1/2), \quad \Psi_{\downarrow} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} (m_s = -1/2) \quad (76)$$

These states are called the spin up and down states respectively.

We have discussed eigenstates of  $\mathbf{L}^2$  and  $L_z$  at the same time. Similarly we can find eigenstates of  $\mathbf{L}^2$  and any component of  $\mathbf{L}$  at the same time. Such an eigenstate can be expressed as a linear combination of the eigenstates of  $\mathbf{L}^2$  and  $L_z$ ;  $\Psi = \sum_m c_{l,m} \psi_{l,m}$ , where  $c_{l,m}$  are appropriately chosen constants and  $\psi_{l,m}$  the eigenstates of  $\mathbf{L}^2$  and  $L_z$  with the quantum numbers  $l$  and  $m$ .

In classical physics the angular momentum can direct in any direction and therefore there exist infinitely many states with different directions of the angular momentum for a given value of its magnitude. Contrary in quantum physics, any state of rotational motion with a given magnitude of angular momentum can be expressed as a linear

combination of the finite number of the eigenstates of  $\mathbf{L}^2$  and  $L_z$  with the quantum numbers  $l$  and  $m$ . For example, the eigenstates of  $S_x$  can be expressed as  $\Psi = 2^{-1/2}(\Psi_{\uparrow} \pm \Psi_{\downarrow})$  whose eigenvalues are  $\pm \hbar/2$ . Here  $\Psi_{\uparrow}$  and  $\Psi_{\downarrow}$  are the spin up and down states with  $m_s = \pm 1/2$ .

Quantum physics provide a new insight about the meaning of energy, linear momentum and angular momentum. Let us consider a wave function  $\Psi(x, y, z, t)$  of a particle. The wave function at a time  $t + \Delta t$  displaced by a small time interval  $\Delta t$  is

$$\begin{aligned} \Psi(x, y, z, t + \Delta t) &= \Psi(x, y, z, t) + \Delta t \partial \Psi(x, y, z, t) / \partial t \\ &= (1 - iE\Delta t / \hbar) \Psi(x, y, z, t) \end{aligned} \quad (77)$$

where we used the substitution  $E = i\hbar\partial_t$ . Thus the time translation of the wave function by  $\Delta t$  is equal to operating  $1 - iE\Delta t / \hbar$  upon the wave function. This is exact when  $\Delta t$  is infinitesimally small.

If we repeat the infinitesimal time translations  $n$  times, we obtain the translation operator  $(1 - iE\Delta t / \hbar)^n$  for time displacement by  $n\Delta t$ . If we take the limit  $n \Rightarrow \infty$  and  $\Delta t \Rightarrow 0$  with  $n\Delta t = T$  kept finite, we obtain the time translation operator for the finite displacement by  $T$ ;

$$\lim_{n \rightarrow \infty} (1 - iET / \hbar n)^n = \exp(-iET / \hbar)$$

Here we used a mathematical formula  $\lim_{n \rightarrow \infty} (1 + x/n)^n = \exp(x)$ . Thus the operator  $\exp(-iET / \hbar)$  is the time translation operator for a finite displacement  $T$ . Similarly  $1 + i\mathbf{p} \cdot \Delta \mathbf{a} / \hbar$  is the spatial translation operator for an infinitesimal displacement  $\Delta \mathbf{a}$ , and  $\exp(i\mathbf{p} \cdot \mathbf{a} / \hbar)$  the spatial translation operator for a finite displacement  $\mathbf{a}$ . Thus, in quantum physics, energy is the generator for time displacement and momentum the generator for spatial displacement.

Also the angular momentum of a particle in quantum physics means a rotation operator for the position of the particle about an axis passing through the origin of the spatial coordinate. If we rotate a position  $(x, y, z)$  by an infinitesimal angle  $\Delta\theta$  about z-axis, it moves to a position  $(x', y', z')$  which is given by  $x' = x - y\Delta\theta$ ,  $y' = y + x\Delta\theta$ ,  $z' = z$ . Then,  $\psi(x', y', z', t) = \psi(x, y, z, t) + \Delta\theta(-y\partial_x + x\partial_y)\psi(x, y, z, t) = (1 + i\Delta\theta L_z / \hbar)\psi(x, y, z, t)$ . In general, the operator  $(1 + i\Delta\vec{\theta} \cdot \mathbf{L} / \hbar)$  is the generator for an infinitesimal rotation  $\Delta\theta$  and  $\exp(i\boldsymbol{\theta} \cdot \mathbf{L} / \hbar)$  the generator for a finite rotation  $\boldsymbol{\theta}$ , where the vectors  $\Delta\boldsymbol{\theta}$  and  $\boldsymbol{\theta}$  express both the direction of the axis of rotation and the magnitude of the rotated angle.

So far we considered that wave functions are time-dependent and follow the Schrödinger equation, while physical quantities such as position, momentum and

angular momentum are operators which are defined in time-independent ways. Instead, we can consider physical quantities as time-dependent ones and wave functions as time-independent ones. If we take the latter view, the equation of motion for a physical quantity  $A$  can be written as

$$dA(t)/dt = (i/\hbar)[H, A(t)] \quad (78)$$

which can be derived from Eq.(65). This is called the Heisenberg equation of motion.

The basic commutation relations between position and momentum are the same with Eq.(66) if we take them at the same time:

$$[x(t), p_x(t)] = [y(t), p_y(t)] = [z(t), p_z(t)] = i\hbar \quad (79)$$

When  $A$  is a function of  $\mathbf{r}$  and  $\mathbf{p}$ , we can solve the Heisenberg equation of motion thereby using the commutation relations (79).

The Heisenberg equations are of the same form with the classical Hamilton's equation of motion, if we replace the Poisson brackets by the corresponding commutators times  $i/\hbar$ :

$$[H, A]_{\text{Poisson}} \Rightarrow (i/\hbar) [H, A], \quad [x_i, p_j]_{\text{Poisson}} \Rightarrow (i/\hbar) [x_i, p_j] \quad (80)$$

Although the Heisenberg formalism using the Heisenberg equation is fully equivalent with the Schrödinger formalism in its content, we shall primarily use the Schrödinger formalism to describe quantum phenomena in this book.

One of the basic ingredients of modern physics is that fundamental particles of the same kind are perfectly identical and indistinguishable with each other. If there are two electrons, they follow the same Schrödinger equation and there is no way to distinguish them from one another. In 1925 Pauli discovered the fundamental principle that governs the electronic configurations of atoms with more than one electron. His exclusion principle states that no two electrons in an atom can exist in the same quantum state.

Let us consider a quantum system which consists of two identical particles. The wave function of the system is described by  $\Psi(1, 2)$ , where 1 and 2 denote all the necessary variables to specify states of the particles 1 and 2. Since the two particles are indistinguishable, it should make no difference in the probability density  $\Psi^*\Psi$  of the system if the two particles are exchanged:

$$\Psi^*(1, 2)\Psi(1, 2) = \Psi^*(2, 1)\Psi(2, 1)$$

From this the wave function  $\Psi(1, 2)$  must satisfy  $\Psi(2, 1) = \exp(i\alpha)\Psi(1, 2)$ , where  $\alpha$  is any real number. Since twice the exchange of the two particles corresponds to no

exchange, we obtain  $\exp(2i\alpha) = 1$ . This leads to  $\exp(i\alpha) = \pm 1$ . Therefore,  $\Psi(1, 2)$  must be either symmetric or antisymmetric under exchange of the two particles:

$$\Psi(1, 2) = \Psi(2, 1) \text{ symmetric, } \Psi(1, 2) = -\Psi(2, 1) \text{ antisymmetric} \quad (81)$$

Contrary to  $\Psi^*\Psi$ , the wave function  $\Psi$  itself is not a measurable quantity, and it can be altered in sign by the exchange of the two particles. The results of experiments on many electron systems such as electronic configurations of multi-electron atoms show that the wave functions of these systems are totally antisymmetric under exchange of any pair of electrons in the systems.

When quantum states of two electrons in an atom are  $\psi_a$  and  $\psi_b$ , the wave function of the two electron system is given as the product of  $\psi_a$  and  $\psi_b$ . Since the wave function must be antisymmetric, it must be written as

$$\Psi(1, 2) = 2^{-1/2} \{ \psi_a(1)\psi_b(2) - \psi_b(1)\psi_a(2) \} \quad (82)$$

where  $2^{-1/2}$  is the normalization factor. The wave function  $\Psi$  vanishes for  $a = b$ , which means that no two electrons can exist in the same atomic orbit. If there exist  $n$  electrons in an atom, the wave function of the  $n$ -electron system is totally antisymmetric, which means that each of the  $n$  electrons must be in a different atomic orbit from the others.

Contrary to electrons, a wave function of a multi-photon system is totally symmetric under exchange of any pair of photons. When two photons are in quantum states  $\psi_a$  and  $\psi_b$ , the two photon wave function is

$$\Psi(1, 2) = 2^{1/2} \{ \psi_a(1)\psi_b(2) + \psi_b(1)\psi_a(2) \} \quad (83)$$

If the two states are identical ( $a = b$ ), the wave function becomes  $\Psi = 2^{1/2}\psi_a(1)\psi_a(2)$ . If the two photons were distinguishable, the wave function should be  $\Psi = \psi_a(1)\psi_a(2)$  without the factor  $2^{1/2}$ . Thus, the probability that the two photons are found in the same quantum state is twice what it is for distinguishable photons. The presence of a photon in a quantum state enhances the probability that other photons occupy the same state and any number of photons can exist in the same quantum state. This is contrary to the case of multi-electron systems where the presence of an electron in a state prohibits other electrons to occupy the same state. In general, the probability for finding  $n$  photons in the same state is enhanced by a factor  $n!$  when compared to the probability for distinguishable particles.

Electrons, protons, neutrons, and any other particle with a half-odd integer spin have totally antisymmetric wave functions. They are called fermions or Fermi-Dirac particles. Contrary to this, photons and any other particle with an integer spin have totally symmetric wave functions. They are called bosons or Bose-Einstein particles.

Ordinary matter consists of electrons, protons and neutrons, all being fermions. The Pauli principle for fermions can give a simple and straightforward explanation for why

more massive objects are larger in size than less massive objects. In general, a more massive object has more fermions in it. If we keep adding more fermions, they have to occupy higher energy states with more spatial extension so that the fermionic configuration of the object is compatible with the exclusion principle. Therefore, the size of the object would become larger as we increase number of fermions.

Statistical properties of multi-particle systems depend much on whether the particles are fermions or bosons. Let us consider multi-particle systems in thermal equilibrium at temperature  $T$ . We denote the number of different states of a single particle whose energy lie between  $\varepsilon$  and  $\varepsilon + d\varepsilon$  by  $g(\varepsilon)d\varepsilon$ . According to Maxwell-Boltzmann's distribution in classical physics, the probability for finding a particle with energy between  $\varepsilon$  and  $\varepsilon + d\varepsilon$  is given by  $g(\varepsilon)e^{-\alpha}e^{-\varepsilon/kT}d\varepsilon$ . The value of  $\alpha$  depends upon the total number of particles  $N$  in the system and is determined by

$$\int g(\varepsilon)e^{-\alpha}e^{-\varepsilon/kT}d\varepsilon = N \quad (84)$$

In quantum physics the probability for finding a boson in quantum states with energy between  $\varepsilon$  and  $\varepsilon + d\varepsilon$  is

$$P(\varepsilon)d\varepsilon = g(\varepsilon)d\varepsilon [e^{\alpha}e^{\varepsilon/kT} - 1]^{-1} \quad (85)$$

which is called the Bose-Einstein distribution for Bose particles. For multi-fermion systems the probability is given by

$$P(\varepsilon)d\varepsilon = g(\varepsilon)d\varepsilon [e^{\alpha}e^{\varepsilon/kT} + 1]^{-1} \quad (86)$$

which is called the Fermi-Dirac distribution for fermions. Short derivations of Bose-Einstein and Fermi-Dirac distributions were given in an earlier chapter (see *section 1*)(see Eqs.(32) and (33)).

For large values of  $\varepsilon$  ( $\varepsilon \gg kT$ ) the two distribution functions coincide with the Maxwell-Boltzmann distribution function, because  $e^{\alpha}e^{\varepsilon/kT} \gg 1$  and the  $\pm$  term in Eqs.(85) or (86) can be neglected. In Fig.12 of the previous chapter ( see *section 1* ) we plotted the three distributions as a function of  $\varepsilon$  for a given value of  $\alpha$ . The Bose-Einstein distribution is always higher than the Maxwell-Boltzmann distribution, while the Fermi-Dirac distribution is always lower.

The quantum nature of multi-particle systems becomes apparent at relatively low temperatures, for which the discrete nature of energy levels is important. This can be shown by the following distribution of electrons in a metal. The Fermi-Dirac distribution plays important roles in understanding various physical properties of multi-electron systems such as electric conductivity of metals due to electrons. Putting  $\alpha = -\varepsilon_F/kT$ , the Fermi-Dirac distribution for fermions can be written as

$$P(\varepsilon) = g(\varepsilon) \left[ \exp\left\{(\varepsilon - \varepsilon_F)/kT\right\} + 1 \right]^{-1} \quad (87)$$

The energy  $\varepsilon_F$  is called the fermi energy of the system. At  $T = 0$ , we obtain  $f(\varepsilon) = 1$  for  $\varepsilon < \varepsilon_F$  and  $f(\varepsilon) = 0$  for  $\varepsilon > \varepsilon_F$ , where  $f(\varepsilon) = P(\varepsilon)/g(\varepsilon)$ . Thus at absolute zero temperature all energy states up to  $\varepsilon_F$  are fully occupied by fermions, while energy states above  $\varepsilon_F$  are all empty. If a system contains  $N$  fermions, we can obtain  $\varepsilon_F$  by filling up its energy states with the  $N$  fermions in order of increasing energy up to  $\varepsilon_F$  starting from the lowest energy state.

As the temperature increases above  $T = 0$  but with  $kT$  still smaller than  $\varepsilon_F$ , some fermions will leave states just below  $\varepsilon_F$  and move into states just above it. The distribution functions of fermions at  $T = 0$  and at a small value of  $T (\ll \varepsilon_F/k)$  are shown in Fig.15.

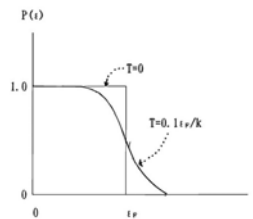


Figure 15. The distribution functions  $P(\varepsilon)$  of fermions at  $T=0$  and a small value of  $T$

Even at room temperature, the Fermi energy of electrons in a metal is much higher than  $kT$ . Thus the energy distribution of electrons in a metal is like the distribution shown in the figure for  $kT \ll \varepsilon_F$ . This has decisive effects on physical properties of metals. For example, only a small fraction of electrons in metals can contribute to electric conductivity of metals. When an electric field is applied to metals, only those electrons near the Fermi energy can contribute to the electric current because other electrons deep below the fermi energy cannot move to higher energy states since they are occupied by other electrons (see *Particles and Fields* ).

For a multi-boson system the distribution function  $P(\varepsilon)$  is given by Eq.(85). Since  $P(\varepsilon)$  must be positive for any value of  $\varepsilon$ ,  $\varepsilon^{-\alpha}$  cannot be greater than  $\exp(\varepsilon_0/kT)$  where  $\varepsilon_0$  is the lowest single particle energy for the bosons. We can take  $\varepsilon_0$  as zero when the volume of the system is sufficiently large. Then, we require that  $\alpha \geq 0$ . As  $\alpha$  approaches 0, the occupation number of the zero-energy state becomes infinitely large. The growth of this occupation number is actually limited by the total number of bosons available, but it can be shown that a significant fraction of the bosons can occupy the lowest energy state. This phenomenon is known as Bose-Einstein condensation, which is the basic cause of superfluidity and superconductivity. We shall describe some of these condensation phenomena in a later chapter ( see *Particles and Fields* ).

Finally we shall mention a few words about the connection between the spin and statistics of the particles. Based upon the present quantum field theories we can prove that particles with an integer spin follow the Bose-Einstein statistics and those with a half-integer spin follow the Fermi-Dirac statistics. These results are obtained based upon the relativistic invariance of the theories and the locality of the field corresponding to the particle.

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### **Biographical Sketch**

**Gyo Takeda**, Professor Emeritus of Tokyo University and Tohoku University, was born in Tokyo 1924. His speciality is the theory of Particle physics and nuclear physics and he also carries out research into neuroscience. He is known as one of the collaborators of Prof. S. Tomonaga's works on the relativistic renormalized theory of quantum electrodynamics. After graduating from Physics Department, University of Tokyo, he has served as an Associate professor, Kobe University, Professor and Director, Institute for Nuclear Studies, University of Tokyo, Professor of Physics and Dean of Faculty of Science, Tohoku University, and a Professor, General Education, Tohoku Gakuin University. Also he served as a research associate of University of Wisconsin and Brookhaven National Laboratory, USA, during the period of 1952-1955 and as a visiting professor of University of Wisconsin and University of California, Berkley, during the period of 1961-1963. He was a member of High Energy Physics Committee of IUPAP(International Union of Pure and Applied Physics) during the period of 1973-1978 and served as the Chairman of the Organizing Committee of the 17th International High Energy Physics Conference held in Tokyo, 1978. He has published many textbooks on general physics, quantum field theory, particle physics, and neuroscience all in Japanese.