## Fu-sui Liu

# Quantum Mechanics Upon Theorems



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## QUANTUM MECHANICS UPON THEOREMS

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PHYSICS RESEARCH AND TECHNOLOGY

## QUANTUM MECHANICS UPON THEOREMS

**FU-SUI LIU** 



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## Preface

Planck proposed the quantum idea in 1900. Now the quantum theory is the most precisely tested and most successful theory in the history of science. As we know, many high science and technology industrials are based on quantum mechanics. In developed countries the output value of these industrials is the 30% of the gross national product (GNP).

Although quantum mechanics is a very important and not a young subject, now quantum mechanics still looks like to cover with mysterious veil or to fall from skies. "Quantum mechanics is very impressive," Einstein wrote in 1926, "But an inner voice tells me that it is not yet the real thing." Bohr said: "Anyone who is not shocked by quantum theory has not understood it." Dirac said: "To improve the quantum mechanics people need a very large *revolution* in basic concepts." Feynman said: "We should always keep in mind the possibility that the quantum mechanics may be fail, since it has certain difficulties with philosophical prejudices that we have about measurement and observation." Feynman also said: "I can safely say that nobody understands quantum mechanics".

This textbook tries to reveal the mysterious veil, and thus makes quantum mechanics a subject easy to be understood, accepted, and mastered. For this goal this textbook proves 52 theorems, 18 corollaries, 1 criterion, and establishes 1 law for *all* basic concepts, pictures, and conclusions in quantum mechanics. The criterion, the law, and half of the theorems and corollaries are given by this textbook at the first time. Except the law, this textbook makes quantum mechanics independent of postulates, axioms, guesses, principles, hypotheses, paradoxes, and assumptions. In one word, quantum mechanics in this and all other textbooks can be called roughly quantum mechanics upon theorems and postulates, respectively.

Let me list *partially* the identical and different points between quantum mechanics upon postulates and theorems.

(1) Quantum mechanics upon postulates contains such as: postulate of operator representation of observable; Schrödinger equation postulate; postulates of three formulations of quantum mechanics postulate; postulate of commutation relation instead of Poison bracket; de Bloglie matter wave hypotheses (i. e., wave-particle duality hypotheses); principle of Heisenberg uncertainty relations; principle of state superposition; wavefunction axiom; identity axiom of multiparticle system. ([1]-[9]).

All the above postulates, axioms, principles, hypotheses become theorems and corollaries.

(2) Some long-standing, big and difficult problems in quantum mechanics upon postulates are completely solved by quantum mechanics upon theorems. For example: (2.1) Quantum mechanics upon postulates does not know the origin of sharp contradiction between quantum mechanics and general theory of relativity, and thinks this contradiction is the rigorous challenge faced by physics in 21 century.

Quantum mechanics upon theorems does.

(2.2) Quantum mechanics upon postulates gives the quantum mechanically theoretical lifetime of free, for example, electron is  $\tau = 10^{-36}$  second [10].

Quantum mechanics upon theorems gives a theorem, according to which  $\tau = \infty$ .

(3) Quantum mechanics upon postulates think that, for example, measurement dependence of quantum mechanics, collapse of wavefunction, ensemble description of wavefunction, environment dependence of decoherence, indistinguishability of identical multiparticle system.

Quantum mechanics upon theorems proves: quantum mechanics is independent of measurement, collapse of wavefunction is not necessary, wavefunction describes individual particle other than particles' ensemble, decoherence is independent of environment, and the particles in identical multiparticle system are only of identity other than the so-called indistinguishability.

(4) Quantum mechanics upon postulates is very difficult to image the picture of waveparticle duality, and thus the wave-particle duality as a concept drifts from a place to place. Quantum mechanics upon theorems proves a theorem of mathematical structure of objects, including big and small massy particle, massless photon and phonon. According to this theorem, any object consists of two parts: substance and wave, and thus the wave-particle duality of object is easy to be imagined.

(5) Quantum mechanics upon theorems proposes some <u>new</u> concepts such as the still more microscopic processes, equiprobability, spontaneous equiprobability symmetry breaking and so on.

Quantum mechanics upon theorems proposes some <u>new</u> viewpoints such as the origins of probability of observed super light speed in tunneling processes and in nonlocality of entangled states.

In one word, at least, the quantum mechanics upon theorems tries to discard the dross and select the essential, and to eliminate the false and to retain the true in the quantum mechanics upon postulates. Note that mast contents in the quantum mechanics upon postulates are correct, and this textbook inherits also many methods and skills of calculations, derivations, arguments, and demonstrations in the quantum mechanics upon postulates.

The best interesting thing in "Quantum Mechanics upon Theorems" is at end of this textbook the exercise:

(i) Would readers, including students and beginners, please argue that quantum mechanics upon theorems will cause fourth science and technology revolution in our world; [The first, second, and third are steam engine (1765, Watt), electric motor (1821, Faraday) $\rightarrow$ applications of electricity (1880, Edison), and computer (1946)  $\rightarrow$ 

internet (1960)→information, respectively.]

(ii) Would readers please appraise classical mechanics, quantum mechanics upon postulates, special and general theory of relativity; (This textbook has introduced history of physics, and hope readers to understand the relations between main theories of physics through this exercise.) (iii) Would readers please estimate the influences of quantum mechanics upon theorems to social science, especially, philosophy.

(iv) Do you agree that the quantum theory from Planck quantum (1900) to basic quantum field theory (1929) cannot be cause of a world science and technology revolution? Why?

The author of this textbook believes that before reading this textbook no one reader believes that this textbook with only no more than 500 pages can cause fourth world science and technology revolution; on the contrary, after reading this textbook, no one reader does not have strong wish and maximum enthusiasm to accomplish the above exercise. Actually, in this preface I just list some obvious features of this textbook. I would like to give readers, including students and beginners, bigger elaboration space and imaginary space.

## Chapter 1

## **Birth of Quantum Mechanics**

#### 1.1. Difficulties of Classical Physics

#### 1.1.1. Introduction

Until the end of nineteenth century, classical physics, including classical mechanics, classical electrodynamics, thermodynamics, classical acoustics, optics, hydromechanics, and classical statistical physics, appeared to be sufficient to explain all physical phenomena. During the latter part of nineteenth century and the early years of twentieth century, the experimental facts mentioned in sections 1.1.2 - 1.1.8 revealed four difficulties:

(1) The observed radioactivity of matter;

(2) The energy of hydrogen atom is discrete;

(3) The electron and other massy particles are of wave property, and the electromagnetic field has particle property;

(4) The uncertainty relations between coordinate and momentum and between energy and time.

All these difficulties required new concepts and ideas radically different from those of classical physics.

Outlined below are the discoveries and events that occurred near the turn of the century that removed some enigmas and led naturally to the development of the quantum mechanics and quantum field theory.

1986	Bacquerel	Radioactive uranium	
1901	Mme. Curie	Radioactive polonium and radium	(1903 Nobel Prize)
1901	Planck	Blackbody radiation	(1918 Nobel Prize)
1905	Einstein	Photoeffect	(1921 Nobel Prize)
1911	Rutherford	Model of atom	
1913	Bohr	Quantum theory of spectra	(1922 Nobel Prize)
1913	Stark	Splitting of spectral line in	
		electric field	(1919 Nobel Prize)

1916	Millikan	Elementary charge of electricity	
		and Photoeffect	(1923 Nobel Prize)
1922	Compton	Scattering photons off electrons	(1927 Nobel Prize)
1925	Pauli	Exclusion principle	(1945 Nobel Prize)
1925	de Bloglie	Matter wave	(1929 Nobel Prize)
1925	Heisenberg	Matrix mechanics	
1926	Schrödinger	Wave mechanics	(1933 Nobel Prize)
1927	Heisenberg	Uncertainty relation	(1932 Nobel Prize)
1927	Davidson	Experiment on wave properties	
	and Germer	of electron	(1937 Nobel Prize)
1927	Born	Statistical interpretation	
		of wavefunction	(1954 Nobel Prize)
1928	Dirac	Relativistic wave mechanics	
		and prediction of positron	(1933 Nobel Prize)
1929	Heisenberg	Basic structure of quantum field	
	and Pauli	theory	
1932	Anderson	Discovery of positron	(1936 Nobel Prize)
1932	Wiener	Path integral method of Brown motion	n
1933	Dirac	Path integral of quantum mechanics	
1948	Feynman,	Path integral formulation of quantum	
	Feynman,	mechanics	
	Schwinger,	Quantum electrodynamics	(1965 Nobel Prize)
	and Tomonaga		

In the remainder of this chapter and other chapters we will illustrate all these topics in more detail.

#### 1.1.2. Radioactive Decay

Radioactivity or Radioactive decay is the process by which an atomic nucleus of an unstable atom loses energy by emitting ionizing particles (ionizing radiation). The emission is spontaneous, in that the atom decays without any physical interaction with another particle from outside the atom [11].

Radioactivity was discovered in 1896 by French scientist Henri Becquerel, while working on phosphorescent materials. During experiments to see if phosphorescent materials would expose photographic materials through black paper in the manner of the recentlydiscovered X-rays, which produced fluorescence, Becquerel used a phosphorescent uranium salt and eventually found that it blackened the plate through paper wrapping, in a desk drawer over a weekend, even without application of light, or production of its phosphorescence. These penetrating radiations, accidentally discovered emanating from uranium minerals, were first called Becquerel rays.

Pierre and Marie Curie soon became clear that the blackening of the plate did not have anything to do with phosphorescence, because the plate blackened when the mineral was in the dark. Non-phosphorescent salts of uranium and metallic uranium also blackened the



Figure 1.1. Spectrum of blackbody radiation. The curves have been discussed to bring out some important features.

plate. It was clear that there is a form of radiation that could pass through paper that was causing the plate to become black.

At first it seemed that the new radiation was similar to the recently-discovered X-rays. Further research by Becquerel, Ernest Rutherford, Paul Villard, Pierre Curie, Marie Curie, and others discovered that this form of radioactivity was significantly more complicated. Different types of decay can occur, producing very different types of radiation. Rutherford was the first to realize that they all occur with the same mathematical exponential formula (see below), and Rutherford and his student Frederick Soddy were first to realize that many decay processes resulted in the transmutation of one element to another. Subsequently, the radioactive displacement law of Fajans and Soddy was formulated to describe the products of alpha and beta decay.

The early researchers also discovered that many other chemical elements besides uranium have radioactive isotopes. A systematic search for the total radioactivity in uranium ores also guided Marie Curie to isolate a new element polonium and to separate a new element radium from barium in 1901. The two elements' chemical similarity would otherwise have made them difficult to distinguish.

#### 1.1.3. Black Body Radiation

When there is an equilibrium between black body (hollow cavity) and thermal radiation, the radiation leaving the hole on a heated hollow cavity is termed as black body radiation. The experimentally observed spectral energy density u(v) of black body radiation as a function of wavelength at different temperatures is shown in Fig. 1.1.

Basing on classical electrodynamics and statistical physics theory, Rayleigh (1900)-Jeans (1905) obtained the spectral distribution of a radiation field in equilibrium at the temperature T

$$u_{rj}(\mathbf{v}) = \frac{8\pi \mathbf{v}^2}{c^3} k_B T \tag{1.1}$$

for low frequencies.  $k_B$  is Boltzmann's constant. c is the speed of light. While Rayleigh-Jean' formula is valid at low frequencies, it is seen to diverge (Historically, this diverge was called ultra-violet catastrophe.) at larger frequencies, where as shown in Fig. 1.1, the observed spectral distribution falls to zero. Basing on thermodynamics theory, Wien (1893) obtained a half-empirical formula

$$u_w(\mathbf{v}) = c_1 \mathbf{v}^3 e^{-c_2 \mathbf{v}/T},\tag{1.2}$$

where  $c_1$  and  $c_2$  are empirical parameters. However, Wien formula has obvious departure from experimental data at low frequencies. Planck (1900) improved the Wien formula, and obtained

$$u_p(\mathbf{v}) = \frac{c_1 \mathbf{v}^3}{e^{c_2 \mathbf{v}/T} - 1},$$
(1.3)

which fits the data at both low and high frequencies very well. Considering the good fitting between Planck's formula and the data of black body radiation, scientists at that time thought that this good fitting was not occasional, there should be a new scientific principle behind the Planck formula, which has not yet been revealed.

#### 1.1.4. Photoelectric Effect

Herz (1887) discovered the photoelectric effect: electrons (which is also called photoelectron) were observed to be ejected from metal when light of an appropriate frequency is incident on its surface. See Fig. 1.2. Further studies were done to learn about the effect observed by Hertz, however it wasn't until 1905 that a theory was purposed that explained the effect completely. The theory was proposed by Einstein and it made the claim that electromagnetic radiation had to be thought of as a series of particles, called photons, which collide with the electrons on the surface and emit them. This theory ran contrary to the belief that electromagnetic radiation was a wave and thus it was not recognized as correct until 1916 when Robert Millikan preformed a series of experiments using a vacuum phototube to confirm the theory. The modern research indicates that if the energy of the photon is less than 100 eV, then we observe the photoeffect. However, if the photon has a lot of energy, Compton scattering (thousands of eV) or pair production (millions of eV) may take place at the same time.

The photoelectric effect (= photoeffect) has the following characteristics:

(1) There exists a critical cutoff frequency  $v_c$ . When  $v < v_c$ , no electrons are liberated from the metal irrespective of the intensity of light;

(2) The energy of photoelectron is dependent only on v, and is independent of the intensity of light. The stronger the latter is, the more the photoelectrons liberated from metal in unit time are;



Figure 1.2. This diagram shows the electron emission induced by light incident upon metal durface.

(3) If  $v > v_c$ , then the photoelectrons appear instantly ( $\approx 10^{-9}$ ) second even when the light intensity is very low.

The first and second characteristics cannot be understood by classical physics in principle.

#### 1.1.5. Compton Effect

Sadler (1912) observed that when a beam of X-rays strikes matter, there was a phenomenon that the wavelength of X-ray becomes longer after scattering. Compton made a series of studies (1923). Compton discovered that some of the X-ray are scattered through an angle. The scattered radiation contains both the same wavelength and the wavelength longer than the wavelength of the incident X-rays. The change of wavelength is called Compton shift. It varies with the scattering angle. The frequency of the scattered radiation is independent of the material.

According to classical electromagnetic theory, the wavelength of scattered wave should be the same as the wavelength of incident wave. Therefore, the classical theory cannot explain Compton effect.

#### 1.1.6. Rule of Atomic Line Spectra

Balmer (1885) discovered that the line emission spectrum of hydrogen atom has the following rule.

$$k = R\left(\frac{1}{2^2} - \frac{1}{n^2}\right),$$
 (1.4)



Figure 1.3. The Balmer series of hydrogen atom spectrum.

where  $k(=1/\lambda = v/c)$  is wavenumber,  $\lambda$  is wavelength, *R* is Ryderberg constant, *R* = 109677.581 cm<sup>-1</sup>, *n*= 3, 4, 5, .... The above spectrum of hydrogen atom is called Balmer series of lines, and is shown in Fig. 1.3. The term in Eq. (1.4) is called spectrum term *T*(*n*).

Based on many observed data, Ritz (1908) discovered combination rule. According to this rule, every kind of atoms has itself spectrum term T(n), and the wavenumber of emission spectrum can be expressed always by

$$k_{mn} = T(n) - T(m).$$
 (1.5)

Then, there is a series of problems: Why the atomic spectrum does not distribute continuously? Why it appears as discrete line spectrum? What is the mechanism of line spectrum? Why the combination rule is so simple? What is the essence of spectrum term?

#### 1.1.7. Stability of Atom

Based on his  $\alpha$  particle scattering of atom, Rutherford (1911) proposed a model for the atom, which is called "planet model of atom" or "nucleus model of atom". According to Rutherford, the atom consists of electrons orbiting around a positive charged nucleus, and the latter's scale is less than  $10^{-12}$  cm.

Although Rutherford model can explain the large angular deflection of  $\alpha$  particle, it still meets difficulty, i. e., the problem of stability of atom. The motion of electrons orbiting around a nucleus is accelerative. According to classical electrodynamics, the accelerated electron would continue to radiate until they had exhausted all the positive energy, would fall into the nucleus, the atom would collapse (Atom's lifetime is only  $10^{-12}$  second in this case.), and in this process atom would a wide continuous spectrum, which also contradicts with the observed sharp line spectrum of atom.

#### 1.1.8. Specific Heat of Solid

In solid every atom makes small oscillation around it equilibrium position, and can treated as a particle with three freedoms. According to the classical statistical mechanics, its average kinetic and potential energy are  $3/2k_BT$ , the total energy is  $3k_BT$ . Therefore, the average thermal energy per one gram atom is  $3Nk_BT = 3RT$ . N=6.023 × 10<sup>23</sup>. N is the Avogadro



Figure 1.4. The variation of specific heat of Einstein solid with temperature.

constant. Thus, the specific heat of solid should be  $C_V = 3R = 5.958$  cal/K, which is called Dulong-Petit empirical rule (1819). However, the observe specific heat at low temperature approaches to zero (See Fig. 1.4).

At that time, no body knew the cause of the zero specific heat at low temperature.

#### 1.2. Planck-Einstein's Quantum Postulate of Light

On October 19, 1900, Planck published a paper on the radiation formula of black body, i. e. Eq. (1.3). Just after 45 days, on December 4, 1900, Planck published a paper to understand the physical meaning of Eq. (1.3). Planck said that if one hypothesized that when the system absorbs or emits radiation, it can only in a unit (or quantum) hv (h is called Planck constant.), then Eq. (1.3) can be derived in theory. Due to that the Planck's light quantum hypothesis cannot be understood by the continuous concept in classical physics, before 1905 there were only a few scientists to note the Planck's non-continuous concept of electromagnetic radiation.

To explain the photoelectric effect, Einstein (1905) hypothesized that light is composed of localized bundles of electromagnetic energy. The bundle was called by Lewis photon (1926). At frequency v, the energy of a photon is E = hv, which is called Planck-Einstein relation. Considering the special theory of relativity, the momentum of a photon p is p = E/c, where E is the energy of a photon. Accepting the concept of photon, the photoelectric effect was readily solved. Although the photon incident upon metal surface can be absorbs by an electron, to eject from the metal the electron needs to overcomes the work function ( $\Phi$ ) of metal. Einstein gave the kinetic energy of ejected electron

$$\frac{1}{2}mv^2 = h\mathbf{v} - \Phi. \tag{1.6}$$

Eq. (1.6) is called Einstein formula. When  $v < v_c = \Phi/h$ , the electron cannot be ejected from the metal, and thus there is no photoelectron. Einstein formula was verified directly by

the Milliken's photoelectric experiment (1916), in which the energy of the most energetic photoelectrons as a function of frequency obeys Eq. (1.6).

Applying the non-continuous concept of energy to the oscillation of atom at equilibrium position in solid, Einstein (1907) solved the observed zero specific heat of solid at low temperature successfully. After Einstein's works, the Planck's light quantum hypothesis caused more attention.

The concept of light quantum and Planck-Einstein relation are verified directly by the Compton effect. Compton suggested that Compton shift came from elastic collision between photon in X-ray and electron (1923). Assume that the momentum and energy in collision are conservative. Due to the recoil of electron, electron takes a part of energy and momentum, and thus the energy and momentum of scattered photon are reduced, i. e. the wavelength of radiation becomes longer.

Comments of this textbook:

(1) The quantum transition theory in chapter 10 proves that the Einstein formula Eq. (1.6) does not hold when the pulse of light is less than the femto second  $(10^{-15} \text{ second})$ .

(2) According to the wavepacket-only theory in chapter 3, any objects, including massy particle and massless photon, consist of various wavepackets. The wavepacket-only theory can prove: (A). The existence of universal Planck constant (See theorem I in chapter 3); (B). In Planck-Einstein relation  $E = hv = \hbar\omega$ ,  $v(k_{\circ}) = \hbar\omega(k_{\circ})$ , where  $k_{\circ}$  is the root-mean-square wavenumber of a photon wavepacket (See corollaries V and VI in chapter 3).

#### **1.3.** Bohr Postulates of Atomic States

To solve the stability of Rotherford's atom model (1911) and the line spectrum of atom (1885, 1908), Bohr (1913) proposed three postulates of atomic states:

(1) First postulate (stable state). The energy of atom is quantized, i. e., atom can only exists in a series of stable states with discrete energies  $(E_1, E_2, E_3, ...)$ .

(2) Second postulate (orbital quantization). The above states are characterized by discrete values of the angular momentum given by the relation:

$$\oint p_{\theta} d\theta = n \cdot h, \tag{1.7}$$

with *n* an integer greater than zero, and the dimension of  $p_{\theta}$  is *energy* × *time*. Eq. (1.7) is called Bohr quantization condition of angular momentum. In these states the atom does not radiate. The line integral follows the electron in one complete orbit around the nucleus.

(3) Third postulate (frequency condition). The change of atomic energy, including emission and absorbtion of photon, can occur only between any two stationary states in terms of quantum transition other than continuous transition.

The energy is conservative in the quantum transition process, i. e., if  $E_n > E_m$ , then the frequency of photon in emission or absorbtion processes is determined by Bohr's frequency

condition

$$h\mathbf{v} = E_n - E_m. \tag{1.8}$$

The first postulate solves the problem on stationariness of atom. The concept of quantization can also solves the problem of the observed zero specific heat of solid at low temperature.

The second and third postulates can explain the Redberg-Ritz composition rule of atomic spectrum. The Redberg-Ritz composition rule of atomic spectrum Eq. (1.5) connects with the frequency condition Eq. (1.8). The physical meaning of spectrum term is  $T(n) = E_n/hc$ , i. e., T(n) connects with the stationary energy of atom  $E_n$ .

Let us recall how the orbital quantization condition Eq. (1.7) leads to a discrete set of energy  $\{E_n\}$ . The energy of a stable hydrogen atom whose electron is moving in circular motion is

$$E = \frac{1}{2}mv^2 - \frac{e^2}{r} = \frac{p_{\theta}^2}{2mr^2} - \frac{e^2}{r}.$$
 (1.9)

The radius r obeys the centripetal condition

$$\frac{mv^2}{r} = \frac{p_{\theta}^2}{mr^3} = \frac{e^2}{r^2}.$$
 (1.10)

So that, with the orbital quantization condition Eq. (1.7)

$$\frac{e^2}{r} = \frac{p_{\theta}^2}{mr^2} = \frac{n^2\hbar^2}{mr^2}.$$
 (1.11)

 $\hbar = h/(2\pi)$  is the (reduced) Planck constant.

$$r_n = \frac{n^2 \hbar^2}{m e^2}.\tag{1.12}$$

These are the quantized values of r at which the electron persists without radiating. The values of the energy at these radii are

$$E_n = -\frac{p_{\theta}^2}{2mr^2} = -\frac{n^2\hbar^2}{2m} \left(\frac{me^2}{n^2\hbar^2}\right)^2 = -\frac{R}{n^2},$$
(1.13)

where *R* is the Ridberg constant:

$$R = \frac{me^4}{2\hbar^2} = 2.18 \times 10^{-11} erg = 13.6 eV.$$
(1.14)

The negative quantity of energy reflects the fact that we are dealing with the bound states. When n = 1, the atom is in ground state and has energy -R. The value of r when the atom is in the ground state is

$$r_1 \equiv a_\circ = \frac{\hbar^2}{me^2} = 5.29 \times 10^{-9} cm.$$
 (1.15)

This is a fundamental length in physics. It is called the Bohr radius.

Of course, Bohr postulates of atomic states cannot determine completely the energy of atom, because it cannot determine the unknown energy constant. To solve this problem, Bohr (1913) proposed correspondence principle, which says that if  $n \to \infty$ , then quantum system approaches to classical system. If the electron and the nucleus of hydrogen atom are infinitely far removed  $(r_n \to \infty)$  and at rest, then there should be no both kinetic and potential energy.  $E_{\infty} = 0$  for a classical system. If we rewrite Eq. (1.13) as  $E_n = -R/n^2 + \text{constant}$ , then Bohr correspondence principle tells us that the constant is zero.

According to Eqs. (1.7) and (1.13), the Balmer Series of lines is generated by transitions to the first n = 2 excited state:

$$h\mathbf{v}_B = E_n - E_2,\tag{1.16}$$

with n > 2.

Comments of this textbook:

(1). Bohr quantum theory of atomic states is only a phenomenological theory. It cannot answer the origin of the non-continuity of atomic energy. The quantum mechanics born in 1925 - 1926 can solve this problem.

(2). In Eq. (1.7)  $p_{\theta}$  is the momentum in polar coordinate. Eq. (1.7) can be written as  $L_n = p_{\theta} = rmv = n\hbar$  where *n* is an integer larger than zero. However, the solution of Schrödinger equation for hydrogen atom in chapter 6 indicates that  $L_l^2 = l(l+1)\hbar^2$  other than  $L_l^2 = l^2\hbar^2$  given by Eq. (1.7).

Using the theory in chapters 3 and 6, one can prove that the difference between  $L_l^2 = l(l+1)\hbar^2$  and  $L_l^2 = l^2\hbar^2$  comes from Heisenberg uncertainty relation.

#### **1.4.** de Bloglie Matter Wave Hypotheses

Inspired by that the light has both wave and particle (photon) properties, de Bloglie imagined that the massy particle (rest mass m > 0) might be have wave property as well as the photon, and proposed matter wave hypotheses (1923).

As we know, the three laws of geometric optics can be expressed by Fermat principle (shortest light range principle), i. e.

$$\delta \int_{A}^{B} \frac{dl}{v} = 0, \qquad (1.17)$$

where v is the speed of light in a medium. Eq. (1.17) means that the practical path of light takes the extreme value of light range  $\int_{A}^{B} dl/v$  in comparison with all the other possible pathes. On the other hand, according to classical mechanics, the practical path of a particle moving in potential field is determined by Maupertuis's least action principle (Refer to section 2.2 of chapter 2), i. e.

$$\delta \int_{A}^{B} p dl = \delta \int_{A}^{B} \sqrt{2m(E-V)} dl = 0.$$
(1.18)

Eq. (1.18) means that the practical path of a particle takes the extreme value of action integral  $\int_{A}^{B} p dl$  in comparison with all other possible pathes.

According to the comparison between Eq. (1.17) and Eq. (1.18), de Bloglie proposed that a massy particle being of energy *E* and momentum *p* connects with a matter wave,

which's frequency and wavelength are

$$\mathbf{v} = \frac{E}{h},\tag{1.19}$$

$$p = \frac{h}{\lambda} = hk, \tag{1.20}$$

where k represents the wavenumber of matter wave. The de Bloglie hypotheses of matter wave consist of the above two equations. According to de Bloglie hypotheses and Bohr's atomic model, the electron in atom, which makes a round motion around the nucleus, should be a stationary wave..

The stationary wave condition requires that the length r of round orbit of electron should be an integer of wavelength, i. e.

$$2\pi r = n\lambda, \tag{1.21}$$

where  $n = 1, 2, 3, \dots$ . From Eqs. (1.20) and (1.21) the angular momentum of electron is

$$J = rp = \frac{n\hbar}{2\pi} = n\hbar. \tag{1.22}$$

Therefore, from the stationary wave condition of matter wave one can obtain the quantization of angular momentum.

Comments of this textbook:

It can be seen from the theorem VI, corollaries VI, VII, and VIII in chapter 3 that:

(1) A particle consists of body-factor and guide-factor. The mass of the particle is carried by the body-factor, and the guide-factor is only a wave, which's action is to guide the body-factor to move. Thus a particle has both particle and wave properties;

(2) The physical meaning of wavenumber  $k_x = p_x/\hbar$  in de Bloglie matter wave hypotheses should be the average wavenumber of wavepacket, and appears in guide-factor, which expresses wave property of a particle;

(3) Any object consists of guide-factor (which is a mathematical function) and bodyfactor (which is the substance of an object, carrying mass and/or charge) is more reasonable. The electron is a rigid (Refer to the comment in the end of this section.) sphere with radius less that  $10^{-18}$  cm. This small rigid sphere cannot absolutely becomes a wave or spreading electron cloud under very weak Coulomb interaction in one atom. (According to the special theory of relativity, the electron has to have structure other than an absolutely rigid body. Otherwise, the propagation speed of interaction acted on an object will surpass light speed.)

#### 1.5. Davidson and Germer Experiment

The wave property in motion of massy particle can be observed only when de Bloglie wavelength ( $\lambda = h/p$ ) is of order or larger than the characteristic dimensions of the massy particle used to investigate it. Since *h* is very small,  $\lambda$  is so small as to preclude the hope observing de Bloglie hypotheses. The wave property in motion of electron was verified directly by Davidson-Germer experiment. A parallel beam of electrons with definite low



Figure 1.5. Schematic diagram of Davidson-Germer experiment.



Figure 1.6. (a). Number of scattered electrons as a function of accelerating voltage for  $\theta = 50^{\circ}$ . (b).Number of scattered electrons as a function of  $\theta$  for accelerating voltage of 54 eV.

energy are incident normal to surface of Ni crystal. See Fig. 1.5. The number  $N(\theta)$  of scattered back at an angle  $\theta$  to the incident direction can be measured by detector. For the periodic distribution of Ni atoms on the surface, the repetition is a = 0.215 nm, which is comparable to the de Bloglie wavelength of the incident electrons.

In the conditions that the electrons are incident normal to the surface and that the de Bloglie matter wave hypotheses are correct, the Ni atomic surface is equivalent to a refraction grating with distance *a*. When

$$a\sin\theta = n\lambda,$$
 (1.23)

the intensity of reflection wave will have extremes (n = 1, 2, 3, ...). Eq. (1.23) is called diffraction condition of grating. From the energy of incident electron and Eq. (1.20) one knows the wavelength of the incident electron  $\lambda = h/p = h/\sqrt{2mE}$ . If the energy of electron is E = 54 eV, then  $\lambda = 0.167$  nm. However, we can obtain an experimental value of  $\lambda_{ex}$ from the observed value of  $N(\theta)$  at  $\theta = 50^{\circ}$  in case of n = 1. See Fig. 1.6. Substituting this



Figure 1.7. Schematic double slit experiment.

wavelength into Eq. (1.23) yields that the peaks of intensity of refraction wave appears at the following directions:

$$\lambda_{ex} = 0.21 nm \times \sin 50^{\circ} = 0.165 nm \approx 0.167 nm.$$
(1.24)

The two values of  $\lambda$  obtained agree to within accuracy of the experiment.

Comments of this textbook:

(1). This experiment demonstrates only that the electron has wave property. This experiment cannot tell us that why the electron is of wave property. Chapter 3 indicates that Davidson-Germer experiment verifies actually that the wavepacket contains a guide-factor, which is a plane wave with wavenumber  $k_{xo}$ .  $k_{xo}$  is the root-mean-square wavenumber of a wavepacket.

#### 1.6. Young's Double Slit Experiment

Suppose that a disturbance propagates from one point to another point in space. What is propagating, waves or particles? A principal distinguishing characteristic is that waves exhibit interference and diffraction, particles do not. Hysterically, the evidence of the wave property of light was deduced from Young's double slit experiment (1804). Experiment with electrons (instead of light) using double slit arrangement (Fig. 1.7) indicates that electron possesses wave-like characteristic.

Consider electrons directed towards double slits A and B in a screen. Let the slit B is closed and slit A is open. By carrying out the experiment for a sufficient time, one obtained a pattern identical with the case when the light is diffracted from a slit A. Similar behavior is observed when A is closed and B is open.

When A and B are both open the final interference pattern should be a simple superposition of the intensities of the blackening on the screen arising when electrons are let through A or B. However, the distribution of intensities of blackening is of completely different character and shows interference pattern. Thus electron, like a wave, possesses interference properties.

A low-intensity double-slit experiment was first performed by G. Taylor in 1909, by reducing the level of incident light until photon emission/absorption events were mostly nonoverlapping. A double slit experiment was not performed with anything other than light until 1961, when Clauss Junsson of the University of Tbingen performed it with electrons. In 2002, Junsson's double slit experiment was voted "the most beautiful experiment" by readers of Physics World.

In 1999, objects large enough to be seen under an electron microscopelbuckyball molecules (diameter about 0.7 nm, nearly half a million times larger than a proton) were found to exhibit wave-like interference.

Variations of the experiment have been done. An important version of this experiment involves single massy particles. Sending them through a double slit apparatus one at a time results in single particles appearing on the screen, as expected. See Fig. 1.8. Remarkably, however, an interference pattern emerges when these particles are allowed to build up one by one. For example, when a laboratory apparatus was developed that could reliably fire one electron at a time through the double slit, the emergence of an interference pattern suggested that each electron was interfering with itself, and therefore in some sense the electron had to be going through both slits at once, an idea that contradicts our everyday experience of discrete objects. This phenomenon has been shown to occur with electrons (See the famous experiment on Ref. [13].). This phenomenon has also been shown to occur with atoms and even some molecules, including buckyballs. So experiments with electrons add confirmatory evidence to the view of Dirac that electrons, protons, neutrons, and even larger entities that are ordinarily called particles nevertheless have their own wave nature and even their own specific frequencies. This experimental fact is highly reproducible. However, the electrons do not arrive at the screen in any predictable order. In other words, knowing where all the previous electrons appeared on the screen and in what order tells us nothing about where any future electron will hit. Also note that if there is a cancelation of waves at some point, that does not mean that a particle disappears; it only means that the probability of a particle's appearing at that point will decrease, and the probability that it will appear somewhere else increases. Thus, we have the appearance of a seemingly causeless selection event in a highly orderly and predictable formulation of the interference pattern. Ever since the origination of quantum mechanics, some theorists have searched for ways to incorporate additional determinants or "hidden variables" that, were they to become known, would account for the location of each individual impact with the target.

The experiment has been performed with particles as large as  $C_{60}$ . Nairz *et al.* (2004) observed that the beam of  $C_{60}$  molecules has the same interference phenomenon like that of electron [14]. In Nairz's experiment the beam of  $C_{60}$  molecules comes from furnace with 1000 K. The most probable velocity of molecules is v = 117 m/s,  $\Delta v/v = 17\%$ . The beam goes through two collimation slits at first. Then the beam hits the SiN<sub>x</sub> grating (the width of every slit is 50 nm, and the distance between slits is 100 nm). Nairz *et al.* obtained a similar interference pattern on screen, as that if the  $C_{60}$  is a de Bloglie matter wave.

Another kind of single photon interference experiment can be found in Ref. [15].

Comments of this textbook:



Figure 1.8. The accumulating electron's buildup of an interference over time in double slit experiment. The number of electrons are just 10. These 10 electrons are distribute on the screen randomly. The diagram corresponding to 70 000 single electrons gives a very clear interference pattern like Fig. 1.7.

We have to point out that if we carry out the single and double slit experiments for single massless photon or single massy particle, instead of a beam with both many photons or many massy particles (electron,  $C_{60}$ , and so on), then at short time the blackening on the screen looks like a random distribution. This phenomenon can only be explained by the composition character of free wavepacket, proved by theorem VI, and law of wavepacket in chapter 3.

#### **1.7.** Establishment of Quantum Mechanics

In 1925 - 1926 two equivalent theoretical formulations: Heisenberg matrix mechanics and Schrödinger wave mechanics were proposed.

Heisenberg (1925), Born (1925), and Jordan (1925) proposed matrix mechanics. In Heisenberg matrix mechanics, any observable physical quantity is assigned by a matrix. Its calculation rule is different from classical physical quantity, e. g., it obeys the canonical communication relation other than the classical Poison bracket.

Based on the enlighten of de Bloglie matter wave idea, Schrödinger (1926) found a wave equation of quantum object. Similarly to the matrix mechanics, many significant problems and difficulties, such as the spectrum of hydrogen atom, were solved by Schrödinger wave equation well. Schrödinger also demonstrated the equivalence of Schrödinger wave mechanics and Heisenbeg matrix mechanics.

In one word, the quantum mechanics was born under the bases of both the discoveries of many difficulties in classical physics and the earlier phenomenological and empirical explorations for these discoveries.

Comments of this textbook:

(1) Although quantum mechanics got extremely brilliant successes in so wide and multitudinous fields, the until now quantum mechanics is still not a truth. We should remember the Feynman's following warn: "We should always keep in mind the possibility that quantum mechanics may fail, since it has certain difficulties with philosophical prejudices that we have about measurement and observation."

(2) Wavepacket-only theory proposed in chapter 3 has proved exactly that:

(a) What does the wave-particle duality mean;

(b) Prove exactly Schrödinger equation;

(c) Why does the wavefunction represents probability amplitude of an object;

(d) Heisenberg uncertainty relations (See next section) are characteristics of one kind of mathematical functions, which  $\in \mathcal{M}(\mathbb{R})$  (Refer to section 2.3 of chapter 2);

(e) Quantum mechanics can be free from all the so-called difficulties, which are thought by some references that the quantum mechanics has to be faced. For example, the quantum measurement and environment influences;

(f) Based just on the theorem of commutation relation in chapter 3, section 5.8 of chapter 5 proves exactly all the three formulations of quantum mechanics: Schrödinger wave mechanics; Heisenberg matrix mechanics; Feynman path integral mechanics.

#### 1.8. Heisenberg Uncertainty Relation

Heisenberg uncertainty relation, put forth in 1927, implies the following:

(1) Experiment cannot simultaneous determine for a particle the exact value of a component of momentum, say  $p_x$ , and also the exact value of the corresponding coordinate x;

(2) Our precision of measurement is inherently limited by the measurement process itself such that

$$\Delta x \Delta p_x \ge \frac{\hbar}{2},\tag{1.25}$$

where the momentum  $p_x$  is known with an uncertainty  $\Delta p_x$  and x at the same time with an uncertainty  $\Delta x$ . Similarly

$$\Delta y \Delta p_y \ge \frac{\hbar}{2}.\tag{1.26}$$

$$\Delta z \Delta p_z \ge \frac{\hbar}{2}.\tag{1.27}$$

(3) Heisenberg feels that there is likewise a minimum for the product of uncertainties of the energy and time

$$\Delta E \Delta t \ge \frac{\hbar}{2}.\tag{1.28}$$

(4) Heisenberg uncertainty relation is not a statement about the inaccuracy of measurement instrument, nor a reflection on the quality of experimental methods. Even with perfect instruments and techniques, the uncertainties are inherent in the nature of things.

Next, we would like to tell you the story about the history of Heisenberg uncertainty relations and the present status [16].

Heisenberg formulated the uncertainty principle at Niels Bohr's institute in Copenhagen, while working on the mathematical foundations of quantum mechanics in 1925, when Heisenberg developed matrix mechanics, which replaced the ad-hoc old quantum theory with modern quantum mechanics. The central assumption was that the classical concept of motion does not fit at the quantum level, and that electrons in an atom do not travel on sharply defined orbits. Rather, the motion is smeared out in a strange way: the Fourier transform of time only involve those frequencies that could be seen in quantum jumps. Heisenberg's paper did not admit any unobservable quantities like the exact position of the electron in an orbit at any time; he only allowed the theorist to talk about the Fourier components of the motion. Since the Fourier components were not defined at the classical frequencies, they could not be used to construct an exact trajectory, so that the formalism could not answer certain overly precise questions about where the electron was or how fast it was going.

In March 1926, working in Bohr's institute, Heisenberg realized that the noncommutativity implies the uncertainty principle. This implication provided a clear physical interpretation for the non-commutativity, and it laid the foundation for what became known as the Copenhagen interpretation of quantum mechanics. Heisenberg showed that the commutation relation implies an uncertainty, or in Bohr's language a complementarity. Any two variables that do not commute cannot be measured simultaneouslythe more precisely one is known, the less precisely the other can be known. Heisenberg wrote:

"It can be expressed in its simplest form as follows: One can never know with perfect accuracy both of those two important factors which determine the movement of one of the smallest particleslits position and its velocity. It is impossible to determine accurately both the position and the speed of a particle at the same instant."

In his celebrated 1927 paper, "On the Perceptual Content of Quantum Theoretical Kinematics and Mechanics", Heisenberg established this expression as the minimum amount of unavoidable momentum disturbance caused by any position measurement, but he did not give a precise definition for the uncertainties  $\Delta x$  and  $\Delta p$ . Instead, he gave some plausible estimates in each case separately. In his Chicago lecture in 1930 he refined his principle:

$$\Delta x \ \Delta p \gtrsim h, \tag{A}$$

Kennard in 1927 first proved the modern inequality:

$$\sigma x \ \sigma p \gtrsim \hbar,$$
 (B)

where  $\hbar = h/2\pi$ , and  $\sigma x$ ,  $\sigma p$  are the standard deviations of position and momentum. Heisenberg himself only proved relation (B) for the special case of Gaussian states in 1930.

On the terminology and translation on the uncertainty relation. Throughout the main body of original 1927 paper, written in German, Heisenberg used the word "Unbestimmtheit" ("indeterminacy") to describe the basic theoretical principle. Only in the endnote did he switch to the word "Unsicherheit" ("uncertainty"). However, when the Englishlanguage version of Heisenberg's textbook, The Physical Principles of the Quantum Theory, was published in 1930, the translation "uncertainty" was used, and it became the more commonly used term in the English language thereafter.

The uncertainty principle is quite counter-intuitive, so the early students of quantum theory had to be reassured that naive measurements to violate it were bound to be always unworkable. One way in which Heisenberg originally illustrated the intrinsic impossibility



Figure 1.9. Heisenberg's gamma-ray microscope for locating an electron. The incoming gamma ray is scattered by the electron up into the microscope's aperture angle  $\theta$ . The scattered gamma-ray is shown in red. Classical optics shows that the electron position can be resolved only up to an uncertainty  $\Delta x$  that depends on  $\theta$  and the wavelength  $\lambda$  of the incoming light.

of violating the uncertainty principle is by using an imaginary microscope as a measuring device. See Fig. 1.9.

Heisenberg imagines an experimenter trying to measure the position and momentum of an electron by shooting a photon at it.

Problem-I: If the photon has a short wavelength, and therefore a large momentum, the position can be measured accurately. But the photon scatters in a random direction, transferring a large and uncertain amount of momentum to the electron. If the photon has a long wavelength and low momentum, the collision does not disturb the electron's momentum very much, but the scattering will reveal its position only vaguely.

Problem II: If a large aperture is used for the microscope, the electron's location can be well resolved (see Rayleigh criterion); but by the principle of conservation of momentum, the transverse momentum of the incoming photon and hence the new momentum of the electron resolves poorly. If a small aperture is used, the accuracy of both resolutions is the other way around. The combination of these trade-offs imply that no matter what photon wavelength and aperture size are used, the product of the uncertainty in measured position and measured momentum is greater than or equal to a lower limit, which is (up to a small numerical factor) equal to Planck's constant. Heisenberg did not care to formulate the uncertainty principle as an exact limit (which is elaborated below), and preferred to use it instead as a heuristic quantitative statement, correct up to small numerical factors, which makes the radically new noncommutativity of quantum mechanics inevitable.

There are some critical reactions for the Heisenberg uncertainty relations.

The Copenhagen interpretation of quantum mechanics and Heisenberg's uncertainty principle were in fact seen as twin targets by detractors who believed in an underlying determinism and realism. According to the Copenhagen interpretation of quantum mechanics, there is no fundamental reality that the quantum state describes, just a prescription for calculating experimental results. There is no way to say what the state of a system fundamentally is, only what the result of observations might be.

Albert Einstein believed that randomness is a reflection of our ignorance of some fundamental property of reality, while Niels Bohr believed that the probability distributions are fundamental and irreducible, and depend on which measurements we choose to perform. Einstein and Bohr debated the uncertainty principle for many years.

The first of Einstein's thought experiments challenging the uncertainty principle went as follows:

Einstein slit. Consider a particle passing through a slit of width d. The slit introduces an uncertainty in momentum of approximately h/d because the particle passes through the wall. But let us determine the momentum of the particle by measuring the recoil of the wall. In doing so, we find the momentum of the particle to arbitrary accuracy by conservation of momentum. Bohr's response was that the wall is quantum mechanical as well, and that to measure the recoil to accuracy the momentum of the wall must be known to this accuracy before the particle passes through. This introduces an uncertainty in the position of the wall and therefore the position of the slit equal to , and if the wall's momentum is known precisely enough to measure the recoil, the slit's position is uncertain enough to disallow a position measurement.

Einstein's box. Bohr was present when Einstein proposed the thought experiment which has become known as Einstein's box. Einstein argued that "Heisenberg's uncertainty equation implied that the uncertainty in time was related to the uncertainty in energy, the product of the two being related to Planck's constant." Consider, Einstein said, an ideal box, lined with mirrors so that it can contain light indefinitely. The box could be weighed before a clockwork mechanism opened an ideal shutter at a chosen instant to allow one single photon to escape. "We now know, explained Einstein, precisely the time at which the photon left the box." "Now, weigh the box again. The change of mass tells the energy of the emitted light. In this manner, said Einstein, one could measure the energy emitted and the time it was released with any desired precision, in contradiction to the uncertainty principle."

Bohr spent a sleepless night considering this argument, and eventually realized that it was flawed. He pointed out that if the box were to be weighed, say by a spring and a pointer on a scale, "since the box must move vertically with a change in its weight, there will be uncertainty in its vertical velocity and therefore an uncertainty in its height above the table... Furthermore, the uncertainty about the elevation above the earth's surface will result in an uncertainty in the rate of the clock," because of Einstein's own theory of gravity's effect on time. "Through this chain of uncertainties, Bohr showed that Einstein's light box experiment could not simultaneously measure exactly both the energy of the photon and the time of its escape." [17]

In 1934 Popper published Zur Kritik der Ungenauigkeitsrelationen (Critique of the Uncertainty Relations) in Naturwissenschaften, and in the same year Logik der Forschung (translated and updated by the author as The Logic of Scientific Discovery in 1959), outlining his arguments for the statistical interpretation. In 1982, he further developed his theory in Quantum theory and the schism in Physics, writing:

"Heisenberg's formulae are, beyond all doubt, derivable statistical formulae of the quantum theory. But they have been habitually misinterpreted by those quantum theorists who said that these formulae can be interpreted as determining some upper limit to the precision of our measurements."

Popper proposed an experiment to falsify the uncertainty relations, though he later with-

drew his initial version after discussions with Weizsocker, Heisenberg, and Einstein; this experiment may have influenced the formulation of the EPR thought experiment.

The Many-worlds interpretation for the uncertainty relations. The many-worlds interpretation originally outlined by Hugh Everett in 1957 is partly meant to reconcile the differences between the Einstein and Bohr's views by replacing Bohr's wave function collapse with an ensemble of deterministic and independent universes whose distribution is governed by wave functions. The uncertainty relations in the many-worlds interpretation follows from each observer within any universe having no knowledge of what goes on in the other universes.

The free will interpretation for the uncertainty relations, i. e., two-stage model of free will. Some scientists including Arthur Compton and Martin Heisenberg [18] have suggested that the uncertainty principle, or at least the general probabilistic nature of quantum mechanics, could be evidence for the two-stage model of free will. The standard view, however, is that apart from the basic role of quantum mechanics as a foundation for chemistry, nontrivial biological mechanisms requiring quantum mechanics are unlikely due to the rapid decoherence time of quantum systems at room temperature. [19]

Comments of this textbook:

(1) The theorem of uncertainty relations in Chapter 3 proves exactly that Heisenberg uncertainty relations are the inherent property of mathematical functions  $\in \mathcal{M}(\mathbb{R})$ , which expresses a space of functions of moderate decrease on Euclidean space (Refer to section 2.3 of chapter 2).

(2) Many references call Heisenberg uncertainty relations Heisenberg uncertainty principle. Considering that the Heisenberg uncertainty relations can be proved exactly by theorem V in chapter 3, we suggest that people abandon the term "Heisenberg uncertainty principle", and use "Theorem of uncertainty relations".

In the above, we give only an initial discussions on the uncertainty relations. After reading chapter 3 I suggest that the readers make an exercise to discuss all the above viewpoints. (The solutions are that all the above viewpoints on Heisenbeg uncertainty relations are not necessary.)

#### **1.9.** Statistical Interpretation of Quantum Mechanics

The statistical (or, ensemble) interpretation of quantum mechanics is about the interpretation of wavefunction. The solution of Schrödinger equation is called wavefunction, and is often expressed by  $\Psi(r,t)$  or  $\psi(r,t)$ . Born suggested in 1927 that, when referred to the propagation of particles,  $|\Psi|^2$  is more appropriately termed a probability density wave quantitatively. The Born's probability density wave postulate states as follows (for example, in Cartesian coordinate space). The wavefunction for a massy particle  $\Psi(x, y, z, t)$  is such that

$$|\Psi(x, y, z, t)|^2 dx dy dz = P dx dy dz, \qquad (1.29)$$

where Pdxdydz is the probability that measurement of the particle's position at time t finds it in the volume element dxdydz about the point x, y, z. According to the Born's
probability density interpretation, Born thought that a wavefunction connects with a statistical ensemble. Now a number of authors support the idea of the above Born's viewpoint [21]. Along this line, Ref. [22] proposed a little different viewpoint. Under the title "What is the meaning of the wavefunction?" and after remarking that "Since the discovery of quantum theory, a very fundamental question has haunted physicists: what is the physical meaning of the wavefunction", Ref. [22] explains how it is possible to extend the usual interpretation of the wavefunction (with a physical meaning by ensemble averages of a large number of identical systems) to an individual or single system. This is done by considering a measurement that lasts a long time, a "protective measurement", during which the wavefunction is prevented form changing appreciably by means of another interaction which is undergoes at the same time [21, 22].

Comments of this textbook:

(1) The statistical interpretation for the wavefunction brings a series of difficulties, such as Einstein even has remarked that quantum mechanics is incapable of describing the behavior of a single system, such as an electron [20].

(2) Although the wavepacket-only theory in chapter 3 will also prove that the probability density is represents by  $|\Psi(x, y, z, t)|^2$ , but the wavefunction belongs to individual particle instead of statistical ensemble. The wavepacket-only theory establishes the probability interpretation in terms of the spontaneous equiprobability symmetry breaking, stated by the law of wavepacket motion.

(3) It is easy to see that that any wavefunction has to connect with an ensemble is without confidence. Because the wavefunction is a solution of a single particle Schrödinger equation, and thus that the wavefunctiin should connect with an ensemble is an "absurd" argument and "strange tale". The idea from statistical interpretation to individual interpretation in Ref. [22] is also nearly without confidence. Hope the readers give detail comments for them after learning chapter 3.

## **1.10.** Exercises and Solutions

(1) Wikipedia gives a very nice summary of the various interpretations for the quantum mechanics [23]). The author of this textbook would like to suggest that after reading the chapter 3 of this textbook make an exercise to discuss all the viewpoints listed in the table of Ref. [23].

## Chapter 2

# **Classical Mechanics and Mathematics**

## 2.1. Introduction

Classical mechanics have three formulations: Newtonian formulation, subsequent Lagrangian formulation and Hamiltonian formulation. In this chapter we will introduce Lagrangian and Hamiltonian formulations of classical mechanism starting from Newtonian formulation. These subsequent reformulations of Newtonian mechanics bring with them a great deal of elegant and computational ease. But our principal interest in reformulations of Newtonian mechanics stems from the importance that they are the ideal springboard from classical to quantum mechanics.

Classical mechanics describes any object by using a function of coordinates and momenta at the same time. However, according to a theorem in chapter 3, any object cannot be described by using both coordinates and momenta at the same time, and can only be described by using either coordinates or momenta. Therefore, any object connects with a function in position space or momentum space. Considering this function, describing an object, should be local, an object can called a wavepacket. Thus, the term "wavepacket" is not a patent of quantum mechanics. In the language using in this textbook,

```
(small or large) object \equiv (small or large) massy or massless particle \equiv
wavepacket;
wavepacket can connect with a mathematical function of spacetime, which
is called wavepacket-function;
wavepacket \equiv wavepacket-function \neq wavefunction;
For convenience of statement,
wavepacket \equiv wavepacket-functioin.
```

We call the theory, which connects any object with a wavepacket wavepacket-only theory. Wavepacket-only theory does not need to know the structure and form of any objects, and, correspondingly, the concretely mathematical form of the wavepacket-functions. The wavepacket-function can represent in principle the distribution of object's mass or charge or energy and so on. The wavepacket-only theory just explores the common and general characteristics of this mathematical function connecting with a wavepacket.

The wavepackets in our exploration can be large or small, and can be heavy or light or even massless. For example, the objects (=wavepackets) can have the following sizes given in Ref. [24].

The lengths *L* of wavepackets (i. e., objects)  $(10^L \text{ cm})$  are:  $\infty$  of radius of the infinite unverse, 28 of radius of the visible unverse, 23 of radius of the Milky Way, 18 of length of light year, 15 of radius of the solar system, 11 of radius of the sun, 9 of radius of the earth, 5 of wavelength of the radio waves,  $3 \rightarrow -1$  of wavelength of sound, 3.75cm of wavelength of the cosmic background radiation, -3 of wavelength of heat radiation,  $4 \times 10^{-7} \rightarrow 8 \times 10^{-7}$  of wavelength of visible light, -7 of radius of molecules, -8 of radius of atoms, -8 of wavelength of X rays, -10 of Compton wavelength of the electron, -13 of radius of protons, -13 of wavelength of cosmic rays, -13 of Compton wavelength of the proton, < -18 of radius of quarks and electrons, -33 of Planck scale, string, quantum graviton, and more less of others [24].

For example, the objects can have the following energy scales given in Ref. [24].

The energy scales *E* of wavepackets (i. e., objects)  $(10^E \text{ GeV}, 1\text{GeV}=1.6 \times 10^{-24} \text{ g})$  are: -8 of binding energy of the electron in the hydrogen atom; energy of chemical processes, -3 of rest energy of the electron, 1 GeV of rest energy of the proton, 2 of rest energy of the vector bosons  $W^+$ ,  $W^-$ ,  $Z^0$ , 3 of weak and electromagnetic interaction decouple at this particle energy, 3 of particle energy at the new CERN accelerator in 2008, 14 of energy consumption of a human being per day, 15 of strong and electroweak energy decouple at this particle energy, 19 of Planck energy, 27 of rest energy of a stone (mass of 1 Kg), 29 of energy production of a hydrogen bomb, 36 of energy production of the sun per day, 52 of rest energy of the earth, 57 of rest energy of the sun, 68 of rest energy of the Milky Way, 79 of rest energy of the visible unverse,  $\infty$  of rest energy of the infinite unverse.

The wavepacket-only theory have many theorems, which will be proved in chapters 3, 4, 5, 9, and 10. These theorems indicate the importance of reformulations of Newtonian mechanics. Next, we list some important points:

(1) The passage from Lagrangian formulation of classical mechanics to Feynman path integral formulation of quantum mechanics is easy;

(2) The passage from Hamiltonian formulation of classical mechanics to Heisenberg matrix mechanics formulation of quantum mechanics is easy;

(3) The passage from Hamiltonian formulation of classical mechanics to Schrödinger wave mechanics formulation of quantum mechanics is easy;

(4) The passages from classical theory, including classical particle theory and classical field theory, to quantum theory, including quantum mechanics and quantum field theory, are based on the same basis.

In terms of classical mechanics and mathematics, introduced just in this chapter, the wavepacket-only theory can make in subsequent chapters that:

(1) The quantum mechanics becomes theories without any assumptions, any hypotheses, any postulates, any axioms, any guesses, any principles, any ambiguous and vague concepts, any paradoxes, and any physical pictures hard to be understood, except one law; (2) The quantum mechanics becomes theory from theorems to theorems, i. e., any things in quantum mechanics can be proved, except one law.

The classical theory includes classical (particle) mechanics, and classical field theory. The quantum theory includes quantum (particle) mechanics, and quantum field theory.

It can be proved that the watershed between classical theory and quantum theory is merely in that: if any object connects with a function of both coordinates and momenta at the same time, then this theory belongs to classical theory; if any object connects with a function of either coordinates or momenta, then this theory belongs to quantum theory. The readers might have heard some conclusions and pictures in quantum mechanics, such as massy particles have wave property, energy quantization and so on. All of these "strange" things come from the theorems proved by the wavepacket-only theory.

From this introduction, the readers will see that the classical theory and mathematics, introduced in this chapter, are important for studying quantum theory. This is the reason why this textbook addresses at first classical analytical mechanics and necessary knowledge of mathematics. I would like to say that if you know classical analytical mechanics very well, then you know quantum mechanics very well.

## 2.2. Foundation of Classical Mechanics

#### 2.2.1. Lagrangian Formulation of Classical Mechanics

In this subsection we will introduce Lagrange function, and derive the Euler-Lagrange equation of motion to replace Newton's second law (i. e., force law).

Suppose that the Lagrange function of system is  $L(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n, t)$  or, for brevity,  $L(q, \dot{q}, t)$ ,  $q_i$   $(n = 1, 2, \dots, n)$  are independent coordinates of system in *n* dimensional configuration space, *n* is the number of degrees of freedom of system,  $\dot{q}_i$  are the generalized velocity. [The term "configuration space" is used even if the *n* coordinates are not Cartesian.  $(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n)$  together construct phase space]. Assume that system is in a conservative potential field *V*, and *T* is the kinetic energy. Define L = T - V. If *V* is explicitly dependent on time *t*, then system is not conservative. Let us study the conservative system for simplicity.

For each path, i. e., trajectory, q(t) connecting point *A* at initial time  $t' = t_i$  and point *B* at final time  $t'' = t_f$ , we define an action  $\mathcal{A}[q(t)]$  as

$$\mathcal{A}[q(t)] = \int_{t_i}^{t_f} L(q, \dot{q}) dt.$$
 (2.2.1.1)

The action can also call the Hamiltonian principal function. We use square brackets to enclose the argument of  $\mathcal{A}$  to remind us that the action  $\mathcal{A}$  depends on an entire path or function q(t), and not just the value of q an some time t. One calls  $\mathcal{A}$  a functional to signify that it is a function of function. The dimension of  $\mathcal{A}$  is angular momentum (i. e., energy×time).

The principle of least action states that: The actual path of a particle is one on which  $\mathcal{A}$  takes a minimum value. (Actually, we will only require that it is an extremum. It is, however, customary to refer to this condition as the principle of least action.)



Figure 2.1. Arbitrary trajectories q(t) going between specific initial and final points, and the extremal trajectory  $q^{ex}(t)$ . The deviation  $\delta q(t)$  is defined as  $\delta q(t)=q(t)-q^{ex}(t)$ .

We will now verify that this principle reproduces Newton's second law.

The mathematical statement of the principle of least action is as follows. Suppose q(t) make an infinitely little variation, i. e.,  $q(t) \rightarrow q(t) + \delta q(t)$ . See Fig. 2.1. Under the condition

$$\delta q(t_i) = \delta q(t_f) = 0, \qquad (2.2.1.2)$$

this principle requires that

$$\delta \mathcal{A} = 0. \tag{2.2.1.3}$$

According to Eq. (2.2.1.3) (principle of least action), one can obtain a differential equation of q(t).

$$\delta \mathcal{A} = \int_{t_i}^{t_f} dt \sum_i \left[ \frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i \right].$$
(2.2.1.4)

Noting that  $\delta \dot{q}_i = \delta dq/dt = d\delta q_i/dt$ , one makes the partial integration for the second term of the right hand side in Eq. (2.2.1.4), and obtains

$$\delta \mathcal{A} = \sum_{i} \int_{t_{i}}^{t_{f}} dt \left[ \frac{\partial L}{\partial q_{i}} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_{i}} \right] \delta q_{i} + \sum_{i} \left[ \frac{\partial L}{\partial \dot{q}_{i}} \delta q_{i} \right]_{t_{i}}^{t_{f}}.$$
 (2.2.1.5)

Substituting Eqs. (2.2.1.2) and (2.2.1.3) into Eq. (2.2.1.5) yields

$$\delta \mathcal{A} = \sum_{i} \int_{t_i}^{t_f} dt \left[ \frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \right] \delta q_i = 0.$$
 (2.2.1.6)

Due to that the  $\delta q_i$  ( $i = 1, 2, \cdot, n$ ) are arbitrary, we have

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left[ \frac{\partial L}{\partial \dot{q}_i} \right] = 0, (i = 1, 2, \cdots, n).$$
(2.2.1.7)

#### Eq. (2.2.1.7) is called Euler-Lagrange equation.

If we take  $q_i$  as Cartesian coordinate  $x_i$ , then

$$L = T - V = \frac{1}{2} \sum_{i} m_{i} \dot{x}_{i}^{2} - V(x_{1}, \cdots, x_{n}).$$
 (2.2.1.8)

Substituting Eq. (2.2.1.8) in Eq. (2.2.1.7) yields Euler-Lagrange equation

$$m_i \ddot{x}_i = -\frac{\partial V}{\partial x_i}, (i = 1, \cdots, n), \qquad (2.2.1.9)$$

i. e., Newton equation. Set

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \tag{2.2.1.10}$$

and

$$F_i = \frac{\partial L}{\partial q_i} \tag{2.2.1.11}$$

stand for the generalized (or canonical) momentum and generalized force corresponding to the generalized (or canonical) coordinate  $q_i$ , respectively. In these conditions, Lagrange equation is formally same as the Newton equation, i. e.,

$$\dot{p}_i = F_i.$$
 (2.2.1.12)

To the readers who wonders why one bothers to even deal with a Lagrangian when all it does is to yield Newtonian force law in the end. I present a few of its main attractions. In comparison with the Newtonian formulation, the Lagrangian formulation of classical mechanics (or Lagrangian mechanics) has the following four features.

First. The Lagrangian formulation is of its closeness to path integral formulation of quantum mechanics.

Euler-Lagrange equation Eq. (2.2.1.7) is a differential equation containing second order derivative of time t over D coordinate variables  $q_i$ . If we are given the initial state variables,  $q_i(0)$  and  $\dot{q}_i(0)$ , these equations can be integrated step by step, just as Newton approach, to determine the trajectory.

In the Lagrangian formulation, for example, the problem of single particle in potential V(x) is posed in a different way: given that the particle is at  $x(t_i)$  and  $x(t_f)$  at times  $t_i$  and t'', respectively, what is it that distinguishes the actual trajectory x(t) from all other trajectories or paths that connect these points  $x(t_i)$  and  $x(t_f)$ ?

The Lagrangian formulation is thus global, in that it tries to determine at one stock the entire trajectory x(t), in contrast to the local approach of Newtonian formulation, which concerns itself with that the particle is going to do in the next infinitesimal time interval.

Second. In the Lagrangian formulation of classical mechanism, one just needs to construct the L, which is a scalar quantity, and all the motion equations can be obtained just by differentiation operations over L. On the contrary, to establish Newton's force equation concerns with the vector operation, and thus is more complicate, especially, in case of curve coordinates.

Third. Although Newton equation Eq. (2.2.1.9) is simpler, but it holds only in Cartesian coordinates. On the contrary, in any coordinate Euler-Lagrange equation Eq. (2.2.1.7) is the same.

Fourth. In Lagrange form, it is easy to analyze conservative quantity. Suppose *L* does not depend on coordinate  $q_i$ , and only depends on  $\dot{q}_i$  (in this case  $q_i$  is called cyclic coordinate). According to Eqs. (2.2.1.7) and (2.2.1.10), one knows that the generalized momentum  $p_i$  is a conservative quantity ( $\dot{p}_i = 0$ ). Due to that in any coordinate system, Lagrange equation Eq. (2.2.1.7) is same, one can choose appropriate coordinate, and thus find the conservative quantity and the symmetry of potential energy.

## 2.2.2. Hamiltonian Formulation of Classical Mechanics

Why it is necessary, or even desirable to recast classical mechanics in Hamiltonian formulation? The answer is that the Hamiltonian equations have an elegant symmetry that the Lagrange equations lack. Another answer, not directly related to the classical mechanics, is that the Hamiltonian is used to write the Heisenberg equation of quantum mechanics, as discussed in section 5.8 of chapter 5.

In the Lagrangian formulation of classical mechanics, the Lagrangian is expressed as a function of canonical coordinates  $q_i$  and generalized velocities  $\dot{q}_i$  ( $i = 1, 2, \dots, n$ ). The canonical momentum is defined as:

$$p_i = \frac{\partial L}{\partial \dot{q}_i}.\tag{2.2.2.1}$$

In Hamiltonian formulation of classical mechanics, the coordinates and momenta in set q, p are lumped together and considered to be coordinates of 2n dimensional space called phase space. The variables  $q_1, \dots, q_n, p_1, \dots, p_n$  are referred to collectively as canonical coordinates of phase space. The  $q_i$  is called the *i*-th canonical coordinate, and  $p_i$  is called *i*-th canonical momentum. The pair  $q_i$ ,  $p_i$  for the same *i* value are called canonical conjugates. Hamiltonian formulation or Hamiltonian mechanics is essentially Newton's second law translated from Lagrangian form into a form appropriate for this phase space. In Hamiltonian mechanics, the  $q_i$  and  $p_i$  are coequal coordinates of phase space. This contrasts with Lagrangian mechanics, where  $p_i$  is defined by Eq. (2.2.2.1),  $p_i(q, \dot{p}, t) = \partial L(q, \dot{q}, t)/\partial \dot{q}_i$ , and therefore cannot be considered an independent variable. The transition from Lagrangian to Hamiltonian mechanics therefore requires a declaration of independence for the  $p_i$  variables. Define the Hamiltonian of system as:

$$H(q,p) = \sum_{i} p_{i} \dot{q}_{i} - L(q, \dot{q}). \qquad (2.2.2.2)$$

Notice that  $q_i, p_i$   $(i = 1, 2, \dots, n)$  are independent variables, i. e., *H* is a function of 2n independent variables. Utilizing Eqs. (2.2.2.1-2), one can obtain

$$\frac{\partial H}{\partial p_i} = \dot{q}_i + \sum_j p_j \frac{\partial \dot{q}_j}{\partial p_i} - \sum_j \frac{\partial L}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial p_i} = \dot{q}_i.$$
(2.2.2.3)

Utilizing Euler-Lagrange equation yields

$$\frac{\partial H}{\partial q_i} = \sum_j p_j \frac{\partial \dot{q}_j}{\partial q_i} - \frac{\partial L}{\partial q_i} - \sum_j \frac{\partial L}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial q_i} = -\frac{\partial L}{\partial q_i} = -\dot{p}_i.$$
(2.2.2.4)

In summary,

$$\dot{q}_i = \frac{\partial H}{\partial p_i},\tag{2.2.2.5}$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad (i = 1, 2, \cdots, n).$$
 (2.2.2.6)

Eqs. (2.2.2.5-6) are the Hamilton canonical equations. The first Hamiltonian equation Eq. (2.2.2.5) provides the same information as Eq. (2.2.2.1), so that information is not lost. But the Hamilton equations are not identities that define their left hand sides ( $\dot{q}_i$  in this case) for all values of q, p, t. They are equations of motion whose solution defines the trajectory  $q_i(t), p_i(t)$  of the mechanical system through phase space. This trajectory is often called the system path, and the Hamilton equations are said to hold only on the system path.

Next we derive the Hamilton canonical equations from the principle of least action. In this case the action is

$$\mathcal{A} = \int_{t_i}^{t_f} dt L = \int_{t_i}^{t_f} dt \left[ \sum_i p_i \dot{q}_i - H(q, p, t) \right], \qquad (2.2.2.7)$$

where  $\mathcal{A}$  is a function of 2n independent variables  $(p_i, q_i)$ . Making variations for  $p_i, q_i$  yields

$$\delta \mathcal{A} = \sum_{i} \int_{t_{i}}^{t_{f}} dt \left[ \dot{q}_{i} \delta p_{i} + p_{i} \delta \dot{q}_{i} - \frac{\partial H(q, p, t)}{\partial q_{i}} \delta q_{i} - \frac{\partial H(q, p, t)}{\partial p_{i}} \delta p_{i} \right].$$
(2.2.2.8)

After the partial integration of the second term in Eq. (2.2.2.8) the second term becomes

$$\int_{t_i}^{t_f} dt p_i \frac{d}{dt} \delta q_i = p_i \delta q_i \big|_{t_i}^{t_f} - \int_{t_i}^{t_f} dt \dot{p}_i \delta q_i = -\int_{t_i}^{t_f} dt \dot{p}_i \delta q_i.$$
(2.2.2.9)

Substituting Eq. (2.2.2.9) into Eq. (2.2.2.8) yields

$$\delta \mathcal{A} = \sum_{i} \int_{t_{i}}^{t_{f}} dt \left[ \left( \dot{q}_{i} - \frac{\partial H}{\partial p_{i}} \right) \delta p_{i} - \left( \dot{p}_{i} + \frac{\partial H(q, p, t)}{\partial q_{i}} \right) \delta q_{i} \right].$$
(2.2.2.10)

According to the principle of least action,  $\delta A = 0$ . Therefore, one obtains the Eqs. (2.2.2.5-6).

If the system is in a conservative field V (V does not depend on time t), then we can demonstrate that

$$H = T + V, \tag{2.2.2.11}$$

where T stands for kinetic energy, and H for energy. The demonstrations are as follows.

In Cartesian coordinates

$$T = \frac{1}{2} \sum_{i} m_i \dot{x}_i^2, \qquad (2.2.2.12)$$

$$p_i = \frac{\partial L}{\partial \dot{x}_i},\tag{2.2.2.13}$$

$$\sum_{i} p_i \dot{x}_i = 2T. \tag{2.2.2.14}$$

From Eqs. (2.2.2.12-14) we have

$$H = \sum_{i} p_{i} \dot{x}_{i} - L = 2T - (T - V) = T + V.$$
(2.2.2.15)

In any curve coordinates, supposing

$$T = \sum_{ij} T_{ij}(q) \dot{q}_i \dot{q}_j, \qquad (2.2.2.16)$$

one still can demonstrates that Eq. (2.2.2.14) holds, and thus the Eq. (2.2.2.11) holds as well.

Both the Lagrangian and Hamiltonian are scalar quantities. The Hamilton equations Eqs. (2.2.2.5-6) should be independent of the choice of coordinates. We can choose appropriate coordinates to give the conservative quantities and symmetries of the system. For example, in *V* (and thus *H*) is not explicitly dependent on time *t*, then from Eqs. (2.2.2.5-6) we have

$$\frac{dH}{dt} = \sum_{i} \left[ \frac{\partial H}{\partial q_{i}} \dot{q}_{i} + \frac{\partial H}{\partial p_{i}} \dot{p}_{i} \right] = \sum_{i} \left[ \frac{\partial H}{\partial q_{i}} \frac{\partial H}{\partial p_{i}} - \frac{\partial H}{\partial p_{i}} \frac{\partial H}{\partial q_{i}} \right] = 0.$$
(2.2.2.17)

Eq. (2.2.2.17) means that *H* (energy) is a conservative quantity. If *H* does not depend on some coordinate  $q_i$ , then  $\dot{p}_i = 0$ , i. e.,  $p_i$  is a conservative quantity. This coordinate is called cyclic coordinate of the system.

## 2.2.3. Poison Bracket

In Hamiltonian mechanics, all physical quantities are represented by phase space function. Assume that F(q, p, t) is such a function. We write the total time derivative of F(q,p,t) in a useful form  $(q = q_1, \dots, q_d \text{ and } p = p_1, \dots, p_d)$ 

$$\dot{F} = \frac{d}{dt}F = \sum_{i=1}^{d} \left(\frac{\partial F}{\partial q_i}\dot{q}_i + \frac{\partial F}{\partial p_i}\dot{p}_i\right) + \frac{\partial F}{\partial t}$$
$$= \sum_{i=1}^{d} \left(\frac{\partial F}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i}\frac{\partial H}{\partial q_i}\right) + \frac{\partial F}{\partial t}.$$
(2.2.3.1)

The sum in Eq. (2.2.3.1) appears frequently enough to merit a special notation for it. It is called Poison bracket {F,H} of two phase space functions F(q, p, t) and H(q, p, t), so that Eq. (2.2.3.1) becomes

$$\dot{F} = \frac{d}{dt}FA = \{F, H\} + \frac{\partial F}{\partial t}.$$
(2.2.3.2)

In Eq. (2.2.3.2) the first and the second term of the right hand side represent the contributions of the explicit time relation and the motion of phase space point, respectively. Eq. (2.2.3.2) implies that a phase space function that is not an explicit function of time twill be a constant of the motion if and only if it has a vanishing Poison bracket with the Hamiltonian. The Poison bracket {A,B} can be defined more generally, for any two phase space functions A(q, p, t) and B(q, p, t),

$$\{F,G\} = \sum_{i}^{n} \left( \frac{\partial F}{\partial q_{i}} \frac{\partial G}{\partial p_{i}} - \frac{\partial F}{\partial p_{i}} \frac{\partial G}{\partial q_{i}} \right).$$
(2.2.3.3)

Note that, since partial derivatives are functions of the same variable set as was the function differentiated, the  $\{F,G\}$  is itself another phase space function.

This definition of Poison bracket implies some useful algebraic properties. First, by construction, the Poison bracket is anti-symmetric in the exchange of the two functions so that for any A and B,

$$\{F,G\} = -\{G,F\}, \text{ and hence } \{F,F\} = 0.$$
 (2.2.3.4*a*)

Also, when F = F(q, p, t), G = G(q, p, t), and C = C(q, p, t) are phase space functions, and  $\alpha$ ,  $\beta$  are numbers or otherwise not functions of q, p, then the following Jacobi identities can be proved,

$$\{F, (\alpha G + \beta C)\} = \alpha \{F, G\} + \beta \{F, C\}.$$
 (2.2.3.4*b*)

$$\{F, GC\} = \{F, G\}C + G\{F, C\}.$$
 (2.2.3.4c)

$$\{F, \{G, C\}\} + \{G, \{C, F\}\} + \{C, \{F, G\}\} = 0.$$
(2.2.3.4*d*)

Here, for example,  $\{F, \{G, C\}\}$  denotes the Poison bracket of function F with the function  $\{G, C\}$  which was obtained by taking the Poison bracket of G and C.

The following identities follow directly from the definition in Eq. (2.2.3.3). If one puts F(q, p, t) and G(q, p, t) equal to any single canonical coordinate or canonical momentum, then, for any choices  $i, j = 1, \dots, n$ , it follows that

$$\{q_i, p_j\} = \delta_{ij}, \{q_i, q_j\} = \{p_i, p_j\} = 0, \qquad (2.2.3.5)$$

where  $\delta_{i,j}$  is called the Kroeneker delta function or Kroeneker notation. Eq. (2.2.3.5) is called fundamental Poison bracket, and are analogous to similar canonical commutation relations in quantum mechanics. In classical mechanics, from Poison bracket one can derive all the dynamical properties of a system. Similarly, in quantum mechanics, from commutation relation one can derive all the dynamical properties of a system as well.

It is easy to show that:

$$\{q_i, F\} = \frac{\partial F}{\partial p_i}, \quad \{p_i, F\} = -\frac{\partial F}{\partial q_i}.$$
 (2.2.3.6)

Utilizing Poisson bracket, the Hamilton canonical equations can be expressed by Poison bracket form. Replacing A(q, p, t) in Eq. (2.2.3.1) by the single variables  $q_i$ ,  $p_i$ , H in succession

$$\dot{q}_i = \{q_i, H\},$$
 (2.2.3.7)

$$\dot{p}_i = \{p_i, H\},$$
 (2.2.3.8)

and

$$\dot{H} = \{H, H\} + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}.$$
(2.2.3.9)

**Poisson Theorem.** If *F* and *G* are the conservative quantities of system, then  $\{F, G\}$  is a conservative quantity as well.

**Proof 1.** Suppose that *F* and *G* does not contain explicitly time *t*. Utilizing Eq. (2.2.3.4d),  $\{F,H\} = 0$ , and  $\{G,H\} = 0$ , one can obtain

$$\{H, \{F, G\}\} = 0, \tag{2.2.3.10}$$

which means that  $\{F, G\}$  is a conservative quantity.

**Proof 2.** If F and G are time-dependent, and conservative, i. e.,

$$\frac{\partial F}{\partial t} + \{F, H\} = 0 \tag{2.2.3.11}$$

and

$$\frac{\partial G}{\partial t} + \{G, H\} = 0. \tag{2.2.3.12}$$

Considering

$$\frac{d}{dt}\{F,G\} = \{\{F,G\},H\} + \frac{\partial}{\partial t}\{F,G\}$$

$$= -\{\{G,H\},F\} - \{\{H,F\},G\} + \left\{\frac{\partial F}{\partial t},G\right\} + \left\{F,\frac{\partial G}{\partial t}\right\}$$

$$= \left\{\frac{\partial F}{\partial t} + \{F,H\},G\right\} + \left\{F,\frac{\partial G}{\partial t} + \{G,H\}\right\}.$$
(2.2.3.13)

According to the assumptions in the theorem, the two terms at the right hand side are zero. Therefore,

$$\frac{d}{dt}\{F,G\} = 0. \tag{2.2.3.14}$$

### 2.2.4. Canonical Transformations

In Hamiltonian formulation of classical mechanics, the freeing of canonical momentum  $p_i$  from the Eq. (2.2.2.1) allows it to be treated as an independent variable on the same footing as the  $q_i$ . This equal status for all the variables of phase space is exploited in the definition of canonical transformations.

As we have mentioned, the form of Lagrange equations is not changed when new generalized coordinates are defined as invertible function of the old coordinates and possibly the time. But Hamiltonian formulation allows a much more richer transformation scheme, called canonical transformations, in which the new coordinates and momenta can depend on both the old coordinates and the old momenta.

What we call extended canonical transformations can be found in special theory of relativity. They permit time to be transformable coordinate and hence allow the Lorentz transformation of special relativity to be canonical. The extended canonical transformation is based on the extended Lagrangian and Hamiltonian theory which treat time as a coordinate rather than as the fixed parameter of nineteenth century physics. This book will not address this extended canonical transformation (Refer to Ref. [25]).

Let us at first introduce the so called point transformation. We have known that Euler-Lagrange equation does not depend on the choice of coordinates, i. e., under the coordinate transformation

$$q_i \to Q_i(q_1, q_2, \cdots, q_n), \quad (i = 1, 2, \cdots, n)$$
 (2.2.4.1)

the Lagrange equation still is in form

$$\frac{\partial L}{\partial Q_i} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{Q}_i} \right) = 0, \quad (i = 1, 2, \cdots, n).$$
(2.2.4.2)

Actually, the *L* in Eq. (2.2.4.2) is  $L(Q, \dot{Q})$ , which's form is different from  $L(q, \dot{q})$ . For brevity, we write  $L(q, \dot{q}) = L(Q, \dot{Q})$ . Under the coordinate transformation in Eq. (2.2.4.1), one can show that

$$p_i \to P_i = \sum_j \frac{\partial q_j}{\partial Q_i} p_j.$$
 (2.2.4.3)

The Eqs. (2.2.4.1) and (2.2.4.3) are called point transformation.

The invariance of the form of Lagrange equations under the point transformation implies that the form of Hamilton equations does not change as well, i. e.,

$$\dot{Q}_i = \frac{\partial H}{\partial P_i} \tag{2.2.4.4a}$$

$$\dot{P}_i = -\frac{\partial H}{\partial Q_i}.$$
(2.2.4.4b)

The point transformation is in *n* dimensional space.

Next, we present a brief introduction to what we call traditional canonical transformations in 2D dimensional phase space [25]. Here, "traditional" means that we do not allow the time to transform. In Hamiltonian mechanics the system is in 2n dimensional phase space. We allow the following more general transformation in 2n dimensional phase space, i. e.,

$$q \to q(Q, P), \quad p \to p(Q, P).$$
 (2.2.4.5)

Of course, arbitrary new 2n variables  $(Q_i, P_i)$   $(i = 1, 2, \cdot, n)$  cannot ensure that the Hamilton canonical equations in Eq. (2.2.4.4) do not change. (For example, Newton equation  $m q = -\partial L/\partial t$  holds only for Cartesian coordinates) If a transformation Eq. (2.2.4.4) can ensure the invariance of the canonical form of Hamilton equations, then this transformation is called canonical transformation.

For a given transformations in Eq. (2.2.4.5), how to judge that whether it is a canonical transformations?

#### Theorem. If

 $\{Q_i, Q_k\} = \{P_i, P_k\} = 0$ 

and

$$\{Q_i, P_k\} = \delta_{ik}, \tag{2.2.4.6}$$

then Eq. (2.2.4.5) is a canonical transformation.

#### Proof. Calculate

$$\dot{Q}_{j} = \sum_{i} \left( \frac{\partial Q_{j}}{\partial q_{i}} \dot{q}_{i} + \frac{\partial Q_{j}}{\partial p_{i}} \dot{p}_{i} \right) = \sum_{i} \left( \frac{\partial Q_{j}}{\partial q_{i}} \frac{\partial H}{\partial p_{i}} - \frac{\partial Q_{j}}{\partial p_{i}} \frac{\partial H}{\partial q_{i}} \right).$$
(2.2.4.7)

Making  $H(q, p) \rightarrow H(Q, P) = H(q, p)$ , we have

$$\frac{\partial H(q,p)}{\partial p_i} = \frac{\partial H(Q,P)}{\partial p_i} = \sum_k \left( \frac{\partial H}{\partial Q_k} \frac{\partial Q_k}{\partial p_i} + \frac{\partial H}{\partial P_k} \frac{\partial P_k}{\partial p_i} \right)$$

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$$\frac{\partial H(q,p)}{\partial q_i} = \frac{\partial H(Q,P)}{\partial q_i} = \sum_k \left( \frac{\partial H}{\partial Q_k} \frac{\partial Q_k}{\partial q_i} + \frac{\partial H}{\partial P_k} \frac{\partial P_k}{\partial q_i} \right).$$
(2.2.4.8)

Substituting Eq. (2.2.4.8) into Eq. (2.2.4.7) yields

$$\dot{Q}_j = \sum_k \left\{ \frac{\partial H}{\partial Q_k} \{ Q_j, Q_k \} + \frac{\partial H}{\partial P_k} \{ Q_j, P_k \} \right\}.$$
(2.2.4.9*a*)

Similarly,

$$\dot{P}_{j} = \sum_{k} \left\{ \frac{\partial H}{\partial Q_{k}} \{P_{j}, Q_{k}\} + \frac{\partial H}{\partial P_{k}} \{P_{j}, P_{k}\} \right\}.$$
(2.2.4.9b)

Using the known conditions, one can conclude the proof. QED.

Note that: Here we do not consider special theory of relativity; If the canonical transformations in Eq. (2.2.4.5) do explicitly depend on time, then the Hamiltonian considered here will be different in the q, p and Q, P systems (For detail, refer to Ref. [25]).

**Jacobi Theorem.** The form of Poisson bracket does not change under the canonical transformation. (Refer to Ref. [1, 25] for the proof of this theorem.)

#### 2.2.5. Jacobi-Hamilton Equation

In subsection 2.2.2 we introduced the principle of least action. The basic idea of this principle is as follows. We have many particle's possible paths, which's initial position  $x(t_i)$  and final position  $x(t_f)$  are given. We make comparisons between the many paths, and choose the path, which has minimum action ( $\delta \mathcal{A} = 0$ . Actually, extreme value of the action is enough.) as the actual path of the particle, and from  $\delta \mathcal{A} = 0$  the Euler-Lagrange equations are derived.

Now, we take a different method to derive the motion equation of particle. Suppose that the q(t) in  $\mathcal{A}$  is just the path determined by the Lagrange equations. Assume that at initial state time  $t_i$  the position of particle is definite [ $\delta q(t_i) = 0$ ], but at final state time t the position of particle is allowed to vary. Thus, the  $\mathcal{A}$  is a function of upper limit q(t) of integration. Then we make variation of q(t) over  $\mathcal{A}[q(t), t]$ , and compare each with others.

$$\delta \mathcal{A} = \delta \int_{t_i}^t L dt = \sum_i \frac{\partial L}{\partial \dot{q}_i} \delta q_i \Big|_{t_i}^t + \sum_i \int_{t_i}^t dt \left[ \frac{\partial L}{\partial q_i} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) \right] \delta q_i$$
$$= \sum_i \frac{\partial L}{\partial \dot{q}_i} \delta q_i(t) = \sum_i p_i \delta q_i. \tag{2.2.5.1}$$

Due to that we look upon  $\mathcal{A}$  as a function of q(t), from Eq. (2.2.5.1) one obtains

$$p_i = \frac{\partial \mathcal{A}}{\partial q_i} \tag{2.2.5.2}$$

and

$$\mathcal{A} = \int_{t_i}^t Ldt, \quad \frac{dS}{dt} = L. \tag{2.2.5.3}$$

From Eq. (2.2.5.3) we have

$$L = \frac{d\mathcal{A}[q(t),t]}{dt} = \sum_{i} \frac{\partial\mathcal{A}}{\partial q_{i}} \dot{q}_{i} + \frac{\partial\mathcal{A}}{\partial t} = \sum_{i} p_{i} \dot{q}_{i} + \frac{\partial\mathcal{A}}{\partial t}.$$
 (2.2.5.4)

Therefore,

$$\frac{\partial \mathcal{A}}{\partial t} = L - \sum_{i} p_i \dot{q}_i = -H(q, p, t).$$
(2.2.5.5)

In Eq. (2.2.5.5)  $p_i = \partial \mathcal{A} / \partial q_i$ , i. e.,

$$\frac{\partial \mathcal{A}}{\partial t} + H\left(q, \frac{\partial \mathcal{A}}{\partial q}, t\right) = 0.$$
(2.2.5.6)

In detail,

$$\frac{\partial \mathcal{A}}{\partial t} + H\left(q_1, \cdots, n, \frac{\partial \mathcal{A}}{\partial q_1}, \cdots, \frac{\partial \mathcal{A}}{\partial q_n}, t\right) = 0.$$
(2.2.5.7)

Eq. (2.2.5.7) is called Jacobi-Hamilton equation. It is a first order partial differential equation satisfied by the action S as action of coordinates  $q_i(t)$  and t. The independent variables are  $q_1, \dots, q_n, t$ . It contains (n + 1) integration constants. Due to that Eq. (2.2.5.7) just contains the first order derivatives of S, one integration constant appears in a sum with other integration constants. Another n integration constants are expressed as  $\alpha_1, \dots, \alpha_n$ .

If *H* does not explicitly contain time t, then Eq. (2.2.5.7) can be made by separation of variables as follows.

$$\mathcal{A}[q(t),t] = \mathcal{A}_{\circ}[q(t)] + f(t).$$
 (2.2.5.8)

Substituting Eq. (2.2.5.8) into Eq. (2.2.5.7) yields

$$H\left[q(t), \frac{\partial \mathcal{A}_{\circ}}{\partial q(t)}\right] + \dot{f}(t) = 0.$$
(2.2.5.9)

Eq. (2.2.5.9) can be rewritten as

$$H\left[q(t), \frac{\partial S_{\circ}}{\partial q(t)}\right] = -\dot{f}(t) \equiv E, \qquad (2.2.5.9)$$

where E is the Hamiltonian which does not explicitly contain time t. However, the q in the Hamiltonian can depend on time t, and thus E still can be depend on time t. From Eq. (2.2.5.9) we have

$$-\dot{f}(t) = E.$$
 (2.2.5.10)

From Eq. (2.2.5.10) we have

$$f(t) = -Et (2.2.5.11)$$

Substituting Eq. (2.2.5.11) into Eq. (2.2.5.8) yields

$$\mathcal{A}[q(t),t] = \mathcal{A}_{\circ}[q(t)] - Et.$$
 (2.2.5.12)

Eq. (2.2.5.9) can be rewritten as

$$H\left[q(t), \frac{\partial \mathcal{A}_{\circ}}{\partial q(t)}\right] = E, \qquad (2.2.5.13)$$

Thus, we have found an integration constant  $E = \alpha_1$ .

To illustrate Jacobi-Hamilton equation we give two examples.

Example 1: Discuss the motion of a particle in potential V[x(t), y(t), z(t)].

Solution: Eq. (2.2.5.12) gives that the action is

$$\mathcal{A}[x(t), y(t), z(t), t] = \mathcal{A}_{\circ}[x(t), y(t), z(t)] - Et.$$
(2.2.5.14)

Substituting Eq. (2.2.5.14) into Eq. (2.2.5.7) yields

$$-E + H\left[q(t), \frac{\partial \mathcal{A}_{\circ}}{\partial q(t)}\right] = 0.$$
(2.2.5.15)

$$H\left[q(t), \frac{\partial \mathcal{A}_{\circ}}{\partial q(t)}\right] = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + V(x, y, z).$$
(2.2.5.16)

Substituting Eq. (2.2.5.2) into Eq. (2.2.5.16) and then Eq. (2.2.5.15) yields

$$\frac{1}{2m}\left\{\left[\frac{\partial\mathcal{A}_{\circ}}{\partial x(t)}\right]^{2} + \left[\frac{\partial\mathcal{A}_{\circ}}{\partial y(t)}\right]^{2} + \left[\frac{\partial\mathcal{A}_{\circ}}{\partial z(t)}\right]^{2}\right\} = E - V[x(t), y(t), z(t)].$$
(2.2.5.17)

Notice that we emphasize the time dependence of x, y, and z.

The momentum of the particle is from Eqs. (2.2.5.2) and (2.2.5.12)

$$p = \nabla \mathcal{A}_{\circ}. \tag{2.2.5.18}$$

Eq. (2.2.5.17) can simply be written as

$$\nabla \mathcal{A}_{\circ} \cdot \nabla \mathcal{A}_{\circ} = |\nabla \mathcal{A}_{\circ}|^{2} = 2m(E - V). \qquad (2.2.5.19)$$

Example 2: Discuss the similarities between geometrical optics (i. e., limit of short wave of wave optics) and the motion of particle in potential field.

Solution: Eq. (2.2.5.19) is similar to the Eikonal equation of geometrical optics. Eikonal equation is

$$|\nabla \mathcal{A}_{\circ}|^2 = n(x, y, z).$$
 (2.2.5.20)

n(x, y, z) stands for the refraction coefficient, and corresponds to  $\sqrt{2m[E - V(x, y, z)]}$ .  $\mathcal{A}_{\circ}$  stands for the phase of wave. In homogeneous medium *n* is a constant, and corresponds to V = constant, i. e., free particle. The equal phase plane is plane cluster, and is given by

$$\mathcal{A}_{\circ} = ax + by + cz + d. \tag{2.2.5.21}$$

The normal direction (a, b, c) of the equal phase (i. e., the direction of  $p = \nabla \mathcal{A}_{\circ}$ ) stands for the propagation direction of the ray, and correspond to that the trajectory of free particle is straight line. Non-homogeneous medium in optics correspond to the particle in external field. In non-homogeneous medium the equal phase plane is the cluster of curved surface, and its normal direction (i. e., the direction of  $\nabla \mathcal{A}_{\circ}$ ) is the propagation direction of ray, and has refraction phenomenon. These similarities between particle mechanics and geometrical optics had been discovered by Hamilton in 1825. However, this discovery did not cause caution, and forgot by peoples. When the wave mechanics was proposed in 1926, peoples began to notice this discovery in 1825. However, the origin existing the similarities has not yet been revealed until now by any theories or ideas. Basing on the wavepacket-only theory (photon and massy particles are wavepacket), the theorem VI in subsection 3.4.1 and the corollary VII in subsection 3.4.5 of chapter 3 proves that both photon and free massy particles have guide-factors, which is plane waves, and the phase is  $\phi$ . The corollary IV in chapter 3 indicates that the momentum  $p = \hbar \nabla \phi$  for both photon and massy particles. The direction of momentum is the propagation direction of wave. For more discussions on this similarity between photon and massy particle see Ref. [109, **?**].

## 2.3. Hilbert Space and Operators

It is the aim of this section to equip you with the necessary mathematical machinery. All the math you need to learn quantum mechanics are developed in this section and in section 2.4. This section will tell you the present available math related to quantum mechanics. In section 2.4 we will demonstrate some new mathematical theorems related quantum mechanics.

## 2.3.1. State Vector and Dirac Notation

It is important to realize that quantum mechanics is a linear theory in which physical state of system is described by vector in complex linear vector space  $\mathbb{V}$ . The vector in linear vector space may represent free particle or particle bound in an atom or particle interacting with other particles or with external fields. The state vector is much like vector in ordinary three dimensional space, following many of the same rules, except that it describes a very complicated physical system.

It is convenient that the mathematical structure of a quantummechanical system will be presented in terms of notations proposed by Dirac.

A physical state in this notation is described by an abstract "ket" vector, |>, designated variously as  $|\alpha>$ ,  $\beta>$ ,  $|\psi>$ ,  $|\phi>$ , and a ket with other appropriate symbols depending on special problem at hand. The kets can be complex. Their conjugates,  $|>^*$ , are designated by < | which are called "bra" vector. The physical interpretation is derived through their so called "representatives" in the coordinate or momentum space or in a space appropriate to the problem under consideration. In this chapter all formulas, notations, and theorems are independent of particular forms of state vector |>. From chapter 3 we will begin to seek particular forms of state vector |> in various problems.

Using the Dirac notations, we can say that a complex linear vector space,  $\mathbb{V}$ , is a collection of |A >, |B >,  $\dots$ , |Z >.

The dimensionality of the linear vector space can be finite (e. g., the spin) or discretely (denumerably) infinite (e. g., the discrete bound state of hydrogen atom) or continuously

(indenumerably) infinite (e. g., a free electron with momentum that takes continuous values).

The vectors  $|\psi\rangle$  have the following important properties (Note that in our language: state vector = state = vector = ket):

- (1)  $\alpha$  and  $c | \alpha >$ , where c is a complex number, describe the same state.
- (2) The bra vector corresponding to  $c | \alpha >$  will be  $c^* < \alpha |$ ;
- (3) The kets follow a linear superposition rule

$$a|\alpha > +b|\beta > = c|\gamma >, \tag{2.3.1.1}$$

where *a*, *b*, *c* are complex numbers. That is, a linear combination of states in vector space is also a state in the same space. This superposition rule corresponding to a very important rule, which is called superposition theorem of state in quantum mechanics.

(4) The inner product (or scalar product or point product) of two states  $|\alpha\rangle$  and  $|\beta\rangle$  is defined as  $\langle\beta|\alpha\rangle$ , which is a complex number and not a vector. We demand that the inner product obeys the following axioms:

- $<\beta|\alpha>^* = <\alpha|\beta>$  (conjugate symmetry or skew-symmetry)
- $< \alpha | \alpha >> 0$  if  $| \alpha >\neq | 0 >$ , = 0 if  $| \alpha >= | 0 >$  (positive definiteness)

•  $< \alpha | (a|\beta > +b|\gamma >) \equiv < \alpha | a\beta + b\gamma > \equiv a < \alpha | \beta > +b < \alpha | \gamma >)$  (linearity in ket or linearity in second argument)

Suppose that **A** and **B** are two vector in three dimensional coordinate space. The definition of inner product is equivalent to  $\langle A|B \rangle = (A,B) \equiv A \cdot B = (A_x,A_y,A_z) \cdot (B_x,B_y,B_z) = A_xB_x + A_yB_y + A_zB_z$ . From this definition of inner product you can verify that the above three axioms of the inner product are satisfied. A vector space with inner product is called inner product space.

(5) The two state vectors are orthogonal if

$$<\alpha|\beta>=0. \tag{2.3.1.2}$$

(6) It is postulated that  $\langle A|A \rangle \ge 0$ . One calls  $\sqrt{\langle A|A \rangle}$  the norm or length of the state vector  $|A \rangle$ . If a state vector  $|A \rangle$  is normalized to unity, then

$$\langle A|A \rangle = 1.$$
 (2.3.1.3)

This state vector is called normalized state vector. If the norm vanishes, then  $|A\rangle = 0$ , in which case  $|A\rangle$  is called null vector.

(7) A set of *d* linearly independent vectors in the *d*-dimensional vector space can be taken as a basis. Any vector in this space,  $|\Psi\rangle$ , can be expressed as

$$|\psi> = \sum_{i=1}^{d} a_i |i>,$$
 (2.3.1.4)

where the vector  $|i\rangle$ 's form a basis, and  $a_i$  is called the component of vector  $|\psi\rangle$  in that basis. If the vector space is continuously (indenumerably) infinite dimensional space

instead of finite or discretely (denumerably) infinite dimensional space, then the summation in Eq. (2.3.1.4) is replaced by integration. If  $|i\rangle$ 's are orthogonal, then  $a_i = \langle i|\psi\rangle$ . It is then stated that  $|a_i|^2$  is the probability that the state  $|\psi\rangle$  will be in the state  $|i\rangle$ . If

$$\langle i|i \rangle = 1$$
 for any *i* and  $\langle i|j \rangle = 0$  for any  $i \neq j$ , (2.3.1.5)

then  $|i\rangle$ 's construct a orthonormal basis.

(8) A state vector may be depend on time, in which case one writes it as  $|i(t)\rangle$ ,  $|\psi(t)\rangle$ , etc. In the following, except when necessary, we will suppress the possible dependence on time.

(9) The product |A > |B > has no meaning unless it refers to two different vector spaces, e. g., one corresponds to spin, the other to momentum, or, if a state consists of two particles described by |A > and |B > respectively.

(10) Since bra vectors are obtained through complex conjugation of the ket vectors, the above properties can be easily extended to the bra vectors.

## 2.3.2. Hilbert Space

We have defined norm or length of vector  $|v\rangle$ , which is denoted by  $||v|| \equiv |v| \equiv \sqrt{\langle v|v\rangle}$ . A complete normed vector space is called a Banach space. We shall not deal with Banach space, but only with those spaces whose norms arise naturally from an inner product. This leads to the following definition: A complete inner product space, commonly denoted by  $\mathcal{H}$ , is called Hilbert space. Hilbert space can be finite dimensional or infinite dimensional. The Hilbert space can be real or complex. According to the definition of norm [Eq. (2.3.1.3)], every inner product space  $\mathfrak{H}$  is a normed space.

(1) The Hilbert space is linear. A function space is linear under the following two conditions: (a). If *a* is a constant and  $\phi$  is any vector of the space, then  $a\phi$  is also an vector of the space; (b). If  $\psi$  and  $\phi$  are any two vectors of the space, then  $\psi + \phi$  is also a vector of the space.

(2) There is an inner (or "dot" or scalar) product,  $\langle \psi | \phi \rangle \equiv (\psi, \phi)$ , for any two vectors in the Hilbert space. For functions defined in the interval  $a \le x \le b$  (if one dimension), we may take

$$\langle \Psi | \phi \rangle = \int_{a}^{b} dx \Psi^{*} \phi.$$
 (2.3.2.1)

The inner product is strictly positive-definite, i. e.,  $\langle \phi | \phi \rangle = 0$  implies  $\phi = 0$ 

(3) Any vector of  $\mathcal{H}$  has norm (length) that is related to the inner product as  $[(norm)(of)(\phi)]^2 = ||\phi||^2 = \langle \phi | \phi \rangle$ .

(4) The Hilbert space  $\mathcal{H}$  is complete. Every Cauchy sequence of function in  $\mathcal{H}$  converges to a vector of  $\mathcal{H}$ . A Cauchy sequence  $\{\phi_n\}$  is such that  $||\phi_n - \phi_l|| \rightarrow 0$  as *n* and *l* approach infinity. Loosely speaking, Hilbert space contains all its limit points.

In the following we give some examples [26, 28].

(1) A vector space  $\mathbb{V}$  over  $\mathbb{R}$  ( $\mathbb{R}$  = real numbers) is a set whose elements (vectors) may be "added" together, and "multiplied" by scalars. Many textbooks and this book sometimes

like to express the vector in this space as X, Y, and so on. For example, an inner product (or scalar product or dot product) on a vector space  $\mathbb{V}$  over  $\mathbb{R}^d$  (d numbers) associates to any pair  $X = x_1 + x_2 + \cdots + x_d$ ,  $Y = y_1 + y_2 + \cdots + y_d$  of vectors in  $\mathbb{V}$  a real number which we denote by (X,Y).

$$(X,Y) = x_1y_1 + \dots + x_dy_d.$$
 (2.3.2.2)

Then

$$||X|| = (X,X)^{\frac{1}{2}} = \sqrt{x_1^2 + \dots + x_d^2},$$
 (2.3.2.3)

which is the usual Euclidean distance, or norm, or length. One often uses the notation |X| instead of ||X||.

(2) The set of functions defined on the interval  $(0 \le x \le a)$  with finite norm

$$||\phi||^2 = \int_0^a dx \phi^* \phi < \infty.$$
 (2.3.2.4)

(3) In applications Hilbert space has many concrete forms. The benefit of using one particular concrete form rather than another is that certain operations may be easier to handle or a calculation may be easier to perform.

One very useful class of concrete Hilbert space is that consisting of so called square integrable functions. Let  $\Omega$  be the real line  $\mathbb{R}$  or an interval on  $\mathbb{R}$ . Mathematicians uses  $\mathcal{L}^2(\Omega)$  to denote the set of complex valued functions on  $\Omega$  for which the integral

$$\int_{\Omega} |f(x)|^2 dx \text{ is finite}$$

To be more precise, functions are required to be measurable and two functions are identified if they are equal almost everywhere. With these conditions,  $\mathcal{L}^2(\Omega)$  is a separable infinite dimensional Hilbert space equipped with an inner product [29]

$$\langle \Psi | \phi \rangle = \int_{\Omega} \Psi^* \phi dx.$$
 (2.3.2.5)

Roughly speaking,  $\mathcal{L}^2(\Omega)$  is a separable infinite dimensional Hilbert space, which is a concrete form of Hilbert space and consist of square-integrable functions.

We recall that if two vectors U and V in three-dimensional vector space are orthogonal to each other, then their inner product vanishes. In a similar vein, two vectors in Hilbert space,  $\phi$  and  $\psi$ , are said to be orthogonal if

$$\langle \psi | \phi \rangle = 0. \tag{2.3.2.6}$$

Furthermore, we recall that the three unit vectors  $e_x$ ,  $e_y$ , and  $e_z$  can span a three dimensional Cartesian space. Similarly, there is a set of vectors that spans Hilbert space. For instance, the Hilbert space whose elements all have the property given by Eq. (2.3.2.5) is spanned by the sequence of functions  $\{\phi_n\}$ , which are the (energy) eigenfunctions of a very simple Hamilton operator. This means that any function  $\phi$  in this Hilbert space may be expanded in a series of the sequence  $\{\phi_n\}$ .

$$\phi(x) = \sum_{n=1}^{\infty} a_n \phi_n(x).$$
 (2.3.2.7)

The geometrical interpretation of Eq. (2.3.2.7) is as follows. The coefficient  $a_n$  is the projection of  $\phi$  onto the vector  $\phi_n$ . Generally, we set that the basis vectors  $\{\phi_n\}$  comprise an orthogonal set. That is,

$$\langle \phi_n | \phi_{n'} \rangle = 0 \quad n \neq n'.$$
 (2.3.2.8)

Two functions  $\phi_1$  and  $\phi_2$  satisfied Eq. (2.3.2.8) are of orthonormality. Furthermore,  $\phi_n$  ia a unit vector, if it has unit length or unit norm

$$\langle \phi_n | \phi_n \rangle = ||\phi||^2 = 1.$$
 (2.3.2.9)

Eqs. (2.3.2.8) and (2.3.2.9) may be combined into a single equation

$$\langle \phi_n | \phi_{n'} \rangle = \delta_{n,n'}. \tag{2.3.2.10}$$

The symbol  $\delta_{n,n'}$  is called Kronecker  $\delta$  function and is defined by

$$\delta_{n,n'} = 0$$
 for  $n \neq n'$ ,  $\delta_{n,n'} = 1$  for  $n = n'$ . (2.3.2.11)

Any sequence of functions that obeys Eq. (2.3.2.10) is called an orthogonal set.

To show that  $a_n$  is the projection of  $\phi$  onto  $\phi_n$ , we first rewrite Eq. (2.3.2.7) by Dirac notation.

$$|\phi> = \sum_{n'} |a_{n'}\phi_{n'}>.$$
 (2.3.2.12)

Then we multiply from the left by  $|\phi_n\rangle$  and use the relation Eq. (2.3.2.10).

$$\langle \phi_n | \phi \rangle = \sum_{n'} \langle \phi_n | a_{n'} \phi_{n'} \rangle$$
$$= \sum_{n'} a_{n'} \langle \phi_n | \phi_{n'} \rangle = \sum_{n'} \delta_{n,n'} = a_n.$$
(2.3.2.13)

Eq. (2.3.2.13) indicates that coefficient  $a_n$  is the inner product between the basis vector  $\phi_n$  and the vector  $\phi$ . Since  $\phi_n$  is a "unit" vector,  $a_n$  is the projection of  $\phi$  onto  $\phi_n$ . The reader should recognize that Eq. (2.3.2.7) to be a discrete Fourier series representation of  $\phi$ , in terms of, for example, the following trigonometric sequence.

$$\phi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right). \tag{2.3.2.14}$$

The eigenfunctions (or eigenvectors) of momentum operator  $p = \hbar k$ :

$$\phi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}, \qquad (2.3.2.15)$$

where k is a continuous variable other then the discrete number n in Eq.(2.3.2.14), can be used to replace  $\phi_n$ .

Let us look if this (continuous) set of functions is an orthogonal set. Towards these ends we form the inner product

$$<\phi_k|\phi_{k'}>=rac{1}{2\pi}\int_{-\infty}^{\infty}dx e^{ix(k'-k)}=\delta(k'-k).$$
 (2.3.2.16)

Here,  $\delta(k' - k)$  is called Dirac delta function [Refer to Eq. (2,3.6.10)]. It follows that the inner product between any two distinct eigenvectors of the operator *p* vanishes.

Any function  $\phi(x)$  in  $\mathcal{L}^2$  may be expanded in terms of the vector set  $\{f_k(x) = 1/(\sqrt{2\pi})\exp(ikx)\}$ . Since this sequence is a continuous set, the expansion is not a discrete summation as in Eq. (2.3.2.7), but an integral. If  $\phi(x)$  is any vector (or, say, any element) of  $\mathcal{L}^2$ , then since  $\{f_k(x)\}$  spans this space, one may write

$$\phi(x) = \int_{-\infty}^{\infty} dk \overline{\phi}(k) \phi_k(x). \qquad (2.3.2.17)$$

This is the Fourier integral representation of  $\phi(x)$ . The coefficient of expansions,  $\overline{\phi}(k)$  is the project of  $\phi(x)$  onto  $\phi_k(x)$ . To exhibit this fact, we first rewrite the last integral in the form

$$|\phi\rangle = \int_{-\infty}^{\infty} dk \overline{\phi}(k) |\phi_k\rangle. \qquad (2.3.2.18)$$

Again, if this equation is compared to Eq. (2.3.2.12), then we see how the summation over discrete  $a_n$  values is replaced by an integration over the continuum of  $\overline{\phi}(k)$  values. If we now multiply Eq. (2.3.2.18) from the left with  $\langle \phi_{k'} |$ , there results

$$< \phi_{k'} | \phi > = \int_{-\infty}^{\infty} dk < \phi_{k'} | \overline{\phi}(k) \phi_k > = \int_{-\infty}^{\infty} dk \overline{\phi}(k) < \phi_{k'} | \phi_k >$$
$$= \int_{-\infty}^{\infty} dk \overline{\phi}(k) \delta(k' - k) = \overline{\phi}(k').$$
(2.3.2.19)

The coefficient of expansion  $\overline{\phi}(k')$  is the inner product between  $\phi_{k'}$  and  $\phi$ .

If X and Y represent two continuous functions in Hilbert space, defined at infinitely large interval, then Eq. (2.3.2.1) becomes

$$(X,Y) \equiv \int_{-\infty}^{\infty} d\tau X^* Y. \qquad (2.3.2.1)'$$

## 2.4. Fourier Transformation

#### 2.4.1. Integration of Functions on Real Line

We begin by extending the notion of integration to functions that are defined on the whole real line. The integral of a continuous functions over  $\mathbb{R}$ , where  $\mathbb{R}$  means real numbers, is [26]

$$\int_{-\infty}^{\infty} dx \Psi(x) = \lim_{N \to \infty} \int_{-N}^{N} dx \Psi(x).$$
(2.4.1.1)

A useful condition for correctness of Eq. (2.4.1.1) is as follows:

A function  $\psi$  defined on  $\mathbb{R}$  is said to be of moderate decrease if  $\psi$  is continuous and there exists a constant A > 0 so that [26]

$$|\Psi(x)| \le \frac{A}{1+x^2} \quad for \quad all \ x \in \mathbb{R}.$$
(2.4.1.2)

This inequality says that  $\psi$  is bounded (by *A* for instance), and also that it decays at infinity at least as fast as  $1/x^2$ , since  $A/(1+x^2) \le x^2$ . For example, the function  $\Psi(x) = 1/(1+x^2)$ 

 $|x|^n$  is of moderate decrease as long as  $n \ge 2$ . Another example is given by the function exp(-a|x|) for a > 0.

We shell denote by  $\mathcal{M}(\mathbb{R})$  the set of functions of moderate decrease on  $\mathbb{R}$ .  $\mathcal{M}(\mathbb{R})$  forms a vector space over  $\mathbb{C}$ , which denotes complex numbers.

## 2.4.2. Definition of Fourier Transform

Suppose that  $\psi(x) \in \mathcal{M}(\mathbb{R})$ . We define its Fourier transform for  $k \in \mathbb{R}$  by

$$\overline{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} dx \Psi(x) e^{-ikx} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \Psi(x) e^{-ikx}.$$
 (2.4.2.1)

Of course,  $|\exp^{-ikx}| = 1$ , so the integrand is of moderate decrease, and the integral makes sense. However, nothing in the definition above guarantees that  $\overline{\psi(k)}$  is of moderate decrease, or has a specific decay. In particular, it is not clear in this context how to make sense of the integral  $\int_{-\infty}^{\infty} dk \overline{\psi}(k) \exp(ikx)$  and the resulting Fourier inversion formula. To remedy this, people often introduce a more refined space of functions considered by Schwartz which is very useful in establishing the initial properties of the Fourier transform [26]. More discussions on the restrictions for Fourier transform can be found in Ref. [27].

This book does not introduce the Schwartz space. We give an additional assumption that the Fourier transform of the function under consideration is of moderate decrease [26]. This assumption, although modest in scope, is nevertheless useful [26].

Theorem of Fourier inversion. If the Fourier transform is defined by Eq. (2.4.2.1), then

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \overline{\Psi}(k) e^{ikx}.$$
 (2.4.2.2)

**Proof.** Substituting Eq. (2.4.2.1) into Eq. (2.4.2.2) yields

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dk\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dx'\psi(x')e^{-ikx'}e^{ikx} = \int_{-\infty}^{\infty}dx'\psi(x')\delta(x-x') = \psi(x)dx'$$

QED.

## 2.5. Mathematical Uncertainty Relations

### 2.5.1. Demonstration

In this section we will prove two mathematical uncertainty relations, and introduce some applications of these uncertainty relations. From the wavepacket-only theory in chapter 3 we will see that the two mathematical uncertainty relations in this section correspond to two (physical) Heisenberg uncertainty relations in many Heisenberg uncertainty relations.

Define a new quantity, variance (which is also called mean-square deviation), of coordinate *x* as follows:

$$(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle = \int_{-\infty}^{\infty} (x - \langle x \rangle)^2 |\Psi(x)|^2 dx, \qquad (2.5.1.1)$$

where  $\langle x \rangle$  represents the average value of x in the function  $\in \mathcal{M}(\mathbb{R})$ . For convenience, we assume that  $\psi(x)$  is normalized:

$$\int_{-\infty}^{\infty} dx |\Psi(x)|^2 = 1, \qquad (2.5.1.2)$$

The Fourier transform of  $\psi(x)$  is

$$\overline{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \Psi(x) e^{-ikx}.$$
(2.5.1.3)

Of course, we can define the variance of k:

$$(\Delta k)^2 = \int_{-\infty}^{\infty} dk (k - \langle k \rangle)^2 |\overline{\Psi}(k)|^2, \qquad (2.5.1.4)$$

where  $\langle k \rangle$  represents the average value of *k* in the Fourier transform  $\overline{\Psi}(x)$ .

**Theorem of uncertainty relation.** If  $\psi(x)$  is a normalized function in  $\mathcal{M}(\mathbb{R})$ , then

$$(\Delta x)^{2} (\Delta k)^{2} = \left[ \int_{-\infty}^{\infty} dx (x - \langle x \rangle)^{2} |\Psi(x)|^{2} \right] \left[ \int_{-\infty}^{\infty} dk (k - \langle k \rangle)^{2} |\overline{\Psi}(k)|^{2} \right] \ge \frac{1}{4},$$
(2.5.1.5*a*)  

$$\Delta x \cdot \Delta k \ge \frac{1}{2},$$
(2.5.1.5*b*)

and equality holds if and only if  $\psi(x) = A \times \exp(-Bx^2)$  where B > 0 and  $A^2 = \sqrt{2B/\pi}$ .

**Proof.** At first we prove that the following equation is same as Eq. (2.5.1.5).

$$\left(\int_{-\infty}^{\infty} dx(x)^2 |\Psi(x)|^2\right) \left(\int_{-\infty}^{\infty} dk(k)^2 |\overline{\Psi}(k)|^2\right) \ge \frac{1}{4}.$$
(2.5.1.6)

We prove a property of Fourier transform:

If

$$\Psi(x) \to e^{-i < k > x} \Psi(x + < x >),$$

then

$$\overline{\Psi}(k) \to \overline{\Psi}(k+\langle k \rangle)e^{i(k+\langle k \rangle)\langle x \rangle}.$$
(2.5.1.7)

The method to prove Eq. (2.5.1.7) is same as that for Eq. (2.4.3.2). Making the transformation of Eq. (2.5.1.7) for Eq. (2.5.1.6) and changing variables, we can obtain Eq. (2.5.1.5). Therefore, we just need to prove Eq. (2.5.1.6).

Beginning with our normalizing assumption  $\int dx |\psi(x)|^2 = 1$ , and assuming that  $\psi(x)$ 

and  $\psi'(x) = d\psi(x)/dx$  are moderate decreasing, an integration by parts gives

$$1 = \int_{-\infty}^{\infty} dx |\Psi(x)|^{2}$$

$$= \int_{-\infty}^{\infty} dx x \frac{d}{dx} |\Psi(x)|^{2} = \int_{-\infty}^{\infty} dx x \frac{d}{dx} [\Psi^{*}(x)\Psi(x)$$

$$= \int_{-\infty}^{\infty} dx (x\Psi'(x)\Psi^{*}(x) + x\Psi'^{*}(x)\Psi(x)) \qquad (2.5.1.8)$$

$$\leq 2 \int_{-\infty}^{\infty} dx |x| |\Psi(x)| |\Psi'(x)|$$

$$\leq 2 \left( \int_{-\infty}^{\infty} dx x^{2} |\Psi(x)|^{2} \right)^{\frac{1}{2}} \left( \int_{-\infty}^{\infty} dx |\Psi'(x)|^{2} \right)^{\frac{1}{2}} \qquad (2.5.1.9)$$

$$= 2 \left( \int_{-\infty}^{\infty} dx x^{2} |\Psi(x)|^{2} \right)^{\frac{1}{2}} \left( \int_{-\infty}^{\infty} dx \frac{d}{dx} \Psi^{*}(x) \frac{d}{dx} \Psi(x) \right)^{\frac{1}{2}}$$

$$= 2 \left( \int_{-\infty}^{\infty} dx x^{2} |\Psi(x)|^{2} \right)^{\frac{1}{2}}$$

$$= 2 \left( \int_{-\infty}^{\infty} dx x^{2} |\Psi(x)|^{2} \right)^{\frac{1}{2}} \left( \int_{-\infty}^{\infty} dk \overline{\Psi}^{*}(k) (-ik) e^{-iks} \sqrt{(2\pi)} \int_{-\infty}^{\infty} dk' \overline{\Psi}(k') (ik') e^{ik's} \right)^{\frac{1}{2}}$$

$$= 2 \left( \int_{-\infty}^{\infty} dx x^{2} |\Psi(x)|^{2} \right)^{\frac{1}{2}} \left( \int_{-\infty}^{\infty} dk \overline{\Psi}^{*}(k) (-ik) \int_{-\infty}^{\infty} dk' \overline{\Psi}(k') (ik') \delta(k-k') \right)^{\frac{1}{2}}$$

$$= 2 \left( \int_{-\infty}^{\infty} dx x^{2} |\Psi(x)|^{2} \right)^{\frac{1}{2}} \left( \int_{-\infty}^{\infty} dk k^{2} |\overline{\Psi}(k)|^{2} \right)^{\frac{1}{2}} . (2.5.1.10)$$

The equality Eq. (2.5.1.9) follows because the Cauchy-Schwartz inequality proves in subsection 2.3.2. The equality Eq. (2.5.1.10) follows from the properties of Fourier transform. Here we concludes the proof of the inequality in the theorem. QED.

If the equality in Eq. (2.5.1.6) holds, then we must also have equality where we applied Cauchy-Schwartz inequality, and as a result we find that  $\psi'(x) = \beta x \psi(x)$  for some constant  $\beta$ . The solutions to this equation are  $\psi(x) = A \exp(\beta x^2/2)$ , where A is a constant. Since we want  $\psi$  to be a function  $\in \mathcal{M}(\mathbb{R})$ , we must take  $\beta = -2B < 0$ , and since we impose the normalized condition, we find that  $A^2 = \sqrt{2B/\pi}$ , as was to be shown.

Let us explain qualitatively that why is  $\langle x \rangle$  our best guess of the position of the particle? Consider the simpler (idealized) situation where we are given that the particle can be found at only finitely many different points,  $x_1, x_2, \dots, x_N$  on the real axis, with  $p_i$  the probability that the particle is at  $x_i$ , and  $p_1 + p_2 + p_3 + \dots + p_N = 1$ . Then, if we knew nothing else, and were forced to make one choice as to the position of the particle, we would naturally take  $\langle x \rangle = \sum_{i=1}^{N} x_i p_i$ , which is the appropriate average of the possible position [26].

Let us define the uncertainty. Having determined that the average position of a function (vividly speaking, a particle or a wavepacket) is  $\langle x \rangle = \overline{x}$ , the resulting uncertainty is defined by the quantity  $\Delta x \equiv \sqrt{(\langle x - \langle x \rangle \rangle)^2}$ . Notice that if  $\psi$  is highly concentrated near  $\langle x \rangle$ , it means that the larger part of the function is near  $\langle x \rangle$ , and so  $\Delta x$  is small,

because most of the contribution to the integral takes place for values of x near  $\langle x \rangle$ . Here we have a small uncertainty. On the other hand, if  $\psi(x)$  is rather flat (that is, the position probability density of single particle is not very concentrated), then the integral in  $\Delta x$  is rather big, because large values of  $(x - \langle x \rangle)^2$  will come into play, and as a result the uncertainty is relatively large.

It is also worthwhile to observe that the average value of  $\langle x \rangle$  is that choice, for which the uncertainty

$$\int_{-\infty}^{+\infty} (x - \langle x \rangle)^2 |\Psi(x)|^2 dx \qquad (2.5.1.11)$$

is the smallest [26]. Indeed, if we try to minimize this quantity by equating to 0 its derivative with respect to  $\langle x \rangle$ , we find that

$$2\int_{-\infty}^{\infty} dx (x - \langle x \rangle) |\Psi(x)|^2 = 0, \qquad (2.5.1.12)$$

which gives  $\langle x \rangle$ .

If a function  $\Psi(t)$  of time and its Fourier transform  $\overline{\Psi}(\omega)$  ( $\omega$  represents angular frequency) are  $\in \mathcal{M}(\mathbb{R})$ , then the theorem can be expressed as

$$(\Delta t)^2 (\Delta \omega)^2 = \left[ \int_{-\infty}^{\infty} dt (t - \langle t \rangle)^2 |\Psi(t)|^2 \right] \left[ \int_{-\infty}^{\infty} d\omega (\omega - \langle \omega \rangle)^2 |\overline{\Psi}(\omega)|^2 \right] \ge \left(\frac{1}{2}\right)^2,$$
(2.5.1.13)

and equality holds if and only if  $\psi(t) = A \times \exp(-Bt^2)$  where B > 0 and  $A^2 = \sqrt{2B/\pi}$ .

Eq. (2.5.1.13) can be called time-frequency uncertainty relation.

#### 2.5.2. Applications of Mathematical Uncertainty Relations

To remove the mysterious feeling to the Heisenberg (physical) uncertainty relations, introduced in chapter 3, we give the following examples to show that even a purely mathematical uncertainty relations have many applications in practices, i. e., in our everyday life we already can meet with may things, which are determined by mathematical uncertainty relations proved here. We hope that after reading these examples, physicists and students do not feel mystery for the Heisenberg physical uncertainty relations. Physical uncertainty relations are merely a characteristic of any functions  $\in \mathcal{MR}$  in essence, and appear in many classical things.

(1) Television and radio broadcasting [30]. The broadcasting uses electromagnetic radiation, with each television or radio channel being broadcast in a narrow range, or band, of frequencies (Not at a particular frequency, as is often considered the case). So, for example, a particular radio station may be using the frequency band from 900 to 910 KHz, corresponding to a range of  $\omega$  from  $5.65 \times 10^6$ /sec to  $5.71 \times 10^6$ /sec. The mean angular frequency of broadcast signal must be about  $5.68 \times 10^6$ /sec. The spread must be less than  $0.03 \times 10^6$ /sec. From the uncertainty relation we obtain that  $\Delta t \ge 17 \times 10^{-6}$  second. In other words, the radio station cannot transmit a signal which lasts less than  $17\mu$ s. This sounds like a very short signal. But a long signal is merely many short signals transmitted successively. Thus, 17  $\mu$ s is a limit on the time resolution of the transmitted signals. The station can transmit no signal with any detail finer than 17  $\mu$ s. Now in order to get reasonably good sound reproduction, the system must be able to transmit pitches as high as the ear can hear, which is around 20 KHz. A sound wave at this frequency has a period of 50  $\mu$ s: just three times the resolution limit of a signal. There is barely room in the frequency band for a good signal [30]. Television systems are even more demanding. Existing European television tubes make up their pictures from 625 lines, scanned 24 times a second. For a good picture, the lines must be able to change sharply in brightness over 1/300 of their length, corresponding to a picture resolution of about 2 mm for a large screen. Thus the television signal must have a time resolution of not worse than  $1/(24 \times 625 \times 300)$  second, or 0.2  $\mu$ s. Indeed for a color signal, three separate lines are sent concurrently–for red, green, and blue picture elements—so the time resolution must be divided by 3. The bandwidth of television broadcasts must be corresponding large.

(2) The mathematical uncertainty relation of frequency(f)-time(t), Eq. (2.5.1.12) ( $\omega = f/(2\pi)$ ), has been used in practice as well. For example, Piano tuner has exploited it for centuries. Piano tuner sounds a vibrating tuning fork of standard frequency in union with a piano note of the same nominal frequency and listens to a beat tone between the struck tune and the tuning fork. If a fork frequency f is 500 Hz and a string frequency f' is 501 Hz, then one beat tone will be heard per second. The goal of the piano tuner rise to reduce the number of beats as much as possible. For example, if the piano tuner tries to achieve an accuracy of  $\Delta f = 0.01$  Hz, then the piano tuner will wait for at least 314 second to be sure no beat had occurred. Piano tuner therefore relies on our mathematical frequency-time uncertainty relation, which clearly means that measurement of the frequency with infinite accuracy requires a infinite time period of measurement, or equivalently, it is impossible within any finite period of time to determine the frequency of the string exactly.

## Chapter 3

# **Wavepacket-Only Theory**

## 3.1. Introduction

The historical experiences and lessons are worthy to notice. Let me tell you a long story on processes of exploration of mankind for the innate character, intrinsic quality, and motion of nature and object. This story can be traced back to remote antiquity [31].

The move towards a rational understanding of nature and object began at least since the book of Shangshu of ancien China (1066-771 BC). In this book the five elements (metal, wood, water, fire, and earth) held by the ancients to compose the physical universe and later used in traditional medicine to explain various physiological and pathological phenomena.

During the Vedic period (1100-500 BC), Indians (Indo-Aryans) had classified the material world into five elements: Earth (Prithvi), fire (Agni), air (Maya) and water (Apa), and ether (Akasha). According to some scholars these five elements or pancha mahabhutas were identified with the various human senses of perception; earth with smell, air with feeling, fire with vision, water with taste and ether with sound. The Buddhist philosophers who came later, rejected ether as an element and replaced it with life, joy and sorrow. In Indian philosophy, Kanada was the first to systematically develop a theory of atomism during the 6th century BC, and it was further elaborated on by the Buddhist atomists Dharmakirti and Dignaga during the 1st millennium CE. Pakudha Kaccayana, a 6th century BC Indian philosopher and contemporary of Gautama Buddha, had also propounded ideas about the atomic constitution of the material world. These philosophers believed that other elements (except ether) were physically palpable and hence comprised miniscule particles of matter. The last miniscule particle of matter which could not be subdivided further was termed Parmanu.

The move towards a rational understanding of nature and object began at 650 BC-480 BC with the Pre-Socratic philosophers in Greece. The philosopher Thales (7th and 6 centuries BC), dubbed "the Father of Science" for refusing to accept various supernatural, religious or mythological explanations for natural phenomena, proclaimed that every event had a natural cause. Thales also made advancements in 580 BC by suggesting that water is the basic element, experimenting with magnets and attraction to rubbed amber, and formulating the first cosmologies. Anaximander, famous for his proto-evolutionary theory, disputed the ideas of Thales and proposed that rather than water, a substance called apeiron was the building block of all matter. Heraclitus (around 500 BC) proposed that the only basic law

governing the universe was the principal of change and that nothing remains in the same state indefinitely. This observation made him one of the first scholars in ancient physics to address the role of time in the universe, one of the most important concepts even in the modern history of physics. The early physicist Leucippus (first half of 5th century BC) adamantly opposed the idea of direct divine intervention in the universe, instead proposing that natural phenomena had a natural cause. Leucippus and his student, Democritus, were the first to develop the theory of atomism-the idea that everything is composed entirely of various imperishable, indivisible elements called atoms.

Aristotle (384 BC-322 BC) promoted the concept that observation of physical phenomena could ultimately lead to the discovery of the natural laws governing them. Aristotle's writings cover physics, metaphysics, poetry, theater, music, logic, rhetoric, linguistics, politics, government, ethics, biology and zoology. He wrote the first work which refers to that line of study as "Physics" (Aristotle's Physics). Aristotle attempted to explain ideas such as motion (and gravity) with the theory of four elements. Aristotle believed that all matter was made up of aether, or some combination of four elements: earth, water, air, and fire. According to Aristotle, these four terrestrial elements are capable of inter-transformation and move toward their natural place, so a stone falls downward toward the center of the cosmos, but flames rise upward toward the circumference. Eventually, Aristotelian physics became enormously popular for many centuries in Europe, informing the scientific and scholastic developments of the Middle Ages. It remained the mainstream scientific paradigm in Europe until the time of Galileo Galilei and Isaac Newton.

Important contributions were made by Ibn al-Haytham (965-1040 AD), a mathematician from Basra, Iraq considered one of the founders of modern optics. Ptolemy and Aristotle theorised that light either shone from the eye to illuminate objects or that light emanated from objects themselves, whereas al-Haytham (known by the Latin name Alhazen) suggested that light travels to the eye in rays from different points on an object. The works of Ibn al-Haytham eventually passed on to Western Europe where they were studied by scholars such as Roger Bacon and Witelo.

Based on Aristotelian physics, Scholastic physics described things as moving according to their essential nature. Celestial objects were described as moving in circles, because perfect circular motion was considered an innate property of objects that existed in the uncorrupted realm of the celestial spheres. The theory of impetus, the ancestor to the concepts of inertia and momentum, was developed along similar lines by medieval (about 1100-1400 AD) philosophers such as John Philoponus and Jean Buridan. Motions below the lunar sphere were seen as imperfect, and thus could not be expected to exhibit consistent motion. More idealized motion in the sublunary realm could only be achieved through artifice, and prior to the 17th century, many did not view artificial experiments as a valid means of learning about the natural world. Physical explanations in the sublunary realm revolved around tendencies. Stones contained the element earth, and earthy objects tended to move in a straight line toward the center of the earth (and the universe in the Aristotelian geocentric view) unless otherwise prevented from doing so.

From 200 BC until 1500 AD, China was the world's most technologically advanced society.

During the 16th and 17th centuries, a large advancement of scientific progress known as the Scientific Revolution took place in Europe. Dissatisfaction with older philosophical approaches had begun earlier and had produced other changes in society, such as the Protestant Reformation, but the revolution in science began when natural philosophers began to mount a sustained attack on the Scholastic philosophical program and supposed

Let me state in more detail the story on the understanding the light and the matter from about more than 300 years ago up to now.

The particles or waves, that the matter and light are, have formed the two poles between which the imagination of physicists has worked. During the three centuries from the end of seventeenth century to 2012, a long struggle had taken place in physics, sometimes acrimoniously, over how to think the world. Newton, for example, thought of the universe in terms of particles.

Newton said: "It seems probable to me, that God in the beginning formed matter in solid, massive, hard, impenetrable, movable particles, of such sizes and figures, and with such other properties, and such proportion to space, as most conduced to the end for which he formed them... [32]."

On Newton's model, everything was particle. Newton contended in 1672 that light was made up of individual particles. In opposition, other physicists felt that part-and perhaps all-of the world could not be so described. They developed a model that emphasized the smooth, unbroken, character of nature, creating a continuum mechanics in which wave phenomena find a natural account. Light above all, with its host of interference effects, seemed especially amenable to a continuum treatment. For example, Hooke (who was utterly despised by Newton) wrote on the wave-like properties of light. In 1801, Thomas Young's double slit experiment demonstrated the wave-like property of light, analogous to sound waves in air, or water waves in a pond.

By 1900 the world of physics was neatly divided into two domains, particle dynamics versus continuum dynamics: particles versus waves, for short. Baseballs and pebbles, on one hand, were particles, obeying the laws of discrete mechanics. Light and sound, on the other hand, were waves, running through the unfragmented media in ether and air. In skipping pebbles at the beach, particles meet waves-but a much more significant meeting between them took place at the dawn of the twentieth century, with birth of quantum mechanics.

Einstein (1905) revisited the theory of light acting as a particle to resolve conflicts between the wave theory of light and certain experimental results such as the photoelectric effect. The initial steps were taken by Planck and Einstein, who suggested that black body radiation and the photoelectric effect were better explained if one thought of light as particle in character. But the real shock came later, when de Bloglie made the even bolder suggestion that matter particles could behave like waves. During the early decades of this century, when the quantum theory was being developed, the evidence for the matter waves was meager. But by to day, with many new experiments, the evidence has become utterly compelling.

Now many physicists accept the viewpoint of "wave-particle duality", which says that light, atom, neutron, and so on have both wave property and particle property. The wave-particle duality looks like to be an indubitable "fact". On that how to understand and to visualize the wave-particle duality different viewpoints are possible.

We list the following two opposite viewpoints.

(1) The quantum mechanics is incomplete. This viewpoint thinks that the reason, that the concepts on the wave-particle duality and so on in quantum mechanics are difficult to be understood, is in the incompleteness of quantum mechanics. Throughout his life, Einstein never accepted the quantum mechanics. He consistently argued that the theory has failed us in an essential respect. Surely something is going on these experiments, he would have claimed, some remarkable processes that accounts for each particle's strange behavior. Quantum mechanics has not told us what that process is, and it is our wish to search for an understanding of this "something". According to Einstein's viewpoint, quantum mechanics, while perfectly adequate so for as it does, simply does not go far enough. It is not telling us everything we demand of a good theory. The quantum mechanics is incomplete.

(2) The quantum mechanics is complete. Bohr championed an opposing viewpoint. According to him, particle interference experiments present us with a state of affairs that is quite literally incomprehensible, at least if we are restricted to conventional ways of thinking. While we naturally wish to build in our minds a picture of the behavior of the particles used in the experiments, we are not going to get our wish-not because we have not yet found the right means, but because the atomic world simply cannot be approached in this manner. Mental pictures draw their elements from our sense world, but nothing like the quantum world has ever appeared to our senses, so how can we expect to make a suitable image if it? Up to the point of the development of scientific knowledge, it has always been possible, to a greater or lesser degree, to build in our minds a visualization image of the working of the world. But, according to Bohr's view, we are now presented with a situation in which such visualization is impossible.

The debate over the completeness of quantum mechanics continued throughout Bohr's and Einstein's lives. Now many physicists think that [35]: "In entering the atomic realm, we have entered a world in which our very ideas of what human knowledge can achieve need revision. Reality can no longer be thought of in the terms we have become used to; new terms need to be invented. Any theory that seeks to comprehend in classical terms what has been going on in our experimental apparatus is guaranteed to fail." Now one new viewpoint exists that would account for the wave-particle duality, which says that electrons, neutrons, atoms, and light are not really behaving in an incomprehensible manner after all. Rather, as they travel towards the experimental apparatus they sense its setup, and they adjust their nature accordingly. If they sense an experiment capable of demonstrating interference (for example, two slit interference), they become waves. But if they sense one capable of demonstrating particle property, they become particles. We might refer to such a viewpoint as a conspiracy theory of physical reality [35]. The quantum mystery which cannot go away (in Feynmans words) of "wave-particle duality" is illustrated in a striking way by the delayed-choice experiment suggested by Wheeler.

In 2000, Kleppner and Jackiw wrote: "Quantum theory is the most precisely tested and most successful theory in the history of science." [34] Although quantum theory got so great success, but many principles and concepts of quantum mechanics, such as wave-particle duality, the statistical interpretation for the wavefunction, Heisenberg uncertainty relations, measurements and so on, contradict seriously with people's everyday life. Therefore, it is difficult to accept these principles and concepts. Bohr said: "Anyone who is not shocked by quantum theory has not understand it." Feynman exhorted us: "We should always keep in

mind the possibility that quantum mechanics may fail, since it has certain difficulties with philosophical prejudices that we have about measurement and observation."

Let me tell you briefly that how does the story on the understanding properties of the light and the matter (including both the small quark and big universe) continue in our "Quantum Mechanics upon Theorems". We list briefly the following six conclusions, proved exactly by the wavepacket-only theory in this textbook. The detail explanations will be given in whole textbook, especially, in chapters 3, 4, 5, 9, and 10. The basic contents, based on quantum mechanics both upon theorems and upon postulates are the same. In the following we well illustrate the differences between the quantum mechanics upon theorems and upon postulates. The main difference between quantum mechanics upon theorems and upon postulates is merely in that the latter's quantum mechanics needs to invoke hypotheses, postulates, axioms, assumptions, guesses, and principles; on the contrary, the former firmly establishes quantum mechanics upon a series of theorems and corollaries, and one law. (In our language, wavepacket-only theory contains quantum mechanics upon theorems, and might contain other as well.)

(1) As is well known, classical mechanics describes any object by using both coordinates and momenta at the same time. However, one theorem of wavepacket-only theory proves that any object can only be described by either coordinates or momenta, and cannot be described by both coordinates and momenta at the same time. Readers might feel that this difference is negligible, and is of no a wee bit of importance. Actually, it is not so! One theorem of wavepacket-only theory proves that the sole watershed between classical mechanics and quantum mechanics is just in this difference "apparently looking like can be neglected". All the marvelous phenomena, such as wave-particle duality, energy quantization, uncertainty relations, come merely from description for any object by (r,t) or (p,t) other than (r, p, t). Vividly speaking, the difference between the quantum theory and the classical theory is merely in that one cannot or can set foot (=wavepacket=object) on two boats (=coordinates and momenta).

(2) Taking the above difference as a staring point, the wavepacket-only theory proves that the wavepacket as a spacetime function consists of body-factor and guide-factor, the body-factor brings all the mass, energy, momentum, spin and so on of the object, the guidefactor is just a mathematical function, which is called wavefunction, does not brings any substance, serves merely as a guide of object's motion. The guide of the guide-factor has equiprobability symmetry, and every time motion of body-factor is a time of spontaneous equiprobability symmetry breaking. In contrast to the wavepacket-only theory, the classical theory cannot give these two factors for object.

(3) Taking this difference as a staring point, the wavepacket-only theory proves commutation relations between coordinate and momentum instead of the Poison bracket in classical mechanics. In quantum mechanics upon postulates, the commutation relation is a hypothesis or postulate. If you ask that why can the quantum mechanics make this hypothesis? Some references's answer is: "Because it fits indirectly experimental facts".

(4) Taking this difference as a staring point, the wavepacket-only theory can prove exactly all the three formulations of quantum mechanics (Heisenberg matrix, Schrödinger wave equation, Feynman path integral). From these three quantummechanical formulations, further one can prove the energy quantization of bound state, the periodic table of elements, and so on. On the contrary, the classical theories can only derive the Newton equation from Poison bracket.

(5) Although the wavepacket-only theory proves, for example, Schrödinger equation, but Newton mechanics is not wrong. The latter can be used as an approximate theory for objects with large scale, high energy, and large mass. (This chapter will give a criterion for classical or quantum mechanics). In this aspect, we recall the special theory of relativity. When we have classical relativistic mechanics, we still say that the classical Newton mechanics is an approximate theory. For example, we say that if the velocity of object is not too high, then the classical Newton mechanics is still a good enough approximate theory.

(6) Although the basis of wavepacket-only theory is very simple (Just that, any objects, including both the massless photon and the massy particle, connect with mathematical functions only of either spacetime variables or momentum-time variables.), but its intensions are very plentiful. The quantum mechanics based on wavepacket-only theory can explain all the experimental facts, including that the until now quantum mechanics can and cannot explain, and gives a clear picture of wave-particle duality of any objects. Based on many theorems and analyses for experimental facts, wavepacket-only theory establishes a law, which states that the motion of any object accepts guide of the guide-factor according to spontaneous equiprobability symmetry breaking. From this law, the wavefunction (=guide-factor) represents a probability amplitude, which is exactly the same as that accepted by all physicists, and the wavefunction describes an individual object, which is different from some references's viewpoint (Some references think that the wavefunction describes an ensemble of particles. Although Ref. [22] mad an effort to start from ensemble interpretation of wavefunction to argue that wavefunction still represents individual object, yet it is not successful.). Both this textbook and many textbooks and references believe that "The God plays dice". However, Einstein said: "I do not believe that the God plays dice."

This chapter has the following arrangement. At first, we prove a theorem which denotes that in nature there is a universal constant, which's dimension is (energy  $\times$  time). For memory, we call this constant Planck constant. As a corollary we prove that how to understand correctly the de Blohlie matter wave, i. e., the wave-particle duality. We extend the two simple mathematical uncertainty relations, proved in section 2.3 of chapter 2 by mathematicians, to more general forms. Combining these mathematical uncertainty relations and the de Bloglie wave corollary and energy-frequency corollary, we prove all Heisenberg (physical) uncertainty relations. In the mean time, we prove some theorems on the operator representation of observable and on the commutation relation between canonical conjugate variable pair. Then, we prove a series of theorems, such as the wavepacket composition theorem. Then, we try to use these theorems to explain all known experimental facts, which the old quantum mechanics can or cannot. Basing on many theorems and analysis for large number of experimental facts, spontaneous equiprobability symmetry breaking motion of object is established as a law. Then we prove that the guide-factor of wavepacket obeys a wave equation, which is called Schrödinger equation for memory. Although our derivation of Schrödonger equation is completely different from the derivation of Schrödinger in 1926, but for the readers' interest we introduce the Schrödinger's work in 1926 and other's approaches to obtain Schrödinger equation. Subsequently, we address and discuss the properties of Schrödinger equation.

In this introduction it is appropriate to write 0-th theorem.

**Theorem 0: Watershed theorem.** There is only one watershed between classical and quantum mechanics. If one describes any object by using both coordinates and momenta at the same time, then this is classical mechanics. If one describes any object by using either coordinates or momenta, and not by both at the same time, then this is quantum mechanics.

Would readers please finish proof for this theorem after learning all this textbook.

This chapter is the center of quantum mechanics upon theorems. If you understand this chapter, then you have understood quantum mechanics basically.

## **3.2.** Existence of Universal Constant

**Theorem I: Existence of universal constant.** The dimension of product of canonical coordinate and canonical conjugate momentum is always (energy × time). In nature there is a universal constant, which's dimension is (energy × time). For memory, we call this constant Planck constant, and is expressed by  $\hbar = h/2\pi$ . (Note that the dimensions of angular momentum and action are (energy × time) as well.)

**Proof.** For that it is easy to be understood by readers, we use the following four steps to prove this theorem. (For the proof one can refer to Ref. [25], although Ref. [25] does not give this theorem.)

(1) First step. We prove that dimension of product of canonical coordinate and canonical conjugate momentum is (energy  $\times$  time). This conclusion can be proved directly from the definition of canonical conjugate momentum. From section 2.2 in chapter 2, we know

$$p_i = \frac{\partial L}{\partial \dot{q}_i},\tag{3.2.1}$$

where  $q_i$  and  $p_i$  are the *i*-th canonical coordinate and canonical conjugate momentum, respectively. In Eq. (3.2.1), the dimension of Lagrangian is (energy), the dimension of  $\dot{q}_i$  is (canonical coordinate/time). Therefore, the dimension of product of canonical coordinate and canonical conjugate momentum is (energy × time). We use  $\hbar$  to denote a constant with dimension *energy* × *time*.

(2) Second step. We prove that the  $\hbar$  is a universal constant. The Lagrangian is a function of coordinates  $s_i$ , velocities  $\dot{s}_i$   $(i = 1, 2, 3, \dots, D)$ , and time *t*. We call this the s-system. According to definition, the canonical conjugate momentum in s-system is

$$P_i = \frac{\partial L}{\partial \dot{s}_i}.$$
(3.2.2)

Let  $(q_1, q_2, q_3, \dots, q_D)$  be any set of *D* independent variables, which we will call the q-system, such that theirs values completely specify all of the s-system values, and vice versa.

We write each of the  $s_i$ , for  $i = 1, 2, \dots, D$ , as a function of these q variables and possible also time t,

$$s_i = s_i(q_1, q_2, \cdots, q_D, t).$$
 (3.2.3)

Under some conditions we have inverse relations for  $j = 1, 2, \dots, D$ ,

$$q_j = q_j(s_1, s_2, \cdots, s_D, t).$$
 (3.2.4)

The canonical conjugate momentum  $p_i$  of canonical coordinate  $q_i$  is defined

$$p_{j} = p_{j}(q, \dot{q}, t) = \frac{\partial L}{\partial \dot{q}_{j}}$$

$$= \sum_{i=1}^{D} \frac{\partial L(s, \dot{s}, t)}{\partial \dot{s}_{i}} \frac{\partial \dot{s}_{i}(q, t)}{\partial \dot{q}_{j}}$$

$$= \sum_{i=1}^{D} P_{i} \frac{\partial}{\partial \dot{q}_{j}} \left( \sum_{l=1}^{D} \frac{\partial s_{i}(q, t)}{\partial q_{l}} \frac{dq_{l}}{dt} + \frac{\partial s_{i}(q, t)}{\partial t} \right)$$

$$= \sum_{i=1}^{D} P_{i} \frac{\partial s_{i}(q, t)}{\partial q_{j}}.$$
(3.2.5)

Similarly,

$$P_i = \sum_{k=1}^{D} p_l \frac{\partial q_j(s,t)}{\partial s_i}.$$
(3.2.6)

Using Eqs. (3.2.3) and (3.2.5), with the notation for a differential at fixed time with  $\delta t = 0$ , the chain rule gives

$$\sum_{j=1}^{D} p_j \delta q_j = \sum_{j=1}^{D} \left( \sum_{i=1}^{D} P_i \frac{\partial s_i(q,t)}{\partial q_j} \right) \delta q_j$$
$$= \sum_{i=1}^{D} P_i \left( \sum_{j=1}^{D} \frac{\partial s_i(q,t)}{\partial q_j} \delta q_j \right) = \sum_{i=1}^{D} P_i \delta s_i.$$
(3.2.7)

We define a constant  $\hbar'$  for *q*-system,  $p_j = \hbar' k_j$ , and a constant  $\hbar''$  for *s*-system,  $P_i = \hbar'' K_i$ . Substituting these definitions into Eq. (3.2.7) yields

$$\sum_{j=1}^{D} p_j \delta q_j \equiv \hbar' \sum_{j=1}^{D} k_j \delta q_j = \sum_{i=1}^{D} P_i \delta s_i \equiv \hbar'' \sum_{i=1}^{D} K_i \delta s_i.$$
(3.2.8)

Because *q*-system is an arbitrary coordinate system, and  $K_i$ ,  $k_j$  are not definite completely, we can set that  $\hbar' = \hbar'' = \hbar$  in Eq. (3.2.8). Then, we have

$$\sum_{j=1}^{D} k_j \delta q_j = \sum_{i=1}^{D} K_i \delta s_i.$$
(3.2.9)

(3) Third step. We prove that  $\hbar$  is a universal constant even we take time as a coordinate. Often, the time's role is as a background parameter. Now, we take the time as a coordinate.
This means that time is removed from its role as a universal background parameter, and elevated to the status of a generalized coordinate with  $q_0 = t$ . When time is a coordinate, the path of particle must be specified by introducing a new background parameter, which is denoted by  $\beta$  [25]. The particle will trace out of a path in an augmented (D+1) dimensional configuration space defined, for all  $j = 0, 1, 2, \dots, D$ , by writing the equations of motion as  $q_j = q_j(\beta)$ , including  $q_0 = q_0(\beta)$  which is the same as  $t = t(\beta)$ .

The dimensions of canonical coordinate  $q_0$  and  $s_0$  are time. The dimensions of canonical conjugate momenta  $p_0$  and  $P_0$  are:

$$p_0(q, \dot{q}) = \frac{\partial L(q, \dot{q}, t)}{\partial \dot{q}_0} = -H(q, \dot{q}, t), \qquad (3.2.10)$$

which denotes that canonical conjugate momentum corresponding to time coordinate is Hamiltonian with minus sign.

We define a constant  $\hbar'$  for *q*-system that  $p_0 = \hbar'\omega_0$ , and a constant  $\hbar''$  for *s*-system that  $P_0 = \hbar''\Omega_0$ . Then, we can prove  $\hbar' = \hbar'' = \hbar$  by the similar method as that in point (2).

(4). Fourth step. Due to  $q_0$  and  $s_0$  are time, and  $p_0$  and  $P_0$  are energy, The points (2) and (3) show that the  $\hbar$  is a universal constant even we take time as a coordinate and energy with minus sign as canonical conjugate momentum [25]. QED.

**Corollary I: Momentum and energy.** Momentum  $p = \hbar k$ . Energy  $E = \hbar \omega$ . The dimensions of k and  $\omega$  are 1/length and 1/time, respectively.

**Proof.** This proof is simple and direct.

From theorem I we have:

(canonical coordinate  $\times$  canoniucal conjugate momentum/ $\hbar$ )

is a quantity without dimension, and the dimension of

(canonical conjugate momentum/ $\hbar$ ) is the inverse of the dimension of (canonical coordinate). Therefore, we have the following conclusion:

If  $q_i$  represents the canonical coordinate, for example, the length x, then the corresponding canonical conjugate momentum is  $p_i = p = \hbar k$ , where k is called wavenumber, and its dimension is 1/length. At this stage, we cannot say more about the physical meaning of k.

If  $q_0$  represents the canonical coordinate, for example, the time *t*, then the corresponding canonical conjugate momentum is  $p_0 = -E \equiv -\omega\hbar$ , where  $\omega$  is called angular frequency, and its dimension is 1/time. At this stage, we cannot say more about the  $\omega$ . QED.

Note that from theorem I we still do not know how to determine the value of the constant. At this stage we just know that, for example, if  $p = \hbar k$ ,  $p = mv_x$  is momentum of x direction, then the dimension of k is 1/length and if energy  $E = \hbar \omega$ , then the dimension of  $\omega$  is 1/time. After establishing the wavepacket law in subsection 3.4.7, we prove a corollary, according to which we know k represents the average wavenumber of a particle (particle=wavepacket). The average wavenumber of a particle can be determined by experiments. Of course, the momentum of a particle can be determined. Thus, from  $p = \hbar k$  the  $\hbar$ is determined. Similarly, we can determine  $\hbar$  from  $E = \hbar \omega$ . The present most precise value is  $\hbar = h/(2\pi) = 1.05457266 \times 10^{-27}$  erg·second. One often calls  $\hbar$  and h Planck constant for memory. Some books also call  $\hbar$  the reduced Planck constant.

# **3.3. Uncertainty Relations**

## 3.3.1. General Theory of Fourier Transformation

#### 3.3.1.1. Four Dimensional Spacetime

Take mathematical function of spacetime,  $\Psi(r,t) \in \mathcal{M}(\mathbb{R})$  as wavepacket-function. This wavepacket-function can be made Fourier expansion. Considering theorem I in last section, we know that the product of canonical conjugate variable pair, i. e., canonical coordinate and canonical conjugate momentum, divided by  $\hbar$ , is without dimension. Therefore, we can take the canonical conjugate variable pair in analytical mechanics as the variable pair in Fourier transformation. We take the plane wave as

$$e^{i(p\cdot r+p_0t)/\hbar} = e^{i(p\cdot r-Et)/\hbar} \equiv e^{i(k\cdot r-\omega t)},$$
 (3.3.1.1.1)

where  $\mathbf{k}$  is called wavevector (or wavenumber vector), and  $\boldsymbol{\omega}$  is called angular frequency.

$$\Psi(r,t) = \Psi(x,y,z,t) = \frac{1}{(2\pi)^{4/2}} \int_{-\infty}^{+\infty} dk d\omega \overline{\Psi}(k,\omega) e^{i(k \cdot r - \omega t)}.$$
 (3.3.1.1.2)

$$\overline{\Psi}(k,\omega) = \overline{\Psi}(k_x, k_y, k_z, \omega) = \frac{1}{(2\pi)^{4/2}} \int_{-\infty}^{+\infty} dr dt \Psi(r, t) e^{-i(k \cdot r - \omega t)}.$$
(3.3.1.1.3)

The notations, dr and dk, when they follow an integral symbol, are merely shorthand notations for dr = dxdydz and  $dk = dk_xdk_ydk_z$ , and the single integral signs preceding drdtand  $dkd\omega$  are shorthand for integrals over all 4-D spacetime and 4-D wavevector  $(k, \omega)$ , respectively.

$$\Psi(r,t) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{+\infty} d\omega \overline{\Psi}(r,\omega) e^{-i\omega t}.$$
 (3.3.1.1.4)

$$\overline{\Psi}(r,\omega) = \overline{\Psi}(x,y,z,\omega) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{+\infty} dt \Psi(r,t) e^{i\omega t}.$$
(3.3.1.1.5)

$$\Psi(r,t) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{+\infty} dk_z \overline{\Psi}(x,y,k_z,t) e^{izk_z}.$$
 (3.3.1.1.6)

$$\overline{\Psi}(x, y, k_z, t) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{+\infty} dz \Psi(x, y, z, t) e^{-izk_z}.$$
(3.3.1.1.7)

The function in Eq. (3.3.1.1.2) is called wavepacket or wavepacket-function in 4 dimensional spacetime. [We would like to stress that quantum mechanics does not need to know the particular or special forms of the wavepackets (=wavepacket-functions) at all. The solutions of Schrödinger equations are called wavefunctions, which is also called guide-factors.] The function in Eq. (3.3.1.1.3) is called a wavepacket in four wavevector (or, momentum) space or Fourier transform of  $\Psi(r,t)$ . Because  $\hbar k = p$ , and **p** represents momentum, we also call the function in Eq. (3.3.1.1.3) a wavepacket in four momentum space. Similarly, we can also define a time function and its Fourier transform (frequency function).

#### 3.3.1.2. Phase and Number of Plane Waves

We show that the number of plane waves, N, and the phases of plane waves,  $\phi$ , can be the variable pair of Fourier transformations. Assume that a function is a direct product of many plane waves. Its form is

$$e^{i(k_1 \cdot r_1 + \phi) + \dots + i(k_N \cdot r_N + \phi)} = e^{i(k_1 \cdot r_1) + \dots + i(k_N \cdot r_N)} e^{iN\phi}.$$
(3.3.1.2.1)

Eq. (3.3.1.2.1) reminds us that  $e^{iN\phi}$  can be made as a basis to expands a function of particle number N,  $\Psi(N)$ . Generally,  $\Psi(N)$  is a complex function of  $N \in \mathbb{Z}$  ( $\mathbb{Z}$  means integers), and can be made Fourier expansion [26].

$$\Psi(N) = \frac{1}{(2\pi)^{1/2}} \int_{-\pi}^{+\pi} d\phi \overline{\Psi}(\phi) e^{iN\phi}.$$
 (3.3.1.2.2)

$$\overline{\Psi}(\phi) = \frac{1}{(2\pi)^{1/2}} \sum_{N=-\infty}^{N=+\infty} \Psi(N) e^{-iN\phi}.$$
(3.3.1.2.3)

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi e^{iM\phi} e^{-iN\phi} = \begin{cases} 0 & if \quad M \neq N \\ 1 & if \quad M = N, \end{cases}$$
(3.3.1.2.4)

# 3.3.1.3. Root-Mean-Square Deviation

The "root-mean-square deviation" of any variable, for examples,  $\Delta k_z$  of  $k_z$ ,  $\Delta x$  of x, are defined as follows.

$$\Delta k_z = \sqrt{\langle (k_z - \langle k_z \rangle)^2 \rangle}.$$
 (3.3.1.3.1)

We have defined that  $\sqrt{\langle (k_z - \langle k_z \rangle)^2 \rangle}$  as uncertainty of a variable in one dimension case in section 2.4 of chapter 2. In high dimension space the generalization is easy.

$$\sqrt{\frac{\int_{-\infty}^{+\infty} dx dy dk_z \overline{\Psi}^*(x, y, k_z, t)(k_z^2 - 2k_z < k_z > + < k_z >^2)\overline{\Psi}(x, y, k_z, t)}{\int_{-\infty}^{+\infty} dx dy dk_z \overline{\Psi}^*(x, y, k_z, t)\overline{\Psi}(x, y, k_z, t)}}, \qquad (3.3.1.3.2)$$

where  $\langle k_z \rangle$  is called "mean value" of  $k_z$ . The "mean-square deviation" is also called variance. Eq. (3.3.1.3.2) is the expression of  $\Delta k_z$ . Note that if  $\Psi$  satisfies normalized condition, then the denominator in Eq. (3.3.1.3.2) is equal to one.

$$\langle k_z \rangle = \frac{\int_{-\infty}^{+\infty} dx dy dk_z \overline{\Psi}^*(x, y, k_z, t)(k_z) \overline{\Psi}(x, y, k_z, t)}{\int_{-\infty}^{+\infty} dx dy dk_z \Psi^*(x, y, k_z, t) \Psi(x, y, k_z, t)}.$$
(3.3.1.3.3)

Note that  $\langle k_z \rangle$  can be a function of *t* through that  $\Psi(x, y, k_z, t)$  is a function of *t*.

$$\Delta x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle}$$
  
=  $\sqrt{\frac{\int_{-\infty}^{+\infty} dx dy dz \Psi^*(x, y, z, t) (x^2 - 2x \langle x \rangle + \langle x \rangle^2) \Psi(x, y, z, t)}{\int_{-\infty}^{+\infty} dx dy dz \Psi^*(x, y, z, t) \Psi(x, y, z, t)}},$  (3.3.1.3.4)

where

$$< x >= \frac{\int_{-\infty}^{+\infty} dx dy dz \Psi^{*}(x, y, z, t)(x) \Psi(x, y, z, t)}{\int_{-\infty}^{+\infty} dx dy dz \Psi^{*}(x, y, z, t) \Psi(x, y, z, t)}.$$
(3.3.1.3.5)

Note that  $\langle x \rangle$  can be a function of *t* through that  $\Psi(x, y, z, t)$  is a function of *t*.

#### 3.3.1.4. From Number to Operator

The two variables in Fourier transformation are called Fourier pair variables. We will prove in this subsubsection that any Fourier pair variables belong to non-commutation variables. Some textbooks like to call the non-commutation incompatible. The examples of such non-commutation pair variables are: any (canonical coordinate) and its (canonical conjugate momentum), any (canonical coordinate) and its (canonical conjugate momentum/ $\hbar$ ), (particle number) and (phase), and so on. Besides these non-commutation pair variables, there are some compositions of Fourier pair variables, which also belong to non-commutation pair variables, and is called Fourier pair variable compositions. For example, the two in the three components of angular momentum vector. In the following we will prove that the commutation relation of the non-commutation pair variables is not equal to zero, and there is the Heisenberg uncertainty relation between non-commutation pair variables.

**Theorem II: Operator representation of observable.** The two variables in Fourier pair variables construct two theirs own spaces. Any variable in its own space is a number, but in space of partner variable is an operator.

Let us at first make some qualitative illustrations for the theorem II. In the integrals of "mean values" of  $k_x^n$ ,  $k_y^n$ , and  $k_z^n$  in **k** space (or wavevector space, or momentum space. Momentum  $p_x = \hbar k_x$ .). The variables  $k_x^n$ ,  $k_y^n$ , and  $k_z^n$  are numbers. The conjugate spaces of  $k_x$ ,  $k_y$ ,  $k_z$  are x, y, z, respectively. In these spaces one can also write equivalent integrals of "mean values" of  $k_x^n$ ,  $k_y^n$ , and  $k_z^n$  according to the following two steps: (a). Transform  $k_x^n$ ,  $k_y^n$ , and  $k_z^n$  into operators  $\partial^n/(i^n\partial x^n)$ ,  $\partial^n/(i^n\partial y^n)$ , and  $\partial^n/(i^n\partial z^n)$ , respectively; (b). These operators have to operate just on  $\Psi$  other than on  $\Psi^*$  in the integral formula of average value. Let us write this theorem with one example.

$$\langle k_x^n \rangle = \frac{\int_{-\infty}^{+\infty} dk_x dy dz \overline{\Psi}^*(k_x, y, z, t) k_x^n \overline{\Psi}(k_x, y, z, t)}{\int_{-\infty}^{+\infty} dk_x dy dz dt \Psi^*(k_x, y, z, t) \Psi(k_x, y, z, t)}.$$
(3.3.1.4.1)

Eq. (3.3.1.4.1) can be changed into

$$< k_{x}^{n} >= \frac{\int_{-\infty}^{+\infty} dx dy dz \Psi^{*}(x, y, z, t) \frac{\partial^{n}}{i^{n} \partial x^{n}} \Psi(x, y, z, t)}{\int_{-\infty}^{+\infty} dx dy dz \Psi^{*}(x, y, z, t) \Psi(x, y, z, t)}.$$
(3.3.1.4.2)

Note the following two points: (1). The theorem II does not need that  $\Psi$  is normalized. If we do normalization, then it is convenient; (2). It is very important to note that in the integrand of Eq. (3.3.1.4.1), which is in wavenumber space, the  $k_x^n$  can be put anywhere because it is just a number (or a special operator = a constant.) However, in conjugate space, i. e., in the position space,  $k_x^n$  is a differential operator, and has to be put in between  $\Psi^*(x)$  and  $\Psi(x)$ . The operator representation of a variable was mentioned in section 2.4 of chapter 2.

**Proof.** The proof for Eq. (3.3.1.4.2) is as follows. We transform the Fourier transforms  $\overline{\Psi}(k_x, y, z, t)$  and  $\overline{\Psi}^*(k_x, y, z, t)$  in Eq. (3.3.1.4.1) into  $\Psi^*(x, y, z, t)$  and  $\Psi(x, y, z, t)$ . The nu-

merator becomes

$$\int_{-\infty}^{+\infty} dk_x dy dz \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{+\infty} dx \Psi^*(x, y, z, t) e^{ik_x x}$$
$$\frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{+\infty} dx' \left[ \frac{\partial^n}{(-i)^n \partial x'^n} e^{-ik_x x'} \right] \Psi(x', y, z, t), \qquad (3.3.1.4.3)$$

where the derivative is only for the factor  $\exp(-ik_x x')$ . The denominator becomes

$$\int_{-\infty}^{+\infty} dk_x dy dz \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{+\infty} dx \Psi^*(x, y, z, t) e^{-ik_x x}$$
$$\frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{+\infty} dx' \Psi(x', y, z, t) e^{ik_x x'}, \qquad (3.3.1.4.4)$$

We have supposed that the function  $\Psi \in \mathcal{M}(\mathbb{R})$ . Therefore,  $\Psi$  and its derivatives at any order approach sufficiently fast to zero at  $x = -\infty$  and  $x = +\infty$ . Making integrations by parts in Eq. (3.3.1.4.3), then Eq. (3.3.1.4.2) becomes

$$\langle k_x^n \rangle = \frac{\int_{-\infty}^{+\infty} dx dy dz \Psi^*(x, y, z, t) \frac{\partial^n}{i^n \partial x^n} \Psi(x, y, z, t)}{\int_{-\infty}^{+\infty} dx dy dz \Psi^*(x, y, z, t) \Psi(x, y, z, t)}.$$
(3.3.1.4.5)

Similarly to Eq. (3.3.1.4.5), we have

$$<\omega^{n}>=\frac{\int_{-\infty}^{+\infty}d\omega\overline{\Psi}^{*}(r,\omega)\omega^{n}\overline{\Psi}(r,\omega)}{\int_{-\infty}^{+\infty}d\omega\overline{\Psi}^{*}(r,\omega)\overline{\Psi}(r,\omega)}$$
$$=\frac{\int_{-\infty}^{+\infty}dt\Psi^{*}(r,t)\frac{\partial^{n}}{((-i)^{n}\partial t^{n})}\Psi(r,t)}{\int_{-\infty}^{+\infty}dt\Psi^{*}(r,t)\Psi(r,t)}.$$
(3.3.1.4.6)

The "mean value" of  $N^n$  can be defined as follows.

$$< N^{n} >= \frac{\sum_{N=-\infty}^{+\infty} \Psi^{*}(N) N^{n} \Psi(N)}{\sum_{N=-\infty}^{+\infty} \Psi^{*}(N) \Psi(N)}.$$
 (3.3.1.4.7)

By using the similar derivations as to obtain Eq. (3.3.1.4.5),  $\langle N^n \rangle$  can also be expressed as

$$< N^{n} >= \frac{\int_{-\pi}^{+\pi} d\phi \overline{\Psi}^{*}(\phi) \frac{\partial^{n}}{((-i)^{n} \partial \phi^{n})} \overline{\Psi}(\phi)}{\int_{-\pi}^{+\pi} d\phi \overline{\Psi}^{*}(\phi) \overline{\Psi}(\phi)}.$$
(3.3.1.4.8)

QED.

In summary,

$$N^n$$
 in N representation  $\rightarrow \frac{\partial^n}{((-i)^n \partial \phi^n)}$  in  $\phi$  representation. (3.3.1.4.9a)

$$\phi^n$$
 in  $\phi$  representation  $\rightarrow \frac{\partial^n}{((i)^n \partial N^n)}$  in N representation. (3.3.1.4.9b)

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$$k^n$$
 in k representation  $\rightarrow \frac{\partial^n}{(i)^n \partial x^n}$  in x representation. (3.3.1.4.9c)

$$\omega^n$$
 in  $\omega$  representation  $\rightarrow \frac{\partial^n}{(-i)^n \partial t^n}$  in t representation. (3.3.1.4.9d)

According to the corollary I,  $\hbar k$  is canonical conjugate momentum of canonical coordinate x, and the energy  $\hbar \omega$  is the minus value of canonical conjugate momentum of canonical coordinate t. Therefore, from Eqs. (3.3.1.4.9b-c) we obtain the operator expressions of the momentum and energy:

$$p^n = (\hbar k)^n$$
 in p representation  $\rightarrow \frac{(\hbar)^n \partial^n}{(i)^n \partial x^n}$  in x representation. (3.3.1.4.9e)

$$E^n = (\hbar \omega)^n$$
 in E representation  $\rightarrow \frac{(\hbar)^n \partial^n}{(-i)^n \partial t^n}$  in t representation. (3.3.1.4.9e)

On the one hand, p and x are the canonical conjugate variables in classical mechanics. On the other hand, p, x are Fourier pair variables in Fourier analysis. Note that in all references the operator representation of observable is given as a postulate.

#### 3.3.1.5. General Inequality of Product of Mean-Square Deviations

To make our statement clear and for the importance in quantum theory, we introduce some definitions.

The commutation relation (=commutator) of operators A and B is defined as [A,B]=AB-BA, which is still an operator. If  $[A,B]\Psi \neq 0$ , then A and B do not commute with each other, and A and B are non-commutation operators. If  $[A,B]\Psi=0$ , then A and B commute with each other, and A and B are commutation operators. More generally, for Fourier pair variable compositions *com*<sub>1</sub> and *com*<sub>2</sub>, if

$$[com_1, com_2]\Psi \equiv (com_1 com_2 - com_2 com_1)\Psi \neq 0, \qquad (3.3.1.5.1)$$

then  $com_1$  and  $com_2$  are non-commutation operators.

If average value of an operator is real, then this operator is called Hermitian operator (Proof is geven in section 5.2). Two variables of Fourier pair variables have real average values. Therefore, they are Hermitian operators. Fourier pair variable compositions consist of Fourier pair variables. Thus, the Fourier pair variable compositions are Hermitian operators as well.

**Theorem III: Non-commutation property.** The product of Fourier pair variables, *AB*, is without dimension, and [A, B] = i.

For Fourier pair variable compositions [A, B] = iC, where C is Hermitian operator.

**Proof.** For convenience, we consider a particular example. The more general proof is easy to obtain. Taking A = x and B = k, one obtains from Eq. (3.3.1.4.9)

$$[x,k]\Psi(x) = \left(x(-i)\frac{d}{dx} - (-i)\frac{d}{dx}x\right)\Psi(x)$$
  
=  $-ix\frac{d\Psi(x)}{dx} + i\frac{d\Psi(x)}{dx} + i\Psi(x) = i\Psi(x).$  (3.3.1.5.2*a*)

Therefore, for A = x and B = k, C = 1 is a special Hermitian operator. The key of this proof is in that one of Fourier pair variables is certainly an operator instead of a number. As an exercise, readers give general proof.

Considering the corollary I (momentum  $p = \hbar k$ ) and Eq. (3.3.1.5.2) yield

$$[x, p] = i\hbar. \tag{3.3.1.5.2b}$$

The Fourier pair variable compositions may be: for example,

(i)  $x^2$  and  $p_x$ ;

(ii) Any two in  $L_x$ ,  $L_y$ , and  $L_z$ . { $L_x$ ,  $L_y$ ,  $L_z$  are the three components of angular momentum [See Eq. (3.3.2.1.2) and section 6.1.1.]}.

The Eq. (6.1.1.9a) in subsection 6.1.1 of chapter 6 proves following formulas:

$$[L_x, L_y] = i\hbar L_z, \quad [L_y, L_z] = i\hbar L_x, \quad [L_z, L_x] = i\hbar L_y \quad (3.3.1.5.2c)(6.1.1.9a)$$

where  $C = L_z$ ,  $L_x$ ,  $L_y$  are Hermitian operators.

Next, let me give more general proof.

Suppose *A* and *B* are the two compositions of any Fourier pair variable compositions. Consider following integral inequality:

$$I(\xi) = (\xi A \Psi + iB \Psi, \xi A \Psi + iB \Psi) = \int |\xi A \Psi + iB \Psi|^2 dx dy dz \ge 0, \qquad (3.3.1.5.2d)$$

where  $\Psi$  is any function,  $\xi$  is any real parameter number. Using the Hermitian property of *A* and *B*, the Eq. (3.3.1.5.2d) can be written as

$$I(\xi) = (\xi A \Psi + iB\Psi, \xi A \Psi + iB\Psi)$$
  
=  $\xi^2 (A\Psi, A\Psi) + i\xi (A\Psi, B\Psi) - i\xi (B\Psi, A\Psi) + (B\Psi, B\Psi)$   
=  $\xi^2 (\Psi, A^2\Psi) + i\xi (\Psi, [A, B]\Psi) + (\Psi, B^2\Psi) \ge 0.$  (3.3.1.5.2e)

Considering that  $\xi$  are real number, Eq. (3.3.1.5.2e) requires  $(\Psi, [A, B]\Psi) = iC$ , where *C* is Hermitian operator. QED.

[A,B] is called commutation relation, which is an operator as well. Because  $[A,B] = iC \neq 0$ , A and B are called non-commutation operators.

**Theorem IV: Preparation for uncertainty relations.** If *W* is a real number, and  $\Delta \alpha$ ,  $\Delta \beta$  are two quantities, which satisfy

$$|\Delta \alpha|^2 - \lambda W + \lambda^2 |\Delta \beta|^2 \ge 0 \tag{3.3.1.5.3}$$

for all real number  $\lambda$ , then the product of these two quantities satisfies

$$|\Delta \alpha|^2 |\Delta \beta|^2 \ge \frac{1}{4} W^2 \tag{3.3.1.5.4}$$

**Proof.** It is easy to confirm that Eq. (3.3.1.5.3) is correct for  $\lambda \to \infty$ . To determine the sign of left hand side of Eq. (3.3.1.5.3) for finite values of  $\lambda$ , let us express Eq. (3.3.1.5.3) in terms of its roots in  $\lambda$ .

$$\lambda^2 |\Delta\beta|^2 - \lambda W + |\Delta\alpha|^2 = |\Delta\beta|^2 (\lambda - \lambda_1) (\lambda - \lambda_2), \qquad (3.3.1.5.5)$$

where  $\lambda_1$  and  $\lambda_2$  are the roots, which we write as

$$\lambda_1 = a_\circ - \Delta \tag{3.3.1.5.6}$$

and

$$\lambda_2 = a_\circ + \Delta, \tag{3.3.1.5.7}$$

where

$$a_{\circ} = \frac{W}{|2\Delta\beta|^2},\tag{3.3.1.5.8}$$

$$\Delta = \frac{\sqrt{W^2 - 4|\Delta\beta|^2 |\Delta\alpha|^2}}{2|\Delta\beta|^2}.$$
(3.3.1.5.9)

Since  $|\Delta\beta|^2$  is positive definite, Eq. (3.3.1.5.5) implies that

$$(\lambda - \lambda_1)(\lambda - \lambda_2) \ge 0.$$
 (3.3.1.5.10)

However, left hand side of Eq. (3.3.1.5.10) is negative for

$$\lambda_1 < \lambda < \lambda_2. \tag{3.3.1.5.11}$$

To solve this apparent contradiction, we substitute Eqs. (3.3.1.5.6) and (3.3.1.5.7) for  $\lambda_1$  and  $\lambda_2$  in the product

$$(\lambda - \lambda_1)(\lambda - \lambda_2) = (\lambda - a_\circ - |\Delta)(\lambda - a_\circ + |\Delta) = (\lambda - a_\circ)^2 - \Delta^2.$$
(3.3.1.5.12)

In order to satisfy Eq. (3.3.1.5.10), the right hand side must be  $\geq 0$ , which implies that  $\Delta^2 < 0$ , i. e.  $\Delta$  is pure imaginary,

$$\Delta = i|\Delta|. \tag{3.3.1.5.13}$$

Hence,

$$(\lambda - \lambda_1)(\lambda - \lambda_2) = (\lambda - a_\circ)^2 + |\Delta|^2.$$
 (3.3.1.5.14)

This is a positive definite quantity. We note that since W is real,  $a_{\circ}$  [defined by Eq. (3.3.1.5.8)] is real. For  $\Delta$  to be a pure imaginary we must have, from Eqs. (3.3.1.5.13) and (3.3.1.5.9),

$$4(\Delta\beta)^2(\Delta\alpha)^2 \ge W^2.$$
(3.3.1.5.15)

Eq. (3.3.1.5.15) concludes the proof of theorem IV. QED.

(

### 3.3.2. Uncertainty Relations

# 3.3.2.1. Theory

**Theorem V: Uncertainty relations.** Suppose that *A* and *B* represent the Fourier pair variable compositions or the Fourier pair variables (or, after we prove that  $p = \hbar k$  represents momentum and  $E = \hbar \omega$  represents energy, considering  $p = \hbar k$ ,  $E = \hbar \omega$ , and so on, the above statement becomes: Suppose that *A* and *B* represent the canonical conjugate pair variables or the canonical conjugate pair variable compositions) and *W* is given by

$$W = i \int_{-\infty}^{+\infty} dx dy dz \Psi^*(x, y, z, t) [A, B] \Psi(x, y, z, t)$$
  
$$\equiv i < \Psi | [A, B] | \Psi >, \qquad (3.3.2.1.1)$$

then

$$(\Delta A)^2 (\Delta B)^2 \ge \frac{|W|^2}{4}.$$
 (3.3.2.1.2)

The lowest bound in Eq. (3.3.2.1.2) is independent of time *t*, although the left hand side of Eq. (3.3.2.1.2) can be dependent on *t* through  $\Psi$ . The often used form of Eq. (3.3.2.1.2) is

$$(\Delta A)(\Delta B) = \sqrt{(\Delta A)^2} \sqrt{(\Delta B)^2} \ge \frac{|W|}{2}.$$
(3.3.2.1.3)

(In history, Heisenberg first proposed the uncertainty relation between coordinate and momentum. This and the following corollaries give a general proof for the uncertainty relations. For memory, we call Eq. (3.3.2.1.3) either uncertainty or Heisenberg uncertainty relation.)

**Proof.** From Eq. (3.3.2.1.1) and theorem III, we know that *W* are real. Theorem IV tells us that if

$$I(\lambda) = |\Delta A|^2 - \lambda W + \lambda^2 |\Delta B|^2 \ge 0$$
 (3.3.1.5.2)(3.3.2.1.4)

holds for any real number  $\lambda$ , then we have

$$|\Delta A|^2 |\Delta B|^2 \ge \frac{1}{4} W^2. \tag{3.3.2.1.5}$$

Now let us prove Eq. (3.3.2.1.4).

$$W' = i \int_{-\infty}^{+\infty} dx dy dz \Psi^*(x, y, z, t) [A - \langle A \rangle, B - \langle B \rangle] \Psi(x, y, z, t)$$
  
=  $i \int_{-\infty}^{+\infty} dx dy dz \Psi^*(x, y, z, t) \{ (A - \langle A \rangle) (B - \langle B \rangle) - (B - \langle B \rangle) (A - \langle A \rangle) \} \Psi(x, y, z, t)$   
=  $i \langle \Psi | [A, B] | \Psi \rangle = W.$  (3.3.2.1.6)

Considering the definitions  $|\Delta A|^2 = \langle (A - \langle A \rangle) \rangle \langle (A - \langle A \rangle) \rangle^*$ ,  $|\Delta B|^2 = \langle (B - \langle B \rangle) \rangle \langle (B - \langle B \rangle) \rangle^*$  and Eq. (3.3.2.1.6), the Eq. (3.3.2.1.4) can be written as

$$I(\lambda) = \int_{-\infty}^{+\infty} dx dy dz \Psi^*(x, y, z, t) |(A - \langle A \rangle) + i\lambda(B - \langle B \rangle)|^2 \Psi(x, y, z, t) \ge 0.$$
(3.3.2.1.7)

Eq. (3.3.2.1.7) holds for any real values of  $\lambda$ . Thus, from theorem IV we prove the theorem V. QED.

**Corollary II: Variables of function.** Any function  $\in \mathcal{M}(\mathbb{R})$  cannot depend on the two variables of Fourier pair variables or the two compositions of the Fourier pair variable compositions commonly at the same time, or, equivalently, any wavepacket-function  $\in \mathcal{M}(\mathbb{R})$  cannot depend on the two variables of canonical conjugate pair variables or the two compositions of canonical conjugate pair variable compositions commonly at the same time.

**Proof.** This corollary is equivalently to say that any function  $\in \mathcal{M}(\mathbb{R})$  cannot depend on the two non-commutation variables at the same time.

The theorem of uncertainty relations [Eq. (3.3.2.1.3)] indicates the existence of lowest bound. If A takes certain value, then  $\Delta A = 0$ , and thus  $\Delta B = \infty$ , which is not reasonable. QED.

Although this Corollary II can be proved very easy, but its significance is significant. As is well known, the Cartesian coordinate  $\mathbf{r}$  and the canonical conjugate momentum  $\mathbf{p}$  are Fourier pair variables. The wavepacket in physics describes an object. The wavepacket in mathematics is a function  $\in \mathcal{M}(\mathbb{R})$ . Corollary II tells us clearly that the function, corresponding to a wavepacket, can only be a function either  $\mathbf{r}$  or  $\mathbf{p}$ , but cannot be a function of both  $\mathbf{r}$  and  $\mathbf{p}$  at the same time.

**Corollary III-1: Object volume.** If any position space function  $\in \mathcal{M}(\mathbb{R})$  represents the distributions of mass or energy or charge or momentum of any object, including both massy and massless particle, then this object has to be three dimensional in position space.

**Proof.** If the object is two dimensional in (x, y) plane, then according to the Heisenberg uncertainty relation theorem, the *z* direction momentum and thus the energy of object are infinite, which is not reasonable.

**Corollary III-2: Zero point energy.** Any object has zero point energy, which is caused by Heisenberg uncertainty relation. This zero point energy is independent of temperature, and is not equal to zero even at 0 K.

**Proof.** From uncertainty relation  $\Delta p \cdot \Delta x \ge \hbar/2$  we deduce that if  $\Delta x < \infty$ , then  $\Delta p > 0$ , which means that the absolute value of momentum and, thus, kinetic energy of any object are larger than zero. This energy is called zero point energy.

In many cases the object is in potential field. The potential energy function is V(x). Next we show that even in potential field, the zero point energy exists still.

Suppose that the *x*-dependence of the potential energy is

$$H = \frac{p^2}{2m} + V(x) = \frac{p^2}{2m} + Ax^n, \quad (n \text{ is real})$$
(3.3.2.1.8)

The average value on any states is

$$< H > = \frac{\langle p^2 \rangle}{2m} + \langle V(x) \rangle = \frac{\langle p^2 \rangle}{2m} + A < |x|^n >$$

$$= \frac{\langle (p - \langle p \rangle)^2 \rangle + \langle p \rangle^2}{2m} + A < [(x - \langle x \rangle)^2 \rangle + \langle x \rangle^2]^{n/2} >$$

$$= \frac{(\Delta p)^2}{2m} + A < [(\Delta x)^2]^{n/2} > = \frac{(\Delta p)^2}{2m} + A < (\Delta |x|)^n >$$

$$\ge \frac{\hbar^2}{8m(\Delta x)^2} + A(\Delta x)^2]^{n/2}.$$
(3.3.2.1.9)

The first and second equalities come from definitions of average values. The third equality comes from  $\langle x \rangle = \langle p \rangle = 0$ . (Since  $\langle x \rangle$  and  $\langle p \rangle$  are independent of each other and of  $(\Delta p)^2$  and  $(\Delta x)^2$ , such a choice is always possible.) The fourth equality comes from the Heisenberg uncertainty relation  $(\Delta p)(\Delta x) \ge \hbar/2$ .

Eq. (3.3.2.1.9) clearly shows that the average value of *H* has minimum value. This minimum value is independent of temperature, and is called called zero point energy. The author of this textbook hopes that when readers know exact zero point energy of harmonic oscillator, seek zero point energy from Eq. (3.3.2.1.9) and make comparison. (The result of comparison is that two expressions are same.) When readers know exact zero point energy of hydrogen atom, seek zero point energy from Eq. (3.3.2.1.9) and make comparison. (The result of result of comparison is that two expressions only have difference of factor 2.)

#### **3.3.2.2.** Various Uncertainty Relations

Mathematician's statement on the uncertainty relations are: "The effective width of function, multiplied by effective width of its Fourier transform, cannot be less than certain minimum value" [26, 30]. However, the Fourier pair variables in mathematician's language are confined only within *position* ~ *wavenumber* and *time* ~ *frequency* [26, 30, 38]. Fourier pair variable compositions (such as  $L_x \sim L_y$ ,  $x \sim p^2$ , and so on have not yet been explored by mathematicians.

Let us prove many uncertainty relations for different Fourier pair variables and Fourier pair variable compositions.

(1) Uncertainty relations between two components of "angular momentum vector". The W in Eq. (3.3.1.2) becomes

$$W = i \frac{1}{\int_{-\infty}^{+\infty} dx dy dz \Psi^*(x, y, z, t) \Psi(x, y, z, t)} \times$$
$$\int_{-\infty}^{+\infty} dx dy dz \Psi^*(x, y, z, t) (L_z L_y - L_y L_z) \Psi(x, y, z, t)$$
$$= \langle L_x \rangle.$$
(3.3.2.2.1)

Substituting  $W = \langle L_x \rangle$  into Eq. (3.3.2.1.3) yields

$$(\Delta L_y)(\Delta L_z) \ge \frac{1}{2} | < L_x > |,$$
 (3.3.2.2.2)

where due to  $\hbar L_x$  is Hermitian operator,  $\langle L_x \rangle$  is real.  $(\Delta L_y)$ ,  $(\Delta L_z)$ , and  $\langle L_x \rangle$  can be dependent on *t* through  $\Psi(r,t)$ .

(2) Position~wavenumber,  $x \sim k_x$ , uncertainty relation. Similarly to "angular momentum", in this case

$$W = i < [x, k_x] >= i < \left[x, \frac{\partial}{i\partial x}\right] >= i^2 = -1.$$
 (3.3.2.2.3)

Substituting |W| = 1 into Eq. (3.3.2.1.3) yields

$$(\Delta x)(\Delta k_x) \ge \frac{1}{2}.$$
 (3.3.2.2.4)

 $(\Delta x)$  and  $(\Delta k_x)$  can be dependent on *t* through  $\Psi$ . However, the right hand side of Eq. (3.3.2.2.4) is independent of *t*.

Here, we give a more direct understanding for the uncertainty relation between x and  $k_x$ . As we know, in the aspect of dimension,  $k_x \propto 1/x$ . Therefore, if  $\Delta x$  is zero, then  $\Delta k_x = \infty$ . Of course, this simple understanding cannot obtain the lowest limit in Eq. (3.3.2.4).

(3) Time~angular frequency uncertainty relation. In this case

$$W = i < [\omega, t] >= i < \left[\frac{\partial}{-i\partial x}, t\right] >= i^2 = -1.$$
 (3.3.2.2.5)

Substituting |W| = 1 into Eq. (3.3.2.1.3) yields

$$(\Delta t)(\Delta \omega) \ge \frac{1}{2}.$$
 (3.3.2.2.6)

Eq. (3.3.2.2.6) is the uncertainty relation of angular frequency-time. Because  $f = \omega/(2\pi)$  the uncertainty relation of frequency-time is

$$(\Delta t)(\Delta f) \ge \frac{1}{4\pi}.\tag{3.3.2.2.7}$$

(4) Number~phase uncertainty relation, i. e.  $N \sim \phi$  uncertainty relation.

$$W = i < [N, \phi] >= i < \left[\frac{\partial}{i\partial\phi}, \phi\right] >= i^2 = -1.$$
(3.3.2.2.8)

Substituting |W| = 1 into Eq. (3.3.2.1.3) yields

$$(\Delta \phi)(\Delta N) \ge \frac{1}{2}.$$
 (3.3.2.2.9)

(5) Position(x)~wavenumber<sup>2</sup>( $k_x^2$ ) uncertainty relation. In this case

$$W = i < [x, k_x^2] >= i < xk_x^2 - k_x^2 x >$$
  
=  $i < xk_xk_x - k_xxk_x + k_xxk_x - k_xk_xx >= i < [x, k_x]k_x + k_x[x, k_x] >$   
=  $i < ik_x + ik_x >= -2 < k_x >$ . (3.3.2.2.10)

Substituting  $|W| = 2| < k_x > |$  into Eq. (3.3.2.1.3) yields

$$(\Delta x)(\Delta k_x^2) \ge | < k_x > |.$$
 (3.3.2.2.11)

(6) Position( $x^2$ )~wavenumber( $k_x$ ) uncertainty relation. In this case

$$W = i < [x^{2}, k_{x}] >= i < x^{2}k_{x} - k_{x}x^{2} >$$
  
=  $i < xxk_{x} - xk_{x}x + xk_{x}x - k_{x}xx >= i < x[x, k_{x}] + [x, k_{x}]x >$   
=  $i < ix + ix >= -2 < x >$ . (3.3.2.2.12)

Substituting |W| = 2| < x > | into Eq. (3.3.2.1.3) yields

$$(\Delta x^2)(\Delta k_x) \ge | < x > |.$$
 (3.3.2.2.13)

#### 3.3.2.3. Heisenberg Uncertainty Relations

From the corollary I we see that *wavenumber*  $\times \hbar = momentum$  and  $\omega\hbar = energy$ . Therefore, the Heisenberg uncertainty relations in subsection 3.3.2.2 can be expressed by other forms.

Eq. (3.3.2.2.2) becomes

$$(\Delta L_y)(\Delta L_z) \ge \frac{\hbar| < L_x > |}{2}. \tag{3.3.2.3.1}$$

The  $k_x$ ,  $k_x$ , and  $k_x$  in Eq. (3.3.2.2.1) are transformed into  $p_x$ ,  $p_x$ , and  $p_x$ .

Eq. (3.3.2.2.4) becomes

$$(\Delta x)(\Delta p_x) \ge \frac{\hbar}{2}.$$
(3.3.2.3.2)

Eq. (3.3.2.2.6) becomes

$$(\Delta t)(\Delta E) \ge \frac{\hbar}{2}.\tag{3.3.2.3.3}$$

Eq. (3.3.2.2.9) still is

$$(\Delta N)(\Delta \phi) \ge \frac{1}{2}. \tag{3.3.2.3.4}$$

Note that Eq. (3.3.2.3.4) does not contain  $\hbar$ .

Eq. (3.3.2.2.11) becomes

$$(\Delta x)(\Delta p_x^2) \ge \hbar | < p_x > |. \tag{3.3.2.3.5}$$

Eq. (3.3.2.2.13) becomes

$$(\Delta x^2)(\Delta p_x) \ge \hbar | < x > |. \tag{3.3.2.3.6}$$

#### 3.3.2.4. Comments on Heisenberg Uncertainty Relations

We make the following ten comments on Heisenberg uncertainty relations.

(1) Subsections 3.3.2.1-3 clearly show that Heisenberg uncertainty relations are inherent characteristics of any function  $\in \mathcal{M}(\mathbb{R})$ . Heisenberg uncertainty relations do not have a wee bit of connections with the so-called non-control disturbance of measurement instruments.

(2) To explain the Heisenberg uncertainty relation, Bohr proposed the so-called complementarity principle in 1927 and accepted by some scientists. According to the so-called complementarity principle, the observables obeying an uncertainty relation are called noncomplementary observables. Although some scientists accepted, but until now the so-called complementarity principle is still an ambiguous and vague concept. No body understands its actual physical meaning. From subsections 3.3.2.1-3 we can understand that quantum mechanics does not need the so-called complementarity principle. The two observables or, equivalently, two dynamical variables in uncertainty relations are only Fourier pair variables or Fourier pair variable compositions multiplied by  $\hbar^n$  ( $n = 1, 2, 3, \dots$ ).

(3) To derive uncertainty relations does not need at all the probability wave hypothesis for the wavefunction, proposed by Born in 1927. The root-mean-square deviation  $\Delta x$  means

that the particle, described by a wavepacket, mainly concentrates in the region  $\Delta x$ . The root-mean-square deviation  $\Delta \hbar k_x = \Delta p_x$  means that the momentum mainly concentrates in the region  $\Delta \hbar k_x$ . The product of  $\Delta x$  and  $\Delta \hbar k_x$  has lowest bound, which is in essence the characteristic of a non-commutation variables or operators, and is called Heisenberg uncertainty relation. The  $\Delta t$  corresponds to the time uncertainty of an object existence. For example, the  $\Delta t$  corresponds to time duration of a signal in radio technology. The  $\Delta E$  corresponds to the energy uncertainty in which the object must have mainly. (The  $\Delta \omega = \Delta E/\hbar$  corresponds to angular frequency width of a signal in radio technology.)

(4) If one tries to use a big wavepacket, to describe the big universe, then it is possible under the condition: the function is  $\in \mathcal{M}(\mathbb{R})$ , i. e., it has Fourier transform.

The reason is as follows. We have to require that the wavepacket as a function and its, at least, first order derivative over coordinate is sufficiently fast to approach zero at  $|r| \rightarrow \infty$  for derivation of uncertainty relation between x and  $k_x$  or  $p_x$ . Note that we can use the function without normalization to derive the Heisenberg uncertainty relations. Therefore, normalization condition does not be a necessary condition for the Heisenberg uncertainty relations.

(5) Let us give the following three examples. The three examples show that different wavefunction or wavepacket-function  $\Psi$  have different lowest bounds for the products of two root-mean-square deviations, and reductions of  $|\Psi(x,t)|^2$  at root-mean-square deviation of x are much different for different functions.

(i) Gaussian wavepacket at t = 0.

$$\Psi(x) = \frac{1}{\pi^{1/4}} e^{-x^2/2}, \qquad (3.3.2.4.1)$$

where the constant factor comes from normalization condition.

$$\Delta x = \sqrt{\int_{-\infty}^{+\infty} dx x^2 |\Psi(x)|^2} = \frac{1}{\sqrt{2}}.$$
(3.3.2.4.2)

$$\overline{\Psi}(k_x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx \Psi(x) e^{-ik_x x} = \frac{1}{\pi^{1/4}} e^{-k_x^2/2}, \qquad (3.3.2.4.3)$$

where the constant factor comes from normalization condition.

$$\Delta k_x = \sqrt{\int_{-\infty}^{+\infty} dk_x k_x^2 |\overline{\Psi}(k_x)|^2} = \frac{1}{\sqrt{2}}.$$
 (3.3.2.4.4)

Therefore, physical position-momentum uncertainty relation is

$$(\Delta x)(\hbar\Delta k_x) = \hbar \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} = \hbar \frac{1}{2}.$$
 (3.3.2.4.5)

The relative value  $|\Psi(x = \Delta x)|^2 / |\Psi(x = 0)|^2$  is 0.60653. The relative value  $|\overline{\Psi}(k_x = \Delta k_x)|^2 / |\overline{\Psi}(k_x = 0)|^2$  is 0.60653. If the normalized Gaussian function is

$$\Psi(x) = \frac{1}{a^{1/2}(2\pi)^{1/4}} e^{-x^2/(2a^2)},$$
(3.3.2.4.6)

$$\Delta x = \sqrt{\int_{-\infty}^{+\infty} dx x^2 |\Psi(x)|^2} = a.$$
(3.3.2.4.7)

$$\overline{\Psi}(k_x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx \Psi(x) e^{-ik_x x} = \sqrt{\frac{2a}{\sqrt{2\pi}}} e^{-a^2 k_x^2}, \qquad (3.3.2.4.8)$$

where the constant factor comes from normalization condition.

$$\Delta k_x = \sqrt{\int_{-\infty}^{+\infty} dk_x k_x^2 |\overline{\Psi}(k_x)|^2} = \frac{1}{2a}.$$
 (3.3.2.4.9)

Therefore, position-momentum uncertainty relation is

$$(\Delta x)(\hbar\Delta k_x) = \hbar a \frac{1}{2a} = \hbar \frac{1}{2}$$
 (3.3.2.4.10)

for any value of *a*.  $\hbar/2$  is the lowest bound for the product in uncertainty relation, and, thus, Gaussian wavepacket is called minimum wavepacket (which was demonstrated in subsections 3.3.2.1-3 by general mathematical formula.) The relative value of  $|\Psi(x)|^2$  at x = 0 and  $\Delta x = a$  is also 0.60653. The relative value of  $|\overline{\Psi}(k_x)|^2$  at  $k_x = 0$  and  $\Delta k_x = 2a$  is also 0.60653.

(ii) One dimensional function at t = 0

$$\Psi(x) = \frac{1}{\sqrt{2}} e^{-|x|/2}.$$
 (3.3.2.4.11)

$$\Delta x = \sqrt{\int_{-\infty}^{+\infty} dx x^2 |\Psi(x)|^2} = \sqrt{\Gamma(3)} = \sqrt{2}.$$
 (3.3.2.4.12)

$$\overline{\Psi}(k_x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx \Psi(x) e^{-ik_x x} = \frac{1}{\pi^{1/2} (0.5^2 + k_x^2)^{1/2}},$$
(3.3.2.4.13)

where the integration formula can be found in Ref. [39].

$$\Delta k_x = \sqrt{\int_{-\infty}^{+\infty} dk_x k_x^2 |\overline{\Psi}(k_x)|^2} = \frac{1}{\sqrt{2}}.$$
 (3.3.2.4.14)

Therefore, physical position-momentum uncertainty relation is

$$(\Delta x)(\hbar\Delta k_x) = \hbar\sqrt{2}\frac{1}{\sqrt{2}} = 1,$$
 (3.3.2.4.15)

where the value of product is larger than 1/2. This means that different function can have different lowest bound. The relative value at x = 0 and  $\Delta x = \sqrt{2}$  is  $|\Psi(x = \sqrt{2})|^2 / |\Psi(x = 0)|^2 = 0.243$ . The relative value at  $k_x = 0$  and  $\Delta k_x = 1/\sqrt{2}$  is  $|\overline{\Psi}(k_x = 1/\sqrt{2})|^2 / |\overline{\Psi}(k_x = 0)|^2 = 0.333$ .

(iii) One dimensional function at t = 0

$$\Psi(x) = \sqrt{\frac{3}{2\Gamma(1/3)}} e^{-|x|^3/2}.$$
(3.3.2.4.16)

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$$\Delta x = \sqrt{\int_{-\infty}^{+\infty} dx x^2 |\Psi(x)|^2} = \sqrt{\frac{1}{\Gamma(1/3)}} = 0.61098.$$
(3.3.2.4.17)

$$\overline{\Psi}(k_x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx \Psi(x) e^{-ik_x x}$$

$$=\frac{2\sqrt{2}}{\pi^{1/2}}\sqrt{\frac{3}{2\Gamma(1/3)}\int_{0}^{+\infty}dx\cos(k_{x}x)e^{-x^{3}/2}}.$$
(3.3.2.4.18)

$$\Delta k_x = \sqrt{\int_{-\infty}^{+\infty} dk_x k_x^2 |\overline{\Psi}(k_x)|^2} = 0.87074.$$
 (3.3.2.4.19)

Therefore, position-momentum uncertainty relation is

$$(\Delta x)(\hbar\Delta k_x) = \hbar(0.61098)(0.87074) = 0.53199\hbar, \qquad (3.3.2.4.20)$$

where the value of product is still larger than  $\hbar/2$ . The relative value at x = 0 and  $\Delta x = 0.61098$  is  $|\Psi(x = 0.61098)|^2/|\Psi(x = 0)|^2 = 0.79607$ . The relative value at  $k_x = 0$  and  $\Delta k_x = 0.87074$  is  $|\overline{\Psi}(k_x = 0.87074)|^2/|\overline{\Psi}(k_x = 0)|^2 = 0.63150$ .

(6) We point out by an exercise in chapter 10 that at present there are many mistakes on deriving and understanding the Heisnberg energy-time uncertainty relation.

(7) Chapter 10 will points out that one cannot confuse the energy-time uncertainty relation with the linewidth-lifetime uncertainty relation. They are different uncertainty relations. The lowest bound of the linewidth-lifetime uncertainty relation depends on the definitions of the lifetime and the linewidth, and its lowest bound can be zero in principle.

(8) To obtain number(N)-phase( $\phi$ ) uncertainty relation, the present methods in some references give many different definitions of the phase operator, and, naturally, the lowest bounds given by different authors are much different. In our derivation, the phase operator's form is definite.

(9) The necessary conditions in deriving uncertainty relation now in some references are to assume that the related quantities are operators, which's commutation relation is not equal to zero. Their method is established on operator representation assumption, and thus precludes us to understand the origin and essence of uncertainty relations. Subsections 3.3.2.1-3 exactly proved that all uncertainty relations are only the methematical characteristics of Fourier pair variables and Fourier pair variable compositions. In essence, Heisenberg uncertainty relations are characteristic of mathematical functions  $\in \mathcal{M}(\mathbb{R})$ . Physicists have to abandon any mysterious feeling for physical uncertainty relations.

(10) In future, the connection between quantum mechanics and mathematics will become more and more close, because many quantummechanical properties are simple mathematical properties of mathematical functions which can make Fourier transformations, or, simply say, which are  $\in \mathcal{M}(\mathbb{R})$ .

# **3.4.** Wavepacket-Only Theory

In this section we will explore the common properties of wavepacket-function, i. e., object. All the following properties of wavepacket-function do not need to concern its particular form; on the contrary, we just require the wavepacket-function is a function either coordinate or momentum, but not both at the same time.

# 3.4.1. Free Wavepacket Compositions

This textbook will establish common wavepacket-only theory on the massy particle (such as electron, sun, Earth, universe) and massless particle (such as photon and phonon), will derive all the three formulations of quantum mechanics, and will explain the relative concepts and pictures through 52 theorems, 15 corollaries, 1 law, and 1 criterion, and, at the same time, without any hypotheses, axioms, postulates, principles, paradoxes (for example Schrödinger cat paradox), guesses, and assumptions except the law.

Classical mechanics describes any object by a function which depends on both coordinates and momenta at the same time. Corollary II tells us that the wavepacket-function can depend on either coordinates or momenta, and cannot depend on both at the same time.

Note that in our textbook we use  $\Psi$  to represent both the wavepacket-function (=wavepacket) and the guide-factor (=wavefunction). Please do not make confusion for them. We always do not need to know the particular form of wavepacket-function. We allow the wavepacket-function is unknown.

In this textbook

objects = massy particles or massless particles, massy particles = electrons, airplanes, the Milky Way, finite Universe,..., massless particles = photons, phonons, graviton,....

In chapters 3 - 10, the wavepacket-only theory will derive whole quantummechanical conclusions and formulas without using a wee bit of particular information on the wavepacket-function form and the structure of object.

For convenience, let wavepacket-function  $\Psi$  satisfy normalization condition, i. e.,

$$\int_{-\infty}^{\infty} |\Psi(r,t)|^2 dr = \int_{-\infty}^{\infty} \Psi^*(r,t) \Psi(r,t) dr = 1.$$
 (3.4.1.1)

If wavepacket-function  $\Psi(r,t)$  satisfies the normalization condition, then, for example,  $m|\Psi(r,t)|^2$  and  $e|\Psi(r,t)|^2$  represent the true mass or charge position (not probability!) density of electron, respectively. If we take out the *m* and *e*, then  $|\Psi|^2$  represents the position density of actual object, which is of extension in position space.

For simplicity, we consider one dimensional wavepacket (in our language, wavepacket  $\equiv$  massy particle and/or massless particle). Suppose that the motion direction of wavepacket is along direction of x, and wavepacket  $\Psi(x)$  can have following Fourier transformation.

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk_x \overline{\Psi}(k_x) e^{ik_x x}, \qquad (3.4.1.2)$$

where  $\overline{\Psi}(k_x)$  satisfies

$$\overline{\Psi}(k_x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx \Psi(x) \mathrm{e}^{-ik_x x}.$$
(3.4.1.3)

From Eqs. (3.4.1.2) and (3.4.1.1) we have

$$\int_{-\infty}^{+\infty} dk_x |\overline{\Psi}(k_x)|^2 = 1.$$
 (3.4.1.4)

Because  $\overline{\Psi}(k_x)$  satisfies normalization condition Eq. (3.4.1.4),  $|\overline{\Psi}(k_x)|^2$  represents density in wavenumber space. If  $k_{xo}$  is defined as

$$k_{xo} = \sqrt{\langle (k_x)^2 \rangle} = \sqrt{\int_{-\infty}^{+\infty} dk_x (k_x)^2 |\overline{\Psi}(k_x)|^2}, \qquad (3.4.1.5)$$

then  $k_{x\circ}$  represents the root-mean-square of wavenumbers of wavepacket.

Let us consider a more general wavepacket-function (for simplicity, we set wavepacket=wavepacket-function)  $\Psi(x,t)$  which can be expressed by Fourier integral.

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk_x \overline{\Psi}(k_x) e^{i[k_x x - \omega(k_x)t]}.$$
(3.4.1.6)

This is general form of wavepacket-function. According to the corollary I, free particle of mass *m* has well defined momentum in, for example, *x* direction  $p = p_x e_x = \hbar k_x e_x$ , and the energy  $E = \hbar \omega = p_x^2/(2m) = \hbar^2 k_x^2/(2m)$ . Thus, the  $\omega(k_x)$  in Eq. (3.4.1.6) as function of  $k_x$  is known.

We make an expansion of  $\omega(k_x)$  around point  $k_{xo}$ .

$$\omega(k_x) = \omega(k_{x\circ}) + \frac{d\omega}{dk_x}\Big|_{k_{x\circ}} (k_x - k_{x\circ}) + \frac{1}{2} \frac{d^2\omega}{dk_x^2}\Big|_{k_{x\circ}} (k_x - k_{x\circ})^2.$$
(3.4.1.7)

To obtain an expansion expression of  $\omega(k_x)$  at  $k_{x\circ}$ , we take its non-relativistic form at first. From  $m = m_{\circ}/\sqrt{1 - v^2/c^2} \approx m_{\circ}$ , we have

$$\omega(k_x) = \frac{1}{\hbar} \frac{p_x^2}{2m} = \frac{1}{\hbar} \frac{\hbar^2 k_x^2}{2m}.$$
(3.4.1.8)

We can also take the relativistic form of  $\omega(k_x)$ . Then

$$\omega(k_x) = \frac{\sqrt{(\hbar k_x)^2 c^2 + m_o^2 c^4}}{\hbar}.$$
(3.4.1.9)

The group velocity  $v_g$  of wavepacket is defined as

$$v_g = \left. \frac{d\omega}{dk_x} \right|_{k_{xo}}.$$
 (3.4.1.10)

For non-relativistic form of  $\omega(k_x)$ 

$$v_{g,n-r} = \frac{\hbar k_{xo}}{m}.$$
 (3.4.1.11)

We would like to remind readers that the next theorem occupies the central position in the wavepacket-only theory.

**Theorem VI: free wavepacket compositions.** A wavepacket in free motion consists of product with three factors: guide-factor; front-factor; and body-factor.

**Proof.** Suppose  $E = \hbar \omega \propto k_x$ .

$$k_x x - \omega(k_x)t = k_x x - [\omega(k_{x\circ}) + v_g(k_x - k_{x\circ})]t, \qquad (3.4.1.12)$$

where  $k_{x\circ}$  is an absolute value of average wavenumber of wavepacket. Thus

$$\Psi(x,t) = e^{ik_{xo}v_g} e^{-i\omega(k_{xo})t} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk_x \overline{\Psi}(k_x) e^{ik_x(x-v_g t)}, \qquad (3.4.1.13)$$

which can be rewritten as

$$\Psi(x,t) = \mathrm{e}^{ik_{x\circ}v_g t} \times \mathrm{e}^{-i\omega(k_{x\circ})t} \times \Psi(x - v_g t, 0).$$
(3.4.1.14)

Set  $x = v_g t + x'$ , where x' represents any point of the wavepacket at t = 0. Substituting  $x - x' = v_g t$  into Eq. (3.4.1.14), we have

$$\Psi(x,t) = e^{ik_{x\circ}x - i\omega(k_{x\circ})t}e^{-ik_{x\circ}x'}\Psi(x',0) \equiv I \times II \times III.$$
(3.4.1.15)

The factors *I*, *II*, and *III* are called guide-factor, front-factor, and body-factor of wavepacket, respectively. It is very important to note that the time-dependence of values of x' and x have not yet been determined uniquely. Let us determine it in terms of mankind practice experience, experiment facts, and mathematics. Because many observed facts tell us that free electrons, protons, neutrinos, big body, and photons can be stable in a quite long time interval, do not spread, and move with a velocity v (in case of photon v = c) as an entity. Therefore, wavepacket-only theory has to think that the free particle does not spread. From Eq. (3.4.1.14) we see that  $v_g$  is the group velocity of free wavepacket. Therefore, we set  $v = v_g$  naturally. This means that if  $v_g \neq 0$ , then  $x' = x'(t = 0) + v_g t$ . Therefore,  $x = x' + v_g t = x'(t = 0) + 2v_g t$ . In case of photon,  $v_g = c$ , thus x = x'(t = 0) + 2ct. The factors I and II are only simple mathematical functions, i. e., plane waves. Therefore, the mass and/or charge and/or energy, and/or momentum can only be carried by factor *III*. This concludes the proof of theorem of wavepacket compositions. QED.

The guide-factor is a plane wave. Let us discuss its phase. Substituting x = x'(t = 0) + 2ct and  $x' = x'(t = 0) + v_g t$  into Eq. (3.4.1.15), we see the following two novel points. First, the concept of phase is still kept. Second, x and x' are time-dependent other than time-independent. Therefore, for the guide-factor the concept of phase velocity is not needed.

For photon  $\omega = ck_x$ , the expansion  $\omega(k_x) = \omega(k_{k\circ}) + c(k_x - k_{x_x\circ})$  is exact. Eq. (3.4.1.15) clearly shows that wavepacket of photon does not spread at all with time. However, if the expressions of  $\omega(k_x)$  are not linearly dependent on  $k_x$ , then we should keep the second and higher order expansions in Eq. (3.4.1.7) to show the non-spreading of free wavepacket (i. e., free particle). The following theorem in section 3.4.2 is devoted to solve this problem.

#### 3.4.2. Non-Spreading of Free Wavepacket

**Theorem VII: Free wavepacket non-spreading.** Free massy wavepacket with central symmetry and massless wavepacket do not spread at all with time.

**Proof.** That the free massless wavepacket (photon and phonon) does not spread at all with time can be obtained directly from theorem VI. Next, we discuss massy particle.

Suppose that there are contributions of second order term in the expansion of  $\omega(k_x)$  as a function of  $k_x$  [See Eq. (3.4.1.7)].

The meaning of central symmetry in one dimensional case, x, is that if the center of coordinate is taken at the center of wavepacket, then the wavepacket is an even function of x. Substituting Eq. (3.4.1.7) into Eq. (3.4.1.6) yields

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk_x \overline{\Psi}(k_x) e^{i[k_x x - \omega(k_{x\circ})t - \nu_g(k_x - k_{x\circ})t - \frac{\nu_{g,s}}{2k_{x\circ}}(k_x - k_{x\circ})^2 t]}.$$
 (3.4.2.1)

Supposing  $x'(t) + v_g t = x(t)$ , Eq. (3.4.2.1) becomes

$$\Psi(x,t) = e^{ik_{x\circ}x - i[\omega(k_{x\circ}) + \frac{k_{x\circ}v_{g,s}}{2}]t} e^{-ik_{x\circ}x'}$$
  
$$= e^{ik_{x\circ}x - i[\omega(k_{x\circ}) + \frac{k_{x\circ}v_{g,s}}{2}]t} e^{-ik_{x\circ}x'} \Psi[(x' + v_{g,s}t), t]. \qquad (3.4.2.2)$$

The definition of  $v_{g,s}$  can be found in Eq. (3.4.1.7).

We see that  $\Psi[(x' + v_{g,s}t), t]$  in Eq. (3.4.2.2) is more complex than  $\Psi(x', 0)$  in Eq. (3.4.1.15). However, we can show that both functions give the exactly same time-dependence for average value of  $\langle (x' + v_{g,s}t)^2 \rangle$ .

$$<[x'(t) + v_{g,s}t]^2 > \equiv <(x'')^2 > = \int_{-\infty}^{+\infty} dx''(x'')^2 \Psi^*(x'',t) \Psi(x'',t).$$
(3.4.2.3)

Eq. (3.4.2.3) becomes

$$<(x'')^{2}>=\frac{1}{2\pi}\int_{-\infty}^{+\infty}dx''(x'')^{2}\int_{-\infty}^{+\infty}dk_{x}\overline{\Psi}^{*}(k_{x})e^{-ik_{x}x''}e^{i\frac{v_{g,s}}{2k_{x\circ}}(k_{x})^{2}t}$$
$$\int_{-\infty}^{+\infty}dk'_{x}\overline{\Psi}(k'_{x})e^{ik'_{x}x''}e^{-i\frac{v_{g,s}t}{2k_{x\circ}}(k'_{x})^{2}}.$$
(3.4.2.4)

For the following calculations we need the particular forms of  $\overline{\Psi}(k_x)$  and  $\overline{\Psi}(k'_x)$ . Let us consider a Gaussian wavepacket.

$$\Psi_{gaussian}(x) = \frac{1}{\sqrt{a}(2\pi)^{1/4}} e^{-\frac{x^2}{4a^2}} = \frac{1}{2\pi} \int_{\infty}^{+\infty} dk_x \overline{\Psi}(k_x) e^{ik_x x}, \qquad (3.4.2.5)$$

and

$$\overline{\Psi}_{gaussian}(k_x) = \sqrt{\frac{2a}{\sqrt{2\pi}}} e^{-a^2 k_x^2}, \qquad (3.4.2.6)$$

where *a* is equal about to the size of a particle. Substituting Eq. (3.4.2.6) into Eq. (3.4.2.4) and finishing the integrations over  $k_x$ ,  $k'_x$  and x'' [39], we obtain

$$<[x''(t)]^2>=a^2+rac{v_{g,s}^2t^2}{4a^2(k_{xo})^2}.$$
 (3.4.2.7)

Substituting Eq. (3.4.2.6) into Eq. (3.3.1.5) yields  $(k_{xo})^2 = 1/(4a^2)$ , and, therefore, Eq. (3.4.2.7) becomes

$$< [x'(t) + v_{g,s}t]^2 > = < [x''(t)]^2 > = a^2 + (v_{g,s}t)^2.$$
 (3.4.2.8)

On the other hand, if we use  $\Psi(x',0)$  instead of  $\Psi[(x'+v_{g,s}t),t]$  to calculate timedependence of  $\langle [x'(t)+v_{g,s}t]^2 \rangle$ , then we obtain

$$< [x'(t) + v_{g,s}t]^2 > = < [x'(t)]^2 > + (v_{g,s}t)^2 = a^2 + (v_{g,s}t)^2.$$
 (3.4.2.9)

In the derivations of Eqs. (3.4.2.8) and (3.4.2.9) we have used the central symmetry of the particle. Considering  $\Psi[(x' + v_{g,s}), t]$  and  $\Psi(x', 0)$  can give the same time-dependence for the average values, we always use  $\Psi(x', 0)$  instead of  $\Psi[(x' + v_{g,s}t), t]$ . This replacement is equivalent to say that the effect of factor  $v_{g,s}$  in the  $x' + v_{g,s}t$  of integrand of  $\Psi[(x' + v_{g,s}t), t]$  is the same as the effect of the explicit *t*-dependent factor  $exp[-iv_{g,s}(k_x)^2t/(2k_{xo})]$  of integrand of  $\Psi[(x' + v_{g,s}t), t]$ . It is obvious that after this replacement, the  $\Psi(x, t)$  in Eq. (3.4.2.2) does not spread. QED.

This theorem indicates also that even we consider the high order approximations in the expansion of  $\omega(k_x)$ , the free wavepacket still consists of factors *I*, *II*, and *III* in Eq. (3.4.2.4).

Some references concluded from Eq. (3.4.2.8) or similar expressions that a wavepacket (which represents a real massy particle and massless photon) in free motion spreads with time certainly, and many wrong concepts are deduced from this wrong conclusion such as the inevitable spreading of a free wavepacket. However, this textbook obtains completely reverse conclusion from Eq. (3.4.2.8). We show that wavepackets with central symmetry in free motion do not spread at all with time.

The some references's reason of the so-called spreading of free wavepacket is as follows. Using the mathematical formula in Ref. [39], one can obtain from Eqs. (3.4.2.1) and (3.4.2.6)

$$|\Psi(x',t)|^2 = \frac{1}{\sqrt{2\pi}\sqrt{a^2 + (v_{g,s}t/2ak_{xo})^2}} e^{-x'^2/\{2[a^2 + (v_{g,s}t/2ak_{xo})^2]\}}.$$
 (3.4.2.10)

Using the  $|\Psi(x',t)|^2$  in Eq. (3.4.2.10), one can find the average value of  $(x' - \langle x' \rangle)^2$ 

$$<(x'-)^2>=a^2+(v_{g,s}t)^2.$$
 (3.4.2.11)

Some references concluded from Eq. (3.4.2.11) that the wavepacket will spread to whole space when  $t \to \infty$ , which contradicts sharply with the our conclusion that every point x' in the body-factor moves uniformly with velocity  $v = v_g$  if the wavepacket (i. e., particle) is free. In our derivation the x' in  $\Psi(x',t)$  of Eq. (3.4.2.11) is a definite function of t, i. e.  $x'(t) = v_g t$ , and the explicit t dependence in  $\Psi(x',t)$  of Eq. (3.4.2.11) cannot determine the time behavior of x'(t). The latter has its own time-linear relation. In our wavepacket-only theory the calculation of  $< (x' - < x' >)^2 >$  has to be as follows

$$<(x'-)^2>=<(v_gt-)^2>\equiv 0\neq a^2+(v_{g,s}t)^2,$$
 (3.4.2.12)

even we use Eq. (3.4.2.10).

In summary, we have the following four conclusions:

(1) The free wavepackets, such as free electrons, protons, atoms, phonons, photons, universe, and any big macroscopic bodies, do not spread with time, which is just as that observed in mankind practices;

(2) The wavenumber of guide-factor of wavepacket is  $k_{xo}$ .  $k_{xo} = p_{xo}/\hbar$ .

(3) The group velocity  $v_g$  of wavepacket and the velocity v of both massy and massless particles are equal each other.

(4) Although photon is not massy particle due to its zero rest mass, the wavepacket of photon does not spread with time. The phonon is also a wavepacket. Ref. [40] thinks that for phonon the wavepacket is a necessary concept. Any object has size or scale in position space, and thus connect with certain position function. It is natural that our universe consists of big and complex wavepacket. In other words, our universe is a wavepacket-only universe. Due to the necessity to explain experiments in section 3.4.7, the motion of wavepacket has to be of some characters. However, considering the conveniences, we will explain these characters in section 3.4.6, and then use these characters to explain experiments.

Considering the above exactly mathematical proofs, the expression of wavepacket given by Eq. (3.4.1.15) is exact. Remember that every point x' in body-factor moves with group velocity  $v_g$ , and  $x' = x'_o + v_g t$ . The x in guide-factor of wavepacket is  $x = x' + v_g t$ . In nonrelativistical quantum mechanics the body-factor of wavepacket is a rigid body without structure, corresponds to particle in classical meaning, such as an electron looks like a rigid sphere. However, in relativistical quantum mechanics, quantum electrodynamics, and quantum field theory, for example, a meson, a quark, or a proton are of structures, which look like a large wavepacket consisted of many small wavepackets. Our theorem of wavepacket compositions still holds water for the quark's and meson's wavepacket in the proton (For this conclusion, please refer to the following corollary VI.). An exact rigid sphere violates the special theory of relativity, because in a rigid sphere the interaction and the action are allowed to propagate with infinitely large speed.

### 3.4.3. Average Wavenumber of Wavepacket

According to the image or picture of free wavepacket in subsection 3.4.1, the guide-factor goes ahead with speed  $2v_g$ , and the front-factor and body-factor go together with speed  $v_g$ .

**Theorem VIII: Average wavenumber and average frequency.** The average wavenumber of wavepacket is  $\langle k_x \rangle = k_{x\circ}$ . The average frequency of wavepacket is  $\langle \omega \rangle = \omega(k_{x\circ})$ .

**Proof.** From Eqs. (3.4.1.15), (3.3.1.4.9c), and definition of average value, we have

$$\langle k_{x} \rangle = \int_{-\infty}^{\infty} dx \Psi^{*}(x,t) k_{x} \Psi(x,t)$$

$$= \int_{-\infty}^{\infty} dx \Psi^{*}(x,t) \frac{\partial}{i\partial x} \Psi(x,t)$$

$$= k_{xo}.$$

$$(3.4.3.1)$$

$$<\omega> = \int_{-\infty}^{\infty} dt \Psi^{*}(x,t) \omega \Psi(x,t)$$
  
= 
$$\int_{-\infty}^{\infty} dt \Psi^{*}(x,t) \frac{\partial}{-i\partial t} \Psi(x,t)$$
  
= 
$$\omega(k_{xo}).$$
 (3.4.3.2)

**Corollary IV: Average momentum and energy.** Average momentum of wavepacket is  $\langle p_x \rangle = \langle \hbar k_x \rangle = \hbar k_{x\circ}$ . Average energy of wavepacket is  $\langle E \rangle = \langle \hbar \omega \rangle = \hbar \omega(k_{x\circ})$ .

**Corollary V: Possible wave property.** A free object (universe, electron, photon, phonon, and so on) has wave property in principle. The wavenumber is determined by (*average momentum*)/ $\hbar$ , and frequency is determined by (*average energy*)/ $\hbar$ . (In history, de Bloglie first proposed the wave property of massy particle as a hypothesis in 1925. This corollary proves that the possible wave property of massy and massless particle.)

In subsection 3.4.7, basing on both inductive method and deductive method, we will establish a law of wavepacket, according to which we prove corollary VIII, which says that massy particle is of wave property, and prove corollary IX, which says that optical and acoustic waves has particle property. According to corollaries VIII and IX, we give the picture of so-called wave-particle duality, shown in the front-cover of this textbook.

#### **3.4.4.** Expressions of Free Wavepacket

#### 3.4.4.1. One Dimensional Cartesian Coordinate and Discrete Values of Wavenumber

According to the corollary I

$$E = \hbar \omega = \frac{h}{2\pi} \omega = hv = \frac{\hbar^2 k^2}{2m}.$$
 (3.4.4.1.1)

$$p = |p| = \hbar |k| = \hbar k. \tag{3.4.4.1.2}$$

We have used the following plane wave

$$\Psi_{k_x}(x,t) = Ae^{ik_x x - i\omega(k_x)t}$$
(3.4.4.1.3)

to expand the wavepacket-function.  $k_x$  represents the wavenumber. The wavenumber can take both discrete and continuous values. "Discrete" or "continuous" depend on two standard prescriptions for the normalization of  $\Psi_{k_x}(x,t)$ .

The first normalization method can be called periodic or discrete or box normalization. Here one divides up the space into units of *L*, with (-L/2 < x < +L/2), and the number of intervals *L* can be infinite.), in which the plane wave  $\Psi_{k_x}(x,t)$  is taken to be periodic, (The second normalization method can be called  $\delta$  function or continuous normalization. See the next.)

$$\Psi_{k_x}(x,t) = Ae^{ik_x x - i\omega(k_x)t} = Ae^{ik_x(x+L) - i\omega(k_x)t} = \Psi_{k_x}(x+L,t).$$
(3.4.4.1.4)

From Eq. (3.4.4.1.4) we know that the wavenumbers k are then discrete, satisfying the relation  $Lk_n = 2\pi n$ , where n is an integer. Thus we have

$$k_n = \frac{2\pi n}{L}, \quad E_n = \frac{2n^2\pi^2\hbar^2}{mL^2}, \quad n = 0, \pm 1, \pm 2, \cdots$$
 (3.4.4.1.5)

The function  $\Psi_{k_x}(x,t)$  becomes

$$\Psi_n(x,t) = Ce^{ik_n x - i\omega(k_n)t}, \quad -\frac{L}{2} < x < \frac{L}{2} \quad . \tag{3.4.4.1.6}$$

For convenience, we use normalization in the traditional manner as follows:

$$\int_{-L/2}^{+L/2} dx \Psi_m^*(x,t) \Psi_n(x,t) = \delta_{mn}.$$
 (3.4.4.1.7)

The normalization constant is found to be  $C = 1/\sqrt{L}$ , and, hence,

$$\Psi_n(x,t) = \frac{1}{\sqrt{L}} e^{ik_n x - i\omega(k_n)t} \equiv \Psi_n(x) e^{\frac{-iE_n t}{\hbar}}, \quad -\frac{L}{2} < x < \frac{L}{2} \quad , \tag{3.4.4.1.8}$$

where  $\omega(k_n) = E_n/\hbar$  is given by Eq. (3.4.4.1.1). When we go to three dimensions, this type of normalization will be extended to the space divided up into units of cubes. This is then called "box normalization". We shall use this term even for normalizing in one or two dimensions. It is easy to show that  $\Psi_n(x)$  satisfies the completeness relation, i. e.,

$$\sum_{n} \Psi_{n}^{*}(x,t) \Psi_{n}(x',t) = \delta(x-x').$$
(3.4.4.1.9)

The second method of normalization involves the entire infinite space  $-\infty < x < +\infty$  by taking  $L \to \infty$ . This method leads to continuous values of  $k_x$ , and is thus called continuous method. Actually, continuous method can be deduced from discrete method. In order to do this we first start with the completeness relation Eq. (3.4.4.1.9) and insert expression Eq. (3.4.4.1.8) for  $\Psi_n(x)$ . The left hand side of Eq. (3.4.4.1.9) is then

$$\frac{1}{L}\sum_{n}e^{ik_{n}(x-x')}.$$
(3.4.4.1.10)

First we note that, since *n* runs over integers, the separation,  $\Delta n$ , between two adjacent values of *n*, is simply given by  $\Delta n = 1$  and so on. Hence,

$$\frac{1}{L}\sum_{n} e^{ik_{n}(x-x')} = \frac{1}{L}\sum_{n} (\Delta n)e^{ik_{n}(x-x')} \\
= \frac{1}{L}\sum_{n} \frac{L(\Delta k_{n})}{2\pi}e^{ik_{n}(x-x')} \\
= \frac{1}{2\pi}\sum_{n} (\Delta k_{n})e^{ik_{n}(x-x')}$$
(3.4.4.1.11)

with  $k_n$  given by Eq. (3.4.4.1.5), we find, therefore, that in the limit when *L* becomes large, the interval extends to  $(+\infty, -\infty)$ , and  $\Delta k_n$  becomes infinitesimal. Therefore,  $k_n$  can be replaced by a continuous variable, which designate as  $k_x$  in the interval  $(-\infty, +\infty)$ . Eq. (3.4.4.1.10), in the limit  $L \to \infty$ , can be written as

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} dk_x e^{ik_x(x-x')}, \qquad (3.4.4.1.12)$$

where we have replaced  $\Delta k_n$  by  $dk_x$  and the sum over *n* by an integral. From the properties of the Dirac  $\delta$  function, the integral above, indeed, reproduces  $\delta(x - x')$ . Thus our results are consistent with the completeness relation Eq. (3.4.4.1.9). We shall, therefore, write the  $\Psi_n(x)$  in Eq. (3.4.4.1.8) in  $(-\infty, +\infty)$  as

$$\Psi_{k_x}(x) = \frac{1}{\sqrt{2\pi}} e^{ik_x x} \quad with \quad p_x = \hbar k_x \quad (-\infty < x < \infty) \quad . \tag{3.4.4.1.13}$$

The completeness relation Eq. (3.4.4.1.9) now reads

$$\int_{-\infty}^{+\infty} dk_x \Psi_{k_x}^*(x) \Psi_{k_x}(x') = \delta(x - x').$$
 (3.4.4.1.14)

The function  $\Psi_{k_x}(x)$  also satisfy the orthogonal condition

$$\int_{-\infty}^{+\infty} dx \Psi_{k_x'}^*(x) \Psi_{k_x}(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dx e^{i(k_x - k_x')x} = \delta(k_x - k_x'), \qquad (3.4.4.1.15)$$

where instead of the Kronecker delta, which appeared for discrete wavenumbers, we have Dirac's  $\delta$  function on the right hand side.

Expression Eq.(3.4.4.1.13) for plane wave corresponds to the second way of normalization method, which here is referred to as  $\delta$  function and continuous normalization. We need to point out that in contrast to the box normalization, the  $\Psi_{k_x}(x)$  here cannot be normalized to unity since for  $k_x = k'_x$ , the right hand side of Eq. (3.4.4.1.15) becomes infinite. This is the price one has to pay by going from box to  $\delta$  function normalization, although both methods are correct for infinite position space.

In summary, a plane wave normalized with  $\delta$  function is

$$\Psi_{k_x}(x,t) = \Psi_{k_x}(x)e^{\frac{-iE_{k_x}t}{\hbar}}, \quad -\infty < x < +\infty \quad , \tag{3.4.4.1.16}$$

where  $E_{k_x} = \hbar^2 k_x^2 / (2m)$ .

# 3.4.4.2. Three Dimensional Cartesian Coordinate and Discrete Values of Wavenumber

In three dimensional case,

$$V = L_x L_y L_z. (3.4.4.2.1)$$

It is enough for expanding the wavepacket-function to use the most simple form of plane wave, which is as follows.

$$\begin{aligned} \Psi_{k_x,k_y,k_z}(x,y,z,t) &= Ae^{i[k_xx+k_yy+k_zz-\omega(k_x,k_y,k_z)t]} \\ &= Ae^{i(k_xx+L_x)}e^{i(k_yy+L_y)}e^{i(k_zz+L_z)}e^{-i\omega(k_x,k_y,k_z,t)} \\ &= \Psi_{k_x,k_y,k_z}(x+L_1,y+L_2,z+L_3,t). \end{aligned}$$
(3.4.4.2.2)

From Eq. (3.4.4.2.2) we know that the wavenumbers  $k_x$ ,  $k_y$ , and  $k_z$  are then discrete, satisfying the relation  $L_x k_{xn} = 2\pi n$ ,  $L_y k_{yl} = 2\pi l$ ,  $L_z k_{zm} = 2\pi m$ , where *n*, *l*, and *m* are an integer. Thus we have

$$k_{xn} = \frac{2\pi n}{L_x}, \quad E_{xn} = \frac{2n^2 \pi^2 \hbar^2}{mL_x^2}, \quad n = 0, \pm 1, \pm 2, \cdots$$
 (3.4.4.2.3)

$$k_{yl} = \frac{2\pi l}{L_y}, \quad E_{yl} = \frac{2l^2 \pi^2 \hbar^2}{mL_y^2}, \quad l = 0, \pm 1, \pm 2, \cdots$$
 (3.4.4.2.4)

$$k_{zm} = \frac{2\pi m}{L_z}, \quad E_{zm} = \frac{2m^2\pi^2\hbar^2}{mL_z^2}, \quad m = 0, \pm 1, \pm 2, \cdots$$
 (3.4.4.2.5)

Note that the *m* in  $k_{zm}$  does not represents mass. The function  $\Psi_{k_x,k_y,k_z}(x,y,z,t)$  becomes

$$\Psi_{nlm}(x, y, z, t) = C e^{ik_{xn}x - \omega(k_{xn})t} e^{ik_{yl}x - \omega(k_{yl})t} e^{ik_{zm}x - \omega(k_{zm})t}$$
  

$$\equiv \Psi_{nlm}(x, y, z) e^{-i\omega(k_{xn})t} e^{-i\omega(k_{yl})t} e^{-i\omega(k_{zm})t}, \qquad (3.4.4.2.6)$$

where

$$\frac{L_x}{2} < x < \frac{L_x}{2}, \quad -\frac{L_y}{2} < y < \frac{L_y}{2}, \quad -\frac{L_z}{2} < z < \frac{L_z}{2}$$
 (3.4.4.2.7)

For convenience, we make box normalization in the traditional manner as that taken in one dimensional case:

$$\int_{-\frac{L_x}{2}}^{+\frac{L_x}{2}} dx \int_{-\frac{L_y}{2}}^{+\frac{L_y}{2}} dy \int_{-\frac{L_z}{2}}^{+\frac{L_z}{2}} dz \Psi_{nlm}^*(x, y, z) \Psi_{n'l'm'}(x, y, z) = \delta_{nn'} \delta_{ll'} \delta_{mm'}.$$
 (3.4.4.2.8)

The normalization constant is found to be  $C = 1/\sqrt{L_x L_y L_z}$ , and, hence,

$$\Psi_{nlm}(x, y, z, t) = \frac{1}{\sqrt{L_x}} e^{ik_{xn}x - \omega(k_{xn})t} \frac{1}{\sqrt{L_y}} e^{ik_{yl}x - \omega(k_{yl})t} \frac{1}{\sqrt{L_z}} e^{ik_{zm}x - \omega(k_{zm})t}$$
$$\equiv \Psi_{nlm}(x, y, z) e^{-i\omega(k_{xn})t} e^{-i\omega(k_{yl})t} e^{-i\omega(k_{zm})t}, \qquad (3.4.4.2.9)$$

where  $\omega(k_{xn}) = E_{xn}/\hbar$  and so on are given by Eq. (3.4.4.1.1). For example,

$$\omega(k_{xn}) = \frac{E_{xn}}{\hbar} = \frac{1}{\hbar} \frac{\hbar^2 k_{xn}^2}{2m}.$$
 (3.4.4.2.10)

It is easy to show that  $\Psi_{nlm}(x, y, z, t)$  satisfies the completeness relation, i. e.,

$$\sum_{nlm} \Psi_{nlm}^*(x, y, z) \Psi_{nlm}(x', y', z') = \delta(x - x') \delta(y - y') \delta(z - z').$$
(3.4.4.2.11)

Let us demonstrate that even in three dimensional case and discrete values of wavenumber, a wavepacket (massy particle and massless photon) consist still of three factors similar to that given by Eq. (3.4.1.15). A wavepacket is a function  $\Psi(x, y, z, t)$ , which can be expanded as follows.

$$\Psi(x, y, z, t) = \sum_{n} \overline{\Psi}(k_{xn}) \frac{1}{\sqrt{L_x}} e^{i[k_{xn}x - \omega(k_{xn}t)]} \sum_{l} \overline{\Psi}(k_{yl}) \frac{1}{\sqrt{L_y}} e^{i[k_{yl}y - \omega(k_{yl}t)]}$$

$$\sum_{m} \overline{\Psi}(k_{zm}) \frac{1}{\sqrt{L_z}} e^{i[k_{zm}z - \omega(k_{zm}t)]}.$$
(3.4.4.2.12)

From Eq. (3.4.4.2.12) we have

$$\sum_{n} |\overline{\Psi}(k_{xn})|^2 = \sum_{l} |\overline{\Psi}(k_{yl})|^2 = \sum_{m} |\overline{\Psi}(k_{zm})|^2 = 1.$$
(3.4.4.2.13)

Because  $\overline{\Psi}(k_{xn})$ ,  $\overline{\Psi}(k_{yl})$ , and  $\overline{\Psi}(k_{zm})$  satisfy normalization conditions Eq. (3.4.4.2.13),  $|\overline{\Psi}(k_{xn})|^2$ ,  $|\overline{\Psi}(k_{yl})|^2$ , and  $|\overline{\Psi}(k_{zm})|^2$  represent probabilities in discrete wavenumber space, respectively. If  $k_{xo}$  is defined as

$$k_{xo} = \sqrt{\langle k_{xn}^2 \rangle} = \sqrt{\sum_{n} k_{xn}^2 |\overline{\Psi}(k_{xn})|^2}, \qquad (3.4.4.2.14)$$

then  $k_{x\circ}$  represents the average value of discrete wavenumbers  $k_{xn}$  of wavepacket. Similarly, we obtain  $k_{y\circ}$  and  $k_{z\circ}$ .

We make an expansion of  $\omega(k_{xn})$  around the point  $k_{xo}$ . [Refer to subsection 3.4.1.]

$$\omega(k_{xn}) = \omega(k_{xo}) + \frac{d\omega}{dk_{xn}}\Big|_{k_{xo}} (k_{xn} - k_{xo}) + \frac{1}{2} \frac{d^2 \omega}{dk_{xn}^2}\Big|_{k_{xo}} (k_x - k_{xo})^2.$$
(3.4.4.2.15)

To obtain an expansion expression of  $\omega(k_{xn})$  at  $k_{x\circ}$ , we can take, for example, the non-relativistic form. According to the de Bloglie relations, given by corollary I, for a non-relativistic particle, and  $m = m_{\circ}/\sqrt{1-v^2/c^2} \approx m_{\circ}$ , we have

$$\omega(k_{xn}) = \frac{1}{\hbar} \frac{p_{xn}^2}{2m} = \frac{1}{\hbar} \frac{\hbar^2 k_{xn}^2}{2m}.$$
 (3.4.4.2.16)

$$\omega(k_{yl}) = \frac{1}{\hbar} \frac{p_{yl}^2}{2m} = \frac{1}{\hbar} \frac{\hbar^2 k_{yl}^2}{2m}.$$
(3.4.4.2.17)

$$\omega(k_{zm}) = \frac{1}{\hbar} \frac{p_{zm}^2}{2m} = \frac{1}{\hbar} \frac{\hbar^2 k_{zm}^2}{2m}.$$
 (3.4.4.2.18)

The group velocities of wavepacket at x, y, and z directions are  $v_{xg}$ ,  $v_{yg}$ , and  $v_{zg}$ , respectively. They are defined as

$$v_{xg} = \left. \frac{d\omega}{dk_{xn}} \right|_{k_{xo}}.$$
(3.4.4.2.19)

$$v_{yg} = \left. \frac{d\omega}{dk_{yl}} \right|_{k_{yo}}.$$
(3.4.4.2.20)

$$v_{zg} = \left. \frac{d\omega}{dk_{zm}} \right|_{k_{zo}}.$$
 (3.4.4.2.21)

The velocity of free wavepacket (free particle) is  $v_g = (v_{xg}, v_{yg}, v_{zg})$ . For the non-relativistic form of  $\omega(k_x)$ 

$$v_{xg,n-r} = \frac{\hbar k_{xo}}{m}, \quad v_{yg,n-r} = \frac{\hbar k_{yo}}{m} \quad v_{zg,n-r} = \frac{\hbar k_{zo}}{m} \quad .$$
 (3.4.4.2.22)

For convenience, we take out the subscripts n - r. For the wavepacket in free motion we can prove the similar theorems as in subsection 3.4.1. For example,

**Theorem IX-1: Wavepacket compositions.** Even we use the plane waves with wavenumbers of discrete values to expand wavepacket-function, a free wavepacket in three dimensional position space still consists of product with three factors: guide-factor; front-factor; and body-factor.

**Proof.** At first we note that for the photon  $\omega = ck$ , there is no the second order term of k. However, for massy particle the second order approximation in Eq. (3.4.4.2.15) is not equal to zero. In this subsection we assume temporarily that the second order approximation term is equal to zero. One exercise requires to prove: If the Eq. (3.4.4.2.15) holds, then a wavepacket in free motion in three dimensional position space and discrete values of wavenumbers still does not spread and consists of product with three factors.

We take

$$k_{xn}x - \omega(k_{xn})t = k_{xn}x - [\omega(k_{x\circ}) + v_{xg}(k_{xn} - k_{x\circ})]t. \qquad (3.4.4.2.23)$$

$$k_{yl}y - \omega(k_{yl})t = k_{yl}y - [\omega(k_{y\circ}) + v_{yg}(k_{yl} - k_{y\circ})]t.$$
(3.4.4.2.24)

$$k_{zm}z - \omega(k_{zm})t = k_{zm}z - [\omega(k_{z\circ}) + v_{zg}(k_{zm} - k_{z\circ})]t.$$
(3.4.4.2.25)

Thus

$$\Psi(x, y, z, t) = e^{i[k_{xo}v_{xg} - \omega(k_{xo})]t} \frac{1}{\sqrt{L_x}} \sum_n \overline{\Psi}(k_{xn}) e^{ik_{xn}(x - v_{xg}t)}$$

$$e^{i[k_{yo}v_{yg} - \omega(k_{yo})]t} \frac{1}{\sqrt{L_y}} \sum_l \overline{\Psi}(k_{yl}) e^{ik_{yl}(y - v_{yg}t)} e^{i[k_{zo}v_{zg} - \omega(k_{zo})]t}$$

$$\frac{1}{\sqrt{L_z}} \sum_m \overline{\Psi}(k_{zm}) e^{ik_{zm}(x - v_{zg}t)}, \qquad (3.4.4.2.26)$$

which can be rewritten as

$$\Psi(x, y, z, t) = e^{i[k_{xo}v_{xg} - \omega(k_{xo})]t} \Psi(x - v_{xg}t, 0) e^{i[k_{yo}v_{yg} - \omega(k_{yo})]t} \Psi(y - v_{yg}t, 0)$$
  
$$e^{i[k_{zo}v_{zg} - \omega(k_{zo})]t} \Psi(z - v_{zg}t, 0). \qquad (3.4.4.2.27)$$

Set  $x = v_{xg}t + x'$ ,  $y = v_{yg}t + y'$ , and  $z = v_{zg}t + z'$ , where x'y'z' represent any point of the wavepacket at t = 0. Introducing x', y', z', Eq. (3.4.4.2.27) becomes

$$\Psi(x, y, z, t) = e^{ik_{\circ} \cdot r} e^{-ik_{x\circ} \cdot r' - i[\omega(k_{x\circ}) + \omega(k_{y\circ}) + \omega(k_{z\circ})]t} \Psi(r', 0)$$
  
$$\equiv I \times II \times III. \qquad (3.4.4.2.28)$$

It is very important to note that the time-dependence of value of r' has not yet been determined solely. Let us determine it in terms of mankind practice and mathematics. Because many observed facts tell us that free electrons, protons, neutrinos, photons, big macroscopic body are stable, do not spread at all, and move with a velocity v (in case of photon c instead of v) as an entirety. Therefore, wavepacket-only theory has to think that the free particle does not spread. From Eq. (3.4.1.15) we see that  $v_g$  is the group velocity of free wavepacket. Therefore, we set  $v = v_g$  naturally. This means that if  $v_g \neq 0$ , then  $x' = x'(t=0) + v_g t$ . Therefore,  $x = x' + v_g t = x'(t=0) + 2v_g t$ . In case of photon,  $v_g = c$ , thus x = x'(t=0) + 2ct. Eq. (3.4.4.2.28) clearly shows that a free wavepacket consists of the same three factors as that in Eq. (3.4.1.15). This concludes the proof. QED.

#### 3.4.4.3. Spherical Coordinates

**Theorem IX-2: Wavepacket compositions.** Even we use the spherical coordinate to expand wavepacket-function, a free wavepacket in three dimensional position space still consists of product with three factors: guide-factor; front-factor; and body-factor.

**Proof.** For the free wavepacket traveling in the *x* direction, the wavepacket is given by Eq. (3.4.1.15).

$$\Psi(x,t) = e^{ik_{xo}x}e^{-i\omega(k_{xo})t}e^{-ik_{xo}x'}\Psi(x',0) = e^{ik_{xo}x}e^{-i\omega(k_{xo})t}e^{-ik_{xo}x'}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}dk_{x}\overline{\Psi}(k_{x})e^{ik_{x}x'}.$$
(3.4.4.3.1)

If we take the wave vector k is in the x direction and the  $\theta$  is the angle between k and **r**. The factors  $exp(ik_xx') = exp(ikr'cos\theta)$  and  $exp(ik_{x\circ}x) = exp(ik_{\circ}rcos\theta)$ . In spherical coordinate

$$e^{ikx'} = e^{ikr'\cos\theta} = \sum_{l=0}^{\infty} (2l+1)i^{l}j_{l}(kr)P_{l}^{m}(\cos\theta)e^{im\phi}$$
  
=  $\sum_{l=0}^{\infty} (2l+1)i^{l}j_{l}(kr)P_{l}(\cos\theta),$  (3.4.4.3.2)

where  $m = 0, \pm 1, \pm 2, \cdots$ . Considering that  $exp(ikr'cos\theta)$  does not depend on  $\phi$ , one must take m = 0. The details of derivations for Eq. (3.4.4.3.2) can be found in chapter 6.  $j_l(kr')$  is spherical Bessel function with  $l = 0, 1.2, \cdots$ ,

$$j_l(kr') = (kr')^l \left(-\frac{d}{kr'd(kr')}\right)^l \frac{\sin(kr')}{kr'}.$$
 (3.4.4.3.3)

 $P_l^m(\theta)$  is Legendre polynomial. For m = 0

$$P_l(\cos\theta) = (-1)^l \frac{1}{2^l l!} \frac{d^l}{d(\cos\theta)^l} [1 - (\cos\theta)^2]^l.$$
(3.4.4.3.4)

$$P_l^m(\cos\theta) = [1 - (\cos\theta)^2]^{\frac{|m|}{2}} \frac{d^{|m|}}{d(\cos\theta)^{|m|}} P_l(\cos\theta).$$
(3.4.4.3.5)

In spherical coordinate

$$\Psi(x,t) = \Psi(r\cos\theta,t)$$
  
=  $e^{ik_{\circ}r\cos\theta}e^{-i\omega(k_{\circ})t}e^{-ik_{\circ}r'\cos\theta}\Psi(r'\cos\theta,0)$   
=  $e^{ik_{\circ}r\cos\theta}e^{-i\omega(k_{\circ})t}e^{-ik_{\circ}r'\cos\theta}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}dk\overline{\Psi}(k)e^{ikr'\cos\theta}.$  (3.4.4.3.6)

Eq. (3.4.4.3.2) can give the expressions in spherical coordinate for the factors exponential factors in Eq. (3.4.4.3.6). Therefore, from Eq. (3.4.4.3.6) we conclude that in spherical coordinate the theorems, proved in subsections 3.4.2 and 3.4.2, on the free wavepacket hold as well as that in Cartesian coordinate.

Eq. (3.4.4.2.27) gives the expression of free wavepacket in three dimensional Cartesian coordinates as follows.

$$\Psi(x, y, z, t) = e^{ik_{\circ} \cdot r} e^{-ik_{\circ} \cdot r' - i[\omega(k_{x\circ}) + \omega(k_{y\circ}) + \omega(k_{z\circ})]t} \Psi(r', 0)$$
  
$$= e^{ik_{\circ} \cdot r} e^{-ik_{x\circ} \cdot r' - i[\omega(k_{x\circ}) + \omega(k_{y\circ}) + \omega(k_{z\circ})]t}$$
  
$$\times \int dk_x dk_y dk_z \overline{\Psi}(k_x, k_y, k_z) e^{ir' \cdot k}, \qquad (3.4.4.3.7)$$

where

$$e^{ik_{\circ}\cdot r} = e^{ik_{\circ}\cos\theta r}, \qquad (3.4.4.3.8)$$

$$e^{-ik_{\circ}\cdot r'} = e^{-ik_{\circ}\cos\theta r'}, \qquad (3.4.4.3.9)$$

**r** and **r'** are in the same direction. In the integrand of Eq. (3.4.4.3.7) we take **r'** as the pole axis, the angle between **r'** and **k** is  $\theta'$ . then we have

$$e^{ik \cdot r'} = e^{ikr'\cos\theta'}.$$
 (3.4.4.3.10)

$$dk_x dk_y dk_z = k^2 \sin\theta dk d\theta d\phi. \qquad (3.4.4.3.11)$$

Substituting Eq. (3.4.4.3.2) into Eqs. (3.4.4.3.8), (3.4.4.3.9), (3.4.4.3.10), and then into Eq. (3.4.4.3.7) yields the expression of free wavepacket in spherical coordinate.

#### 3.4.4.4. Wavepacket-Only Theory of System Consisting of Many Different Particles

**Theorem IX-3: Wavepacket compositions.** For a system consisting of many different particles the wavepacket composition theorem VI is still correct.

**Proof.** A system consisting of many different particles can be looked as a system consisting of many separated and different wavepackets. Assume that we have two free wavepacket (i. e., two free particles)  $\Psi(r_1)$  and  $\Phi(r_2)$ . Of course, the wavepacket of two particles is

$$\Psi(r_1, r_2, t) = \Psi(r_1, t)\Phi(r_2, t)$$

$$= \frac{1}{\sqrt{2\pi^3}} \int dk_1 \overline{\Psi}(k_1) e^{ik_1 \cdot r_1} e^{-i\omega(k_1)t} \frac{1}{\sqrt{2\pi^3}} \int dk_2 \overline{\Phi}(k_2) e^{ik_2 \cdot r_2} e^{-i\omega(k_2)t}$$
$$= e^{ik_{1\circ} \cdot r_1 - i\omega(k_{1\circ})t} e^{-ik_{1\circ} \cdot r_1'} \Psi(r_1', 0) e^{ik_2 \cdot r_2 - i\omega(k_{2\circ})t} e^{-ik_{2\circ} \cdot r_2'} \Phi(r_2', 0).$$
(3.4.4.4.1)

For this two different wavepackets we can also use relative coordinates:

$$r = r_1 - r_2$$
 relative coordinate . (3.4.4.2)

$$R = \frac{1}{2}(r_1 + r_2)$$
 mass center coordinate. (3.4.4.4.3)

$$k = \frac{1}{2}(k_1 - k_2)$$
  $\hbar k$  relative momentum . (3.4.4.4.4)

$$K = k_1 + k_2 \quad \hbar K \quad total \quad momentum \; .$$
 (3.4.4.4.5)

Using relative coordinates, Eq. (3.4.4.1) can be rewritten as

$$\Psi(r_1, r_2, t) = \Psi(R, r, t)$$

$$= \frac{1}{2\pi^3} \int dK \int dk \overline{\Psi}(K, k) e^{iK \cdot R + ik \cdot r} e^{-i\omega(K)t - i\omega(kt)}$$

$$= e^{iK_\circ \cdot R} e^{-i\omega(K_\circ)t} e^{ik_\circ \cdot r} e^{-i\omega(k_\circ)t} e^{-iK_\circ \cdot R'} e^{-ik_\circ \cdot r'} \Psi(R', r', 0). \qquad (3.4.4.4.6)$$

Eq. (3.4.4.6) shows that in relative coordinates the theorem of wavepacket constitution Eq.(3.4.1.4) does not change.

Here, we just would like to mention that if the many identical single particle wavefunctions are together, then there might be some new physical requirements for the multiparticle wavefunction. Chapter 9 will prove that if many identical single particle guide-factors (guide-factor=wavefunctiion) are put together, then what the total multiparticle wavefunction should be?

# 3.4.5. Schrödinger Equation Determining Wavefunction

In this subsection we prove that the basic equation of quantum mechanics, i. e., Schrödinger equation, is the equation determining guide-factor ( $\equiv wave function$ ). Note that, for brevity, we use  $\Psi$  to represent both the wavefunction and wavepacket. However, we have to remember that the both are much different. If the  $\Psi$  appears in the Scrödinger equation, then it represents the wavefunction (i. e., guide-factor) definitely. In case of non-zero potential, although the guide-factor is not a plane wave, but the wavefunction and the guide-factor are still the same thing, i. e., the solution of Schrödinger equation.

# 3.4.5.1. One Dimensional Time-Dependent Schrödinger Equation of Free Wavepacket

We shall derive one dimensional time-dependent Schrödinger equation satisfied by guidefactor.

Eq. (3.4.1.15) gives general expression of one dimensional free wavepacket, which is

$$\Psi(x,t) = e^{ik_{xo}x - i\omega(k_{xo})t} \times e^{-ik_{xo}x'} \times \Psi(x',0)$$
  
$$\equiv I \times II \times III$$
  
$$\equiv \Psi(x,t) \times II \times III. \qquad (3.4.5.1.1)$$

In Eq. (3.4.5.1.1) we use  $\Psi(x,t)$  to represent the guide-factor. It is easy to verify the guide-factor *I* in Eq. (3.4.5.1.1) satisfies the following differential equation.

$$i\hbar\frac{\partial}{\partial t}e^{ik_{xo}x-i\omega(k_{xo})t} = \hbar\omega(k_{xo})e^{ik_{xo}x-i\omega(k_{xo})t} = \frac{\hbar^2 k_{xo}^2}{2m}e^{ik_{xo}x-i\omega(k_{xo})t}$$
$$= \frac{p^2}{2m}e^{ik_{xo}x-i\omega(k_{xo})t}$$
$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}e^{ik_{xo}x-i\omega(k_{xo})t}.$$
(3.4.5.1.2)

Considering new  $\Psi(x,t)$  in the third equality of Eq. (3.4.5.1.1), Eq. (3.4.5.1.2) can be written as

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t). \qquad (3.4.5.1.3)$$

Eq. (3.4.5.1.3) is the one dimensional time-dependent guide-factor equation of free wavepacket. This equation is called one dimensional time-dependent Schrödinger (wave) equation of free particle. The solution of this equation is called wavefunction. We should remember that Schrödinger equation in Eq. (3.4.5.1.3) is derived by wavepacket-only theory. Note that  $\Psi(x,t)$  in Schrödinger equation represents just the wavefunction (i. e., guide-factor of wavepacket) instead of wavepacket. Do not confuse the meanings of  $\Psi$  in different cases, because we use the same notation  $\Psi$  to represent both wavepacket-function and wavefunction.

# 3.4.5.2. Three Dimensional Time-Dependent Schrödinger Equation of Non-Free Wavepacket

**Theorem X: Schrödinger equation.** The guide-factor (=wavefunction) of wavepacket in potential V(r,t) satisfies generally the three dimensional time-dependent differential equation

$$i\hbar\frac{\partial}{\partial t}\Psi(r,t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r,t)\right]\Psi(r,t).$$
(3.4.5.2.1)

Eq. (3.4.5.2.1) is called Schrödinger equation, because Schrödinger proposed this equation in 1926.

**Proof.** The expression of a three dimensional free wavepacket is given by Eq. (3.4.4.2.27), which is

$$\begin{split} \Psi(x,y,z,t) &\stackrel{V=0}{=} e^{ik_{\circ}\cdot r - i\omega(k_{\circ})t} \times e^{-ik_{\circ}\cdot r'} \times \Psi(r',0) \\ &\stackrel{V=0}{\equiv} I \times II \times III \\ &\stackrel{V\neq0}{\equiv} \Psi(r,t) \times II \times III, \end{split}$$
(3.4.5.2.2)

where  $\Psi(r,t)$  in the third line of Eq. (3.4.5.2.2) corresponds to the guide-factor *I* in the second lines.

Let me argue that the reasonableness of the third line in Eq. (3.4.5.2.2). The terms *II* and *III* are independent of *t*. Therefore, we can think that the terms *II* and *III* are in potential field V = 0, and all the variations in case of  $V \neq 0$  appear in term *I*.

It is easy to verify that in case of V = 0, guide-factor I satisfies the following three dimensional differential equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(r,t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(r,t), \qquad (3.4.5.2.3)$$

where  $\Psi(r,t)$  represents the guide-factor (=wavefunction) other than the wavepacket and the body-factor! Eq. (3.4.5.2.3) is the three dimensional time-dependent guide-factor equation of free wavepacket, and is called three dimensional time-dependent Schrödinger equation of free particle.

Let us seek the equation satisfied by  $\Psi(x,t)$  in case of  $V(r,t) \neq 0$ . Theorem II in subsection 3.3.1.4 has proved that in spacetime representation

$$p \equiv \hbar k \to -i\hbar \nabla, \quad E \to i\hbar \frac{\partial}{\partial t},$$
 (3.4.5.2.4)

where *E* represents the total energy of the system.

ThusEq. (3.4.5.2.3) can formally be written as

$$E_{total}\Psi = \frac{p^2}{2m}\Psi = E_{kinetic}\Psi.$$
 (3.4.5.2.5)

If  $V \neq 0$ , then Eq. (3.4.5.2.5) is transformed naturally into

$$E_{total}\Psi = (E_{kinetic} + V)\Psi = E_{total}\Psi.$$
(3.4.5.2.6)

Considering the operator representations in Eq. (3.4.5.2.3) yields Eq. (3.4.5.2.1). QED.

Eq. (3.4.5.2.1) is called three dimensional time-dependent Schrödinger equation of the guide-factor of a non-free wavepacket. (guide-factor=wavefunction).

In section 5.8 of chapter 5 Schrödinger equation will be derived just from the proved commutation relation  $[x, p] = i\hbar$ . Due to that these derivation steps in section 5.8 of chapter 5 are more complex, we introduce here the above simple method to prove schrödinger equation.

**Corollary VI: Wavepacket non-spreading.** Any wavepacket never spreads in weak external field.

**Proof.** Look at the third equality of Eq. (3.4.5.2.1). The prominent character of this formula is that all the *x*- and *t*-dependences of wavepacket-function are contained just in the guide-factor. The substance of object exists in the the body-factor, which just contains x'(t).

Eq. (3.4.5.2.6) tells us that in external potential field, the guide-factor has variation, and the body-factor still keeps its original form. In other word, all the influences of potential field are just onto the guide-factor, and the body-factor does not suffer any perturbation. Therefore, the body-factor never spreads, which means wavepacket non-spreading.

This corollary needs weak field condition. If the field is strong enough, then the object can be broken and so on.

**Corollary VII: General wavepacket compositions.** The wavepacket (= object = particle = wavepacket-function) in potential field consists still of the three factors as the case of V(r,t) = 0. The sole difference is that the guide-factor in cases of  $V \neq 0$  obeys Schrödinger equation of  $V \neq 0$ .

**Proof.** This corollary comes from the third line of Eq. (3.4.5.2.2) and Eq. (3.4.5.2.1).

# 3.4.6. Other Methods to Obtain Schrödinger Equation

Although this textbook does not use the methods in subsections 3.4.6.1-2, but, considering to widen the readers' outlook, we introduce them here. Please make comparisons with the method in subsection 3.4.5.2. From these comparisons you will see that the way of science is tortuous, but the prospects are bright.

#### 3.4.6.1. Derivation of Schrödinger in 1926

Under the elicitation of Planck's (1900) and Einstein's (1905) quantum theory of light, de Bloglie proposed in 1925 that the massy particle has wave property. The next problem is how to establish an equation to describe the law of wave motion for a massy particle.

The physical idea of Schrödinger to derive this equation in 1926 is as follows. In the wave optics the wave of light is described by the following function:

$$Z = ae^{i\phi}, (3.4.6.1.1)$$

where *a* is amplitude, and  $\phi$  is phase. The variation of the phase relates with the wavelength. In physics, the light line in the geometric optics moves along the shortest path (Fermat principle). In mathematics, the Fermat principle is equivalent to that the phase variation is minimum. In view of this comparison, Schrödinger guessed that the phase of light wave might be equivalent to the Hamilton principle function or, say, action  $\mathcal{A}$  (for action see section 2.2 of chapter 2). Schrödinger tried to use the following function:

$$\Psi = Re^{i\frac{A}{\hbar}} \tag{3.4.6.1.2}$$

to describe the wave motion of a massy particle. Here, the appearance of  $\hbar$  in Eq. (3.4.6.1.2) is to make the phase without dimension. Schrödinger is familiar with Jacobi-Hamilton equation of particle.

$$\frac{\partial \mathcal{A}}{\partial t} + \frac{1}{2m} \left(\frac{\partial \mathcal{A}}{\partial x}\right)^2 + V(x) = 0.$$
(3.4.6.1.3)

Eq. (3.4.6.1.3) is energy conservative due to the time-independence of V(x). The first term equals -E, second term equals kinetic energy, and third term is potential field. Considering Eq. (3.4.6.1.2), Schrödinger guessed that

$$\frac{\partial \mathcal{A}}{\partial x} = -\frac{i\hbar}{\Psi} \frac{\partial \Psi}{\partial x}.$$
(3.4.6.1.4)

Considering the possibility of complex  $\Psi$ , Eq. (3.4.6.1.3) was rewritten as

$$-E + \frac{1}{2m} \left(\frac{\partial \mathcal{A}}{\partial x}\right)^* \left(\frac{\partial \mathcal{A}}{\partial x}\right) + V(x) = 0.$$
 (3.4.6.1.5)

Substituting Eq. (3.4.6.1.4) into Eq. (3.4.6.1.5) yields

$$[V(x) - E]\Psi^*\Psi + \frac{\hbar^2}{2m} \left(\frac{\partial\Psi^*}{\partial x}\right) \left(\frac{\partial\Psi}{\partial x}\right) = 0.$$
(3.4.6.1.6)

Schrödinger used the  $\mathcal{L}$  to express the left hand side of Eq. (3.4.6.1.6), took the  $\mathcal{L}$  as a Lagrangian density, which is a function of general coordinates:  $\Psi$ ,  $\Psi^*$ ,  $\partial \Psi / \partial x$ , and  $\partial \Psi^* / \partial x$ , and defined action

$$\mathcal{A} = \int_{t_1}^{t_2} dt L = \int_{t_1}^{t_2} \int_V dx \mathcal{L}$$
$$= \int_{t_1}^{t_2} \int_V dt dx \left\{ [V(x) - E] \Psi^* \Psi + \frac{\hbar^2}{2m} \left( \frac{\partial \Psi^*}{\partial x} \right) \left( \frac{\partial \Psi}{\partial x} \right) \right\}.$$
(3.4.6.1.7)

Eq. (3.4.6.1.7) is same as Eq. (2.2.8.2.4). Using the method from action to Euler-Lagrange equation Eq. (2.2.8.2.8), Schrödinger obtained corresponding Euler-Lagrange equation, which is

$$\frac{\partial \mathcal{L}}{\partial \Psi^*} - \frac{\partial}{\partial x} \left[ \frac{\partial \mathcal{L}}{\partial (\partial \Psi^* / \partial x)} \right] = 0, \qquad (3.4.6.1.8)$$

i. e.,

$$[V(x) - E]\Psi - \frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = 0, \qquad (3.4.6.1.9)$$

which is just the time-independent Schrödinger equation, i. e., the energy eigenequation of a particle in potential V(x). (For this subsubsection readers can see Refs. [1, 41])

Comments of this textbook for the works of Schrödinger in 1926:

Without any doubt, Schrödinger's works in 1926 is great, and promotes the development of quantum theory. The historical experiences are worth to notice. Next, we make some analyses for Schrödinger's works in 1926.

Classical mechanics is possible to calculate, for example, the vibrational models of a string, membrane, or resonator by solving a wave equation, subject to certain boundary conditions. At a very beginning of the development of quantum mechanics (1926), one was faced with the problem of finding a wave equation satisfied by wavefunction describing massy particle after proposition of the de Bloglie matter wave hypotheses. At the beginning time, one had to search for parallels in classical mechanics, and tried to "derive" the desired equation on the basis of plausible arguments. Such a wavefunction equation, not derived but guessed at intuitiveness, would then be a postulate of quantum mechanics, and its validity would have to be verified by experiments.

For the wavepacket-theory, the situation is much different. Just basing on the commutation relation  $[x, p] = i\hbar$ , proved by theorem III, the wavepacket-only theory will prove exactly in section 5.8 of chapter 5 all the three different formulations of quantum mechanics (Schrödinger wave equation, Heisenberg matrix, Feynman path integral) instead of any guesses.

#### 3.4.6.2. Another Method to Derive Time-Dependent Schrödinger Equation

Now let us introduce an another method to derive time-dependent Schrödinger equation, often being used in until now many textbooks [4]. This method requires to make three assumptions.

(i) First assumption. Assume that the equation has a plane wave solution, i. e., the solution  $\Psi(r,t)$  is

$$\Psi(r,t) = Ae^{i(k \cdot r - \omega t)}.$$
 (3.4.6.2.1)

In one dimensional case, Eq. (3.4.6.2.1) takes the form

$$\Psi(x,t) = Ae^{i(k_x x - \omega t)}.$$
 (3.4.6.2.2)

(ii) Second assumption. Use the de Bloglie matter wave hypotheses, mentioned in chapter 1, i. e.,  $p = \hbar k$  and  $E = \hbar \omega$ . Therefore,

$$\Psi(r,t) = A e^{i(p \cdot r - Et)/\hbar}.$$
(3.4.6.2.1)'

In one dimensional case, Eq. (3.4.6.2.1) takes the form

$$\Psi(x,t) = Ae^{i(k_x x - \omega t)} = Ae^{i(p_x x - Et)/\hbar}.$$
(3.4.6.2.2)'

If an equation is correct, then substituting Eqs. (3.4.5.6.1-2)' into it, we should get an equality. To find the wave equation conveniently in this method, we give the following differentiations with respect to x, y, z, and t of  $\Psi$  in Eqs. (3.4.6.2.1-2)'.

$$\frac{\partial}{\partial t}\Psi = -\frac{i}{\hbar}E\Psi, \quad \frac{\partial^2}{\partial t^2}\Psi = -\frac{1}{\hbar^2}E^2\Psi.$$
(3.4.6.2.3)

$$\frac{\partial}{\partial x}\Psi = \frac{i}{\hbar}p_x\Psi, \quad \frac{\partial^2}{\partial x^2}\Psi = -\frac{1}{\hbar^2}p_x^2\Psi. \tag{3.4.6.2.3}'$$

$$\frac{\partial}{\partial y}\Psi = \frac{i}{\hbar}p_y\Psi, \quad \frac{\partial^2}{\partial y^2}\Psi = -\frac{1}{\hbar^2}p_y^2\Psi. \tag{3.4.6.2.3}''$$

$$\frac{\partial}{\partial z}\Psi = \frac{i}{\hbar}p_z\Psi, \quad \frac{\partial^2}{\partial z^2}\Psi = -\frac{1}{\hbar^2}p_z^2\Psi. \tag{3.4.6.2.3}$$

The form of the wave equation applicable to many classical waves (electromagnetic wave, transverse waves on a string, plane sound waves in a gas, and so on) is

$$\frac{\partial^2 \Psi}{\partial t^2} = v^2 \frac{\partial^2 \Psi}{\partial x^2}, \qquad (3.4.6.2.4)$$

where v is real constant equal to the wave velocity. Substituting Eq. (3.4.6.2.3) into Eq. (3.4.6.2.4) yields

$$-E^2 \Psi = -v^2 p_x^2 \Psi. \tag{3.4.6.2.5}$$

$$E = v|p_x|. \tag{3.4.6.2.6}$$

From Eqs. (3.4.6.2.5) and (3.4.6.2.6)

$$E = \hbar v |k_x|. \tag{3.4.6.2.7}$$
For a non-relativistic free particle of mass m, the kinetic energy is

$$E = \frac{p_x^2}{2m}.$$
 (3.4.6.2.8)

The difference between Eqs. (3.4.6.2.8) and (3.4.6.2.7) shows that the wave equation Eq. (3.4.6.2.4) cannot be the wave equation governing the wavefunctions. We have thus to discard the differential equation Eq. (3.4.6.2.4).

It is observed that to get Eq. (3.4.6.2.8) other than Eq. (3.4.6.2.7), the differential equation should have first order derivative with respect to *t* and second order derivative with respect to *x*, that is

$$\frac{\partial \Psi}{\partial t} = \beta \frac{\partial^2 \Psi}{\partial x^2}, \qquad (3.4.6.2.9)$$

where  $\beta$  is a constant. Substituting Eq. (3.4.6.2.3) into Eq. (3.4.6.2.9) yields

$$-iE\Psi = -\beta \frac{p_x^2}{\hbar}\Psi, \qquad (3.4.6.2.10)$$

$$\beta = \frac{iE\hbar}{p_x^2}.$$
 (3.4.6.2.11)

From Eqs. (3.4.6.2.8) and (3.4.6.2.11) we have

$$\beta = \frac{i\hbar}{2m}.\tag{3.4.6.2.12}$$

Substituting Eq. (3.4.6.2.12) into Eq. (3.4.6.2.10) yields

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}.$$
(3.4.6.2.13)

Eq. (3.4.6.2.13) is Schrödinger equation satisfied by plane wave.

(iii). Third assumption. Assume that in potential field, i. e., when

$$E = \frac{p_x^2}{2m} + V(x,t) = \omega_{kin}(k_{xo})\hbar + V(x,t), \qquad (3.4.6.2.14)$$

the Eq. (2.4.1.13) can be extended to

$$i\hbar\frac{\partial\Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right)\Psi,$$
(3.4.6.2.15)

which is the desired one dimensional time-dependent Schrödinger equation for a wavefunction.

Comments:

Although the Eq. (3.4.6.15) is same as that from the wavepacket-only theory, but this another method requires three assumptions. The first assumption in this another method corresponds to the conclusion proved by theorem VI. The second assumption in this another method corresponds to the conclusion proved by corollaries I and IV. The third assumption in this another method is not an assumption in the wavepacket-only theory, because the wavepacket-only theory has proved that  $i\hbar\partial/\partial t$  represents the total energy, and  $-\hbar^2\nabla^2/(2m)$  just represents kinetic energy.

# 3.4.7. Wavepacket Motion Law and Explanations for Experiments

To connect a theory with experimental facts is very important because

(1) Any theory has to be verified by experiments; Practice is the only standard to test truth;

(2) The processes to use a theory to explain experimental facts are also processes to improve theory.

(3) The theory can predict new phenomena, some in which might be important for mankind life and science.

The quantum mechanics, based on wavepacket-only theory, has to explain, at leat, all the five experiments in sections 3.4.7.1-5. In these processes of our explanations, we use both inductive and deductive methods to find some necessary relations between the guide-factor and the body-factor of wavepacket. Let us interpret these necessary relations in detail as follows.

We have known that the body-factor is the substance of wavepacket, and the guide-factor is only a mathematical wavefunction (a plane wave for free particle). Does the guide-factor have positive action for wavepacket's motion? Let us seek the guide-factor's action. We make the following analyses:

(1) It is very important to note that according to the wavepacket composition theorems, the time variation appears just in the guide-factor. Therefore, we must have to connect the particle's motion with the guide-factor, i. e., the motion of body-factor has to obey guide of the guide-factor.

(2) On other hand, if the body-factor's motion obeys the guide of the guide-factor, then the particle is of wave property. Many experiments have observed this wave property.

(3) Further, we have known that the guide-factor can be a complex function. The body-factor cannot follow the guide of any complex functions. Therefore, we have to think that the body-factor obeys the guide of square of absolute value of the guide-factor.

(4) How does the guide-factor guide the body-fsactor's motion? In experiments of interference pattern of particles through double slit, the squares of absolute values of the guide-factor have a distribution on the screen in experiments. This distribution can be calculated because the guide-factor is a known plane wave in the double slit experiments. We have known that Born's probability density interpretation of wavefunction fits experimental facts, although the Born's connection between wavefunction and ensemble does not accepted by all physicists. Next, we hope: (i). That the Born's probability density interpretation of wavefunction is still correct; (ii). Wavefunction describes individual object other than ensemble. We find that if the guide of the guide-factor for motion of the body-factor is of equiprobability symmetry, and every time motion of the body-factor is a spontaneous equiprobability symmetry breaking, then our hopes (i) and (ii) can be realized, and the explanations for experimental facts, such as the interference pattern of particles through a double slit, can be done well.

To understand the following statement, readers need to read the subsection 3.5.3 at the

first.

Let us illustrate the equiprobability symmetry in detail. For convenience of statement, assume that the values of coordinate x on screen and observed square of absolute value of the guide-factor as a function of x take integers instead of actual continuous values. Suppose that the possible position number (i. e., the values of x) on double slit experimental screen in the Fig. 1.7 of chapter 1 are 17, and they are

$$x_1, x_2, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}, x_{13}, x_{14}, x_{15}, x_{16}, x_{17}.$$
(3.4.7.1)

The values of square of absolute value of the guide-factor on these 17 positions are

$$n_1 = 2, n_2 = 1, n_3 = 0, n_4 = 2, n_5 = 4, n_6 = 2, n_7 = 0, n_8 = 4, n_9 = 8,$$
  
 $n_{10} = 4, n_{11} = 0, n_{12} = 2, n_{13} = 4, n_{14} = 2, n_{15} = 0, n_{16} = 1, n_{17} = 2.$  (3.4.7.2)

The total value of squares of absolute values of the guide-factor on these 17 positions are 38. For statement convenience, we say 38 units. Of course, one body-factor can only choose one unit in the 38 units in every time motion. But, what is the choosing rule? This is a very important problem. We can look for the answer just from many experiments. The experiments of interference pattern of particles through double slit in Fig. 1.7 of chapter 1 and next subsection 3.4.7.1 can have many ways. For example, the particles can be electron, neutron, quite big molecule  $C_{60}$ , and photon. For example again, all the particles go through the double slit at the same time, or at one time just one particle goes through the double slit (Of course, in this way, one should do the same experiment, for example,  $N \times 38$  times. N is big integer.). According to analysis for large amount of experimental data, obtained in interference pattern of particles through double slit, we find that the body-factors choose one unit from the 38 units with equiprobability. The reason to conclude the equiprobability is as follows. When experimentalist made, for example,  $10 \times 38$ experiments of interference pattern of particles through a double slit, and every time experiment uses just one particle, the observed particle number distribution on the screen is nearly proportional to  $n_1 = 2, n_2 = 1, n_3 = 0, n_4 = 2, n_5 = 4, n_6 = 2, n_7 = 0, n_8 = 4, n_9 = 1, n_8 =$  $8, n_{10} = 4, n_{11} = 0, n_{12} = 2, n_{13} = 4, n_{14} = 2, n_{15} = 0, n_{16} = 1, n_{17} = 2$ . In the past 200 years this kind of experiments for photon (from 1804) and massy particle (from 1961) has been done more than, for example, 10<sup>3</sup> times, and the conclusions are same. The large amount of experiments indicate that the body-factors choose, for example, one unit in the 38 units with equiprobability. The subsequent question is that although the body-factor motion is of equiprobability symmetry, but the body-factors cannot remain in a undecided state in a long time, when the body-factor needs to make just one choice in, for example, the 38 units of the guide-factor. It is obviously that the body-factors will make choice without a wee bit of hesitations. Thus, the choice has occur in a uniquely way, i. e., spontaneous equiprobability symmetry breaking.

Based on the necessary of explaining large amount of experimental facts and on the wavepacket composition theorems, we deduce and induct a law of wavepacket motion:

#### Wavepacket motion law.

Any objects, including both massy and massless particles, are wavepackets.

Any objects have both wave and particle (corpuscle) properties because theirs wavepackets consist of guide-factor (which is also called wavefunction) and body-factor (which is substance of the object).

The motion of the body-factor accepts guide of the guide-factor. This guide is of equiprobability symmetry.

The actual motion of the body-factor is determined by spontaneous equiprobability symmetry breaking.

This spontaneous equiprobability symmetry breaking process is a still more microscopic process. In essence, this process is stochastic or random. In this process the momentum conservation, the energy conservation, the general and special theory of relativity and so on, determined by theories belonging to determinism, might be violated.

The equiprobability symmetry and spontaneous equiprobability symmetry breaking appear often in macroscopic phenomena and human society as well.

Example 1. Let us look at the macroscopic spontaneous magnetization phenomenon. In some solids individual ions have non-vanishing vector magnetic moments. Above a critical temperature  $T_c$ , the directions of vectors of magnetic moments are random, and thus the total magnetic moment is zero. However, below  $T_c$  the total magnetic moment is not zero, which is called spontaneous magnetization. For an isotropic system, the direction of spontaneous magnetization of a ferromagnetic body is of equiprobability. Therefore, no people knows this direction before appearance of the spontaneous magnetization.

Example 2. lottery ticket. Every equal-value lottery ticket is of equal probability to draw a prizewinning in a lottery. However, to draw a prizewinning in a lottery occurs in a way of spontaneous equiprobability symmetry breaking.

**Corollary VIII: Matter wave.** Massy particle (rest mass  $\neq 0$ ) has wave property. The wavenumber of the matter wave is  $k = p/\hbar$ , where k and p represent the average wavenumber and momentum of the marry particle, respectively. The angular frequency of the matter wave is  $\omega = E/\hbar$ , where  $\omega$  and E represent the average angular frequency and momentum of the marry particle, respectively.

**Proof.** From theorem I we know energy  $E = \hbar \omega$  and momentum  $p = \hbar k$ .

From theorem VI we know that a free wavepacket has a guide-factor, which is a plane wave. This plane wave has angular frequency  $\omega$  and wavenumber *k*.

From theorem VIII and corollary IV we know that the k and  $\omega$  appearing in the guide-factor are the average wavenumber and angular frequency of the wavepacket of massy particle, respectively.

From wavepacket motion law we know that the guide-factor guides the particle's motion according to spontaneous equiprobability symmetry breaking rule. Therefore, the k and  $\omega$  in the guide-factor con be observed. QED.

This corollary is equivalent to the de Bloglie matter wave hypotheses introduced in section 1.4 of chapter 1.

Corollary IX: Wave quantum property. Wave, such as light and acoustic wave, has

**Corollary IX: Wave quantum property.** Wave, such as light and acoustic wave, has quantum property. The energy and momentum of wave quantum are  $E = \hbar \omega$  and  $p = \hbar k$ , respectively. The wavenumber of the wave quantum is k, which is the average wavenumber of the wave quantum. The angular frequency of the wave quantum is  $\omega$ , which is the average angular frequency of the wavepacket of wave quantum.

**Proof.** From theorem I we know energy  $E = \hbar \omega$  and momentum  $p = \hbar k$ .

From theorem VI we know that a free photon and phonon wavepacket has a guidefactor, which is a plane wave. This plane wave has angular frequency  $\omega$  and wavenumber k.

From theorem VIII and corollary IV we know that the k and  $\omega$  appearing in the guidefactor are the average wavenumber and angular frequency of the wavepacket of wave quantum, respectively.

From wavepacket motion law we know that the guide-factor guides the wavepacket's motion according to spontaneous equiprobability symmetry breaking rule. Therefore, the k and  $\omega$  in the guide-factor can be observed. QED.

This corollary is equivalent to the Planck-Einstein quantum postulate of light introduced in section 1.2 of chapter 1.

# 3.4.7.1. Interference Pattern of Particles through a Grating or Double Slit

Wave propagation can be well explained by the Huygens-Fresnel principle. According to this principle, each point along the wave-front can act as a source of secondary waves. The Huygens-Fresnel principle is the very good method to explain the formation of wave diffraction or interference on the screen behind single or double slit and grating. Therefore, the formation of interference pattern on the screen (See Fig. 1.7.), when a beam of massy particles passes through a double slit or a grating, is a signature of that wave property of particle.

Recently, the interference pattern was observed in beam of big molecules of  $C_{60}$  [14, 42]. Refs. [14, 42] detected the central maximum and two first-order interference peaks in the pattern. The molecules had a most probable velocity of 117 meters per second, which correspond to a de Bloglie wavelength of wavepacket of 0.0047 nm. On the  $C_{60}$  grating interference experiment, Ref. [42] made the following three conclusions.

First, one of the deepest mysteries of quantum mechanics is that an interference pattern is formed even if there is only one particle in experimental set-up at any given time. All their observations support the viewpoint that each  $C_{60}$  interferes with itself only.

Second, the interactions of  $C_{60}$  with environment, such as the spontaneous emission of photons by the thermally exited molecules, could not reveal which slits they had passed through. Even the merely small possibility of being able to know which slits the particle passes through would be enough to wipe out the interference pattern. This phenomenon also observed in many other references.

Third, the same interference pattern for  $C_{60}$  molecules, that contained one or two atoms of  ${}^{13}C$  (the heavy isotope of carbon), can also be observed.

The above experimental results are easy to be explained by wavepacket motion law,

because the wavepacket itself contains purely plane wave factor, i. e. guide-factor, which's expression is like the light wave. The pattern is determined by the square of absolute value of the superposition of two plane waves, coming from the two slits, on the screen. (For grating, coming from the all slits) According to the wavepacket-only theory a free single  $C_{60}$ molecule has a guide-factor, which is a plane wave just like the light wave. After through the two slits or many slits, the guide-factor consists of the superposition of two or many waves. According to the equiprobability symmetry, the motion of the body-factor of wavepacket is determined by the square of the absolute value of the superposition of two or many waves. Similarly to the light wave, at the screen we observe a interference pattern. The two or many waves come from one free individual particle, and thus the interference on the screen is self-interference. If at every time just one individual  $C_{60}$  molecule goes from the source, and goes through the two or many slits, then according to equiprobability symmetry the individual particle will take a position on the screen due to spontaneous equiprobability symmetry breaking. Because one molecular cannot gives a interference pattern, we shall see on the screen that the  $C_{60}$  molecules look like to distribute on the screen randomly at the beginning step of the experiment. However, after longer time many  $C_{60}$  molecules will give on the screen a pattern exactly like the interference pattern determined by the interference of two or many plane waves. If we know that which slit does the  $C_{60}$  molecule pass through, then the equiprobability symmetry will be destroyed, and therefore the  $C_{60}$  molecule will move deterministically, and the interference pattern will be wiped out. If the  $C_{60}$  molecules contain one or two atoms of heavy isotope of carbon, then the the average wavenumber of  $C_{60}$  molecule has only a little change, and therefore the guide-factors have only a little change. Naturally, the interference pattern coming from different  $C_{60}$  molecules has only a little change.

#### 3.4.7.2. Interference Pattern of Photon through Grating or Double Split

Let us look at that how does the wavepacket-only theory explain the light interference. The observed single x-ray photon interference through a grating is as follows [43]. For photon  $\omega(k_x) = k_x c$ , and the group velocity of photon wavepacket  $v_g = c$ . The compositions of the photon wavepacket are the same as the massy particle. Therefore, the explanation for  $C_{60}$  in section 3.4.7.1 can be used to photon as well, and all the results in Ref. [43] can be explained. The number  $n_{emi}$  of photons emitted from light source is always larger than the number  $n_{pas}$  of photons which pass through the grating.  $n_{pas}/n_{emi} < 1$  is called light pupil function or screen function [44]. The equiprobability symmetry can explain  $n_{pas}/n_{emi} < 1$ . Some photons, emitted from source, will distribute on the grating uniformly because the squares of absolute value of plane wave at any point y, z on the grating are the same. Some photons will be obstructed by the non-slit parts on the grating. According to the equiprobability symmetry

$$\frac{n_{pas}}{n_{emi}} = \frac{W_{sp}}{W_{sp} + W_{sd}} < 1, \tag{3.4.7.2.1}$$

where  $W_{sp}$  is the width of slit, and  $W_{sb}$  is the distance between two nearest neighbor slits on the grating.

From subsections 3.4.7.1-2, we know that the wave property of photon and massy particle are exactly the same.

#### 3.4.7.3. Polarized Photon Experiment

To clearly explain the polarized photon experiment, let us at first learn the language of optics to make some preparations.

Assume that a so-called monochromatic light propagates along z direction, and the electric field intensity is

$$E = E_x \exp[i(k_z z - \omega t)]e_x + E_y \exp[i(k_z z - \omega t)]e_y, \qquad (3.4.7.3.1)$$

where

$$E_x = E_x^{\circ} \exp(i\alpha_x), \quad E_y = E_y^{\circ} \exp(i\alpha_y) \quad . \tag{3.4.7.3.2}$$

If  $E_y = 0$  and  $E_x = 0$ , then they are x- and y-linearly-polarized light, respectively. If  $E_x = E_y$ , then it is 45°-linearly-polarized light. If  $E_y = E_x \exp(i\pi/2)$  and  $E_y = E_x \exp(-i\pi/2)$ , then they are right and left dextrorotatory circle-polarized light, respectively.

The experimental results of polarized photon (or light) passing through polarizer (i. e., crystal tournaline thin piece) are as follows. Take the crystal axis of the polarizer to be along *x* direction. If incident photon is a x-linearly-polarized, then it can pass through the polarizer without a bit of absorptions. If incident photon is a y-linearly-polarized, then it is absorbed by the polarizer, and cannot pass through the polarizer. For the 45°-linearly-polarized photon (Note that photon is a wavepacket.), if at every time just set one single photon to pass through polarizer, then at the initial time, when there are only a few photons which pass through polarizer randomly. Just after a long time, when many single photons pass through polarizer, one can observe that half of photons pass as x linearly-polarized photon [1].

Let us use our wavepacket-only theory to explain above experimental results, and answer the question having not yet been answered by modern quantum mechanics. The photon as a quantum has an extension in position space. Photon is a wavepacket as well as electron. Considering wavepacket in Eq. (3.4.1.15), the formulas in Ref. [44], and that the light wave is a transverse wave, the wavepacket of the linearly-polarized photon is described by

$$\Psi(z,t) = (E_x e_x + E_y e_y) e^{ik_{zo}z - i\omega(k_{zo})t} e^{-ik_{zo}z'} \Psi(z',0), \qquad (3.4.7.3.3)$$

where z is the propagation direction of photon, and  $E_x$ ,  $E_y$  just belong to one photon. The  $\Psi(z,t)$  is called x- or y-linearly-polarized (or plane-polarized) photon wavepackets, and is a vector in the (x,y) plane. If  $E_x = E_y$  in Eq. (3.4.7.3.3), then  $\Psi(z,t)$  is called 45°-linearly-polarized photon wavepacket. According to  $(E_x e_x + E_y e_y) \cdot (E_x e_x + E_y e_y) = E_x^2 + E_y^2$  and the equiprobability symmetry, the body-factor of wavepacket will take x- or y-linearly-polarization with equiprobability before entering the polarizer. If one just observes a few photons, then the numbers of x- and y-linearly-polarized (or plane-polarized) photon (wavepackets) might be not equal to each other due to the fluctuation caused by the spontaneous equiprobability symmetry breaking. So, the experimental results of polarized photons of both a few and many single photon can be explained by our wavepacket-only theory well. Zeng proposed a question in 2010 in Ref. [1], i. e., how does the photon change its polarized state from 45°-linearly-polarized to x- or y-linearly-polarized, when the photon passes through the polarizer. The answer of our wavepacket-only theory is as

follows. When the guide-factor of  $45^{\circ}$ -linearly-polarized photon wavepacket meets polarizer, the body-factor will have the equal choice for the x- and y-linearly-polarized state. According to the equiprobability symmetry when the body-factor of wavepacket arrives in the polarizer, the body-factor of wavepacket will have the same probability to choose the xor y-linearly-polarized state. Therefore, according to wavepacket-only theory, there is no the so-called question that how does the photon change its polarized state in the polarizer, because before entering in the polarizer the probability already is definited.

### 3.4.7.4. Delayed-Choice Experiment

"Wave-particle duality" of light has dumbfounded physical scientists for more two centuries. Newton contended in 1672 that light was made up of individual particles while Hooke (who was utterly despised by Newton) wrote on the wave-like properties of light. In 1801, Thomas Young's double slit experiment demonstrated the wave-like properties of light. In 1905, Einstein revisited the theory of light acting as a particle to resolve conflicts between the wave theory of light and certain experimental results such as the photoelectric effect. The quantum mystery which cannot go away (in Feynmans words) of "wave-particle duality" is illustrated in a striking way by the delayed-choice thought experiment suggested by Wheeler [45, 46, 47]. In Wheeler's words: "We hope to choose whether the individual photons should act schizophrenically or not." [48] In this experiment [45], the configuration of a two-path interferometer is chosen after a single-photon pulse has entered it: either the interferometer is closed (i.e., the two paths are recombined), and the interference is observed, or the interferometer remains open and the path followed by the photon is measured. Refs. [45, 46] report an almost ideal realization of that Wheeler's experiment, where the light pulses are true single photons, allowing unambiguous which-way measurements, and the interferometer, which has two spatially separated paths, produces high visibility interference. Measurements in the closed configuration show interference with a visibility of 94%, while measurements in the open configuration allow us to determine the followed path with an error probability lower than 1% [45].

Wheeler's delayed choice thought experiment put the wave-particle complementarity principle of quantum mechanics to the test. The corresponding interpretation of the experiments is still a matter of debate. Some physicists are attempting to find a classical interpretation completely ignoring quantum mechanics altogether, while others consider the experiment relevant to explaining quantum decoherence. As with many classic thought problems, the realization of Wheeler's delayed choice experiment has answered one question and created several new ones. How does light know when to display wave-like or particle-like properties? Present popular answer to this was that the light can "sense" what the experiment is attempting to measure. Based on the initial "feel", light would decide whether or not it will display wave-like or particle-like behavior before entering the experiment. This hypothesis is aptly named the "conspiracy" theory [49].

The experimental results in Refs. [45, 46] on Wheeler's thought experiment can be explained by the wavepacket-only theory very easily. The single photon is emitted from source. The guide-factor (plane wave) in Eq. (3.4.1.15) will separate into two parts, one part goes through the splitter, and one part is reflected by the splitter. The body-factor of wavepacket will move according to the equiprobability symmetry and spontaneous

equiprobability symmetry breaking. At last the two parts of the guide-factor will arrive at end point, and have interference. The body-factor of wavepacket will take the direction and the position according to the equiprobability symmetry and spontaneous equiprobability symmetry breaking. Thus the wavepacket-only theory can explain experimental results exactly. In our wavepacket-only theory the body-factor of wavepacket of individual photon itself moves as an entity in Wheeler's thought experiment.

# **3.4.7.5.** Interference of Refraction Wave of Electron on Surface of Single Crystal and One Prediction

In the wavepacket-only theory the wavepacket of electron consists of three factors given by Eq. (3.4.1.15). The direct verification for existence of the guide-factor and the equiprobability symmetry is the interference experiment of electron on the surface of a single crystal, made by Davidson-Germer and Thompson [50, 51, 52] (See section 1.5.). The wavepacket-only theory explains the Davidson-German experiment as follows. The guide-factor of free electron wavepacket, which is exactly a plane wave, can give the intensity distribution of refraction wave of this plane wave, and the body-factor of wavepacket moves according to the equiprobability symmetry and spontaneous equiprobability symmetry breaking. If the electron beam contains many electrons, then we observed the interference pattern of refractory electrons, which is the same as that observed by Davidson-Germer.

The guide-factor of the free wavepacket is just a plane wave in essence. Therefore, it cannot been observed. However, its intensity distribution is proportional to the distribution of "rooms in a hotel", in which the wavepacket body-factor as a guest can reside according to the equiprobability symmetry and spontaneous equiprobability symmetry breaking. The body-factor of a wavepacket represents the rigid electron sphere with radius  $< 10^{-18}$  cm. If we do single electron experiment for a long time instead of an electron beam containing many electrons, then the wavepacket-only theory predicts that initial observed distribution of refraction electrons will be random due to the fluctuation caused by the spontaneous equiprobability symmetry breaking. However, after a long time we can see the interference pattern in Davidson-Germer experiment clearly.

# 3.4.7.6. Experiment of Partial Stop of C<sub>60</sub> Molecules at Grating

To let readers believe the equiprobability symmetry in the wavepacket-only theory deeply, we design the following thought experiment. According to the equiprobability symmetry, mentioned in the beginning of subsection 3.4.7, if a wavepacket moves along x direction, then the body-factor of wavepacket can take any value of (y, z) plane with equiprobability before passing through the grating. The widths of slit and non-slit on the grating are 50 nm and 50 nm [42], respectively. Only half  $C_{60}$  molecules can pass the slits of the grating to give the interference pattern, and half  $C_{60}$  molecules are stopped by the non-slit parts on grating. This particle stop phenomenon was already observed in photon interference experiments mentioned in subsection 3.4.7.2.

#### 3.4.8. Properties of Wavefunction

#### 3.4.8.1. Normalization

The guide-factor (= wavefunction)  $\Psi(x)$  can be normalized. Due to the equiprobability symmetry, the square of absolute value of guide-factor  $|\Psi(x)|^2$ , represents the probability density if values of x are continuous and the probability if the values of x are discrete. For convenience, we often think that the wavefunction is normalized. The definition of normalization is, for example,

$$\int_{a}^{b} dx |\Psi(x)|^{2} = 1, \qquad (3.4.8.1.1)$$

where a and b can be finite or infinite. More normalization methods can also be found in sections 5.1 and 5.4 of chapter 5. The equiprobability symmetry gives the normalized guide-factor the following physical meaning:

The probability of the body-factor to appear in all the domain of the guide-factor is 1;

The probability of the body-factor to appear in small range  $x \to x + dx$  is  $|\Psi(x)|^2 dx \equiv \rho(x) dx$ . Therefore,  $|\Psi(x)|^2$  represents probability density.

In momentum space

$$\Psi(x) \to \overline{\Psi}(k_x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \Psi(x) e^{-k_x x}.$$
 (3.4.8.1.2)

In momentum space the guide-factor still is a guide-factor.

The probability of the body-factor to appear in the momentum domain of the guidefactor is 1;

The probability of the body-factor to appear in small range  $k_x \to k_x + dk_x$  is  $|\overline{\Psi}(k_x)|^2 dk_x \equiv \rho(k_x) dk_x$ . Therefore,  $|\overline{\Psi}(k_x)|^2$  represents probability density in momentum space  $(p_x = \hbar k_x)$ .

#### 3.4.8.2. Individual Interpretation for Wavefunction

Some references think that the wavefunction represents statistical ensemble behavior of large number of identical particles other than the individual behavior of one particle.

Wavepacket-only theory thinks that the wavefunction (i. e., guide-factor) represents the individual behavior of one particle other than the statistical ensemble behavior of large number of particles, i. e., the wavepacket-only theory gives the individual interpretation of wavefunction. The reason of our individual interpretation is obvious. From the beginning of this chapter to now we have proved the wavepacket compositions, derived the Schrödinger equation, and deduced the character of wavepacket. All these things do not have a wee bit of connections with other particles or with the so-called statistical ensemble. We cannot absolutely right now connect our single particle wavepacket guide-factor and body-factor quite unaccountably with other particles or with the so-called statistical ensemble.

According to the statistical interpretation of wavefunction,  $\rho(x) \equiv |\Psi(x)|^2$  represents position probability density of appearance of the single particle. In this aspect of probability density, both our individual interpretation and the statistical interpretation are the same formally. But, there are two differences between them: (i) The latter thinks that  $|\Psi|^2$  describes the behavior of ensemble of large number of particles, and the former thinks  $|\Psi|$  describes still the behavior of the single particle;

(ii) The latter is a purely phenomenological hypothesis. Although the latter says that it gives a statistical interpretation, actually, the latter does not know more reasons for his statistical interpretation besides that if it represents probability, then it has to connect with an ensemble. On the contrary, our individual interpretation comes from theorems proved and from analysis for large amount of experimental data. Why the probability in the wavepacket-only theory does not require to connect with an ensemble? Because the the wavepacket-only theory uses the spontaneous equiprobability symmetry breaking concept, and thus does not need to invoke the ensemble concept.

#### 3.4.8.3. Comments for Wavefunction Collapse

There are many arguments on the wavefunction collapse, which was proposed by von Neumann in 1932 [53, 55, 56, 57, 21]. The so-called collapse of wavefunction says: for example, if a wavefunction (i. e., guide-factor) is  $\Psi(x)$ , and one finds that the value of momentum of a particle is  $p_{x1} = \hbar k_{x1}$ , then the wavefunction (guide-factor) collapses from  $\Psi(x)$  to  $Aexp(-ik_{x1}x)$ . The origin of this collapse might be non-control distribution of measurement processes.

Our comment on the wavefunction collapse is as follows.

The wavefunction  $\Psi(x)$  can be transformed from x representation to  $k_x = p_x/\hbar$  representation.

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk_x \overline{\Psi}(k_x) e^{ik_x x}.$$
(3.4.8.3.1)

 $|\overline{\Psi}(k_x)|^2$  represents the momentum probability density of appearance of single particle. In detail,  $|\overline{\Psi}(k_x)|^2 dk_x$  represents the momentum probability of appearance of single particle between  $p_x = \hbar k_x$  and  $p_x + \Delta p_x = \hbar k_x + \hbar \Delta k_x$ . If one measures the single particle's momentum, and obtains value  $p_{x_1} = \hbar k_{x_1}$ , then this just means that the single particle takes a special value of many momentum values, provided by the guide-factor (i. e., wavefunction), according to spontaneous equiprobability symmetry breaking. For a wavepacket there are at least two factors: guide-factor and body-factor. If single particle takes special value  $p_{x_1} = \hbar k_{x_1}$  contained in wavefunction, then this does not mean that all other values of momentum, contained in the wavefunction, do not exist or vanish. In our everyday life, Neumann's wavefunction collapse looks like that: Neumann (a single particle) touches the tail (special momentum value) of a big elephant (the wavefunction), then Neumann concludes that the big elephant becomes elephant's tail. Another our everyday life example to indicate the mistake of wavefunction collapse is as follows. The hotel looks like a wavefunction. The guest looks like a single particle. We always cannot say that if a guest chooses a room in the hotel, then the hotel becomes one room chosen by the guest. We always cannot say that if there is no guest in the hotel, then the hotel does not exist.

The origin of mistake in the wavefunction collapse is simply due to confusing the guidefactor with the body-factor of wavepacket. In our wavepacket-only theory, in measurement processes, apparatus and instruments are purely classical, and there are no a wee bit of necessities to consider the so-called non-controllable disturbance of measurement apparatuses.

#### 3.4.8.4. On Phase Velocity of Guide-Factor

There are two discussions on the concept of phase velocity in case of the guide-factor as a plane wave.

First, the guide-factor in Eq.(3.4.1.15) is  $\exp\{i[k_{x\circ}x - \omega(k_{x\circ})t]\}$ . Considering  $x = 2v_g t$  yields

$$e^{\{i[k_{x\circ}x - \omega(k_{x\circ})t]\}} = e^{\{i[k_{x\circ}2v_g - \omega(k_{x\circ})]t\}}.$$
(3.4.8.4.1)

Eq. (3.4.8.4.1) clearly shows that the phase is dependent linearly on time *t*. Although the phase-equal plane at any time can exist, but there should be no velocity of equal-phase plane, because the phase is a monotonous increasing function.

Second, in some references the method to determine the so-called phase velocity  $v_p$  is as follows. At first, some references assume that  $k_{xo}x - \omega(k_{xo})t$  is a time-independent constant C. Then, some references obtain

$$\frac{dC}{dt} = \frac{d[k_{x\circ}x - \omega(k_{x\circ})t]}{dt} = k_{x\circ}\frac{dx}{dt} - \omega(k_{x\circ}) = 0.$$
(3.4.8.4.2)

Some references define that the so-called phase velocity  $v_p$  is dx/dt, and from Eq. (3.4.8.4.2) obtain the phase velocity

$$v_{p,some\ references} = \frac{dx}{dt} = \frac{\omega(k_{x\circ})}{k_{x\circ}}.$$
 (3.4.8.4.3)

If we take  $\hbar\omega(k_{xo}) = (\hbar k_{xo})^2/(2m)$  in Eq. (3.4.8.4.3), then  $v_{p,some\ references} = \hbar k_{xo}/(2m) = v_g/2$ . Thus, the phase velocity of the guide-factor of wavepacket described by Eq. (3.4.8.4.2) is less than the group velocity of the same wavepacket, i. e., the propagation velocity of phase is less than the moving velocity of wavepacket. The diffraction and inference phenomena of massy particle and massless photon in our wavepacket-only theory come from that the guide-factor is a plane wave. If the phase of the plane wave is behind the wavepacket-body, then there are no diffraction and inference phenomena of massy particle.

Therefore, we conclude that for the guide-factor there is no the concept of phase velocity.

# 3.5. Schrödinger Equation

#### 3.5.1. One Dimensional Time-Independent Schrödinger Equation

Consider a system in which the potential is time-independent. In one dimensional case V(r) = V(x). Schrödinger equation is

$$i\hbar\frac{\partial\Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi.$$
 (3.5.1.1)

Because V(x) is time-independent,  $\Psi(x,t)$  can be written as

$$\Psi(x,t) = \Psi(x)F(t).$$
(3.5.1.2)

Substituting Eq. (3.5.1.2) into Eq. (3.5.1.1) and then dividing both sides by  $\Psi(x)F(t)$  yield

$$i\hbar \frac{1}{F(t)} \frac{dF(t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{1}{\Psi(x)} \frac{d^2}{dx^2} \Psi(x) + V(x).$$
(3.5.1.3)

Each side of Eq. (3.5.1.3) is equal to certain function F' of x and t. The left hand side does not depend on x, so F' is independent of x. The right hand side does not depend on t, so F' is independent of t. Since F' is independent of both variables x and t, F' must be a constant. We denote this constant by E. Equating the left hand side of Eq. (3.5.1.3) to E yields

$$i\hbar \frac{1}{F(t)} \frac{dF(t)}{\partial t} = E.$$
(3.5.1.4)

After integration

$$F(t) = e^{-iEt/\hbar}.$$
 (3.5.1.5)

Equating the right hand side of Eq. (3.5.1.3) to E yields

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) \equiv H\Psi(x) = E\Psi(x).$$
(3.5.1.6)

Eq. (3.5.1.6) is called time-independent Schrödinger equation for determining the wavefunction (i. e., the guide-factor) of a particle with mass *m* and moving in time-independent potential V(x). From Eq. (3.5.1.6), *E* has dimension of energy. We should take that *E* is the energy of the particle, and is called eigenenergy. The *H* is called Hamiltonian. The  $\Psi(x)$  is called eigenfunction.

From Eqs. (3.5.1.5) and (3.5.1.2)

$$\Psi(x,t) = e^{-iEt/\hbar} \Psi(x).$$
 (3.5.1.7)

The wavefunction  $\Psi(x,t)$  corresponds to state of constant energy.

Let us here give an simple example to look for  $\Psi(x)$  in Eq. (3.5.1.7). Suppose that a particle with mass *m* is constrained to move between two impenetrable walls which are a distance *a* apart. The corresponding potential has the values

$$V(x) = \infty \quad (x \le 0, x \ge a) \quad (domain \quad 1)$$
  

$$V(x) = 0 \quad (0 \le x \ge a) \quad (domain \quad 2)$$
(3.5.1.8)

This form of V(x) is known as one-dimensional box. According to Eq. (3.5.1.6), the Hamiltonian for this problem is as follows.

$$H_1 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \infty \ (x \le 0, \ x \ge a) \ (domain \ 1)$$
(3.5.1.9)

$$H_2 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \quad (0 \ge x \ge a) \quad (domain \ 2). \tag{3.5.1.10}$$

In domain 1 the time-independent Schrödinger equation gives  $\phi(x) = 0$ . The reasons are as follows. For any finite energy *E*, in this domain Eq. (3.5.1.9) reads

$$H_1\phi(x) = E\phi(x).$$
 (3.5.1.11)

Since  $\phi(x)$  and *E* are finite, the right hand side of Eq. (3.5.1.11) is finite. Therefore, the left hand side has to be finite as well, and  $\phi(x)$  must vanish in the domain 1.

That the  $\phi(x) = 0$  in domain 1 implies that there is no the guide-factor, and thus the body-factor of wavepacket has no probability in domain 1. The domain 1 is called "forbidden domain" where  $E < V(x) = \infty$ . Certainly, this is the case in domain 1 for any finite energy *E*.

In domain 2 the time-independent Schrödinger equation Eq. (3.5.1.10) is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi_n(x) = E_n\phi_n(x).$$
(3.5.1.12)

The subscript *n* is an anticipation of a discrete energy spectrum  $E_n$  and eigenfunctions  $\phi_n(x)$ . The wavefunction is continuous. Therefore, it must be at x = 0 and x = a

$$\phi_n(0) = \phi_n(a) = 0. \tag{3.5.1.13}$$

which is called boundary conditions. To solve Eq. (3.5.1.12), we rewrite it in the form

$$\frac{d^2\phi_n(x)}{dx^2} + k_n^2\phi_n(x) = 0.$$
(3.5.1.14)

$$k_n^2 = \frac{2mE_n}{\hbar^2}.$$
 (3.5.1.15)

Eq. (3.5.1.15) is merely a change of variables from energy  $E_n$  to wavenumber  $k_n$ . The solution to Eq. (3.5.1.14) appears as

$$\phi_n(x) = Asink_n x + Bcosk_n x. \tag{3.5.1.16}$$

The boundary conditions Eq. (3.5.1.13) give

$$B = 0. \tag{3.5.1.17}$$

$$A\sin k_n a = 0. \tag{3.5.1.18}$$

Eq. (3.5.1.18) serves to determine the eigenvalues  $k_n$ .

$$k_n a = n\pi, \quad n = 0, 1, 2, \cdots$$
 (3.5.1.19)

This is equivalent to the requirement that an integer number of half-wavelengths,  $n \times \lambda/2$ , fit into the width *a*.

The spectrum of eigenvalues is discrete. To find the constant *A* in Eq. (3.5.1.18), we normalize  $\phi_n(x)$ .

$$\int_0^a dx \phi_n^2 = 1. \tag{3.5.1.20}$$

The normalization condition is convenient for quantum mechanics. According to the equiprobability principle and after normalization,  $|\phi_n(x)|^2 dx$  represents the probability of body-factor of wavepacket at  $x \to x + dx$ . This normalization of  $\phi(x)$  requires that the  $\phi_n(x)$ 

is square-integrable. For convenience, one always makes the normalization expressed by Eq. (3.5.1.20). From Eq. (3.5.1.20) one obtains  $A = \sqrt{2/a}$ , and

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right). \tag{3.5.1.21}$$

Substituting Eq. (3.5.1.19) into Eq. (3.5.1.15) yields

$$E_n = n^2 E_1 \equiv n^2 \frac{\hbar^2 k_1^2}{2m} = n^2 \frac{\hbar^2 \pi^2}{2ma^2}.$$
 (3.5.1.22)

The eigenstate corresponding to n = 0 is  $\phi_0(x) = 0$ . This, together with the solution in domain 1, gives  $\phi_0(x) = 0$  over the whole x axis, which means that there is no particle (body-factor of wavepacket) to take the state  $\phi_0(x)$ . This is equivalent to the statement that the particle does not exist in the n = 0 state. Another argument that disallows the n = 0 state follows from Heisenberg uncertainty relation of energy-time (See section 3.3).

#### 3.5.2. Stationary State

Using Eq. (3.5.1.7) yields

$$|\Psi(x,t)|^2 = |\Psi(x)|^2.$$
(3.5.2.1)

The probability density occupied by body-factor of wavepacket is then independent of time. A particle in such a state will remain in that state until it is acted upon by some external object that forces the particle out of that state. The solution of Schrödinger equation for time-independent potential is called stationary state. The stationary state is a state with well defined energy, *E* being the definite value of its energy. For a stationary state,  $\Psi(x,t)$  equals a function of time multiplied by a function of particle coordinate,  $\Psi(x)$ , which is called an eigenfunction (or eigenvector) of Hamiltonian *H*.

$$H\Psi(x) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\Psi(x,t) = E\Psi(x).$$
 (3.5.2.2)

Eq. (3.5.2.2) is called the eigenequation of Hamiltonian.  $\Psi(x)$  is called eigenfunction of Hamiltonian.

#### 3.5.3. Superposition of States

It is better to put this subsection 3.5.3 after subsection 3.4.5 and before subsection 3.4.7. If we put subsection 3.5.3 in that way, then we address the law in subsection 3.4.7 easily. Considering the superposition of states is an important property of Schrödinger equation, we put it still here. Schrödinger equation is linear in  $\Psi(x,t)$ . As a result, its solutions  $\Psi(x,t)$  satisfy superposition theorem which can also be called superposition theorem of states or wavefunctions or guide-factors. Note that the wavepacket-function is not the solution of Schrödinger equation, and thus do not satisfy superposition theorem. In all other textbooks the superposition theorem is called superposition principle. The proof of state superposition theorem is very simple, and is given as follows. **Theorem XI: State superposition.** Linear composition of possible states (= wavefunctions = solutions of Schrödinger equation = guide-factors $\neq$ wavepacket-function) is also a possible state. In mathematics, if  $\Psi_i(x,t)$ ,  $(i = 1, 2, \dots, N)$  satisfy Schrödinger equation Eq. (3.4.5.2.1)

$$\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{dx^2} - V(x,t)\right]\Psi_i(x,t) = 0, \quad (i = 1, 2, \cdots, N)$$
(3.5.3.1)(3.4.5.2.1)

then the wavefunction

$$\Psi(x,t) = \sum_{i=1}^{n \le N} c_i \Psi_i(x,t)$$
(3.5.3.2)

also satisfies Schrödinger equation Eq. (3.5.3.1).

**Proof.** From Eq. (3.5.3.2) and Eq. (3.5.3.1) we have

$$\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{dx^2} - V(x,t)\right]\Psi(x,t) = \sum_{i=1}^{n \le N} \left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{dx^2} - V(x,t)\right]\Psi_i(x,t) = 0.$$
(3.5.3.3)

Therefore,  $\Psi(x,t)$  is the solution of the Schrödinger equation as well. QED.

The key to prove the state superposition theorem is in that the Schrödinger equation is a linear equation. Because the superposition property of wavefunctions can be proved, it is better to call it superposition theorem instead of superposition principle.

**Corollary X: Interference between component states.** There are interference between component states of superposition state, or say, the state superposition is a coherent superposition.

**Proof.** See Eq. (3.5.3.2). The  $\Psi(x,t)$  satisfies Schrödinger equation, and thus it is guidefactor of wavepacket. According to wavepacket motion law, the probability density of an object to appear in  $x \to x + dx$  at time t is  $|\Psi(x,t)|^2 = |\sum_{i=1}^N c_i \Psi_i(x,t)|^2 \neq \sum_{i=1}^N |c_i \Psi_i(x,t)|^2$ , i. e., the cross terms of the components are of contributions to the total probability.

For example, See Young's double slit experiment in Fig. 1.7 [5]. The incident wavefunction of free electron is plane wave,  $\psi = A \exp[i(ky - \omega t)]$ , incident direction is y, the x direction is perpendicular to the slits, and the two slits are  $S_1$  and  $S_2$ , which are distance a apart. At a distance d parallel to it is a row of detectors that measures the intensity as a function of the position x measured along the fluorescent screen. Simply, d is the perpendicular distance between slit surface and screen (Refer to Fig. 3.1 (a) in Ref. [5]).

If we first keep only  $S_1$  open, the incident wavefunction will come out of  $S_1$  and propagate radially outward. One may think of  $S_1$  as the virtual source of this wavefunction  $\psi_1$ , which has the same frequency and wavelength as the incident wavefunction. The intensity pattern  $I_1 = |\psi_1|^2$  is registered by the detectors. Similarly, if  $S_2$  is open instead of  $S_1$ , the wavefunction  $\psi_2$  produces the pattern  $I_2 = |\psi_2|^2$ . In both cases the arrival of energy at the detectors is a smooth function of *x* and *t*.

Now if both  $S_1$  and  $S_2$  are opened, both wavefunctions  $\psi_1$  and  $\psi_2$  are present and produce an intensity pattern, according to optics,  $I_{1+2} = |\psi_1 + \psi_2|^2$ . According to theorem *XI*,  $\psi_1 + \psi_2$  is also a state of the incident free electron.

The interesting thing is that  $I_{1+2} \neq I_1 + I_2$ , but rather the interference pattern shown in Fig. 1.7. The ups and downs are due to the fact that wavefunctions  $\Psi_1$  and  $\Psi_2$  have to travel different distance  $d_1$  and  $d_2$  (Refer to the nice Fig. 3.1 in Ref. [5].) to arrive at some given x and thus are not always in step. In particular, the maxima correspond to the case  $d_1 - d_2 = n\lambda$  (*n* is integer.  $\lambda$  is the wavelength of the incident plane wavefunction.  $d_1$  and  $d_2$  are the distances from slits to the common point x on the screen, respectively.), when the wavefunctions arrive exactly in step, and the minima correspond to the case  $d_1 - d_2 = (2n+1)/2\lambda$ , when the plane wavefunction are exactly out of step. In terms of the phases  $\phi_1$  and  $\phi_2$ ,  $\phi_2(x) - \phi_1(x) = 2n\pi$  at a maximum and  $\phi_2(x) - \phi_1(x) = (2n+1)\pi$  at a minimum. One can easily show that the spacing  $\delta x$  between two adjacent maxima is  $\delta x = \lambda d/a$ .

The feature to take special notability is that if  $x_{min}$  is an interference minimum, there is more electron flowing into  $x_{min}$  with just one slit open than with both. In other words, the opening of an extra slit can actually reduce the electron flow into  $x_{min}$ .

From these facts of electron and photon double slit experiment Born (1927) drew the following conclusion: with each free electron or photon is associated a wavefunction  $\psi$ , called probability amplitude or simply amplitude, whose modulus squared  $|\psi|^2$  gives the probability of finding the particle at *x*. [Strictly speaking, we must do not refer to  $|\psi|^2$  as the probability for a given *x*, but rather as the probability density at *x* since *x* is continuous variable.]

# 3.5.4. Requirements for Wavefunction

The wavefunction can be a complex function in principle, and therefore the wavefunction itself cannot be observed directly. The square of absolute value  $|\Psi(x,t)|^2$  evaluated at a particular position and at a particular time is proportional to the position probability density of appearance of body-factor at that time. The position probability density is positive and real, and is equal to  $\Psi^*(x,t)\Psi(x,t)$ . Although the wavefunction (guide-factor of wavepacket) can take negative values, but position probability density is always positive. Due to that  $|\Psi(x,t)|^2$  represents position probability density, the wavefunction should be square-integrable, and thus belongs to  $\mathcal{L}^2$ . The wavefunction can be described by both position space and momentum space, and belongs to  $\mathcal{M}(\mathbb{R})$ . Generally speaking, the solution (i. e., wavefunction) of time-independent Schrödinger equation must satisfy the following physical conditions or requirements. The requirements for wavefunctions can be called boundary conditions.

(1) The wavefunction must be continuous and single valued.

(2)  $\partial \Psi / \partial x$ ,  $\partial \Psi / \partial y$ , and  $\partial \Psi / \partial z$  must be continuous and single valued everywhere. There is an exception, which is given at the end of this subsection.

(3) The integral of square modulus of wavefunction over all values x must be finite.

$$\int \Psi^* \Psi dx = finite, \qquad (3.5.4.1)$$

i. e., the wavefunction must be square-integrable. This condition means that wavefunction can be normalized, i. e., wavefunction must go to zero as  $x(y,z) \to \pm \infty$  in order that  $\int |\Psi|^2 d^3r$  over all space is a finite constant.

These requirements for the wavefunction ensure that the position probability density of appearance of body-factor of wavepacket in the vicinity of any point is unambiguously defined and continuous rather than having two or more possible values. If  $\Psi$  and  $(\partial \Psi/\partial x)$ are not single valued and finite, then the same is true for  $\Psi(x,t)$  and  $\partial \Psi/\partial t$ , since the given formula for calculating the average values of position and momentum contains  $\Psi(x,t)$  and  $\partial \Psi(x,t)/\partial t$ .

The first order derivative of the wavefunction with respect to position coordinates must be continuous every where except where there is an infinite discontinuity in the potential. We know that any function always has an infinite derivative whenever it has a discontinuity. Let us consider the time-independent Schrödinger equation in one dimension.

$$\frac{d^2\Psi}{dx^2} = \frac{2m}{\hbar^2} (V - E)\Psi.$$
 (3.5.4.2)

If V, E, and  $\Psi$ , and  $(d^2\Psi/dx^2)$  is finite, then this in turn requires  $d\Psi/dx$  to be continuous. A finite discontinuity in  $d\Psi/dx$  implies an infinite discontinuity in  $d^2\Psi/dx^2$ . Some special V(x) in the Schrödinger equation may have this discontinuity. For example, for the step square potential

$$V(x) = \begin{cases} V_1 & x < a \\ V_2 & x > a \end{cases}$$
(3.5.4.3)

The theorem XIII-5 in chapter 4 says that if  $(V_1 - V_2)$  is finite, then  $\Psi(x)$  and  $d\Psi(x)/dx$  are continuous. However, if  $[(V_1 - V_2) \rightarrow \pm \infty]$ , then this theorem does not hold water.

#### 3.5.5. Observable as Operator

The terminology "dynamical variable" or (physical) "observable" is generally used for a physical quantity that can be determined experimentally. For brevity, some times we call the dynamical variable simply the quantity. We have seen that a quantity has to be expressed by an operator. For example, the momentum in coordinate representation (See section 3.3) is an operator, and the energy in time representation is an operator. For the convenience of studying quantum mechanics, here we give a complete discussion on operator.

(1) An operator O is a mathematical terminology that transforms a function  $\phi$  into another function  $\Psi$ . We have known the following five operators in position space: coordinate **r** (a special operator, i. e., a number operator in position space), momentum operator  $(\hbar/i)\nabla$ , kinetic energy operator  $(-\hbar^2/2m)\nabla^2$ , potential operator V(r,t) (a special operator, i. e., a number operator in position space), and Hamiltonian operator  $H = (-\hbar^2/2m)\nabla^2 + V(r,t)$ . They correspond to dynamical variables: position **r**, momentum **p**, kinetic energy *T*, potential energy V(r,t), and total energy *H*, respectively.

(2) The form of operator for a dynamical variable depends on space used to express the dynamical variable. For example, section 3.2 tells us that if we use momentum space, then the form of momentum operator will be simply represented by the number momentum itself. Similarly, if we use position space, then the form of position operator will be simply represented by the number position itself.

(3) Dynamical variables correspond to linear operators. An operator O is called a linear operator if it satisfies two criteria:  $O(c\phi) = cO\phi \equiv \Psi$  and  $O(c_1\phi_1 + c_2\phi_2) = c_1O\phi_1 + c_2O\phi_2 = c_1\Psi_1 + c_2\Psi_2$ , where *c*'s are complex constants. The examples of linear operators are differential operator, position operator etc. Nonlinear operators are, for example,  $\sqrt{some}$  (take the root of *some*) and  $[some]^2$  (take the square of *some*). We do not study nonlinear operator.

(4) In formula  $H\Psi = E\Psi$ , we have defined that  $\Psi$  is the eigenfunctions of Hamiltonian. Generally speaking, we can define the eigenfunctions and eigenvalues of any operator O. The definitions are as follows. When an operator acting on a function yields a constant times the function, we call the function eigenfunction and the constant the corresponding eigenvalue. Let the function is  $\Psi$  and the operator is O

$$O\Psi = o\Psi, \tag{3.5.5.1}$$

where o is a complex number. Eq. (3.5.5.1) defines the eigenvalue equation. For a given operator O many eigenfunctions may exist so that

$$O\Psi_i = o_i \Psi_i, \tag{3.5.5.2}$$

where  $\Psi_i$  are the eigenfunctions, and  $o_i$  are the corresponding eigenvalues. Each eigenfunction of O is unique. If two or more eigenfunctions have the same eigenvalues, then the eigenvalue is said to be degenerate. Let  $\Psi_1$  and  $\Psi_2$  are eigenfunctions of the operator O with the eigenvalue o, i. e.,

$$O\Psi_1 = o\Psi_1.$$
 (3.5.5.3)

$$O\Psi_2 = o\Psi_2.$$
 (3.5.5.4)

This eigenvalue is said to be doubly degenerate. The eigenvalue can be also three-, tour-,  $\cdots$ , *n*-fold degenerate. The eigenvalue is nondegenerate, if there is only one eigenfunction corresponding to the eigenvalue.

If  $\Psi_1$  and  $\Psi_2$  are eigenfunctions of *O* with the same eigenvalue, then their linear composition is also an eigenfunction, that is,

$$\Psi = c_1 \Psi_1 + c_2 \Psi_2. \tag{3.5.5.5}$$

$$O\Psi = O(c_1\Psi_1 + c_2\Psi_2) = c_1O\Psi_1 + c_2O\Psi_2 = o(c_1\Psi_1 + c_2\Psi_2) = o\Psi.$$
 (3.5.5.6)

If a state (= wavefunction = guide-factor)  $\Phi$  is not any one in the eigenstates of operator O, but is a state which can be expressed by a superposition of eigenstates  $\Psi_1, \Psi_2, \Psi_3, \cdots$ , then the state  $\Phi$  consists of many eigenstates of operator O according to definite proportionality. O represents both operator and quantity, for brevity.

(5) We hope that readers feel that it is a natural thing to represent a dynamical variable [or (physical) observable] in terms of operators. The basic reason to represent a dynamical variable by an operator is just a mathematical requirement. The theorem proved in subsection 3.3.1.4 of chapter 3, is independent of physics, and is just dependent on the mathematics.

# 3.5.6. Probability Current Density of Single Particle

The position probability density occupied by the body-factor of wavepacket (= position probability density of the single particle) is

$$\rho(r,t) = \Psi^*(r,t)\Psi(r,t). \tag{3.5.6.1}$$

$$\frac{\partial}{\partial t} \int d^3 r \rho(r,t) = \frac{\partial}{\partial t} \int d^3 r \Psi^*(r,t) \Psi(r,t) = \int d^3 r \left( \frac{\partial \Psi^*}{\partial t} \Psi + \Psi^* \frac{\partial \Psi}{\partial t} \right).$$
(3.5.6.2)

The time-dependent Schrödinger equation can be written as

$$\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m} \bigtriangledown^2 \Psi - \frac{i}{\hbar} V(x, t) \Psi.$$
(3.5.6.3)

Substituting Eq. (3.5.6.3) and its conjugate into Eq. (3.5.6.2) yields

$$\frac{\partial}{\partial t} \int d^3 r \rho(r,t) = -\frac{i\hbar}{2m} \int d^3 r \left[ \Psi(\nabla^2 \Psi^*) - \Psi^*(\nabla^2 \Psi) \right].$$
(3.5.6.4)

Substituting the vector identity

$$\nabla \cdot [\Psi^* \nabla \Psi - \Psi \nabla \Psi^*] = \Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^*$$
(3.5.6.5)

into Eq. (3.5.6.4) yields

$$\frac{\partial}{\partial t} \int d^3 r \rho(r,t) = \int d^3 r \nabla \cdot \left[ \frac{i\hbar}{2m} (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) \right].$$
(3.5.6.6)

We define probability current density or probability density flux, J, of single particle J(r,t) as

$$J(r,t) = -\frac{i\hbar}{2m} (\Psi^* \bigtriangledown \Psi - \Psi \bigtriangledown \Psi^*). \qquad (3.5.6.7)$$

mJ(r,t) is called mass probability current density of single particle with total mass m.

Substituting Eq. (3.5.6.7) into Eq. (3.5.6.6) yields

$$\frac{\partial}{\partial t} \int_{V} d^{3}r \rho(r,t) + \int_{V} d^{3}r \bigtriangledown J = 0.$$
(3.5.6.8)

According to Gauss theorem, the surface integral of the component of any vector V along the outward normal taken over a closed surface S is equal to the integral of the divergent of V taken over the volume V enclosed by the surface S, that is,

$$\int_{V} d^{3}r \nabla \cdot V = \int_{S} d^{2}s \cdot V, \qquad (3.5.6.9)$$

where  $d^2s$  is a vector whose magnitude is equal to an element  $d^2s$  on the surface S. Substituting Eq. (3.5.6.9) into Eq. (3.5.6.8) yields

$$\frac{\partial}{\partial t} \int_{V} d^{3}r \rho(r,t) = -\int_{S} d^{2}s \bigtriangledown J.$$
(3.5.6.10)

The left hand side of Eq. (3.5.6.10) represents the increase of the rate of total probability that the particle appears in closed volume *V*. The right hand side of Eq. (3.5.6.10) (Note the minus sign!) represents the rate of the probability, entering in volume *V* trough the closed surface *S*.

Let the volume V is extended to the entire space. The S in Eq. (3.5.6.10) then recedes to infinity. Since  $\Psi$  is square integrable, it vanishes at large distances so that surface integral in Eq. (3.5.6.10) is equal to zero. The Eq. (3.5.6.10) is then

$$\frac{\partial}{\partial t} \int_{V} d^{3}r \rho(r,t) = 0, \qquad (3.5.6.11)$$

that is, normalization integral  $\int_{-\infty}^{\infty} d^3 r \rho(r,t)$  is independent on time *t*. If a wavefunction is normalized at initial time, then this wavefunction will always be normalized.

Using Eq. (3.5.6.9), Eq. (3.5.6.8) can be written as

$$\frac{\partial}{\partial t}\rho(r,t) + \nabla \cdot J(r,t) = 0.$$
(3.5.6.12)

By analogy with charge conservation in electrodynamics and with the equation of continuity in hydromechanics, Eq. (3.5.6.12) can be interpreted as the conservation of position probability density occupied by the body-factor of wavepacket, and is called continuity equation. Eq. (3.5.6.7) can also be written as

$$J(\mathbf{r},t) = Re\left(\Psi^*\frac{\hbar}{im}\nabla\Psi\right).$$
(3.5.6.13)

The operator  $\hbar \bigtriangledown /i$  represents momentum **p** therefore,  $\hbar \bigtriangledown /(im)$  represents the velocity of the particle, since p/m = v. However, one cannot naively think that **J** corresponds to product of the velocity and the position probability, and that velocity is equal to  $J/\rho$ . Since  $\Psi$  and  $\bigtriangledown \Psi$  are continuous function of **r**, therefore  $\rho(\mathbf{r},t)$  and  $\mathbf{J}(\mathbf{r},t)$  have no discontinuous change distribution as **r** varies.

The dimension of J(r,t) in Eq. (3.5.6.7) is cm<sup>-2</sup>sec<sup>-1</sup>. Note that the one dimensional form of Eq. (3.5.6.7) is

$$J_x = -\frac{\hbar}{2mi} \left( \Psi^* \frac{d\Psi}{dx} - \Psi \frac{d\Psi^*}{dx} \right).$$
(3.5.6.14)

The dimension of  $J_x$  is sec<sup>-1</sup>, which is different from the three and two dimensional J(r,t) in dimension. It is reasonable to call  $J_x$  probability current. However, for convenience, we often still uniformly call  $J_x$  probability current density.

# 3.5.7. More about Average Values

At first consider the average or expectation value of x for a single particle in one dimensional wavefunction state  $\Psi(x,t)$ , which represents the wavefunction other than the wavepacket. The one dimensional particle is a line particle. The  $|\Psi(x,t)|^2$  represents the position probability density. The  $|\Psi(x,t)|^2 dx$  will take different values at different interval  $dx \rightarrow x + dx$ , and thus the contribution of different intervals will be different. The probability of a line particle at  $x \rightarrow x + dx$  and t is

$$|\Psi(x,t)|^2 dx. \tag{3.5.7.1}$$

Thus the average value of *x*, symbolized by  $\langle x \rangle$ , is

$$\langle x \rangle = \int_{-\infty}^{\infty} dx x |\Psi(x,t)|^2.$$
 (3.5.7.2)

Note that if  $|\Psi(x,t)|^2$  is an even function, then  $\langle x \rangle = 0$ . Therefore, one often uses  $\sqrt{\langle x^2 \rangle}$  to represent the average value of *x*.

For three dimensional case, the probability of the three dimensional particle at  $x \rightarrow x+dx$ ,  $y \rightarrow y+dy$ ,  $z \rightarrow z+dz$ , and *t* is

$$|\Psi(x,y,z,t)|^2 dx dy dz.$$
 (3.5.7.3)

Thus for three dimensional case

$$\langle x \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dy dz x |\Psi(x, y, z, t)|^2.$$
(3.5.7.4)

The average value of some physical quantity A that is a function of x, y, and z is

$$\langle A(x,y,z) \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dy dz A |\Psi(x,y,z,t)|^{2}$$
$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dy dz \Psi^{*} A \Psi.$$
(3.5.7.5)

In general, the property A depends on both coordinates and momenta, that is,

$$A = A(x, y, z, p_x, p_y, p_z).$$
(3.5.7.6)

Remember that we have used position space to find average values. The momentum in position space is an operator instead of a numerical value (Number is sometimes called special operator). Thus

$$\langle A(x, y, z, p_x, p_y, p_z) \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dy dz \Psi(x, y, z, t)$$

$$A\left(x, y, z, \frac{\hbar}{i} \frac{\partial}{\partial x}, \frac{\hbar}{i} \frac{\partial}{\partial y}, \frac{\hbar}{i} \frac{\partial}{\partial z}\right) \Psi(x, y, z, t).$$

$$(3.5.7.7)$$

The A under the integral notation is an operator corresponding to the observable A.

For N-particle case, the formula of average value is naturally extended to

$$\langle A \rangle = \int d\tau \Psi^* A \Psi,$$
 (3.5.7.8)

where  $d\tau$  indicates a definite integral over the full range of 3N coordinates. In the above expression the operator A is sandwiched between  $\Psi^*$  and  $\Psi$ . The quantity  $\Psi^*A\Psi$  is not the same as  $A\Psi^*\Psi$  or  $\Psi^*\Psi A$ . On right hand side of the Eq. (3.5.7.8) at first A operates on  $\Psi$  to produce a new function which is then multiplied by  $\Psi^*$ . One then integrates over all the coordinate space to produce  $\langle A \rangle$ . If the functions are not normalized, then the average value of A is

$$\langle A \rangle = \frac{\int d\tau \Psi^* A \Psi}{\int d\tau \Psi^* \Psi},$$
 (3.5.7.9)

Note that if  $\Psi$  does not satisfy the normalized condition, then all formulas of average values have to have a denominator  $\int d\tau |\Psi|^2$ .

# 3.6. Quantum or Classical Mechanics

# 3.6.1. Criterion

The watershed theorem tells us that:

If you connect an object (such as universe, electron, quark, photon) with a function of both coordinates or momenta at the same time, then you can prove that the equation of motion is decided by Poison bracket, and you can further prove Newton equation and further you can derive a series of properties of the object, and you call this object the classical object.

If you connect an object (such as universe, electron, quark, photon) with a function of either coordinates or momenta, then you can prove that the equation of motion is decided by commutation relations instead of Poison bracket (See section 5.8 of chapter 5), and you can further prove all the three formulations of quantum mechanics instead of Newton equation and further you can derive a series of the object's properties (such as energy quantization of a bound state, tunneling effect, and so on), and you call this object the quantum object instead of classical object.

We know that the series of classical theories are not wrong. They are approximately good enough in some cases. The calculations and treatments using classical theory are much easier than the calculations and treatments using quantum theory. Now we propose a question: When we have to use the exact, correct, but much trouble quantum theory? To answer this question we give the following criterion and two corollaries.

**Criterion: Criterion of quantum or classical mechanics.** Suppose that the system is one dimensional.

$$\begin{cases} \lambda_{x} > L_{x} \\ or, \ equivalently, \\ h > mv_{xg}L_{x} \end{cases} \ quantum \ effect \ prevails \ over \ classical \ effect, \qquad (3.6.1.1) \\ \begin{cases} \lambda_{x} << L_{x} \\ or, \ equivalently, \\ h << mv_{xg}L_{x} \end{cases} \ classical \ effect \ prevails \ over \ quantum \ effect, \qquad (3.6.1.2) \\ \begin{cases} \lambda_{x} << L_{x} \\ or, \ equivalently, \\ or, \ equivalently, \\ mv_{xg} < h < 10nv_{xg}L_{x} \end{cases} \ quantum \ effect \ still \ manifests \ a \ little, \qquad (3.6.1.3) \end{cases}$$

where  $\lambda_x$ ,  $L_x$ , m,  $v_{xg}$ , and h are the average wavelength, size, group velocity in x direction of wavepacket, and Planck constant, respectively.

**Proof.** The guide-factor and the body-factor of wavepacket represent the wave and particle property of wavepacket, respectively. The guide-factor is a wave with wavelength  $\lambda_x = 2\pi/k_{xo} = h/(mv_g)$ . If  $\lambda_x = h/(mv_{xg}) > L_x$ , i. e., the size of body-factor of wavepacket is less than the wavelength of wavepacket, then this means that the wave property of wavepacket will prevail over the particle property of wavepacket. If the wave property of an object is clear, then the object will manifest quantum property.

On the contrary, if  $\lambda_x = h/(mv_{xg}) \ll L_x$ , i. e., the size of body-factor of wavepacket is much larger than the wavelength of wavepacket, then this means that the particle property of wavepacket will prevail over the wave property of wavepacket. If the wave property of an object cannot manifest, and thus cannot be observed, then the object will appear as a classical object, and obey classical mechanics.

**Corollary XI:** If  $h \rightarrow 0$ . If  $h \rightarrow 0$ , then even a microscopic particle such as electron obeys classical mechanics. On the contrary, so long as *h* is big enough, then even our Earth has to obey quantum mechanics.

**Corollary XII: Velocity and mass effects.** From  $h < mv_{xg}L_x$  we see that the larger the  $v_{xg}$  or *m* are, the weaker the quantum mechanical effects are, i. e., the high velocity and large mass of particle does not benefit quantummechanical effect.

If a macroscopic particle with mass of one gram and with  $v_{xg} = 1$  cm per second, then the condition for that the quantummechanical effect prevails over the classical mechanical effect in x direction is the particle's length  $L_x < 6.6 \times 10^{-27}$  cm, which is too short. The actual size of this particle is much much larger than this value of  $L_x$ . Therefore, the properties of the so-called macroscopic particle always corresponds to the average values of quantum mechanics, and thus there is no quantummechanical wave effect, i. e., the classical effect prevails over the quantum effect.

If  $\lambda_x \ll L_x$ , then we call this object macroscopic object. If  $L_x \ll 10\lambda_x$ , then we call it microscopic object.

Here, we would like to mention our viewpoint coming from this criterion and the zero theorem.

Classical physics includes: Newton classical mechanics, special and general theory of relativity, and so on. In these theories, any objects are described by both momenta and coordinates at the same time, the variations of objects are deterministic, there are no coherence between two macroscopic objects, and so on.

Quantum physics includes: quantum mechanics, quantum field theory, and so on. In these theories, any objects cannot be described by both momenta and coordinates at the same time, the variations of objects are stochastic, there are coherence between two microscopic objects (except macroscopic quantum phenomena), and so on.

# 3.6.2. Ehrenfest Theorem

Theorem XII: Ehrenfest average value theorem. Newton equations, written in the forms

$$\frac{dr}{dt} = \frac{p}{m} \tag{3.6.2.1}$$

and

$$\frac{dp}{dt} = -\bigtriangledown V, \tag{3.6.2.2}$$

are exactly satisfied by the average values of corresponding operators ( $\mathbf{p}$ ,  $\mathbf{r}$ , V) on wavefunction (guide-factor). Here, V represents real potential energy. (Ehrenferst proved

this theorem in 1927.)

**Proof.** Set  $\Psi$  represent the wavefunction. Consider the average value of x

$$\langle x \rangle = \int d^3 r \Psi^* x \Psi. \tag{3.6.2.3}$$

$$\frac{d \langle x \rangle}{dt} = \frac{d}{dt} \int d^3 r \Psi^* x \Psi = \int d^3 r \left( \frac{\partial \Psi^*}{\partial t} x \Psi + \Psi^* x \frac{\partial t}{\Psi} \right)$$
(3.6.2.4)

From Schrödinger equation Eq. (3.4.5.2.1), its conjugate equation, and Eq. (3.6.2.4), we have for real potential V

$$\frac{d \langle x \rangle}{dt} = \frac{i\hbar}{2m} \int d^3r \left[ \Psi^* x(\nabla^2 \Psi) - (\nabla^2 \Psi^*) x \Psi \right].$$
(3.6.2.5)

From Green's theorem we have

$$\int_{volume} d^3 r(u \bigtriangledown^2 v - v \bigtriangledown^2 u) = \int_{surface} d^2 s \cdot (u \bigtriangledown v - v \bigtriangledown u).$$
(3.6.2.6)

If  $u = \Psi^*$  and  $v = x\Psi$ , then from Eq. (3.6.2.6) we have

$$\int_{volume} d^3 r [\Psi^*(\bigtriangledown^2 x \Psi) - x \Psi(\bigtriangledown^2 \Psi^*)]$$
  
= 
$$\int_{surface} d^2 s \cdot [\Psi^*(\bigtriangledown x \Psi) - x \Psi(\bigtriangledown \Psi^*)]. \qquad (3.6.2.7)$$

If the integration is carried over the entire space and the wavefunction vanishes at infinity, then the surface integral approaches zero and hence from Eq. (3.6.2.7)

$$\Psi^* \bigtriangledown^2 (x\Psi) = x\Psi \bigtriangledown^2 \Psi^*. \tag{3.6.2.8}$$

Substituting Eq. (3.6.2.8) into Eq. (3.6.2.5) yields

$$\frac{d \langle x \rangle}{dt} = \frac{i\hbar}{2m} \int d^3r \left[ \Psi^* x(\nabla^2 \Psi) - \Psi^* \nabla^2 \left( x\Psi \right) \right].$$
(3.6.2.9)

Using  $\bigtriangledown^2(x\Psi) = 2 \triangledown \Psi + x \triangledown^2 \Psi$ , Eq. (3.6.2.9) becomes

$$\frac{d \langle x \rangle}{dt} = \frac{i\hbar}{2m} \int d^3r \left[ \Psi^* x(\nabla^2 \Psi) - \Psi^* (2 \nabla \Psi + x \nabla^2 \Psi) \right]$$
  
=  $-\int d^3r \Psi^* \frac{i\hbar}{m} \nabla \Psi.$  (3.6.2.10)

Eq. (3.6.2.10) can be written as

$$m\frac{d < x >}{dt} = , \tag{3.6.2.11}$$

where  $p_x = \hbar \partial / (i \partial x)$ . Eq. (3.6.2.11) is the quantum counterpart of the *x* component of Newton equation Eq. (3.6.2.1).

Let us now consider

$$\frac{d < p_x >}{dt} = \frac{d}{dt} \int d^3 r \Psi^* \frac{\hbar}{i} \frac{\partial \Psi}{\partial x} = \frac{\hbar}{i} \int \left[ \Psi^* \frac{\partial}{\partial x} \left( \frac{\partial \Psi}{\partial t} \right) + \frac{\partial \Psi^*}{\partial t} \frac{\partial \Psi}{\partial x} \right].$$
(3.6.2.12)

Substituting Schrödinger equation Eq. (3.4.5.2.1) and its conjugate equation into right hand side of Eq. (3.6.2.12) yields

$$\frac{d < p_x >}{dt} = -\int d^3 r \left[ \Psi^* \frac{\partial}{\partial x} (V\Psi) - V\Psi^* \frac{\partial\Psi}{\partial x} \right] -\frac{\hbar^2}{2m} \int d^3 r \left[ \frac{\partial\Psi}{\partial x} (\nabla^2 \Psi^*) - \Psi^* \nabla^2 \left( \frac{\partial\Psi}{\partial x} \right) \right].$$
(3.6.2.13)

Using  $u = \partial \Psi / \partial x$  and  $v = \Psi^*$  in Green's theorem Eq. (3.6.2.6) yields

$$\int_{volume} d^3 r \left[ \frac{\partial \Psi}{\partial x} (\nabla^2 \Psi^*) - \Psi^* \nabla^2 \left( \frac{\partial \Psi}{\partial x} \right) \right]$$
$$= \int_{surface} d^2 s \cdot \left[ \frac{\partial \Psi}{\partial x} \nabla \Psi^* - \Psi^* \nabla \frac{\partial \Psi}{\partial x} \right].$$
(3.6.2.14)

If the integration is carried over the entire position space and the wavefunction vanishes at infinity, then the surface integral approaches zero. Thus the second term on the right hand side of Eq. (3.6.2.14) vanishes and we have

$$\frac{d \langle p_x \rangle}{dt} = -\int d^3 r \left( \Psi^* \frac{\partial V}{\partial x} \Psi \right) = -\left\langle \frac{\partial V}{\partial x} \right\rangle.$$
(3.6.2.15)

The Eq. (3.6.2.15) is the counterpart of the *x* component of Newton equation Eq. (3.6.2.2). Eqs. (3.6.2.11) and (3.6.2.15), together with the similar ones for the *y* and *z* components, constitute the mathematical formulation of the theorem of average value.

The connection of quantum mechanics with classical mechanics can be more close in some cases. If the potential is linear or square (for example, oscillator), i. e.  $V(x) = a + bx + cx^2$ . We make Tailor expansion at  $\langle x \rangle$  for V, then we have

$$\frac{\partial V}{\partial x} = \left. \frac{\partial V(x)}{\partial x} \right|_{} + (x - \langle x \rangle) \left. \frac{\partial^2 V}{\partial x^2} \right|_{} + \frac{1}{2} (x - \langle x \rangle)^2 \left. \frac{\partial^3 V(x)}{\partial x^3} \right|_{} + \cdots \left. (3.6.2.16) \right.$$

Considering  $\langle x - \langle x \rangle \ge 0$ , from Eq. (3.6.2.16) we have

$$\frac{\overline{\partial V}}{\partial x} = \frac{\partial V(x)}{\partial x}\Big|_{} + \overline{(x - \langle x \rangle)^2} \frac{\partial^3 V(x)}{\partial x^3}\Big|_{} + \cdots$$
(3.6.2.17)

If the  $V(x) = a + bx + cx^2$  in Eq. (3.6.2.17), then Eq. (3.6.2.15) becomes

$$m\frac{d^2 \langle x \rangle}{dt^2} = \frac{d \langle p_x \rangle}{dt} = -\frac{\partial V(x)}{\partial x}\Big|_{\langle x \rangle}.$$
(3.6.2.18)

Eq. (3.6.2.18) shows that the motion of average values of the particle position obeys exactly Newton equation for some special potential.

# 3.6.3. Still More Microscopic Process

(1) Some references think that there is a sharp contradiction between general theory of relativity and quantum mechanics, and that this contradiction is a rigorous challenge faced by mankind in 21 century [1, 58].

The wavepacket-only theory thinks that the above so-called "rigorous challenge" has been solved by wavepacket-only theory completely. For the so-called "challenge" in Refs. [1, 58], wavepacket-only theory makes following analysis. When quantum mechanics writes Hamiltonian to establish equation of motion of the particle (i. e., Schrödinger equation), quantum mechanics requires that the particle obeys the general theory of relativity, such as the weak equivalence principle, rigorously and exactly. In this aspect, there is no any contradiction between quantum mechanics and general theory of relativity.

The wavepacket-only theory thinks that after solving Schrödinger equation and finding out the solution (i. e., the wavefunction or, say, the guide-factor), the body-factor of wavepacket obeys the guide of the wavefunction according to spontaneous equiprobability symmetry breaking. This process is a still more microscopic process, and is a stochastic procees. For this process, general theory of relativity cannot say anything (General theory of relativity belongs to one kind of deterministic theories.). The quantum theory is a theory, which can describe stochastic processes, and thus goes beyond the scope of general theory of relativity, or, is higher than the general theory of relativity. In this aspect, we cannot say that there is a contradiction between quantum theory and general theory of relativity, because the latter is powerless and helpless for the spontaneous equiprobability symmetry breaking. The so-called "contradiction" in Refs. [1, 58] looks like the following question in our everyday life: one person asks: "Why does guest in room of hotel and the hotel's room do not obey the same rule?" This is obviously a stupid question because guest is a person, and room is a nonliving matter. Thus, this question itself in Refs. [1, 58] is not reasonable. guest=peaple=body-factor)  $\neq$  hotel=guide-factor=wavefunction because guide-factor  $\neq$  body-factor. The action of guide-factor is to guide a spontaneous equiprobability symmetry breaking motion of body-factor. Both special and general theory of relativity study the motion roles satisfying determinism. In the following we will give many examples to interpret that the action of wavefunction violates the general theory of relativity.

Actually, all potentials in Schrödinger equation are written by Newton mechanics (if low velocity) and the weak equivalent principle. Therefore, there is no contradiction between quantum mechanics and general theory of relativity. Let us give an example. The cold neutrons in the Earth's gravitational field are allowed to fall along z direction towards a horizontal mirror put on the Earth' surface. The cold neutron potential is  $V = m_{neutron}gz$ . Let us recall how to obtain this potential expression. The neutron receives force  $-dV/dz = -m_{neutron,gravitationalg}$ . However, if a neutron has acceleration g, then according to Newton second law the neutron receives force  $-m_{neutron,inertialg}$ . When one writes the expression of the potential in gravitational field in Schrödinger equation, one always uses the weak equivalent principle of general theory of relativity, i. e.,  $m_{neutron,inertial} = m_{neutron,gravitational} = m_{neutron}$ . Therefore, from the aspect of establishment of Schrödinger equation, the wavepacket-only theory requires any objects to obey the weak equivalent principle, i. e., there is no any contradiction between wavepacket-only theory and general theory of relativity.

However, we have to note that although Hamiltonian of wavepacket obeys general theory of relativity and so on, but the actual motion of particle obeys the equiprobability symmetry and spontaneous equiprobability symmetry breaking law. The wavepacket motion law has no direct connection with general theory of relativity and so on. According to equiprobability symmetry, the actual motion is decided by the square of absolute value of the guide-factor. If, for example, the energy connected with a wavefunction might be discrete, then the actual motion of the particle will be jumping or hopping. This actually observed motion is a result of wavepacket motion law. (The particle jumping motion in gravitational field was observed, which will be introduced in subsection 4.5.2 of chapter 4.) Both the equiprobability symmetry and spontaneous equiprobability symmetry breaking are independent of general theory of relativity, Maxwell equation, and so on. However, when we write Schrödinger equation, we have to think that the particle's Hamiltonian obeys general theory of relativity, and so on. Thus, the actual quantummechanical motion of a body-factor of particle and the weak equivalent principle obeyed by the Hamiltonian of particle are two different things. In other words, general theory of relativity and the still more microscopic process are independent of each other. The law of wavepacket motion is a law, which all particles, including Earth, the sun, quark, meson, neutrino, photon, phonon, electron, and so on, have to obey. The spontaneous equiprobability symmetry breaking is a new process.

Let us look at the cold neutron falling experiment in more detail. The falling neutron experiment on Earth's surface has non-continuous energy levels (Energy quantization of bound state. See chapter 4). Experiment showed that the falling neutrons really do not move continuously along the vertical direction, but rather jump from one height to another hight [36]. Although the falling cold neutron jumps from one height to another hight, but when we write Hamiltonian in the motion equation of the wavepacket, we have to use rules such as Newton laws and the weak equivalent principle. But, the quantum state or wavefunction or guide-factor determined by Schrödinger equation does not obeys weak equivalent principle and so on.

The prominent character of the still more microscopic processes is the equiprobability symmetry and spontaneous equiprobability symmetry breaking, which is a new symmetry and rule obeyed by objects. We can say that quantum mechanics (or more generally speaking, wavepacket-only theory) needs the general theory of relativity, but wavepacket-only theory gives new motion rule of object. Therefore, in aspect of theoretical administrative levels, the wavepacket-only theory is higher than the general theory of relativity.

Next, we list some properties of wavefunction, which violate weal equivalence principle [1, 30].

(i) The wavelength of de Bloglie wave of free massy particle is  $\lambda = h/p = h/(mv)$ , which is dependent on the mass *m*. Therefore, all phenomena on diffraction and interference are related to mass;

(ii) The radius of hydrogen atom is  $r_n = n^2 a = n^2 \hbar^2 / (me^2)$ , *n* is the principal quantum number, and  $a = \hbar^2 / (me^2)$  is the Bohr radius, dependent on the electron mass *m*. If we use Schrödinger equation to calculate motion of a particle with mass *m* in gravitational field of a body with huge mass *M*, then the radius of the circle trajectory of the particle *m* is  $r_n = n^2 a = n^2 \hbar^2 / (mGMm)$  (in which  $e^2 \to GMm$ ). The  $r_n$  depends on the *m*. However, according to the weak equivalence principle, the acceleration  $\ddot{r} = -\nabla \phi(r)$  ( $\phi$  is the gravitational potential

energy) should be independent of mass of the particle;

(iii) The uncertainty relations do not obey general theory of relativity. For example,  $\Delta x \cdot \Delta p = m\Delta x \cdot \Delta v = \geq \hbar/2$ .  $\Delta x \cdot \Delta v$  is dependent on *m*;

(iv) In gravitational field  $V = m\phi$ , Schrödinger equation is

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + m\phi\right)\Psi_n = E_n\Psi_n$$

can be rewritten as

$$\left(-\frac{\hbar^2}{2m^2}\nabla^2+\phi\right)\Psi_n=\frac{E_n}{m}\Psi_n.$$

Therefore, the energy of particle and the wavefunction are both dependent on mass *m*. However, according to the weak equivalence principle, the particle energy  $E = mv^2/2 + m\phi$ . E/m should be independent of *m*.

(v) Weak equivalence principle for elementary particle in quantum state might be violated by some direct observations. Quantum states of neutrons in gravitational and centrifugal potentials can be considered the first direct demonstration of the weak equivalence principle of the general relativity for an object (a particle) in a pure quantum state. The current accuracy of such a comparison is limited by the precision of the gravitational experiment, but it will be significantly improved in the near future. In the classical case, the weak equivalence principle has been verified with the best accuracy  $10^{-12}$ , using macroscopic bodies. The accuracy of measurements with atoms,  $7 \times 10^{-9}$ , is very high as well. Concerning elementary particles, the best accuracy  $3 \times 10^{-4}$  has been achieved with neutrons. However, a known contradiction occurs in the analysis of another neutron experiment, where a gravitationally induced phase shift was measured in a neutron interferometer. Accounting for dynamical diffraction effects in the silicon of neutron interferometer results in a formal violation of the weak equivalence principle. This statement was followed by a series of more precise experiments, where a small deviation was also measured. Although the most probable reason for this deviation is apparently some methodical error, an increase in accuracy of neutron experiments by a few orders of magnitude would help clarify the current contradiction. Such an improvement could be achieved in planned experiments with a neutron interferometer of another type, or in precision experiments with gravitational quantum states of neutrons in the spectrometer. For this point (v) please refer to Ref. [36].

(2) Chapter 10 and many other references such as [103, 6] prove that in some quantum transition processes the energy is conditionally not conservative more or less, and, especially, point out that there are already some experimental data on the light absorption in semiconductor which require the explanation of energy nonconservation.

(3) As is well known, the general and special theories of relativity are compatible with the energy conservation. If the energy conservations are violated by quantum mechanics more or less in principle, then, at least, we can say that the general and special theory of relativity are violated indirectly by the still more microscopic processes in quantum mechanics.

In one word, the wavepacket-only theory is a theory more higher and more prominent in scientific administrative levels in comparison with general and special theories of relativity, and thus general and special theories of relativity shouldn't interfere with the spontaneous equiprobability symmetry breaking in wavepacket-only theory. Why? Because the wavepacket-only theory is based basically on the exact mathematics, and is thus more basic.

# 3.7. Exercises and Solutions

(1) Use the uncertainty relation to estimate the characteristic energies of particles in different levels.

#### Solution:

First level. For atom, molecular, and nuclei, the non-relativistic energy formula can be used, i. e.

$$E \approx \frac{p^2}{2m} \approx \frac{\Delta p}{2m}.$$

For atom,  $\Delta x \approx 10^{-8}$  cm, the energy of electron is

$$E \approx \frac{\hbar^2}{2m_e(\Delta x)^2} \approx 4eV.$$

For comparison, the binding energy of an electron in hydrogen is 13.6 eV ( $\approx 4 \text{ eV}$ ).

Second level. For nuclei with middle size  $\Delta x \approx 6 \times 10^{-13}$  cm, the energy of neutron or proton is

$$E \approx \frac{\hbar^2}{2m_{n,p}(\Delta x)^2} \approx 1 MeV.$$

We note in passing that this is a far from academic exercise. The energy we have obtained, which is the typical energy obtained from nuclear reactions, is some five million times greater than our earlier estimate of the typical energy of an electron in an atom, which is the typical energy obtainable from chemical reactions. This is the origin of the terrible destructiveness of nuclear, as opposed to the conventional, weapons.

Third level. In particle physics, the size of particle is  $\Delta x \le 10^{-13}$  cm. Use approximate relativistic formula

$$E \approx pc \approx c(\Delta p) \approx \frac{c\hbar}{(\Delta x)} \approx 0.2 GeV.$$

(2) Ref. [60] tells us that the phase  $\phi$  quantization is one of the frontier problems in quantum mechanics. Ref.[60] states: (i). Assume  $[\hat{N}, \hat{\phi}] = i$ ; (ii). Set  $a = e^{i\hat{\phi}}\sqrt{\hat{N}}$  and  $a^+ = \sqrt{\hat{N}}e^{-i\hat{\phi}}$ , then  $\hat{N} = a^+a = \sqrt{\hat{N}}e^{-i\hat{\phi}}e^{i\hat{\phi}}\sqrt{\hat{N}}$ . However, the average value of commutation relation is

$$< N | [\hat{N}, \hat{\phi}] | N > = < N | \hat{N} \hat{\phi} | N > - < N | \hat{\phi} \hat{N} | N >$$
  
=  $N < N | \hat{\phi} | N > - < N | \hat{\phi} | N > N = 0 \neq i.$  (2.1)

It is obvious that to explain the contradiction, we need that  $\exp(i\hat{\phi})$  is not an unitary operator. To solve the contradiction revealed by Eq. (2.1), the present references proposed two theories: SG and PB. In SG theory, Boson number can be arbitrary, but the phase operator does not have unitary property. On the contrary, in PB theory, Boson number has upper limit, but the phase operator keeps unitary property. Would reader please propose a method to make every thing OK.

Solution: Eq. (3.3.1.4.9b) is

$$\phi$$
 in  $\phi$  representation  $\rightarrow \frac{\partial}{i\partial N}$  in N representation. (3.3.1.4.9b)(2.2)

From Eq. (2.2) we can prove

$$[\hat{N}, \hat{\phi}] = i.$$

$$\exp(i\hat{\phi}) \times \exp(-i\hat{\phi}) = \exp\left(i\frac{\partial}{i\partial N}\right) \times \exp\left(-i\frac{\partial}{i\partial N}\right) = 1.$$

Eq. (3.3.1.2.3) shows that *N* is an arbitrary integer number. In our method, Eq. (2.1) in Ref. [60] is wrong.

$$\begin{split} < N|[\hat{N}, \hat{\phi}]|N > &= < N|\hat{N}\hat{\phi}|N > - < N|\hat{\phi}\hat{N}|N > \\ &= N < N|\frac{\partial}{i\partial N}|N > - < N|\frac{\partial}{i\partial N}N|N > \\ &= N < N|\frac{\partial}{i\partial N}|N > - N < N|\frac{\partial}{i\partial N}|N > - < N|\frac{1}{i}|N > \\ &= i \neq N < N|\hat{\phi}|N > - < N|\hat{\phi}|N > N \end{split}$$

(3) Newton said that our universe need "fist driving force of God". Do you believe?

Solution:

No. I do not believe. I can give two parallel reasons.

First. The theorem of uncertainty relation proves that if any big or small body is in rest, then its momentum will be infinite. That is the body itself can produce motion.

Second. The law of wavepacket tells us that any body can have spontaneous equiprobability symmetry breaking. This breaking process does not need any force, it is spontaneous.

(4) Einstein said on quantum mechanics that "I do not believe: God plays dice." Do you agree?

#### Solution:

No. I do not agree. The spontaneous equiprobability symmetry breaking process is a process to dice.

(5) In section 3.8 I said: "The uncertainty principle is quite counter-intuitive, so the early students of quantum theory had to be reassured that naive measurements to violate it were bound to be always unworkable. One way in which Heisenberg originally illustrated the intrinsic impossibility of violating the uncertainty principle is by using an imaginary microscope as a measuring device. See Fig. 1.9." Do you think that it is correct that the Heisenberg's explanation for uncertainty relation by using thought microscopic experiment?

Solution:

No, it is not correct completely. This thought experiment indicates that even Heisenberg at that time did not understand the physics of uncertainty relation correctly. As explanation and derivation in this chapter, we know that the uncertainty relation does not connect with any kind of measurements, and is an intrinsic characteristic of an object. If we can put an electron on a plate, that the electron cannot have certain position. On the contrary, it will move around an equilibrium position. Sometime the electron moves to east spontaneously with very high speed v. In principle, v can surpass light speed c, which's reason is simple, because the law of wavepacket is the higher law of nature than the special theory of relativity. Sometime the electron moves to west spontaneously with very low speed v. But, the product of the root-mean-square values of coordinate and momentum has lowest bound. The momentum uncertainty of the electron under the thought microscope does not come from the randomly scattering photons.

(6) In section 1.8 you can also see that there were tit-for-tat arguments between Einstein and Bohr on the uncertainty relation. Please join these arguments, review both Einstein's and Bohr's viewpoints, and propose yours viewpoint.

(7) Ref. [60] gave a typical and representative statement for the superposition of states, which is: "One of the arresting features of quantum mechanics is that particles or system of particles do not have in general definite attributes. When we express the wavefunction as

$$\Psi = c_1 \Psi_1 + c_2 \Psi_2$$

where  $\psi_1$  and  $\psi_2$  are eigenfunctions of an operator  $A_{op}$  corresponding to an observable A, we are saying that before we make a measurement of A the particle does not have a definite value of that attributes. The probability that a measurement yields  $a_1$  is, of course,  $c_1^2$ . After a measurement yielding  $a_1$ , the wavefunction collapses to  $\psi_1$ , since a measurement of Aimmediately thereafter again yields the value  $a_1$ . How this collapse happens is a mystery. It is referred as the measurement problem."

Please use the wavepacket-only theory to review the above statement.

Solution:

In the language of the wavepacket-only theory, wavepacket=object=massy particle (e.g., electron, cat, sun, universe) and massless particle (e.g., photon, phonon). The wavepacket-only theory proves that wavepacket consists of two factors: guide-factor and body-factor. The body-factor carries the substance, such as mass, charge, and spin, of the object, and the guide-factor is only a function, which is often called wavefunction. Although the guide-factor is only a mathematical function, which is determined by Schrödinger wave equation, but is is necessary for an object, because the motion of body-factor obeys the guide of the guide-factor according to the spontaneous equiprobability symmetry breaking law.

In the wavepacket-only theory, the statement in exercise should be:

"One of the arresting features of quantum mechanics is that the object consists of two parts: body-factor and guide-factor(=wavefunction). The guide-factor does not have in general definite attributes. When the guide-factor is in state  $\Psi$ 

$$\Psi = c_1 \Psi_1 + c_2 \Psi_2$$

general definite attributes. When the guide-factor is in state  $\Psi$ 

$$\Psi = c_1 \Psi_1 + c_2 \Psi_2$$

where  $\psi_1$  and  $\psi_2$  are eigenfunctions of an operator  $A_{op}$  corresponding to an observable A, we are saying that before the body-factor takes  $a_1$  and  $a_2$  the guide-factor does not have a definite value of that attributes. According to the spontaneous equiprobability symmetry breaking, the probability that the body-factor takes  $a_1$  is  $c_1^2$ . After that the body-factor takes  $a_1$ , the guide-factor(=wavefunction) accomplishes its guide action or task. This process does not mean that the guide-factor collapses to  $\psi_1$ ; on the contrary, this process means that the body-factor takes value  $a_1$  of the observable A with probability  $c_1^2$ . A measurement of Aimmediately thereafter this process yields the value  $a_1$  with probability 1. Therefore, there is no any mystery in this process. In the wavepacket-only theory, the body-factor's motion has no a wee bit of connections with measurement."

From the above discussions, you can see that the wavepacket-only theory requires that quantum mechanics abandons the viewpoints of wavepacket collapse and measurement-dependence of quantum mechanics.

(8) Schrödinger cat is an unsolved basic problem of quantum mechanics. Although Schrödinger cat has been observed in experiments such as Refs. [61, 62] and even in macroscopic superconducting system in Ref. [63], but Schrödinger cat has not yet been observed in a macroscopic non-superconducting system.

Please use the wavepacket-only theory to argue that Schrödinger macroscopic cat is a pseudo-proposition.

Foe convenience of readers, at first I summarize the present research situations on Schrödinger cat (For detail refer to Ref. [64]).

Schrödinger's cat is a thought experiment, sometimes described as a paradox, devised by Austrian physicist Schrödinger in 1935. It illustrates what he saw as the problem of Copenhagen interpretation of quantum mechanics applied to everyday objects, resulting in a contradiction with common sense. The scenario presents a cat that might be alive or dead, depending on an earlier random event. Although the original "experiment" was imaginary, similar principles have been researched and used in practical applications. The thought experiment is also often featured in theoretical discussions of the interpretations of quantum mechanics. In the course of developing this experiment, Schrödinger coined the term Verschrönkung (entanglement).

(A) Origin and motivation. Schrödinger intended his thought experiment as a discussion of EPR article/named after its authors Einstein, Podolsky, and Rosen/in 1935. EPR article highlighted the strange nature of quantum entanglement, which is a characteristic of a quantum state that is a combination of the states of two systems (for example, two subatomic particles), that once interacted but were then separated and are not each in a definite state. Copenhagen interpretation implies that the state of the two systems undergoes collapse into a definite state when one of the systems is measured. Schrödinger and Einstein exchanged letters about Einstein's EPR article, in the course of which Einstein pointed out that the state of an unstable keg of gunpowder will, after a while, contain a superposition of both exploded and unexploded states. To further illustrate, Schrödinger describes how one could, in principle, transpose the superposition of an atom to large-scale systems. He proposed a scenario with a cat in a sealed box, wherein the cat's life or death depended on the state of a subatomic particle. According to Schrödinger, the Copenhagen interpretation implies that the cat remains both alive and dead (to the universe outside the box) until the box is opened. Schrödinger did not wish to promote the idea of dead-and-alive cats as a serious possibility; quite the reverse, the paradox is a classic reductio ad absurdum. The thought experiment illustrates quantum mechanics and the mathematics necessary to describe quantum states. Intended as a critique of just the Copenhagen interpretation (the prevailing orthodoxy in 1935), the Schrödinger cat thought experiment remains a typical touchstone for limited interpretations of quantum mechanics. Physicists often use the way each interpretation deals with Schrödinger's cat as a way of illustrating and comparing the particular features, strengths, and weaknesses of each interpretation.

(B) The thought experiment. Schröinger wrote:

One can even set up quite ridiculous cases. A cat is penned up in a steel chamber, along with the following device (which must be secured against direct interference by the cat): in a Geiger counter, there is a tiny bit of radioactive substance, so small that perhaps in the course of the hour, one of the atoms decays, but also, with equal probability, perhaps none; if it happens, the counter tube discharges, and through a relay releases a hammer that shatters a small flask of hydrocyanic acid. If one has left this entire system to itself for an hour, one would say that the cat still lives if meanwhile no atom has decayed. The psi-function of the entire system would express this by having in it the living and dead cat (pardon the expression) mixed or smeared out in equal parts. It is typical of these cases that an indeterminacy originally restricted to the atomic domain becomes transformed into macroscopic indeterminacy, which can then be resolved by direct observation. That prevents us from so naively accepting as valid a "blurred model" for representing reality. In itself, it would not embody anything unclear or contradictory. Schrödinger's famous thought experiment poses the question, when does a quantum system stop existing as a superposition of states and become one or the other? (More technically, when does the actual quantum state stop being a linear combination of states, each of which resembles different classical states, and instead begins to have a unique classical description?) If the cat survives, it remembers only being alive. But explanations of the EPR experiments that are consistent with standard microscopic quantum mechanics require that macroscopic objects, such as cats and notebooks, do not always have unique classical descriptions. The thought experiment illustrates this apparent paradox. Our intuition says that no observer can be in a mixture of stateslyet the cat, it seems from the thought experiment, can be such a mixture. Is the cat required to be an observer, or does its existence in a single well-defined classical state require another external observer? Each alternative seemed absurd to Albert Einstein, who was impressed by the ability of the thought experiment to highlight these issues. In a letter to Schrödinger dated 1950, he wrote:

You are the only contemporary physicist, besides Laue, who sees that one cannot get around the assumption of reality, if only one is honest. Most of them simply do not see what sort of risky game they are playing with reality/reality as something independent of what is experimentally established. Their interpretation is, however, refuted most elegantly by your system of radioactive atom + amplifier + charge of gunpowder + cat in a box, in which the psi-function of the system contains both the cat alive and blown to bits. Nobody really doubts that the presence or absence of the cat is something independent of the act of observation.

Note that no charge of gunpowder is mentioned in Schrödinger's setup, which uses a Geiger counter as an amplifier and hydrocyanic poison instead of gunpowder. The gunpowder had been mentioned in Einstein's original suggestion to Schrödinger 15 years before, and apparently Einstein had carried it forward to the present discussion.

(C) Interpretations of the experiment. Since Schrödinger's time, other interpretations of quantum mechanics have been proposed that give different answers to the questions posed by Schrödinger's cat of how long superpositions last and when (or whether) they collapse.

(C.1) Copenhagen interpretation. Main article: Copenhagen interpretation The most commonly held interpretation of quantum mechanics is the Copenhagen interpretation. In the Copenhagen interpretation, a system stops being a superposition of states and becomes either one or the other when an observation takes place. This experiment makes apparent the fact that the nature of measurement, or observation, is not well-defined in this interpretation. The experiment can be interpreted to mean that while the box is closed, the system simultaneously exists in a superposition of the states "decayed nucleus/dead cat" and "undecayed nucleus/living cat," and that only when the box is opened and an observation performed does the wave function collapse into one of the two states.

However, one of the main scientists associated with the Copenhagen interpretation, Niels Bohr, never had in mind the observer-induced collapse of the wave function, so that Schrödinger's Cat did not pose any riddle to him. The cat would be either dead or alive long before the box is opened by a conscious observer. Analysis of an actual experiment found that measurement alone (for example by a Geiger counter) is sufficient to collapse a quantum wave function before there is any conscious observation of the measurement. The view that the "observation" is taken when a particle from the nucleus hits the detector can be developed into objective collapse theories. In contrast, the many worlds approach denies that collapse ever occurs.

(C.2) Many-worlds interpretation and consistent histories. The quantum-mechanical "Schrödinger's cat" paradox according to the many-worlds interpretation. In this interpretation, every event is a branch point. The cat is both alive and dead/regardless of whether the box is opened/but the "alive" and "dead" cats are in different branches of the universe that are equally real but cannot interact with each other. In 1957, Hugh Everett formulated the many-worlds interpretation of quantum mechanics, which does not single out observation as a special process. In the many-worlds interpretation, both alive and dead states of the cat persist after the box is opened, but are decoherent from each other. In other words, when the box is opened, the observer and the already-dead cat split into an observer looking at a box with a dead cat, and an observer looking at a box with a live cat. But since the dead and alive states are decoherent, there is no effective communication or interaction between them.

When opening the box, the observer becomes entangled with the cat, so "observer states" corresponding to the cat's being alive and dead are formed; each observer state is entangled or linked with the cat so that the "observation of the cat's state" and the "cat's state" correspond with each other. Quantum decoherence ensures that the different outcomes have no interaction with each other. The same mechanism of quantum decoherence

is also important for the interpretation in terms of consistent histories. Only the "dead cat" or "alive cat" can be a part of a consistent history in this interpretation.

Roger Penrose criticizes this:

"I wish to make it clear that, as it stands, this is far from a resolution of the cat paradox. For there is nothing in the formalism of quantum mechanics that demands that a state of consciousness cannot involve the simultaneous perception of a live and a dead cat". However, the mainstream view (without necessarily endorsing many-worlds) is that decoherence is the mechanism that forbids such simultaneous perception.

A variant of the Schrödinger's Cat experiment, known as the quantum suicide machine, has been proposed by cosmologist Max Tegmark. It examines the Schrödinger's Cat experiment from the point of view of the cat, and argues that by using this approach, one may be able to distinguish between the Copenhagen interpretation and many-worlds.

(C.3) Ensemble interpretation. The ensemble interpretation states that superpositions are nothing but subensembles of a larger statistical ensemble. The state vector would not apply to individual cat experiments, but only to the statistics of many similarly prepared cat experiments. Proponents of this interpretation state that this makes the Schrödinger's cat paradox a trivial non-issue.

This interpretation serves to discard the idea that a single physical system in quantum mechanics has a mathematical description that corresponds to it in any way.

(C.4) Relational interpretation. The relational interpretation makes no fundamental distinction between the human experimenter, the cat, or the apparatus, or between animate and inanimate systems; all are quantum systems governed by the same rules of wavefunction evolution, and all may be considered "observers." But the relational interpretation allows that different observers can give different accounts of the same series of events, depending on the information they have about the system. The cat can be considered an observer of the apparatus; meanwhile, the experimenter can be considered another observer of the system in the box (the cat plus the apparatus). Before the box is opened, the cat, by nature of it being alive or dead, has information about the state of the apparatus (the atom has either decayed or not decayed); but the experimenter does not have information about the state of the box contents. In this way, the two observers simultaneously have different accounts of the situation: To the cat, the wavefunction of the apparatus has appeared to "collapse"; to the experimenter, the contents of the box appear to be in superposition. Not until the box is opened, and both observers have the same information about what happened, do both system states appear to "collapse" into the same definite result, a cat that is either alive or dead.

(C.5) Objective collapse theories. According to objective collapse theories, superpositions are destroyed spontaneously (irrespective of external observation) when some objective physical threshold (of time, mass, temperature, irreversibility, etc.) is reached. Thus, the cat would be expected to have settled into a definite state long before the box is opened. This could loosely be phrased as "the cat observes itself," or "the environment observes the cat."

Objective collapse theories require a modification of standard quantum mechanics to allow superpositions to be destroyed by the process of time evolution.

(C.6) The decoherence (or say, localization) of macroscopic system, caused by the inevitable interaction of the macroscopic system with the environment [116]. This paper
confirms through theirs numerical calculations for the influence on a macroscopic system by the scattering of the microscopic particles in the environment [which contains at least  $10^3$  microscopic particles (photons and so on) per cm<sup>3</sup>] that the decoherence, or say, localization of a macroscopic system comes from this scattering influence.

## Solution:

The wavepacket-only theory thinks that just the (C.6)'s illustration for Schrödonger cat in all the six illustrations is better, although it is still wrong. The following proof also negatives any form of so called inevitable environment influence, for example, the influence in Ref. [69].

For convenience, suppose that the cat is one dimensional. Let us estimate the cat's minimum momentum.

$$(\Delta p_x) \geq \frac{\hbar}{2(\Delta x)}.$$

According to the present measurement technique of length, if the cat's  $(\Delta x) \ge 10^{-4} cm$ , then we can measure. Therefore, it becomes

$$(\Delta p_x) \geq \frac{\hbar}{2 \times 10^{-4}}.$$

The cat's de Bloglie wavelength is

$$\lambda_x \leq 4\pi \times 10^{-4} \ cm \ll L_x \approx 20 \ cm,$$

where  $L_x$  represents the size of the cat. According to the criterion of quantum or classical object, it can be concluded that the cat is a classical object, and thus there is no the interference state of alive and dead cat. Therefore, "Schrödinger cat" is a pseudo-proposition. The decoherence of a macroscopic object does not be caused by the influence of environment; on the contrary, this decoherence is an intrinsic characteristic of a macroscopic object.

Although Schrödinger cat paradox is one in the frontier problems of quantum mechanics [60], but in our wavepacket-only theory it can be proved exactly and easily by one theorem and one criterion that the Schrödinger macroscopic cat paradox is a pseudo-proposition.

(9) To describe the classical Kepler motion, the Ruterger-Lenz vector M is introduced instead of L. The importance of  $\mathbf{M}$  can be found in Ref. [60].

$$M = \frac{1}{m}p \times L - k\frac{r}{r},\tag{9.1}$$

where *m* is the point mass, angular momentum  $L = r \times p$ , the central force field V(r) = -k/r, for example, for the hydrogen-like ion,  $k = Ze^2$ . Its extension in quantum mechanics is

$$M = \frac{1}{2m} \left[ p \times L - L \times p \right] - k \frac{r}{r}.$$
(9.2)

The M satisfies the following canonical commutation relations:

$$[M_x, M_y] = -\frac{2i\hbar}{m} HL_z, \ [M_x, L_x] = 0, \ [M_x, M_y] = i\hbar M_z, \ [M_z, M_z] = i\hbar M_y, \tag{9.3}$$

where

$$H = \frac{1}{2m}p^2 - \frac{k}{r}.$$
 (9.4)

The Heisenberg uncertainty relation is

$$(\Delta M_x)(\Delta M_y) \ge \frac{1}{2}| < -2iHL_z > | if \hbar = m = Ze^2 = 1.$$
 (9.5)

Prove one of the canonical commutation relations, and the Heisenberg uncertainty relation.

Solution:

(A) Using the formula, given by Eq. (9.3.1.4.9.d), one can prove the commutation relations.

(B) Using Theorem V, one can prove the Heisendberg uncertainty relation.

(10) Ref. [70] listed many quantum paradoxes. Please, in terms of the wavepacket-only theory, prove exactly that quantum mechanics is without a wee bit of paradoxes.

(11) It is concluded that the state of a particle with zero energy cannot exist in the infinitely deep pit with finite width a. Give an argument from Heisenverg uncertainty relation in section 3.3.

## Solution:

The energy of the particle in the pit is entirely kinetic, in turn, implies that the particle is in a state of absolute rest ( $\Delta p = 0$ ). From physical uncertainty relation ( $\Delta p$ )( $\Delta x$ )  $\geq (\hbar/2)$ . If  $\Delta p = 0$ , then  $\Delta x = \infty$ . Therefore, The state with E = 0 is an illegitimate state of affairs for a particle constrained in a finite domain.

(12) The quantum of gravitational field has not yet been observed by any experiment. Argue that if it exists really, then the quantum cannot be monotonous.

#### Solution:

Any object, including a quantum, has to be a wavepacket. Heisenberg uncertainty relation does not allow that it is a point without size. Heisenberg uncertainty relation  $(\Delta t)(\Delta \omega) \ge 1/2$ . Because the time duration of a signal cannot be infinitely long, thus the gravitational quantum cannot be monotonous.

(13) The size of superstring is Planck length  $10^{-33}$  cm. Estimate its energy connected with Heisenberg uncertainty relation.

#### Solution:

In the string theory the strings can constitute any particles such as quark, electron, and proton. The size of string is equal to about  $10^{-33}$  cm. Some authors even think that the string theory might be the last theory on nature and unverse [71]. The string has at least to be described by a mathematical function satisfying not too harsh terms,

which's requirement is independent of any physical principles, rules, laws, and theorems. Therefore, the string has to satisfy Heisenberg uncertainty relation, which requires the string to have  $\Delta x \times \Delta p_x \ge \hbar/2$ . From  $\Delta x = 10^{-33}$  cm we obtain  $\Delta p_x \ge 10^{33}\hbar/2$ . Even we neglect the rest mass of superstring, the energy of superstring is  $E = 1.5 \times 10^{16}$  erg. The size of electron is  $\Delta x = 10^{-18}$  cm. Therefore,  $\Delta p_x = 5 \times 10^{-9}$  for electron. The energy of electron is thus  $\sqrt{p_x^2 c^2 + m_0^2 c^4} \propto 8 \times 10^7$  erg. Here, we derive a doubtful conclusion from the string theory. That is, although many superstrings constitute an electron, but the energy of electron is less than the (energy of string) $\times 10^{-9}$ . The other problem of superstring theory is as follows. If the superstring is one dimensional along x axis, then  $\Delta y = 0$ , and  $\Delta p_y = \infty$ . Obviously, the latter equality is not reasonable in mathematics.

(14) Assume that a particle with negligible mass is confined in a box, the size of which is around 1  $fm = 10^{-15}m$ . Use Heisenberg uncertainty relation to estimate the energy of the confined particle.

Solution:

 $(\Delta x)(\Delta p_x) \geq \hbar/2.$   $\Delta p_x \geq 10^{-27} erg.second/(2 \times 10^{-13} cm).$   $E \approx c(\Delta p_x) \geq 5 \times 10^{-15} \times 3 \times 10^{10} = 1.5 \times 10^{-4} erg \approx 100 MeV.$ 

(15) For photon,  $\Delta \phi = 10^{-4} rad$ , what is  $\delta N$ ?

Solution:  $(\Delta N)(\Delta \phi) \ge \frac{1}{2}$ . Thus,  $\Delta N \ge 10^4/2 = 5 \times 10^3$ .

Note:  $\Delta N$  may be made vanishingly small at the expense of very large phase  $\Delta \phi$ . The obtained field is called "squeezed light". The field is squeezed in the sense that intensity fluctuations are vanishing small [6].

(16) The size of atom is approximately  $10^{-8}$  cm. To locate an electron within the atom, one should use electromagnetic radiation of wavelength not longer than, say,  $\lambda = 10^{-9}$  cm.

(a) What is the energy of a photon with such a wavelength (in eV)?

(b) What is the uncertainty in the electron's momentum if we are certain about its position by  $10^{-9}$  cm?

Solution:

(a) The energy of a photon is  $\hbar \omega = \hbar c 2\pi/\lambda = 1.9 \times 10^{-7} \text{ erg} \approx 1.2 \times 10^5 \text{ eV.}$  (b). From  $(\Delta x)(\Delta p_x) \ge \hbar/2$  we have the uncertainty in the electron's momentum  $\Delta p_x \ge 5 \times 10^{-19}$  g.cm/sec.

(17) There is a small dust,  $mass \approx 10^{-12}$  g, radius  $r \approx 10^{-4}$  cm, velocity  $v \approx 0.1$  cm/sec, momentum  $p \approx 10^{-13}$  g.cm/sec. Suppose its position uncertainty is  $\Delta x = 10^{-8}$  cm. Find its momentum uncertainty  $\Delta p$ .

Solution:

 $\Delta p \geq \hbar/[2(\Delta x) \approx 10^{-19} \text{ g.cm/sec.} \quad \Delta p/p \approx 10^{-6}$ , which is a very small magnitude. Therefore, in practice people does not need to consider the effect of uncertainty relation of the dust, and the dust can be described quite well at the same time by position and momentum or velocity.

(18) Estimate the size of particle in terms of the momentum uncertainty.

Solution:

By "size" we mean  $\Delta x$  in the sense of the uncertainty relations. According to this uncertainty relation

$$\Delta x \approx \frac{\hbar}{\Delta p}.$$

A typical value of  $\Delta p$  is given by the momentum mv of the particle. The maximum possible value of the velocity according to the special theory of relativity is the velocity of light c. The minimum value of  $\Delta x$  is then

$$(\Delta x)_{min} \approx \frac{\hbar}{mc}.$$

Therefore, one does not think of a particle of mass *m* as a point particle but rather as an object with a finite size,  $\hbar/mc$ . This is also called Compton wavelength characteristic of that particle and it enters into calculations whenever a length scale for the particle appears.

(19) Just use the uncertainty relations to estimate Bohr radius and ground state energy of hydrogen atom.

Solution:

Classically, an electron of charge -e orbiting around of charge e would lose energy due to radiation and eventually fall into the proton. This is, of course, in contradiction to the observed fact that the electron executes stable orbits. This is explained quantum-mechanically in the simplest terms through the uncertainty relations.

The total energy E of the electron is a sum of the kinetic energy  $mv^2/2$  and the potential energy, which in the case of hydrogen is just the Coulomb potential. Thus, writing the kinetic energy in terms of p = mv, the momentum, we have

$$E = \frac{p^2}{2m} - \frac{e^2}{r},$$

where *r* is the distance between the proton and electron. Taking  $\Delta p \approx p$  and  $\Delta r \approx r$ , uncertainty relation says that

$$pr \approx \hbar$$
.

Thus, as r for the electron gets small due to the Coulomb attraction, p becomes large due to the uncertainty relation. In other words, as the attractive Coulomb potential moves the electron towards the proton, the increasing kinetic energy pushed the electron away from the system. The electron will then settle down at a minimum of the total energy. We can obtain this minimum by writing

$$E = \frac{\hbar^2}{2mr^2} - \frac{e^2}{r}$$

and then taking

$$\frac{\partial E}{\partial r} = 0.$$

This gives

$$-\frac{\hbar^2}{mr^2} + \frac{e^2}{r^2} = 0.$$

We find

$$r_{min}=\frac{\hbar^2}{me^2}.$$

This is, indeed, the Bohr radius of the hydrogen atom, which is designated as  $a_{\circ}$ . Substituting this in the expression of *E*, we obtain

$$E = -\frac{me^4}{2\hbar^2}.$$

(20) Assume that an one dimensional particle has certain momentum  $p_{\circ}$ , and its wavefunction is  $\Psi_{p_{\circ}}(x) = exp(ip_{\circ}x)/\hbar)/\sqrt{2\pi\hbar}$ , which are called eigenvalue and eigenstate of momentum, respectively.

(a) Discuss the uncertainty relation;

(b) Find the form of this quantum state in momentum space.

Solution:

(a)  $p = p_{\circ}$  means the uncertainty of momentum  $\Delta p = 0$ .  $|\Psi_{p_{\circ}}(x)|^2$  means that the particle exists in infinitely large position space. Thus  $\Delta x = \infty$ , which fits the uncertainty relation of position momentum uncertainty relation;

(b) According to the definition of transformation of a function from position space into momentum space, the Fourier transform of  $\Psi_{p_{\circ}}(x) = exp(ip_{\circ}x)/\hbar/\sqrt{2\pi\hbar}$  is

$$\phi_{p_{\circ}}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx e^{i\frac{p_{\circ}x}{\hbar}} / \sqrt{2\pi\hbar} e^{-i\frac{px}{\hbar}} = \delta(p - p_{\circ})$$

(21)  $\Psi_{x_o}(x) = \delta(x - x_o)$  describes the quantum state of an one dimensional particle with certain position  $x = x_o$ , which are called eigenstate and eigenvalue of position (coordinate), respectively.

(a) Discuss the uncertainty relation;

(b) Write this quantum state in momentum space.

Solution:

(a)  $x = x_{\circ}$  means the uncertainty of position  $\Delta x = 0$ . Thus  $\Delta p = \infty$ ; (b)

$$\phi_{x_{\circ}}(p) = \frac{1}{\sqrt{2\pi\hbar}} e^{-i\frac{x_{\circ}p}{\hbar}}.$$

(22) In the so-called "Quantum Land", a strange land, where  $\hbar = 10^4$  erg.sec, melons with a very hard peel are grown. They have a diameter of approximately 20 cm, the mass density is 1 g/cm<sup>3</sup>, and contain seeds with a mass of around m = 0.1 g [2].

Problems:

(a) Why do we have to be careful when cutting open melons grown in Quantum Land?

(b) How big the recoil of a melon at the reflection of a "visual" photon of 628 nm wavelength?

Solution:

(a) From the uncertainty relation of position-momentum follows for the momentum of uncertainty of the melon seeds  $\Delta p \ge \hbar/(2 \times 20) \approx 10^8$  g.cm.ses<sup>3</sup> and therefore their velocity uncertainty is  $\Delta v \ge \Delta/m \approx 1000$  cm.sec<sup>-1</sup>. The seeds leave the melon with this (mean) velocity when it is cut open.

(b) A photon of wavelength  $\lambda = 628$  nm has the momentum  $p = \hbar (2\pi/\lambda) = 10^9$  g.cm.sec<sup>-1</sup> and the energy  $E = pc = 3 \times 10^{19}$  erg. The mass of melon is  $M \approx (3\pi/4)10^3 \times 1$  g.cm<sup>-3</sup>  $\approx 4$  kg, its rest energy is  $Mc^2 = 36 \times 10^{24}$  erg; hence we can calulate nonrelativistically. Let the collision be elastic. The momentum of the melon after the collision is approximately  $2p = 2 \times 10^9$  g.cm.sec<sup>-1</sup>. This corresponds to a velocity  $v_{melon} = 5$  km.sec<sup>-1</sup> which is less than the escape velocity from the Earth. The collision of melon with such a photon would be rather unpleasant for a human being.

(23) Show that in three dimensional case, the position-momentum uncertainty relation may be written

$$(\Delta r)^2 (\Delta p)^2 \ge \frac{9}{4}\hbar^2, \tag{23.1}$$

where

$$(\Delta r)^2 = \langle (r - \langle r \rangle)^2 \rangle, \quad (\Delta p)^2 = \langle (p - \langle p \rangle)^2 \rangle.$$
 (23.2)

Solution:

Working in the frame where  $\langle p \rangle = \langle r \rangle = 0$ , we have  $(\Delta r)^2 = \langle r^2 \rangle$ ,  $(\Delta p)^2 = \langle p^2 \rangle$ . The resulting nine Cartesian products separate into two groups as follows:

$$(\Delta r)^{2} (\Delta p)^{2} = [(\Delta x \Delta p_{x})^{2} + \cdots] + [(\Delta x \Delta p_{y})^{2} + (\Delta y \Delta p_{x})^{2} + \cdots].$$
(23.3)

The first bracketed terms give

$$[(\Delta x \Delta p_x)^2 + \cdots] \ge \frac{3}{4}\hbar^2.$$
(23.4)

In the second bracketed six terms, with  $\Delta p_y \ge \hbar/\Delta y$ , etc., we write

$$\left[(\Delta x \Delta p_y)^2 + (\Delta y \Delta p_x)^2 + \cdots\right] \ge \left(\frac{\hbar}{2}\right)^2 \left[\left(\frac{\Delta x}{\Delta y}\right)^2 + \left(\frac{\Delta y}{\Delta x}\right)\right] + \cdots$$
(23.5)

As  $z + z^{-1} \ge 2$ , for all positive *z*, we find

$$[(\Delta x \Delta p_y)^2 + (\Delta y \Delta p_x)^2 + \cdots] \ge 6 \left(\frac{\hbar}{2}\right)^2.$$
(23.6)

Adding both contributions give the desired result.

(24) According to the meson theory of nuclear force, the long range part of the nuclear force is determined by the exchanging  $\pi$  meson. The  $\pi$  meson's mass is  $m_{\pi} \sim 270 m_e$ .

Estimate the force range  $r_{\circ}$  of the nuclear force.

Solution: The concerning energy uncertainty is

$$\Delta E \sim m_{\pi} c^2$$
.

The momentum uncertainty is

$$\Delta p \sim \Delta E/c \sim m_{\pi}c$$

The position uncertainty is

$$\Delta x \sim r_{\circ} \sim \hbar/\Delta p \sim \hbar/m_{\pi}c \approx 1.4 fm \ (1.4 \times 10^{-15}m)$$

(25) In monochromatic plane wave  $\Psi_{p_o}(x) = \exp(ip_o x)/\sqrt{2\pi\hbar}$ , the particle has definite momentum  $p = p_o$ , which is called eigenstate of position space. Find its expression  $\phi_{p_o}(p)$  in momentum space.

Solution: At first expand  $\Psi_{p_{\circ}}(x)$  in momentum-space

$$\Psi_{p_\circ}(x) = rac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dp \phi_{p_\circ}(p) e^{ip_\circ x}.$$

Then

$$\phi_{p_{\circ}}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \Psi_{p_{\circ}}(x) e^{-i\frac{p_{\circ}x}{\hbar}} = \delta(p - p_{\circ}).$$

(26)  $\Psi_{x_o}(x) = \delta(x - x_o)$  describes a particle with definite position  $x_o$ , which is called the eigenstate of the particle in position space, and eigenvalue is  $x_o$ . Find the expression of this state in momentum space.

Solution:

$$\phi_{x_{\circ}}(p) = \frac{1}{\sqrt{2\pi\hbar}} e^{-ix_{\circ}p}$$

(27) A quantum state in position space is  $\Psi(r)$ . The position average value of particle is  $\langle r \rangle = \int d^3 r r \Psi^*(r) \Psi(r)$ . Calculate  $\langle r \rangle = \overline{r}$  in momentum space.

Solution:

First expand  $\Psi(r)$  and  $\Psi^*(r)$  in momentum space. Second, substituting these expansions into the definition expression of  $\langle r \rangle$  yields

$$\langle r \rangle = \overline{r} = \int d^3 p \phi^* p i \hbar \bigtriangledown_p \phi(p).$$

That is, in momentum space **r** should be an operator  $\hat{r} = i\hbar \nabla_p$ . From this example we know that the operator of an observable is a requirement of mathematics. **r** in position space is a number (a special operator). However, it has to be expressed by a operator in

momentum space.

(28) In non-local potential V(r, r'), Schrödinger equation is

Find the requirement of conservation of probability density of single particle for the non-local potential.

Solution:  $V(r,r') = V^*(r',r).$ 

(29) Suppose that the Hamiltonian of N particle system is

$$H = -\sum_{i=1}^{N} \frac{\hbar^2 \bigtriangledown_i^2}{2m} + \sum_{i < j}^{N} v_{ij}(r_i - r_j|).$$

 $\Psi(r_1, r_2, \cdots, r_N, t)$  is the state function of the system. Define

$$\rho(r,t) = \sum_{i} \rho_{i}(r,t)$$
  
=  $\int d^{3}r_{2} \cdots d^{3}r_{N} \Psi^{*} \Psi + \int d^{3}r_{1} d^{3}r_{3} \cdots d^{3}r_{N} \Psi^{*} \Psi + \cdots$ 

$$j(r,t) = \sum_{i} j_{i}$$

$$= \frac{\hbar}{2im} \int d^{3}r_{2} \cdots d^{3}r_{N} (\Psi^{*} \bigtriangledown_{1} \Psi - \Psi \bigtriangledown_{1} \Psi^{*})$$

$$+ \frac{\hbar}{2im} \int d^{3}r_{1} d^{3}r_{3} \cdots d^{3}r_{N} (\Psi^{*} \bigtriangledown_{2} \Psi - \Psi \bigtriangledown_{2} \Psi^{*}).$$

Prove

$$\frac{\partial \rho}{\partial t} + \bigtriangledown \cdot j = 0.$$

Solution: Refer to the case of single particle.

(30) Is the wavefunction of a single particle  $\Psi(x) = x$  correct?

#### Solution:

No. It does not satisfy the normalization condition, i. e.

$$\int_{-\infty}^{\infty} dx \Psi^* \Psi \neq 1.$$

(31) At t = 0, the particle in a stationary state is described by a linear composition of two lowest energy states  $\Psi(x, 0) = A\Psi_{E_1}(x) + B\Psi_{E_2}(x)$ . Calculate the wavefunction  $\Psi(x, t)$ .

Solution:

Using the time dependence of stationary eigenstate, we have

$$\Psi(x,t) = Ae^{-\frac{iE_1t}{\hbar}}\Psi_{E_1} + Be^{-\frac{iE_2t}{\hbar}}\Psi_{E_2}.$$

(32) The sun light power per cm<sup>2</sup> on the Earth surface is 100 mW. Assume that the average energy of photon wavepacket in sun light is 1.56 eV. Find the number *n* of photons of the sun light on the Earth surface per cm<sup>2</sup> per second.

Solution:  $n = 4 \times 10^{17} / (cm^2.sec).$ 

(33) Consider a situation where it is equally likely that an electron has momentum  $\pm p_{\circ}$ . Measurement at a given instant of time finds the value  $+p_{\circ}$ . A student concludes that the electron must have had this value of momentum prior to measurement. Is the student correct?

Solution:

Our answer is that the student is correct. It is obvious that the given information indicates that the electron was in a superposition state prior to measurement. This superposition state shows that the both possibilities, that electron takes  $+p_{\circ}$  and  $-p_{\circ}$ , are equal to 0.5, which does not depend on measurement. The practical electron will take a momentum according to equiprobability symmetry and spontaneous equiprobability symmetry breaking, which does not depend on measurement as well.

For this exercise, Ref. [3] gives an opposite answer. Please make comment.

Some textbooks of quantum mechanics think also that the student is incorrect. They think: "The given information indicates that the electron was in a superposition state prior to measurement. In quantum mechanics one cannot rely on the premise of inference." [6] Please also make comment.

(34) Prove that in case of discrete values of wavenumbers, a wavepacket in free motion in three dimensional position space does not spread.

(35) Is there a possibility that the electron obeys the classical mechanics?

Solution:

The mass and size of an electron are  $m_{\circ} = 9.1 \times 10^{-28}$  g and  $L = 10^{-18}$  cm. According to the criteria, if

$$v_g > \frac{h}{mL},\tag{35.1}$$

then the electron obeys the classical mechanics. Considering special theory of relativity, Eq. (35.1) becomes

$$v_g > \frac{h\sqrt{1-v_g^2/c^2}}{m_o L} = 7.3 \times 10^{18} \sqrt{1-v_g^2/c^2}.$$

$$v_g > c \sqrt{\frac{7.3^2 \times 10^{36}}{1 + 7.3^2 \times 10^{36}}}$$

(36) The size of superstring is the Planck length  $10^{-33}$ , the velocity at the parts of ends of superstring is light speed c. So short length contains at least energy  $E = 1.6 \times 10^{16}$  erg (the estimation from uncertainty relation). The superstring can constitute any particles such as quark, electron, and proton. Some authors even think that the superstring theory might be the last theory on nature and unverse.

Discuss the condition that the superstring obeys classical mechanics.

## Solution:

We assume the velocity of entirety of superstring  $v_g = 10^5$  cm/sec. From the criterion in section 3.4, the condition should be

$$m > \frac{h}{v_g L_x} = 66(g).$$
 (36.1)

(37) Suppose that the potential is a separable potential in Cartesian coordinates, i. e.,

$$V(r) = V_1(x) + V_2(y) + V_3(z).$$
(37.1)

Seek the general form of stationary wavefunction.

Solution:

The Schrödinger equation in Cartesian coordinates is

$$-\frac{\hbar d^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \Psi(x, y, z) + V(x, y, z) \Psi(x, y, z) = E \Psi(x, y, z).$$
(37.2)

Considering that the potential is of the separable form, the solution of Eq. (37.2) is also separable, i. e.,

$$\Psi = X(x)Y(y)Z(z). \tag{37.3}$$

Substituting Eq. (37.3) into Eq. (37.2) yields

$$-\frac{\hbar d^2}{2m} \left( YZ \frac{^2X}{dx^2} + XZ \frac{d^2Y}{dy^2} + XY \frac{d^2Z}{dz^2} \right) + [V_1 + V_2 + V_3] XYZ = EXYZ.$$
(37.4)

This equation can be reduced further by dividing it by XYZ to obtain

$$-\frac{\hbar d^2}{2m} \left( \frac{1}{X} \frac{d^2 X}{dx^2} + \frac{1}{Y} \frac{d^2 Y}{dy^2} + \frac{1}{Z} \frac{d^2 Z}{dz^2} \right) + V_1 + V_2 + V_3 = E.$$
(37.5)

Now combining the terms with individual variables yields

$$\left[-\frac{\hbar d^2}{2m}\frac{1}{X}\frac{d^2X}{dx^2} + V_1\right] + \left[-\frac{\hbar d^2}{2m}\frac{1}{Y}\frac{d^2Y}{dy^2} + V_2\right] + \left[-\frac{\hbar d^2}{2m}\frac{1}{Z}\frac{d^2Z}{dz^2} + V_3\right] = E.$$
 (37.6)

Eq. (37.6) can be written in three one dimensional equations.

$$-\frac{\hbar d^2}{2m}\frac{d^2X}{dx^2} + V_1 X = E_1 X.$$
(37.7)

$$-\frac{\hbar d^2}{2m}\frac{d^2Y}{dy^2} + V_1 Y = E_2 Y.$$
(37.8)

$$-\frac{\hbar d^2}{2m}\frac{d^2 Z}{dz^2} + V_3 Z = E_3 Z.$$
(37.9)

$$E = E_1 + E_2 + E_3. \tag{37.10}$$

If  $X_i(x)$ ,  $Y_j(y)$ , and  $Z_k(z)$  are the solutions with eigenvalues  $E_{1i}$ ,  $E_{2j}$ , and  $E_{3k}$ , respectively for the Eqs. (37.7-8), then the solution for the three dimensional system is

$$\Psi_{ijk}(x, y, z) = X_i(x)Y_j(y)Z_k(z), \qquad (37.11)$$

with energy eigenvalues

$$E_{ijk} = E_{1i} + E_{2j} + E_{3k}. ag{37.12}$$

(38) Ref. [72, 21] tells us that the decoherence (i. e., there is no interference between two macroscopic object) is a present hot open problem. Now the nearly common viewpoint is that the interference loss comes from the environment influence on macroscopic objects.

Do you agree? Why?

#### Solution:

No. Would reader please write reasons according to the criterion of quantum or classical mechanics. Please give the picture of decoherence.

## Chapter 4

# **Stationary states of One Dimension System**

## 4.1. General Properties

Both classical and quantum mechanics use function to describe object. This function is a localized mathematical function  $\in \mathcal{M}(\mathbb{R})$ . If a particle with mass *m* moves along *x* axis and in potential V(x), then Schrödinger equation is

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x,t).$$
(4.1.1)

The solution of Schödinger equation is called wavefunction or guide-factor. The bodyfactor of wavepacket will move according to equiprobability symmetry and spontaneous symmetry breaking. For stationary state (i. e., a quantum state being of certain energy), the expression of wavefunction is

$$\Psi(x,t) = \Psi(x)e^{-i\frac{Et}{\hbar}}.$$
(4.1.2)

Substituting Eq. (4.1.2) into Eq. (4.1.1) yields

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\Psi(x) = E\Psi(x).$$
(4.1.3)

 $V(x) = V^*(x)$ , that is, V(x) is real. (Generally, in quantum mechanics potential V(x) is taken as real quantity to ensure that the eigenvalue of energy is real.) (For the theorems XIII-1 - XIII-6 and the corollaries in this section refer Ref. [1].)

**Theorem XIII-1.** If  $\Psi(x)$  is a solution of Eq. (4.1.3), and eigenvalue is *E*, then  $\Psi^*(x)$  is also a solution, and its eigenvalue is also *E*.

**Proof.** The complex conjugate of Eq. (4.1.3) is

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V^*(x)\right]\Psi^*(x) = E^*\Psi^*(x).$$
(4.1.4)

Considering  $V^*(x) = V(x)$  and  $E^* = E$  yields

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\Psi^*(x) = E\Psi^*(x).$$
(4.1.5)

QED.

**Corollary XIII.** If for some E the solution of Eq. (4.1.3) is not degenerate (i. e. just has one independent solution), then the solution can be taken as real except a constant real or complex factor. QED.

**Proof.** If  $\Psi(x)$  is a solution with energy *E* and the energy level is not degenerate, then  $\Psi^*(x)$  and  $\Psi(x)$  describe the same quantum state. Thus,  $\Psi^*(x) = C\Psi(x)$ . Its complex conjugate is  $\Psi(x) = C^*\Psi^*(x) = |C|^2\Psi(x)$ . Therefore, |C| = 1 and  $C = e^{i\alpha}$ .  $\alpha$  is real number. For convenience, we take  $\alpha = 0$ , then  $\Psi^*(x) = \Psi(x)$  which means that  $\Psi(x)$  is a real function.

**Theorem XIII-2.** Suppose that V(x) is invariant under space reflection, V(-x) = V(x). If  $\Psi(x)$  is a solution of Eq. (4.1.3) and its energy is *E*, then  $\Psi(-x)$  is also a solution with energy *E*.

**Proof.** When  $x \to -x$ ,  $d^2/dx^2 \to d^2/d(-x)^2 = d^2/dx^2$ . Suppose V(-x) = V(x). Eq. (4.1.3) becomes

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\Psi(-x) = E\Psi(-x).$$
(4.1.6)

Eq. (4.1.6) shows that  $\Psi(-x)$  is also a solution of Eq. (4.1.3), and its energy is *E* as well. The reflection operator (parity operator) *P* is defined by

$$P\Psi(r) = \Psi(-r). \tag{4.1.7}$$

Thus the reflection operator reverse the sign of each cartesian coordinate. The operator is equivalent to an inversion of the coordinate system through origin.

**Corollary XIV.** If V(x) is invariant under space reflection, and  $\Psi(x)$  is not degenerate, then  $\Psi(x)$  has definite parity.

**Proof.** Because in this case  $\Psi(-x)$  and  $\Psi(x)$  represent the same solution, i. e.,  $P\Psi(x) \equiv \Psi(-x)$  and  $\Psi(x)$  represent the same quantum state. The difference between them is at the largest a constant factor *C*. Therefore, if  $\Psi(x)$  is an eigenfunction of *P*, then the eigenvalue equation is

$$P\Psi(x) = C\Psi(x). \tag{4.1.8}$$

Operating with P again yields

$$P^2\Psi = C(P\Psi) = C^2\Psi = \Psi.$$
(4.1.9)

 $C^2 = 1$ ,  $C = \pm 1$ . The eigenfunction corresponding to the eigenvalue 1 is called function of even parity (for example,  $P\Psi(x) = \Psi(x)$ ). The eigenfunction corresponding to the eigenvalue -1 is called function of odd parity (for example,  $P\Psi(x) = -\Psi(x)$ ). One dimensional harmonic oscillator and one dimensional symmetric square well belong to these case. QED.

For the case of degeneracy of energy levels, the energy eigenstate does not definitely have certain parity. Theorem XII-3 can solve this problem.

**Theorem XIII-3.** If V(-x) = V(x), then for any energy eigenvalue *E*, one can always find a group of complete solutions of Schrödinger equation. Every solution has certain parity.

**Proof.** If  $\Psi(x)$  is a solution of Eq. (4.1.3) and has no certain parity, then according to theorem XIII-2  $\Psi(-x)$  is also a solution of Eq. (4.1.3), and is different from  $\Psi(x)$  (although both refer to same *E*.) Therefore, we can construct

$$f(x) = \Psi(x) + \Psi(-x), \quad g(x) = \Psi(x) - \Psi(-x) \quad , \tag{4.1.10}$$

where f(x) and g(x) are solutions of Eq. (4.1.3), both refer to the same *E*, have definite parities (f(-x) = f(x), g(-x) = -g(x)), and their linear superposition can express  $\Psi(x)$  and  $\Psi(-x)$ 

$$\Psi(x) = \frac{1}{2}[f(x) + g(x)], \quad \Psi(-x) = \frac{1}{2}[f(x) - g(x)] \quad , \tag{4.1.11}$$

**Theorem XIII-4.** For some energy eigenvalue E, one can always find a group of complete real solutions, i. e., any solution with energy E can be expressed as a linear superposition of these real solutions in the group.

**Proof.** Suppose that  $\Psi(x)$  is a solution with energy eigenvalue *E*. If it is real, then one can refer this solution to the group of real solutions. If it is complex solution, according to theorem XIII-1,  $\Psi^*(x)$  is also a solution with energy eigenvalue *E*. According to the superposition theorem of solutions of linear differential equation,

$$\alpha(x) = \Psi(x) + \Psi^*(x), \quad \beta(x) = -i[\Psi(x) - \Psi^*(x)]$$

are also solutions of Eq. (4.1.3), and are real.  $\alpha(x)$  and  $\beta(x)$  have energy *E*, and independent each other.  $\Psi(x)$  and  $\Psi^*(x)$  can be expressed as linear superposition of  $\alpha(x)$  and  $\beta(x)$ . That is

$$\Psi = \frac{1}{2} [\alpha(x) + i\beta(x)], \quad \Psi^* = \frac{1}{2} [\alpha - i\beta(x)]$$

QED.

**Theorem XIII-5.** If V(x) is step square potential, i. e.,

$$V(x) = \begin{cases} V_1, & x < a \\ V_2, & x > a \end{cases}$$
(4.1.12)

and  $V_2 - V_1$  is finite, then energy eigenfunction  $\Psi(x)$  and its derivative  $\Psi'(x)$  are continuous certainly.

**Proof.** According to Eq. (4.1.3),

$$\frac{d^2}{dx^2}\Psi(x) = -\frac{2m}{\hbar^2} [E - V(x)]\Psi(x).$$
(4.1.13)

In the region where V(x) is continuous,  $\Psi(x)$  and  $\Psi'(x)$  are continuous obviously. However, at the point x = a of the step jump of V(x),  $V(x)\Psi(x)$  has finite change. At  $x \sim a$  we do integration over  $a - \varepsilon < x < a + \varepsilon$  ( $\varepsilon \rightarrow 0^+$ ) for Eq. (4.1.13), and we obtain

$$\Psi'(a+\varepsilon) - \Psi'(a-\varepsilon) = -\frac{2m}{\hbar^2} \lim_{\varepsilon \to 0^+} \int_{a-\varepsilon}^{a+\varepsilon} dx [E-V(x)] \Psi(x).$$
(4.1.14)

Due to the finiteness of  $[E - V(x)]\Psi(x)$ , the right hand side of Eq. (4.1.14) is zero. Therefore,

$$\Psi'(a+\varepsilon) = \Psi'(a-\varepsilon), \qquad (4.1.15)$$

that is,  $\Psi'(x)$  is continuous at the step jump point (x = a) of potential V(x). Thus  $\Psi(x)$  is continuous as well. QED.

**Theorem XIII-6.** If for one dimensional particle  $\Psi_1(x)$  and  $\Psi_2(x)$  are the solutions of Eq. (4.1.3), and belong to the same energy, then

$$\Psi_1\Psi_2' - \Psi_2\Psi_1' = constant. \tag{4.1.16}$$

Proof. According to the hypotheses of this theorem

$$\Psi_1'' + \frac{2m}{\hbar^2} [E - V(x)] \Psi_1(x) = 0.$$
(4.1.17)

$$\Psi_2'' + \frac{2m}{\hbar^2} [E - V(x)] \Psi_2(x) = 0.$$
(4.1.18)

From  $\Psi_1 \times (4.1.17) - \Psi_2 \times (4.1.18)$  one obtains  $\Psi_1 \Psi_2'' - \Psi_2 \Psi_1'' = 0$ , that is,  $(\Psi_1 \Psi_2' - \Psi_2 \Psi_1')' = 0$ . After integration one obtains

$$\Psi_1\Psi_2' - \Psi_2\Psi_1' = constant, \qquad (4.1.19)$$

where the constant is independent of x. QED.

## 4.2. Infinite Square Well and Discrete Spectrum

Particle in an one dimensional box [also known as the infinite potential well or infinite square (rectangular) well] is defined as a particle confined in a box where it experiences no force, that is, the potential energy is constant or zero. At the walls of the box the potential is infinitely large. Therefore, the particle is constrained to remain in the box (infinite square well). Section 3.5 of chapter 3 calculated the one dimensional infinite and asymmetric (i. e. V(x) = 0 for 0 < x < a and  $V(x) = \infty$  for x < 0 and x > a) well, and gave the eigenenergy and eigenfunction, respectively.

Now let us study the infinite and symmetric square well. The potential is

$$V = 0 \ for \ -\frac{a}{2} < x < \frac{a}{2}, \tag{4.2.1a}$$

$$V = \infty \ for \ x \le -\frac{a}{2}, \ x \ge \frac{a}{2}.$$
 (4.2.1b)

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2} [E - V]\Psi = 0.$$
(4.2.2)

In the region -a/2 < x < a/2 where V = 0, Eq. (4.2.2) is

$$\frac{d^2\Psi}{dx^2} + \frac{2mE}{\hbar^2}\Psi = 0. \tag{4.2.3}$$

$$\frac{d^2\Psi}{dx^2} + k^2\Psi = 0,$$
 (4.2.4)

where

$$k^2 = \frac{2mE}{\hbar^2}.\tag{4.2.5}$$

The general solution of Eq. (4.2.4) is

$$\Psi(x) = Asin(kx) + Bcos(kx). \tag{4.2.6}$$

Since the wavefunction vanishes outside the well, the requirement that the wavefunction be continuous gives

$$\Psi(x) = 0 \quad at \quad x = \pm \frac{a}{2}$$
 (4.2.7)

From Eqs. (4.2.7) and (4.2.6) at x = a/2

$$\Psi(x = a/2) = Asin(ka/2) + Bcos(ka/2) = 0.$$
(4.2.8)

From Eqs. (4.2.7) and (4.2.6) at x = -a/2

$$\Psi(x = -a/2) = Asin(-ka/2) + Bcos(ka/2) = 0.$$
(4.2.9)

Eqs. (4.2.9) and (4.2.8) can be expressed in the matrix form

$$\begin{pmatrix} \sin(ka/2) & \cos(ka/2) \\ -\sin(ka/2) & \cos(ka/2) \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = 0.$$
(4.2.10)

For nontrivial solution to this set of homogeneous equation in *A* and *B*, the determinant of the coefficients vanishes, that is,

$$2sin(ka/2)cos(ka/2) = sin(ka) = 0$$
(4.2.11)

or

$$ka = n\pi, \tag{4.2.11}'$$

where *n* is an integer. Now *A* and *B* both cannot be set to zero, since this would give the physically uninteresting solution  $\Psi = 0$  everywhere. Further both sin(ka/2) and cos(ka/2)

cannot be zero for a given value of k and E. There are then two possible classes of solutions. For the first class

$$A = 0$$
 and  $cos(ka/2) = 0$  (4.2.12)

and for the second class

$$B = 0$$
 and  $sin(ka/2) = 0$ . (4.2.13)

Thus  $ka/2 = n\pi/2$  where *n* is an odd integer for the first class and even integer for the second class. Thus

$$\Psi(x) = B\cos(n\pi x/a) \quad n \quad odd \tag{4.2.14}$$

$$\Psi(x) = Asin(n\pi x/a) \quad n \quad even \tag{4.2.15}$$

and Eqs. (4.2.11) and (4.2.5) give

$$k^2 = \frac{2mE}{\hbar^2} = \frac{n^2 \pi^2}{a^2},$$
(4.2.16)

and

$$E = \frac{n^2 \pi^2 \hbar^2}{2ma^2}.$$
 (4.2.17)

n = 0 gives the physically uninteresting result  $\Psi = 0$  and the solutions for negative value of *n* are not linearly independent of those for positive. The energy given by Eq. (4.2.17) is the same as that in section 3.5 calculated for one dimensional infinite and asymmetric (i. e. V(x) = 0 for 0 < x < a and  $V(x) = \infty$  for x < 0 and x > a) well.

To obtain A, we normalize the function in Eq. (4.2.15)

$$A^*A \int_{-a/2}^{a/2} dx \sin^2 \frac{n\pi x}{a} = 1.$$
 (4.2.18)

Eq.(4.2.18) yields

$$A^*A = \frac{2}{a}, \quad A = \sqrt{\frac{2}{a}}.$$
 (4.2.19)

To obtain B, we normalize the function in Eq. (4.2.14)

$$B^*B \int_{-a/2}^{a/2} dx \cos^2 \frac{n\pi x}{a} = 1.$$
 (4.2.20)

Eq.(4.2.20) yields

$$B^*B = \frac{2}{a}, \quad B = \sqrt{\frac{2}{a}}.$$
 (4.2.21)

For convenience, we take A and B are real numbers. The functions in Eqs. (4.2.14) and (4.2.15) are

$$\Psi_{n}(x) = \begin{cases} \sqrt{\frac{2}{a}} \cos \frac{n\pi x}{a} & n = 1, 3, 5, \cdots \text{ even parity } |x| < \frac{a}{2} \\ \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} & n = 2, 4, 6, \cdots \text{ odd parity } |x| < \frac{a}{2} \\ 0 & |x| \ge \frac{a}{2} \end{cases}$$
(4.2.22)

	x	$-\infty \rightarrow -a$	$-a \rightarrow 0$	$0 \rightarrow a$	$a \rightarrow \infty$
$a, step \ potential, E > V$	V(x)	0	0	V	V
$a, step \ potential, E < V$	V(x)	0	0	V	V
b, barrier potential, E > V	V(x)	0	V	V	0
b, barrier potential, E < V	V(x)	0	V	V	0
$c, well \ potential, E > 0$	V(x)	0	-V	-V	0

 Table 4.1. Forms of potentials

## 4.3. One Dimensional Potential Barrier and Well

## 4.3.1. Basic Rules

In one dimensional experiment (potential barrier, well, and step), the energy E > 0 of the incident single particle is known in addition to the structure of the potentials, V(x) (In the table 4.1, we take V > 0.).

In this section we have to remember clearly the following three points proved in chapter 3.

First, the incident single particle is a free wavepacket E > 0, and its expression is given by Eqs. (3.4.1.14-15), which is

$$\Psi(x,t) = e^{ik_{xo}x - i\omega(k_{xo})t} e^{-ik_{xo}x'} \Psi(x',0).$$
(4.3.1.1)

The first factor

$$I = e^{ik_{xo}x - i\omega(k_{xo})t} \tag{4.3.1.2}$$

is called guide-factor. The velocity of the wavepacket is  $v_g = \hbar k_{xo}/m$ .  $x = 2v_g t$ .  $x' = v_g t$  if at t = 0 the particle is at the origin point of coordinate system. The second factor

$$II = e^{-ik_{xo}x'} (4.3.1.3)$$

is called front-factor. The momentum of wavepacket is  $\hbar \times k_{x\circ} = mv_g$ . The third factor

$$III = \Psi(x', 0) \tag{4.3.1.4}$$

is called body-factor. From  $x' = v_g t$  and  $x = 2v_g t$  we know that the guide-factor goes always ahead, and the other two factors of wavepacket go always behind. The time producing reflection or transmission, is the time when the guide-factor arrives at the boundary of barrier or well or step.

Second,  $\Psi(x',0)$  is called body-factor of wavepacket. We allow that  $\Psi(x',o)$  can be a complex function. A complex function cannot corresponds to an observable quantity. Therefore, in practice we use  $\Psi^*(x',0)\Psi(x',0) = |\Psi(x',0)|^2$ . The body-factor of wavepacket is substance of wavepacket, carries mass and/or charge, spin, and so on, and when we write Hamiltonian of wavepacket, we use classical mechanics (if  $v_g << c$ ), special theory of relativity, Maxwell equation set, weak equivalent principle of general theory of relativity, and so on. Third, the actual motion of body-factor of wavepacket obeys equiprobability symmetry and spontaneous equiprobability symmetry breaking, i. e., the square of absolute value of guide-factor gives the position probability density or discrete spectrum probability.

We solve these kinds of problems always through four steps.

First step. We write Shrödinger equation, and solve Schrödinger equation in every domain of potential barrier or well or step potential to obtain the guide-factors (i. e., wavefunctions) of incident, reflected, and transmitted wavepacket;

Second step. According to the equiprobability symmetry and spontaneous equiprobability symmetry breaking we have to obtain the squares of absolute values of incident, reflected, and transmitted wavefunctions, which are expressed as  $|A|^2$ ,  $|B|^2$ , and  $|C|^2$ , respectively;

Third step. According to definitions calculate the reflected R and transmitted T coefficients. According to the equiprobability symmetry and spontaneous equiprobability symmetry breaking, these coefficients represent the probability of motion of body-factor.

Fourth step. Derive the expressions of the wavepacket in different domains. Please remember

wavepacket=wavepacket-function=object=particle

=guide-factor×front-factor×body-factor

=wavefunction×front-factor×body-factor.

The first, second, and third steps are explained very well in many textbooks such as Ref. [3]. However, the until now all references and textbooks have not yet give the avove fourth step.

## 4.3.2. Potential Step

We study two configurations of potential steps.

(1). Let us consider the first configuration of a simple step potential (barrier), E > V (see Table 4.1a.up).

First step. Actually, the true incident free particle is a free wavepacket including three factors given by Eq. (4.3.1.1). However, at the first step, we only seek the guide-factor given by Eq. (4.3.1.2), which is a plane wave. The so-called wavefunction,  $\Psi$  for all x, is just guide-factor. The potential function is zero for x < 0 and is a constant V > 0 for  $x \ge 0$ . The incident plane wave, i. e., wavefunction comes from  $x = -\infty$ . To construct wavefunction  $\Psi$  as a function of x (See Table 4.1a.up), we divide the x axis into two domains: region I in x < 0 and region II in x > 0.

In region I, V = 0, the time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\Psi_{I,xx} = E\Psi_I. \tag{4.3.2.1}$$

The subscript x denotes differentiation. In this region I, the energy is entirely kinetic. If we

set

$$\frac{\hbar^2 k_{1xo}^2}{2m} = E, \tag{4.3.2.2}$$

then Eq. (4.3.2.1) becomes

$$\Psi_{I,xx} = -k_{1xo}^2 \Psi_I \quad in \quad region \quad I \tag{4.3.2.3}$$

In region II, the potential is a constant V > 0, corresponding to repulsive force, and the time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\Psi_{II,xx} = (E - V)\Psi_{II}.$$
(4.3.2.4)

The kinetic energy, connected with wavenumber, decreases by V, and is given by

$$\frac{\hbar^2 k_{2x\circ}^2}{2m} = E - V. \tag{4.3.2.5}$$

In terms of  $k_{2x\circ}$ , Eq. (4.3.2.4) becomes

$$\Psi_{II,xx} = -k_{2xo}^2 \Psi_{II} \quad in \quad region \quad II \tag{4.3.2.6}$$

 $\Psi_I$  and  $\Psi_{II}$  are the general solutions of Eqs. (4.3.2.3) and (4.3.2.6), respectively.

$$\Psi_I = A e^{ik_{1xo}x} + B e^{-ik_{1xo}x}.$$
(4.3.2.7)

$$\Psi_{II} = Ce^{ik_{2xo}x} + De^{-ik_{2xo}x}.$$
(4.3.2.7)'

Since the term  $Dexp(-ik_{2x\circ}x) = Dexp[ik_{2x\circ}(-v_gt)]$  represents a wave emanating from the right (that is, from  $x = +\infty$ ), and there is no such wave, we may conclude that D = 0. The interpretations of the remaining A, B, and C terms are as follows.

$$\Psi_{I,inc} = A e^{ik_{1xo}x - i\omega_{1}t}, \quad \hbar \omega_{1} = E_{inc} = \frac{\hbar^{2}k_{1xo}^{2}}{2m} \quad , \tag{4.3.2.8}$$

$$\Psi_{I,ref} = Be^{-ik_{1xo}x - i\omega_{1}t}, \quad \hbar\omega_{1} = E_{ref} = \frac{\hbar^{2}k_{1xo}^{2}}{2m} = E_{inc} \quad , \qquad (4.3.2.8)'$$

$$\Psi_{II,trans} = Ce^{ik_{2xo}x - i\omega_2 t}, \quad \hbar\omega_2 = E_{trans} = \frac{\hbar^2 k_{2xo}^2}{2m} + V = E_{inc} = \hbar\omega_1 \quad , \qquad (4.3.2.8)''$$

where subscripts *inc*, *ref*, and *trans* represent incident, reflected, and transmitted guidefactors, respectively. Considering time uniformity, the energy is conservative (Refer to section 5.6 of chapter 5). Energy is conserved across the potential hill so that the angular frequency remains constant ( $\omega_1 = \omega_2$ ). The change in wavenumber *k* corresponds to changes in momentum and kinetic energy, connected with wavenumber, of wavepacket (particle). Note that  $\Psi_{I,inc}$ ,  $\Psi_I$  and  $\Psi_{II}$  (with D = 0) in first step represents only the guidefactors, which are solutions of Schrödinger equation for potential curve depicted in Table 4.1a.up.

Second step. Since the wavefunction and its derivative are continuous at the point x = 0, where  $\Psi_I$  and  $\Psi_{II}$  join, it is required that

$$\Psi_I(0) = \Psi_{II}(0). \tag{4.3.2.9}$$

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$$\frac{\partial}{\partial x}\Psi_I(0) = \frac{\partial}{\partial x}\Psi_{II}(0). \tag{4.3.2.9}'$$

These equalities give the relations

$$A + B = C. \tag{4.3.2.10}$$

$$A - B = \frac{k_{2xo}}{k_{1xo}}C.$$
 (4.3.2.10)'

Solving for C/A and B/A yields

$$\frac{C}{A} = \frac{2}{1 + k_{2x\circ}/k_{1x\circ}},\tag{4.3.2.11a}$$

$$\frac{B}{A} = \frac{1 - k_{2xo}/k_{1xo}}{1 + k_{2xo}/k_{1xo}}.$$
(4.3.2.11b)

Third step. Subsection 3.5.6 in chapter 3 gives current expression. (If the system is three dimensions, then Eq. (3.5.6.14) gives the current density.) Substituting Eq. (4.3.2.8) into Eq. (3.5.6.14) yields

$$J_{inc} = \frac{\hbar}{2mi} 2ik_{1xo}|A|^2.$$
(4.3.2.12*a*)

$$J_{trans} = \frac{\hbar}{2mi} 2ik_{2x\circ}|C|^2.$$
(4.3.2.12b)

$$J_{ref} = \frac{\hbar}{2mi} 2ik_{1xo}|B|^2.$$
(4.3.2.12c)

It should be noted that these current relations of a single particle are formally similar to the classical single particle current  $J = \rho v$ , with  $\rho = |\Psi|^2$  and  $v = \hbar k/m$ . The wavefunctions in this first step: incident, reflected, and transmitted wavefunctions represent just the guide-factor of incident, reflected, and transmitted wavepacket, respectively. The three wavefunctions are plane wave other than the complex wavepacket representing the single particle.

The transmission coefficient T and reflection coefficient R are defined as the transmitted and reflected probability of incident particle. The often used formulas of R and T are as follows.

$$T \equiv \left| \frac{J_{trans}}{J_{inc}} \right|, \tag{4.3.2.13a}$$

$$R \equiv \left| \frac{J_{ref}}{J_{inc}} \right|. \tag{4.3.2.13b}$$

Substituting Eq. (4.3.2.12) into Eq. (4.3.2.13) gives

$$T = \left|\frac{C}{A}\right|^2 \frac{k_{2xo}}{k_{1xo}},$$
 (4.3.2.14*a*)

$$R = \left|\frac{B}{A}\right|^2. \tag{4.3.2.14b}$$



Figure 4.1. T and R versus  $k_{2x\circ}/k_{1x\circ}$ . Note that in Fig. 4.1 we use  $k_2/k_1$  to express  $k_{2x\circ}/k_{1x\circ}$ .

Substituting Eq. (4.3.2.11) into Eq. (4.3.2.14) gives

$$T = \frac{4k_{2xo}/k_{1xo}}{(1+k_{2xo}/k_{1xo})^2},$$
(4.3.2.15*a*)

$$R = \left| \frac{1 - k_{2xo}/k_{1xo}}{1 + k_{2xo}/k_{1xo}} \right|^2.$$
(4.3.2.15*b*)

The ration  $k_{2x\circ}/k_{1x\circ}$  is obtained from Eqs. (4.3.2.2) and (4.3.2.5).

$$\left(\frac{k_{2x\circ}}{k_{1x\circ}}\right)^2 = 1 - \frac{V}{E}.$$
(4.3.2.16)

In the present case  $E \ge V$ , so  $0 \le k_{2x\circ}/k_{1x\circ} \le 1$ . For  $E \gg V$ ,  $k_{2x\circ}/k_{1x\circ} \to 1$  and  $T \to 1$ ,  $R \to 0$ . There is the total transmission and zero reflection. On the other hand, for E = V,  $k_{2x\circ}/k_{1x\circ} = 0$  and T = 0, R = 1. There is zero transmission and total reflection. The *T* and *R* curves for the simple step potential are sketched in Fig. 4.1.

For all values of  $k_{2x\circ}/k_{1x\circ}$ ,

$$T + R = 1. \tag{4.3.2.17}$$

Fourth step. Some references think that this step potential problem has been solved completely by the above three steps, and stop the derivations. On the contrary, this textbook thinks that the problem has not yet been solved completely. For example, some references think that the reflected and transmitted waves are plane waves. As we know, the square of absolute value of plane wave is a constant independent of space position. Therefore, according to probability density interpretation for the square of absolute value of wavefunction no person knows that where are the reflected and transmitted particles. However, our wavepacket-only theory will continue the derivations to answer the following questions:

- (1) Where are the particle;
- (2) What are the velocities of reflected and transmitted particles;

(3) What are the expressions of the particles in all regions. (Note that particle=wavepacket)

It is obvious that the incident wavepacket (particle) cannot be separated into two wavepackets. It can only become one of the transmitted and reflected wavepackets with definite probabilities determined according to T and R. If there are 100 same incident particles, and they make incidence separately and individually, then just after finishing all the incidences we can find out that the number of reflected and transmitted particles are about 100R and 100T, respectively. At the beginning of the incidences the numbers of reflected and transmitted particles are a few, and we cannot find out the rule. (Refer to the double slit experiment in many time single particle experiments.)

Let us write the expression of transmitted wavepacket. We show in next that  $k_{2xo}$  is average wavenumber of transmitted wavepacket. According to Eq. (4.3.2.8)

$$\Psi_{trans}(x,t) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dk_{2x} b_{trans}(k_{2x}) e^{i[k_{2x}x - \omega_2(k_{2x})t]}.$$
(4.3.2.18)

Substituting the plane wave in Eq. (4.3.2.18) into time-dependent Schrödinger equation yields

$$\omega_2(k_{2x}) = \frac{1}{\hbar} \left( \frac{\hbar^2 k_{2x}^2}{2m} + V \right) = \frac{1}{\hbar} \left( \frac{\hbar^2 k_{2x}^2}{2m} \right) + \frac{V}{\hbar} \equiv \omega_2'(k_{2x}) + \frac{V}{\hbar}.$$
 (4.3.2.19)

Substituting Eq. (4.3.2.19) into Eq. (4.3.2.18) yields

$$\Psi_{trans}(x,t) = e^{-i\frac{Vt}{\hbar}} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dk_{2x} b_{trans}(k_{2x}) e^{i[k_{2x}x - \omega_2'(k_{2x})t]}.$$
(4.3.2.20)

Using the same method as that in section 3.5, Eq. (4.3.2.20) can be rewritten as

$$\Psi_{trans}(x,t) = e^{ik_{2x\circ}x - i[\omega_{2}'(k_{2x\circ}) + \frac{V_{t}}{\hbar}]t} e^{-ik_{2x\circ}x'} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dk_{2x} b_{trans}(k_{2x}) e^{i[k_{2x}x']}$$
$$\equiv e^{ik_{2x\circ}x - i[\omega_{2}'(k_{2x\circ}) + \frac{V}{\hbar}]t} e^{-ik_{2x\circ}x'} \Psi_{trans}(x',0), \qquad (4.3.2.21)$$

where  $x = 2v_{g,trans}t$ . As we know,  $v_{g,trans} = \partial \omega'(k_{2x})/\partial x$  at  $k_{2x} = k_{2x\circ}$  is the group velocity of the transmitted wavepacket. Eq. (4.3.2.16) has been given the relation between  $k_{1x\circ}$  and  $k_{2x\circ}$ , which is

$$k_{2x\circ} = k_{1x\circ} \sqrt{1 - \frac{V}{E}} = k_{1x\circ} \sqrt{1 - \frac{V2m}{\hbar^2 k_{1x\circ}}}.$$
(4.3.2.22)

From Eq. (4.3.2.22) we see that the group velocity of the transmitted wavepacket or velocity of the transmitted particle is less that of the incident particle.

Let us write the expression of the reflected wavepacket. We have to note that the  $k_1$  in Eq. (4.3.2.8) represent actually  $k_{1xo}$ .  $k_{1xo}$  is the average wavenumber of the incident wavepacket. We can understand that  $-k_{1xo}$  is average wavenumber of the reflected wavepacket. To make sure, we make the following derivations. According to section 3.5 of chapter 3 and Eq. (4.3.2.8)

$$\Psi_{ref}(x,t) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dk_{1x} b_{ref}(k_{1x}) e^{i[-k_{1x}x - \omega_1(k_{1x})t]}.$$
(4.3.2.23)

Substituting the plane wave in Eq. (4.3.2.23) into time-dependent Schrödinger equation yields

$$\omega_1(k_{1x}) = \frac{1}{\hbar} \left( \frac{\hbar^2 k_{1x}^2}{2m} \right).$$
(4.3.2.24)

Substituting Eq. (4.3.2.24) into Eq. (4.3.2.23) yields

$$\Psi_{ref}(x,t) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dk_{1x} b_{ref}(k_{1x}) e^{i[-k_{1x}x - \omega_1(k_{1x})t]}.$$
(4.3.2.25)

Using the same method as to derive Eq. (2.3.2.4), Eq. (4.3.2.25) can be rewritten as

$$\Psi_{ref}(x,t) = e^{i[-k_{1xo}x - \omega_{1}(k_{1xo})t]} e^{ik_{1xo}x'} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dk_{1x} b_{ref}(k_{1x}) e^{i[-k_{1x}x']}$$
  
$$= e^{i[-k_{1xo}x - \omega_{1}(k_{1xo})t]} e^{ik_{1xo}x'} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dk_{1x} b_{ref}(k_{x}) e^{i[-k_{1x}x']}$$
  
$$\equiv e^{-ik_{1xo}x - i\omega_{1}(k_{1xo})t} e^{ik_{1xo}x'} \Psi_{ref}(x',t), \qquad (4.3.2.26)$$

where  $x = 2v_{g,ref}t = 2\hbar(-k_{1x\circ})t/m = -2v_{g,inc}t$ , and  $v_{g,ref}$  is the group velocity of the reflected wavepacket. In physics, we know that the body-factor of incident and reflected wavepacket should be same, i. e., the forms of  $b_{ref}(k_x)$  and  $b_{inc}(k_{1x})$  as function of  $k_{1x}$  are same. In mathematics, Schrödinger equation in region I just tells us the changes of the factor  $\exp\{-i[k_{1x}x - \omega_1(k_{1x})t]\}$  in region I, and tell us nothing about  $b_{ref}$ . In physics, we take  $b_{ref}(k_{1x}) = b_{inc}(k_{1x})$  obviously.

(2) Let us consider the second configuration of a simple potential step (barrier), E < V (see Table 4.1a.down).

First step. Once again, the x domain is divided into two regions: region  $I \ x < 0$  and region  $II \ x > 0$ .

In region I the Schrödinger equation becomes

$$\Psi_{I,xx} = -k_{1x\circ}^2 \Psi_I, \qquad (4.3.2.27)$$

where

$$\frac{\hbar^2 k_{1xo}^2}{2m} = E. \tag{4.3.2.28}$$

In region II the Schrödinger equation becomes

$$\Psi_{II,xx} = \kappa^2 \Psi_{II}, \tag{4.3.2.29}$$

where

$$\frac{\hbar^2 \kappa^2}{2m} = V - E > 0. \tag{4.3.2.30}$$

The kinetic energy in region II is negative  $(-\hbar^2 \kappa^2/2m < 0)$ . In classical physics region II is a forbidden domain. In quantum mechanics, however, it is possible for particle to penetrate the barrier. One obtains

$$\Psi_I = A e^{ik_{1xo}x} + B e^{-ik_{1xo}}. \tag{4.3.2.31a}$$

$$\Psi_{II} = Ce^{-\kappa x}.\tag{4.3.2.31b}$$

Second step. Continuity of  $\Psi$  and  $\Psi_x$  at x = 0 gives

$$A + B = C. (4.3.2.32a)$$

$$A - B = i \frac{\kappa}{k_{1x\circ}} C. \tag{4.3.2.32b}$$

Solving for C/A and B/A yields

$$\frac{C}{A} = \frac{2}{1 + i\kappa/k_{1xo}}, \quad \frac{B}{A} = \frac{1 - i\kappa/k_{1xo}}{1 + i\kappa/k_{1xo}}.$$
(4.3.2.33)

The coefficient B/A is of the form  $z^*/z$ , where z is a complex number. It follows that |B/A| = 1, so

$$R = \left|\frac{B}{A}\right|^2 = 1, \quad T = 0$$
 (4.3.2.34)

Eq. (4.3.2.34) indicates that there is total reflection; hence the transmission must be zero.

Third step. To obtain the latter result analytically from our equations above, we must calculate the transmitted current. The function is of the form of a complex amplitude times a real function of x Eq. (4.3.2.31). Such wavefunctions do not represent propagating waves. They are sometimes called evanescent waves. That they carry no current is most simply seen by constructing  $J_{trans}$  [refer to Eq. (2.3.3.14)].

$$J_{trans} = \frac{\hbar}{2mi} |C|^2 \left( e^{-\kappa x} \frac{\partial}{\partial x} e^{-\kappa x} - e^{-\kappa x} \frac{\partial}{\partial x} e^{-\kappa x} \right) = 0.$$
(4.3.2.35)

We conclude that T = 0. T = 0 means that there is no the transmitted wavepacket, i. e., the transmitted particle. The total reflection means that, according to spontaneous equiprobability symmetry breaking, every incident wavepacket (particle) becomes reflected wavepacket (particle).

Fourth step. The expression of the reflected wavepacket is same as that given by Eq. (4.3.2.26).

## 4.3.3. Rectangular Potential Barrier and Well

The scattering configuration, we now wish to examine, is shown in Table 4.1b. This configuration can be called rectangular or square barrier or well. In physics, rectangular barrier and well are equivalent to that the incident particle touches repulsive and attractive force, respectively. We will study three types.

(1) The first configuration is that the energy of the single particle (wavepacket) is greater than the hight of the potential barrier E > V.

First step. we study the guide-factor, which obeys time-independent Schrödinger equation. For the case at hand there are three relevant domains (see Table 4.1b.up).

Region I: 
$$x < -a$$
,  $V = 0$ , . (4.3.3.1*a*)

Region II:  $-a \le x \le +a$ , V > 0, and constant. (4.3.3.1b)

Region III: a < x, V = 0, . (4.3.3.1c)

The solutions in each of the three domains are

$$\Psi_I = A e^{ik_{1xo}x} + B e^{-ik_{1xo}x}, \quad \frac{\hbar^2 k_{1xo}^2}{2m} = E \quad . \tag{4.3.3.2a}$$

$$\Psi_{II} = Ce^{ik_{2xo}x} + De^{-ik_{2xo}x}, \quad \frac{\hbar^2 k_{2xo}^2}{2m} = E - V \quad . \tag{4.3.3.2b}$$

$$\Psi_{III} = F e^{ik_{1xo}}, \quad \frac{\hbar^2 k_{1xo}^2}{2m} = E \quad . \tag{4.3.3.2c}$$

$$(ak_{1xo})^2 - (ak_{2xo})^2 = \frac{2ma^2V}{\hbar^2} \equiv \frac{g^2}{4}.$$
 (4.3.3.3)

The parameter g contains all the barrier (or well) characteristics. The Eq. (4.3.3.3) (conservation of energy) reveals the simple manner in which  $ak_{1x\circ}$  and  $ak_{2x\circ}$  are related.

The permitted values of  $k_{1xo}$  (and therefore *E*) comprise positive unbounded continuum. For each such eigen- $k_{1xo}$ -value, there is corresponding eigenstate ( $\Psi_I$ ,  $\Psi_{II}$ ,  $\Psi_{III}$ ) which is determined in terms of the coefficients, (B/A, C/A, D/A, F/A). Knowledge of these coefficients gives the scattering parameters

$$T = \left|\frac{F}{A}\right|^2, \quad R = \left|\frac{B}{A}\right|^2. \tag{4.3.3.4}$$

Second step. The coefficients are determined from the boundary conditions at x = a and x = -a,

$$e^{-ik_{1x\circ}a} + \left(\frac{B}{A}\right)e^{ik_{1x\circ}a} = \left(\frac{C}{A}\right)e^{-ik_{2x\circ}a} + \left(\frac{D}{A}\right)e^{ik_{2x\circ}a}.$$
(4.3.3.5*a*)

$$k_{1x\circ}\left[e^{-ik_{1x\circ}a} - \left(\frac{B}{A}\right)e^{ik_{1x\circ}a}\right] = k_{2x\circ}\left[\left(\frac{C}{A}\right)e^{-ik_{2x\circ}a} - \left(\frac{D}{A}\right)e^{ik_{2x\circ}a}\right].$$
(4.3.3.5b)

$$\left(\frac{C}{A}\right)e^{ik_{2x\circ}a} + \left(\frac{D}{A}\right)e^{-ik_{2x\circ}a} = \left(\frac{F}{A}\right)e^{ik_{1x\circ}a}.$$
(4.3.3.5c)

$$k_{2x\circ}\left[\left(\frac{C}{A}\right)e^{ik_{2x\circ}a} - \left(\frac{D}{A}\right)e^{-ik_{2x\circ}a}\right] = k_{1x\circ}\left(\frac{F}{A}\right)e^{ik_{1x\circ}a}.$$
(4.3.3.5d)

These are four linear, algebraic, inhomogeneous equations for the four unknowns: (B/A), (C/A), (D/A), and (F/A). Solving the last two for (D/A) and (C/A) as functions of (F/A) and substituting into the first two permits one to solve for (B/A) and (F/A). These appear as

$$\frac{F}{A} = e^{-2ik_{1x\circ}a} \left[ \cos(2k_{2x\circ}a) - \frac{i}{2} \left( \frac{k_{1x\circ}^2 + k_{2x\circ}^2}{k_{1x\circ}k_{2x\circ}} \right) \sin(2k_{2x\circ}a) \right]^{-1}.$$
(4.3.3.6*a*)

$$2\frac{B}{A} = i\frac{F}{A}\frac{k_{2x\circ}^2 - k_{1x\circ}^2}{k_{1x\circ}k_{2x\circ}}sin(2k_{2x\circ}a).$$
(4.3.3.6b)

Third step. The transmission coefficient is most simply obtained from the second of these, together with the relation

$$T + R = \left|\frac{F}{A}\right|^2 + \left|\frac{B}{A}\right|^2 = 1.$$
 (4.3.3.7)

Thus we have

$$\frac{1}{T} = \left|\frac{A}{F}\right|^2 = 1 + \frac{1}{4} \left(\frac{k_{1x\circ}^2 - k_{2x\circ}^2}{k_{1x\circ}k_{2x\circ}}\right)^2 \sin^2(2k_{2x\circ}a).$$
(4.3.3.8)

Rewriting  $k_{1xo}$  and  $k_{2xo}$  in terms of E and V as given by Eq. (4.3.3.2), one obtains

$$\frac{1}{T} = 1 + \frac{1}{4} \frac{V^2}{E(E-V)} \sin^2(2k_{2x\circ}a), (E > V).$$
(4.3.3.9)

The reflection coefficient R = 1 - T. According to the equiprobability symmetry and spontaneous equiprobability symmetry breaking *T* is the probability of transmission of the body-factor, and *R* is the probability of reflection of the body-factor.

Fourth step. From Eq. (4.3.3.2) and the last two equations of Eq. (4.3.3.5), we obtain

$$\frac{C}{D} = \frac{1 + \frac{k_{1xo}}{k_{2xo}}}{1 - \frac{k_{1xo}}{k_{2xo}}} e^{-i2k_{2xo}a}$$

$$= \frac{1 + \sqrt{\frac{E}{E-V}}}{1 - \sqrt{\frac{E}{E-V}}} e^{-2ia\frac{\sqrt{2m(E-V)}}{\hbar}}$$

$$= \begin{cases} \infty, \quad D = 0, \quad if \quad V = 0 \\ -1, \quad C = -D, \quad if \quad E \to V > 0 \end{cases}$$
(4.3.3.10)

The physical meaning of Eq. (4.3.3.10) is obvious. If V = 0, then there should be no reflected wave in region *II*. If  $E \rightarrow V > 0$ , then the amplitudes of both reflected and transmitted waves are equal to each other in region *II*.

=

From Table 4.1b.up and Eq. (4.3.3.2) one obtains that the reflected wavepacket is the same as that given by Eq. (4.3.2.26), and the transmitted wavepacket is the same as given by Eqs. (3.4.1.4) or (4.3.1.1). The wavepacket,  $\Psi_{II}$ , in region *II* can be obtained as follows. From Eq. (4.3.1.1) we know that the incident free wavepacket is

$$\Psi_{I,inc}(x) = e^{i[k_{1xo}x - \omega(k_{1xo})t]} e^{-ik_{1xo}x'} \Psi(x',0)$$
  
=  $e^{i[k_{1xo}x - \omega(k_{1xo})t]} e^{-ik_{1xo}x'} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk_{1x} b(k_{1x}) e^{ik_{1x}x'},$  (4.3.3.11)

where  $E = \hbar^2 k_{1xo}^2 / 2m$ .

From physics, we know that the wavepackets in region I and III are free wavepacket, which is given by Eqs. (3.4.1.4) and (4.3.1.1). We just need to determine the wavepacket in region II,  $\Psi_{II}(x,t)$ . Let us write the general forms of the wavepackets in regions *I*, *II*, and *III*.

$$\Psi_{I}(x,t) = A\Psi_{I,inc} + B\Psi_{I,ref} 
\equiv Ae^{i[k_{1x\circ}x - \omega(k_{1x\circ})t]}e^{-ik_{1x\circ}x'}\Psi_{I}(x',0) 
+ Be^{i[-k_{1x\circ}x - \omega(k_{1x\circ})t]}e^{ik_{1x\circ}x'}\Psi_{I}(-x',0).$$
(4.3.3.12*a*)

$$\begin{split} \Psi_{II}(x,t) &= C\Psi_{II,inc} + D\Psi_{II,ref} \\ &\equiv Ce^{i[k_{2xo}x - \omega(k_{2xo})t]} e^{-ik_{2xo}x'} \Psi_{II}(x',0) \\ &+ De^{i[-k_{2xo}x - \omega(k_{2xo})t]} e^{ik_{2xo}x'} \Psi_{II}(-x',0). \end{split}$$
(4.3.3.12b)

$$\Psi_{III}(x,t) = F \Psi_{III,trans}$$
  
$$\equiv F e^{i[k_{1xo}x - \omega(k_{1xo})t]} e^{-ik_{1xo}x'} \Psi_I(x',0). \qquad (4.3.3.12c)$$

Considering that any wavefunction and its first derivative with respect to x are continuous at boundaries (Here they are x = -a and x = a.), from Eq. (4.3.3.12) we obtain the same relations between A, B, C, D, and F as that given by Eqs. (4.3.3.5), (4.3.3.2). Solving these equations yields the wavepacket in region II,  $\Psi_{II}(x,t)$ .

$$\Psi_{II}(x,t) = A \left\{ \frac{C}{A} e^{i[k_{2xo}x - \omega(k_{2xo})t]} e^{-ik_{2xo}x'} \Psi_I(x',0) + \frac{D}{A} e^{i[-k_{2xo}x - \omega(k_{2xo})t]} e^{ik_{2xo}x'} \Psi_I(x',0) \right\},$$
(4.3.3.13)

where

$$\frac{C}{A} = \frac{F}{A} e^{ik_{1xo}a} \left(1 + \frac{k_{1xo}}{-k_{2xo}}\right) \frac{e^{-ik_{2xo}a}}{2},$$
(4.3.3.14)

$$\frac{D}{A} = \frac{F}{A} e^{ik_{1xo}a} \left(1 - \frac{k_{1xo}}{k_{2xo}}\right) \frac{e^{-ik_{2xo}a}}{2},$$
(4.3.3.15)

and F/A was given by Eq. (4.3.3.6).  $k_{1xo} = \sqrt{2mE}/\hbar$ .  $k_{2xo} = \sqrt{E-V}/\hbar$ . Often, A = 1. Therefore, from Eq. (4.3.3.15) the wavefunction in region II consists of two known wavepackets.

If we just need the probability of reflection and transmission of a free incident particle, then it is enough to know R and T, and it is not useful to know the wavefunction in the region II.

(2) The second configuration is that the energy of the free incident single particle (wavepacket) is less than the hight of the potential barrier E < V, as depicted in Table 4.1b.down.

First step. The structure of the solutions Eq. (4.3.3.2) is still appropriate, with the simple modification

$$ik_2 \to \kappa, \quad \frac{\hbar^2 \kappa^2}{2m} = V - E > 0.$$
 (4.3.3.16*a*)

$$(ak_{1xo})^2 + (a\kappa)^2 = \frac{2ma^2V}{\hbar^2} = \frac{g^2}{4}.$$
(4.3.3.16b)

This latter statement of energy conservation indicates that the variables  $ak_{1xo}$  and  $a\kappa$  lie on a circle of radius g/2.

The permitted  $k_{1xo}$ -values now comprise a bounded continuum, so that the eigenenergies

$$E = \frac{\hbar^2 k_{1xo}^2}{2m} \tag{4.3.3.17}$$

also comprise a bounded continuum.

Second and third steps. The algebra leading to Eq. (4.3.3.6) remains unaltered so that the transmission coefficient for this case is obtained by making the substitution of Eq. (4.3.2.22) into Eq. (4.3.3.8). We also recall that sin(iz)=isinh(z). Thus we have

$$\frac{1}{T} = 1 + \frac{1}{4} \left( \frac{k_{1xo}^2 + \kappa^2}{k_{1xo}\kappa} \right)^2 \sinh^2(2\kappa a).$$
(4.3.3.18)

Rewriting  $k_{1x0}$  and  $\kappa$  in terms of E and V as given by Eq. (4.3.3.16), one obtains

$$\frac{1}{T} = 1 + \frac{1}{4} \frac{V^2}{E(V-E)} sinh^2(2\kappa a) \quad E < V.$$
(4.3.3.19)

Eq. (4.3.3.19) indicates that in the domain E < V, T < 1. The limit that  $E \rightarrow V$  deserves special attention. With

$$\frac{V-E}{V} = \frac{\hbar^2 \kappa^2}{2mV} \equiv \varepsilon \to 0 \tag{4.3.3.20}$$

one obtains

$$T = \frac{1}{1 + g^2/4} + 0(\varepsilon) < 1.$$
(4.3.3.21)

$$g^2 \equiv \frac{2m(2a)^2 V}{\hbar^2}.$$
 (4.3.3.21)

The expression  $0(\varepsilon)$  represents a sum of terms whose value goes to zero with  $\varepsilon$ . We conclude that for scattering from a potential barrier, the transmission is less than unity at E = V. For example, if  $g^2 = 16$ , then  $T = 0.2 \ll 1$ .

Returning to the case E > V, Eq. (4.3.3.9) indicates that T = 1 when  $sin^2(2k_{2xo}a) = 0$ , or equivalently when

$$2ak_{2x\circ} = n\pi \quad (n = 1, 2, \cdots) \quad .$$
 (4.3.3.22)

Setting  $k_{2x\circ} = 2\pi/\lambda$ , the latter statements is equivalent to

$$2a = n\left(\frac{\lambda}{2}\right). \tag{4.3.2.23}$$

When the barrier width 2a is an integer number of half-wavelength,  $n(\lambda/2)$ , the barrier becomes transparent to the incident particle, that is, T = 1. This is analogous to the case of total transmission of light through thin reflecting layers.

Written in terms of *E* and *V*, the requirement for perfect transmission, Eq. (4.3.3.22), becomes

$$E - V = n^2 \left(\frac{\pi^2 \hbar^2}{8a^2 m}\right) = n^2 E_1, \qquad (4.3.3.24)$$

where  $E_1$  is the ground state energy of an one dimensional box of width 2a [see Eq. (4.3.2.21), and note that the barrier width in this equation is a].

Eqs. (4.3.3.9) and (4.3.3.19) give the transmission coefficient T, as a function of E, V, and the barrier width 2a. The former of these indicates that  $T \rightarrow 1$  with increasing energy of incident particle. The transmission is unity for the values of E given by Eq. (4.3.3.24). Eq. (4.3.3.19) gives T for  $E \leq V$ . The transmission is zero for E = 0 and is less than 1 for E = V. Eq. (4.3.3.10) can give a physical interpretation for T < 1 when E = V.

The fact that *T* does not vanish for E < V is a purely quantum mechanical result. This phenomenon of particle passing through barrier higher than their own incident energy is known as tunneling effect. This tunneling effect leads to the emission of  $\alpha$  particle from a nucleus and field emission of electron from a metal surface in the present of a strong electric field.

Let us make an estimation for the transmission coefficient T given by Eq. (4.3.3.18). If  $2\kappa a >> 1$ , then  $sinh 2\kappa a \approx e^{2\kappa a}/2 >> 1$ . Eq. (4.3.3.18) can be expressed approximately as

$$T \approx \frac{16k_{1xo}^{2}\kappa^{2}}{(k_{1xo}^{2} + \kappa^{2})^{2}}e^{-4\kappa a}$$
$$= \frac{16E(V-E)}{V}e^{-4a\sqrt{2m(V-E)/\hbar}}.$$
(4.3.3.25)

From Eq. (4.3.3.25) we see that *T* connects closely with barrier width 2a, V - E, and particle mass *m*. Therefore, in macroscopic experiment, it is difficult to observe the phenomenon of penetrating barrier of particle. For example, for electron and proton, if E = 1 eV, V = 2 eV,  $2a = 2 \times 10^{-8}$  cm, then Eq. (4.3.2.25) gives  $T \approx 0.51$  and  $T \approx 2.6 \times 10^{-38}$ , respectively. However, for electron, if  $2a = 5 \times 10^{-8}$  cm, then  $T \approx 0.024$ .

Fourth step. Now we look for the expressions of the wavepackets in every region. From physics, we know that the wavepackets in region I and III are free wavepackets [Refer to Eqs. (3.4.1.4) and (4.3.1.1)]. We just need to determine the wavepackets in region II,  $\Psi_{II}(x,t)$ . We have to write the wavepackets in every regions exactly. Let us write the general forms as follows.

$$\Psi_{I}(x,t) = Ae^{i[k_{1x\circ}x - \omega(k_{1x\circ})t]}e^{-ik_{1x\circ}x'}\Psi_{I}(x',0) + Be^{i[-k_{1x\circ}x - \omega(k_{1x\circ})t]}e^{ik_{1x\circ}x'}\Psi_{I}(-x',0).$$
(4.3.3.26*a*)

$$\Psi_{II}(x,t) = Ce^{\kappa x - i\omega_{II}(\kappa)t}e^{-\kappa x'}\Psi_{II}(x',0) + De^{-\kappa x - i\omega_{II}(\kappa)t}e^{\kappa x'}\Psi_{II}(-x',0).$$
(4.3.3.26b)

$$\Psi_{III}(x,t) = F e^{i[k_{1x\circ}x - \omega(k_{1x\circ})t]} e^{-ik_{1x\circ}x'} \Psi_I(x',0).$$
(4.3.3.26c)

The particle's energies at region I and II are conservative. Referring to Eq. (4.3.3.16) yields  $\hbar\omega_{II}(\kappa) = -\hbar^2 \kappa^2 / (2m) + V = \hbar^2 k_{1xo}^2 / (2m) = E = \hbar\omega(k_{1xo})$ . Referring to Eq. (4.3.3.5), we have the following boundary conditions.

$$e^{-ik_{1x\circ}a} + \left(\frac{B}{A}\right)e^{ik_{1x\circ}a} = \left(\frac{C}{A}\right)e^{-\kappa a} + \left(\frac{D}{A}\right)e^{\kappa a}.$$
(4.3.3.27*a*)

$$ik_{1x\circ}\left[e^{-ik_{1x\circ}a} - \left(\frac{B}{A}\right)e^{ik_{1x\circ}a}\right] = i(-i\kappa)\left[\left(\frac{C}{A}\right)e^{-\kappa a} - \left(\frac{D}{A}\right)e^{\kappa a}\right].$$
(4.3.3.27b)

$$\left(\frac{C}{A}\right)e^{\kappa a} + \left(\frac{D}{A}\right)e^{-\kappa a} = \left(\frac{F}{A}\right)e^{ik_{1x\circ}a}.$$
(4.3.3.27c)

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$$i(-i\kappa)\left[\left(\frac{C}{A}\right)e^{\kappa a} - \left(\frac{D}{A}\right)e^{-\kappa a}\right] = ik_{1x\circ}\left(\frac{F}{A}\right)e^{ik_{1x\circ}}.$$
(4.3.3.27d)

Comparing Eq. (4.3.3.27) with Eq. (4.3.3.5), we find that if  $k_{2x\circ} \rightarrow -i\kappa$ , then Eq. (4.3.3.5) becomes Eq. (4.3.3.27). Therefore, we make  $k_{2x\circ} \rightarrow -i\kappa$  in Eqs. (4.3.3.14) and (4.3.3.15), and obtain

$$\frac{C}{A} = \frac{F}{A} e^{ik_{1xo}a} \left(1 + \frac{k_{1xo}}{-i\kappa}\right) \frac{e^{-\kappa a}}{2}, \qquad (4.3.3.28)$$

$$\frac{D}{A} = \frac{F}{A} e^{ik_{1x\circ}a} \left(1 - \frac{k_{1x\circ}}{-i\kappa}\right) \frac{e^{\kappa a}}{2},\tag{4.3.3.29}$$

where the F/A in Eq. (4.3.3.6) becomes

$$\frac{F}{A} = e^{-2ik_{1x\circ}a} \left[ \cos(-i2\kappa a) - \frac{i}{2} \left( \frac{k_{1x\circ}^2 - \kappa^2}{-ik_{1x\circ}\kappa} \right) \sin(-i2\kappa a) \right]^{-1}.$$
(4.3.3.30)

Substituting Eq. (4.3.3.30) into Eqs. (4.3.3.28) and (4.3.3.29) and then into Eq. (4.3.2.26) yield the wavepacket in region *II*. If we just need the probability of reflection and transmission of a free incident particle, then it is enough to know *R* and *T*, and it is not useful to know the wavepacket in the region II.

The present research situation on this barrier tunneling problem in academic circle is as follows. There are still no an accepted theory, an accepted physical essence of tunneling time, and an accepted wavepacket in barrier region [73]. Some authors [74, 75] analyzed the following experimental facts:

(i). Several photon tunneling experiments have revealed considerably higher tunneling speeds than vacuum light speed c. For example, v = 4.7 c, 10 c;

(ii). The phonons after tunneling do not have the change of theirs frequencies. This means that one can listen the superluminal music, and this superluminal music had been listened;

(iii). There is a Hartman effect: No time is lost in the tunnel behavior. The related experimental data are as follows. If the length of the barrier is doubled, then the tunneling time remain the same;

(iv). The tunneling times of, for example, photon, electron, phonon,  $\alpha$ -particle, depend only on energy or frequency of particle, and do not on the kind of the barriers,

and guessed:

(i). The tunneling process is as follows. The tunneling particle interacts for a certain time at the entrance of the tunnel before it either turn back or transverse the barrier;

(ii). When the particle in inner part of barrier, the tunneling particle moves with infinite speed, and looks like through a space with zero time.

Until now, the above two points (i) and (ii) are in arguments of physicists, and thus the tunneling process still is an open problem. Ref. [76] (2013) points out: "It is possible for spin zero particles to travel faster than the speed of light when tunneling. This apparently violates the principle of causality, since there will be a frame of reference in which it arrives

before it has left. However, careful analysis of transmission of wavepacket shows that there is actually no violation of relativity theory." More recently experimental tunneling time data of phonons, photons, and electrons are published by Ref.[77].

Although our wavepacket-only theory supports the above two guesses (i) and (ii) as well, the reasons are different from Ref. [76]. Next, we introduce our arguments. In the barrier domain, the wavefunction is exponential decaying. But, the body-factor keeps always its original form, and accepts the guide of guide-factor according to the spontaneous equiprobability symmetry breaking. This spontaneous equiprobability symmetry breaking. This spontaneous equiprobability symmetry breaking process is a stochastic process. The speed of tunneling body-factor can surpass the light speed, or even can be infinite, because it belongs to a more microscopic process. There is only one point to add to the (i) and (ii): According to the spontaneous equiprobability symmetry breaking law, the body-factor within the barrier still has possibility to turn back with infinite speed as a reflecting particle.

(3). The third configuration is rectangular well, which is depicted in Table 4.1c. (In case of E > 0 and V < 0, it is called Ramsauer effect.) The rectangular well can be called also square well.

First-third steps. Once again Eq. (4.3.3.2) is used with the modification

$$\frac{\hbar^2 k_{2xo}^2}{2m} = E - V = E + |V|.$$
(4.3.3.31)

The transmission coefficient Eq. (4.3.3.9) becomes

$$\frac{1}{T} = 1 + \frac{1}{4} \frac{V^2}{E(E+|V|)} \sin^2(2k_{2x\circ}a) \quad E \ge 0.$$
(4.3.3.32)

Again there is perfect transmission when an integral number of half-wavelength fit the well width.

$$2ak_{2xo} = n\pi$$
 (*n* = 1.2,···) . (4.3.3.33)

This condition may also be cast in terms of the eigenenergies of one dimensional box of width 2a:

$$E + |V| = n^2 E_1. \tag{4.3.3.34}$$

From Eq. (4.3.3.32) we see that  $T \to 1$  with increasing incident energy. At E = 0, T = 0. Thus we obtain an idea of the shape of T versus E. The transmission is zero for E = 0 and rises to the first maximum (unity) at  $E = E_1 - |V|$ . It has successive maxima of unity at the values given by Eq. (4.3.3.34), and approaches 1 with growing incident energy E. The phenomenon that T = 1 in case of  $E = -|V| = n^2 E_1$  is called resonance transmission.  $E = -|V| + n^2 E_1$  is called resonance energy.

Fourth step. The wavepacket,  $\Psi_{II}(x)$ , in region *II* consist of two wavepackets. If we take  $k_{2x\circ} = \sqrt{2m(E+|V|)}/\hbar$  other than  $k_{2x\circ} = \sqrt{2m(E-|V|)}/\hbar$ , then Eqs. (4.3.3.13-15) gives the  $\Psi_{II}(x)$ . (See Table 4.1c.)

The preceding theory of scattering of particle by a potential well has been used as model for scattering of low-energy electrons from atoms. The attractive well represents the field of the nucleus, whose positive charge becomes evident when the scattering electrons penetrate the shell structure of the atomic electrons. The reflection coefficient is a measure of scattering cross section. Experiments in which this cross section is measured (for rare gas atoms) detect a low-energy minimum which is consistent with the first maximum that T goes through for typical values of well depth and width according to the model above, Eq. (4.3.3.32). The transparency to low-energy electrons of rare gas atoms is known as the Ramsauer effect.

The student should not lose sight of the following fact. For any of the solutions to scattering problems considered in sections 4.2 and 4.3, we only found out the guide-factor (wavefunction) of the wavepackets. The guide-factor obeys Schrödonger equation. The Hamiltonian in Schrödinger equation is of the form

$$H = \frac{p^2}{2m} + V(x), \qquad (4.3.3.35)$$

with the potential in Table 4.1. In cases of V < E, the wavenumber of guide-factor represents the average wavenumber of a wavepacket. In each case considered (except V > E, such as the tunneling through barrier), the spectrum of energies is a continuum, the kinetic energy connected with wavenumber is  $E_{kin} = \hbar^2 k_{xo}^2 / (2m)$ . For each value of  $k_{1xo}$  of incident particle, a corresponding set of coefficient ratios (B/A, C/A for simple step and B/A, D/A, C/A, F/A for the rectangular potential barriers and wells) are determined. The coefficient  $|A|^2$  is equal to position probability density occupied by the body-factor of wavepacket. (Suppose that the guide-factor of incident wavepacket is normalized.) These coefficients then determine the motions of the wavepackets according to equiprobability symmetry and spontaneous symmetry breaking. The guide-factor of a wavepacket in free motion is in unbound state or scattering state. A continuous spectrum is characteristic of unbound states, while a discrete spectrum is characteristic of bound states. The guide-factors of particle in box, harmonic oscillator and so on are in bound states. The another characteristic of wavefunction (guide-factors) of incident, reflected, and transmitted wavepacket in scattering states is that these wavefunctions have finite value for  $t \to \pm \infty$ . (Refer to Ref. [3] for subsection 4.3.3)

## 4.4. One Dimensional Harmonic Oscillator

## 4.4.1. Harmonic Oscillator Potential

The harmonic oscillator is a system in which a particle of mass m subjects to a linear restoring force **F** proportional to the displacement from the equilibrium position  $r_e$ .

$$F = -K(r - r_e). \tag{4.4.1.1}$$

The proportionality constant K is known as force constant (or spring constant). Eq. (4.4.1.1) is Hooke law. The minus sign indicates that force is in the direction opposite to direction of the displacement. The potential energy V(x) near equilibrium position can be expressed in

Taylor series, with  $r - r_e = x$  as

$$V(x) = V(0) + \frac{dV}{dx}\Big|_{0} x + \frac{1}{2!} \frac{d^{2}V}{dx^{2}}\Big|_{0} x^{2} + \cdots$$
 (4.4.1.2)

The potential at x = 0, that is, V(0) can be taken as zero. The first order derivative term is also absent because the slope is zero at the minimum in V(x). The second derivative term

$$\frac{1}{2} \frac{d^2 V}{dx^2} \bigg|_0 x^2 = \frac{1}{2} K x^2, \qquad (4.4.1.3)$$

where *K* is force constant.

The potential energy in Eq. (4.4.1.2), after ignoring cubic and higher terms in x, is given by

$$V(x) = \frac{1}{2}Kx^2 = \frac{1}{2}m\omega^2 x^2 > 0.$$
(4.4.1.4)

$$\omega = \sqrt{\frac{K}{m}}.\tag{4.4.1.5}$$

The  $\omega$  in Eq. (4.4.1.5) is called natural frequency of classical harmonic oscillator. The V(x) given by Eq. (4.4.1.5) is called one dimensional harmonic potential.

## 4.4.2. One Dimensional Harmonic Oscillator

We use coordinate representation. The time-independent Schrödinger equation of one dimensional harmonic oscillator, which means that a particle with mass m in potential field given by Eq. (4.4.1.4), is

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2} \left[ E - \frac{1}{2} K x^2 \right] \Psi = 0, \qquad (4.4.2.1)$$

where E is the energy, and  $\Psi$  represents wavefunction (guide-factor of wavepacket) other the wavepacket itself. Eq. (4.4.2.1) can also be called energy eigenequation of one dimensional harmonic oscillator. For brevity, let  $\omega$  represents angular frequency and

$$\lambda = \frac{2m}{\hbar^2}E, \quad \alpha^2 = \frac{mK}{\hbar^2} = \frac{m^2\omega^2}{\hbar^2}, \quad (4.4.2.2)$$

then Eq. (4.4.2.1) is written as

$$\frac{d^2\Psi}{dx^2} + (\lambda^2 - \alpha^2 x^2)\Psi = 0, \qquad (4.4.2.3)$$

with the boundary condition  $\Psi \to 0$  as  $|x| \to \infty$ , which means that a perfect potential of one dimensional harmonic oscillator is an infinitely deep potential well, and thus there are only bound states. The Eq. (4.4.2.3) has two asymptotical solutions for very large value of |x|  $(x^2 >> \lambda^2/\alpha^2)$ .

$$\Psi(x) = e^{\pm \alpha x^2/2}.$$
(4.4.2.4)

Of the two asymptotic solutions in Eq. (4.4.2.4) the  $\exp(\alpha x^2/2)$  is unsatisfactory as a bound state, since it tends rapidly to infinity with increasing value of |x|. Thus we abandon it. Let

$$\xi = \sqrt{\alpha}x. \tag{4.4.2.5}$$

$$\Psi(\xi) = e^{-\alpha x^2/2} f(x) = e^{-\xi^2/2} H(\xi).$$
(4.4.2.6)

Substituting Eqs. (4.4.2.5) and (4.4.2.6) into Eq. (4.4.2.3) yields

$$H''(\xi) - 2\xi H'(\xi) + \left(\frac{\lambda}{\alpha} - 1\right) H(\xi) = 0.$$
(4.4.2.7)

For  $|\xi| < \infty$ , the Eq. (4.4.2.7) can be solved by assuming a power series of the form

$$H(\xi) = \sum_{s=0}^{\infty} a_s \xi^s.$$
 (4.4.2.8)

Substituting Eq. (4.4.2.8) into Eq. (4.4.2.7) yields

$$\sum_{s=0}^{\infty} s(s-1)a_s \xi^{s-2} + \sum_{s=0}^{\infty} \left(\frac{\lambda}{\alpha} - 1 - 2s\right) a_s \xi^s = 0.$$
(4.4.2.9)

In order for Eq. (4.4.2.9) to vanish for all values of  $\xi$ , that is, for  $H(\xi)$  to be a solution of Eq. (4.4.2.7) the coefficients of individual power of  $\xi$  must vanish separately, i. e.

$$1 \times 2a_2 + \left(\frac{\lambda}{\alpha} - 1\right)a_\circ = 0, \ 2 \times 3a_3 + \left(\frac{\lambda}{\alpha} - 1 - 2\right)a_1 = 0 \ etc.$$

In general

$$(s+1)(s+2)a_{s+2} + \left(\frac{\lambda}{\alpha} - 1 - 2s\right)a_s = 0.$$
 (4.4.2.10)

Eq. (4.4.2.10) is called recursion formula. Using this,  $a_2, a_3, \cdots$  can be calculated in terms of  $a_{\circ}$  and  $a_1$ , which are arbitrary. If  $a_{\circ}$  is set to be zero, then only odd powers appear. If  $a_1$  is set to be zero, then only even powers appear. For large values of *s* in Eq. (4.4.10)

$$\frac{a_{s+2}}{a_s} = \frac{\left(2s+1-\frac{\lambda}{\alpha}\right)}{(s+1)(s+2)}\bigg|_{s\to\infty} = \frac{2s}{s^2} = \frac{2}{s}.$$
(4.4.2.11)

It is seen that this behavior is the same as that of the series for

$$e^{\xi^2} = 1 + \xi^2 + \frac{\xi^4}{2!} + \dots + \frac{\xi^s}{(s/2)!} + \frac{\xi^{s+2}}{[(s/2)+1]!} + \dots$$
(4.4.2.12)

The ratio of the coefficient  $\xi^{s+2}$  and  $\xi^s$  in Eq. (4.4.2.12) is 2/s for large values of s. Thus  $H(\xi)$  behaves like  $\exp(\xi^2)$ .

The function in Eq. (4.4.2.6) behaves like an  $\exp(\xi^2/2)$ , which increases with increasing value of  $\xi^2$  or increasing value of x, thus making it unacceptable as a bound state wavefunction. Therefore, we choose the values of the energy parameter, which will cause the series
for  $H(\xi)$  to break off after a finite number of terms. This yields a satisfactory wavefunction of bound state, because the negative exponential factor  $\exp(-\xi^2/2)$  will cause the wavefunction to approach zero for large value of  $\xi$ . The value of  $\lambda$ , which cause the series to break off after the n terms, can be found from Eq. (4.4.2.11).

$$\lambda = (2n+1)\alpha. \tag{4.4.2.13}$$

Substituting the definitions of  $\lambda$  and  $\alpha$  in Eq. (4.4.2.2) into Eq. (4.4.2.13) yields the energy eigenvalues of harmonic oscillator

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \tag{4.4.2.14}$$

The possible energy levels of the harmonic oscillator are restricted to the infinite discrete set of values given by Eq. (4.4.2.14) with  $n = 0, 1, 2, \cdots$ .

Thus the wavefunction of bound state (eigenfunction) is

$$\Psi_n(x) = \Psi_n(\xi) = N_n e^{-\xi^2/2} H_n(\xi), \qquad (4.4.2.15)$$

where  $H_n(\xi)$  is Hermite polynomial of *n*-th degree in  $\xi$  and  $N_n$  is a normalization constant of  $\Psi_n$ ,  $\Psi_n$  is a real function, and satisfies

$$\int_{-\infty}^{+\infty} dx \Psi_n^* \Psi_n = 1.$$
 (4.4.2.16)

The value of  $N_n$ , which makes the above condition true, is

$$N_n = \left[ \left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \frac{1}{2^n n!} \right]^{\frac{1}{2}}.$$
 (4.4.2.17)

To obtain the normalization constant in Eq. (4.4.2.17), consider two generating functions

$$S(\xi,s) = \sum \frac{H_n(\xi)}{n!} s^n = e^{[\xi^2 - (s-\xi)^2]} e^{[-s^2 + 2s\xi]}.$$
(4.4.2.18)

$$T(\xi,t) = \sum \frac{H_m(\xi)}{m!} t^n = e^{[\xi^2 - (t-\xi)^2]} e^{[-t^2 + 2t\xi]}.$$
(4.4.2.19)

and

$$\int_{-\infty}^{\infty} d\xi ST e^{-\xi^2} = \sum_{n} \sum_{m} s^n t^m \int d\xi \frac{H_n(\xi) H_m(\xi)}{n! m!} e^{-\xi^2}.$$
(4.4.2.20)

Substituting Eqs. (4.4.2.18) and (4.4.2.19) into the left hand side of Eq. (4.4.2.20) yields

$$\int_{-\infty}^{\infty} d\xi e^{-s^2 - t^2 + 2s\xi + 2t\xi - \xi^2} = e^{2st} \int_{-\infty}^{\infty} d(\xi - s - t)e^{[-(\xi - s - t)^2]}$$
$$= e^{2st}\sqrt{\pi}$$
$$= \sqrt{\pi} \left(1 + \frac{2st}{1!} + \frac{2^2s^2t^2}{2!} + \frac{2^3s^3t^3}{3!} + \dots + \frac{2^ns^nt^n}{n!} + \dots\right).$$
(4.4.2.21)

Considering coefficients of  $s^n t^n$  in the two equal series expansions Eqs. (4.4.2.20) and (4.4.2.21) yields for  $m \neq n$ 

$$\int_{-\infty}^{\infty} d\xi H_n(\xi) H_m(\xi) e^{-\xi^2} = 0$$
(4.4.2.22)

and for m = n

$$\int_{-\infty}^{\infty} d\xi H_n(\xi) H_n(\xi) e^{-\xi^2} = 2^n n! \sqrt{\pi}.$$
(4.4.2.23)

Therefore

$$\int_{-\infty}^{\infty} dx \Psi_n^*(x) \Psi_m(x) = \frac{N_n N_m}{\sqrt{\alpha}} \int_{-\infty}^{\infty} d\xi H_n(\xi) H_m(\xi) e^{-\xi^2}$$
$$= \frac{N_n N_m}{\sqrt{\alpha}} 2^n n! \sqrt{\pi} \delta_{mn}. \qquad (4.4.2.24)$$

For  $n \neq m$ ,  $\delta_{mn} = 0$  and therefore

$$\int_{-\infty}^{\infty} dx \Psi_n^*(x) \Psi_m(x) = 0.$$
 (4.4.2.25)

For n = m,  $\delta_{mn} = 1$  and therefore

$$\int_{-\infty}^{\infty} dx \Psi_n^*(x) \Psi_m(x) = \frac{N_n^2}{\sqrt{\alpha}} 2^n n! \sqrt{\pi} = 1.$$
 (4.4.2.26)

Eq. (4.4.2.26) gives Eq. (4.4.2.17).

The wavefunction in Eq. (4.4.2.15) becomes

$$\Psi_n(x) = \left[ \left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \frac{1}{2^n n!} \right]^{\frac{1}{2}} e^{-\xi^2/2} H_n(\xi).$$
(4.4.2.27)

The wavefunction in Eq. (4.4.2.27) is either even or odd, depending to *n*. The functions  $\Psi_{2n}$  are even [that is,  $\Psi_{2n}(-x) = \Psi_{2n}(x)$ ] and  $\Psi_{2n+1}(x)$  are odd [that is,  $\Psi_{2n+1}(-x) = -\Psi_{2n+1}(x)$ ] as Hermite polynomial  $H_{2n}(x)$  are even and  $H_{2n+1}(x)$  are odd.

The wavefunctions of harmonic oscillator at lowest four energy levels

$$\Psi_{\circ}(\xi) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\xi^2/2} = H_{\circ}(x)e^{-\alpha x^2/2}.$$
(4.4.2.28)

$$\Psi_1(\xi) = \left(\frac{\alpha}{4\pi}\right)^{1/4} 2\xi e^{-\xi^2/2} = H_1(x)e^{-\alpha x^2/2}.$$
(4.4.2.28)'

$$\Psi_2(x) = \left(\frac{\alpha}{64\pi}\right)^{1/4} (4\xi^2 - 2)e^{-\xi^2/2} = H_2(x)e^{-\alpha x^2/2}.$$
(4.4.2.28)"

$$\Psi_3(x) = \left(\frac{\alpha}{2304\pi}\right)^{1/4} (8\xi^3 - 12\xi)e^{-\xi^2/2} = H_3(x)e^{-\alpha x^2/2}.$$
 (4.4.2.28)'''

 $\Psi_n(x)$  is a wavefunction corresponding to energy eigenvalue  $E_n$ , and not degenerate. According to the corollary of theorem XII-2,  $\Psi_n(x)$  has definite parity. Actually, from the property of  $H_n(x)$ , one can show that

$$\Psi_n(x) = (-1)^n \Psi_n(x). \tag{4.4.2.29}$$

Let us discuss the ground state. First, the energy of ground state is

$$E_{\circ} = \frac{\hbar\omega}{2}.\tag{4.4.2.30}$$

It is not equal to zero, and it is called zero point energy. This is the minimum vibrational energy, that the oscillator may have at 0 K. The existence of zero point energy can be explained by uncertainty relation.

Second, the position probability density of particle (wavepacket) in ground state is

$$|\Psi_{\circ}(x)|^{2} = \left(\frac{\alpha}{\pi}\right)^{1/2} e^{-\alpha x^{2}}.$$
(4.4.2.31)

This is Gaussian type distribution. The position probability density, occupied by the particle, at x = 0 is the largest. Due to the particle energy  $E_{\circ} = \hbar \omega/2$ , it is not difficult to show that at  $x = 1/\sqrt{\alpha} = \sqrt{\hbar/(m\omega)}$ 

$$V(x = 1/\sqrt{\alpha}) = E_{\circ} = \hbar\omega/2.$$
 (4.4.2.32)

 $1/\sqrt{\alpha}$  is called characteristic length of harmonic oscillator. According to the viewpoint of classical mechanics the harmonic oscillator in ground state is allowed to exist in  $|x| \le 1/\sqrt{\alpha}$  (that is,  $\xi \le 1$ ), and the region in  $|x| > 1/\sqrt{\alpha}$  belongs to forbidden domain of classical mechanics. However, according to quantum mechanics the particle (that is, the harmonic oscillator) can have certain probability in  $|x| > 1/\sqrt{\alpha}$ , which is

$$\frac{\int_{1/\sqrt{\alpha}}^{+\infty} dx |\Psi_{\circ}(x)|^2}{\int_0^{+\infty} dx |\Psi_{\circ}(x)|^2} = \frac{\int_{1/\sqrt{\alpha}}^{+\infty} dx e^{-\alpha x^2}}{\int_0^{+\infty} dx e^{-\alpha x^2}} \approx 16\%.$$
 (4.4.2.33)

This is a quantum effect or, equivalently speaking, an effect of wavepacket-only theory, corresponding to that the particle can penetrate a finite barrier. For subsection 4.4.2 refer to Ref. [4].

#### 4.4.3. Operator Method

In this subsection we shell take harmonic oscillator as example to illustrate that Heisenberg matrix (or, operator) mechanics formulation of quantum mechanics can also be used to solving the harmonic oscillator problem. In references this method is called operator or ladder or algebraic method. This subsection derives the eigenvalues of harmonic oscillator. In subsection 5.8.1.2 we seek the eigenfunctions of harmonic oscillation problem.

We turn to general solutions of Schrödinger equation Eq. (4.4.2.1). Eq. (4.4.2.1) can be rewritten as

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}Kx^2 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \qquad (4.4.3.1)$$

where p is momentum operator,

$$\omega = \sqrt{\frac{K}{m}} \tag{4.4.3.2}$$

is the natural frequency, and x can take positive or negative values in the range  $-\infty < x < +\infty$ . Since the force constant in Eq. (4.4.3.2) is positive, the eigenvalues of the Hamiltonian would be positive, i. e.,

$$E_n > 0.$$
 (4.4.3.3)

The operator method involves the operators

$$a = \frac{1}{\sqrt{2}} \sqrt{\frac{m\omega}{\hbar}} \left( x + \frac{ip}{m\omega} \right) \equiv X + iP, \qquad (4.4.3.4a)$$

$$a^{+} = \frac{1}{\sqrt{2}} \sqrt{\frac{m\omega}{\hbar}} \left( x - \frac{ip}{m\omega} \right) \equiv X - iP, \qquad (4.4.3.4b)$$

where X and P are Hermitian operators.

Inasmuch as  $a \neq a^+$ , a is non-Hermitian operator. The properties that these operators have been determined through the fundamental commutator relation

$$[x, p] = i\hbar.$$
 (4.4.3.5)

Let us using Eq. (4.4.3.5) to show that

$$[a,a^+] = aa^+ - a^+a = 1.$$
 (4.4.3.6)

$$aa^{+} = (X+iP)(X-iP) = X^{2} - iXP + iPX + P^{2}$$
  
=  $X^{2} + P^{2} - i[X,P].$  (4.4.3.7)

$$[X,P] = \sqrt{\frac{m\omega}{2\hbar}} x \frac{p}{2m\hbar\omega} - \frac{p}{2m\hbar\omega} \sqrt{\frac{m\omega}{2\hbar}} x$$
$$= \frac{1}{2\hbar} (xp - px) = \frac{1}{2\hbar} [x,p] = \frac{i\hbar}{2\hbar} = \frac{i}{2}.$$
(4.4.3.8)

Substituting Eq. (4.4.3.8) into Eq. (4.4.3.7) yields

$$aa^{+} = X^{2} + P^{2} - i[X, P] = X^{2} + P^{2} - i\frac{i}{2} = X^{2} + P^{2} + \frac{1}{2}.$$
 (4.4.3.9*a*)

Similarly,

$$a^{+}a = X^{2} + P^{2} - \frac{1}{2}.$$
(4.4.3.9b)

Substituting Eqs. (4.4.3.8) and (4.4.3.9) into Eq. (4.4.3.6), one knows that Eq. (4.4.3.6) holds. The inverse of Eq. (4.4.3.4) is

$$X = \frac{a+a^+}{2},\tag{4.4.3.10a}$$

$$P = \frac{a - a^+}{2i}.$$
 (4.4.3.10b)

With the aids of Eq. (4.4.3.9) and the definitions of X and P, the Hamiltonian for the harmonic oscillator in Eq. (4.4.3.1) becomes

$$H = \hbar \omega (X^2 + P^2) = \hbar \omega \left( a^+ a + \frac{1}{2} \right).$$
 (4.4.3.11)

In this manner we see that the problem of finding the eigenvalues of H has been transformed into finding eigenvalues of operator

$$N \equiv a^+ a,$$
 (4.4.3.12)

where N is called number operator.

Let  $\psi_n$  be the eigenfunction of N corresponding to the eigenvalue n, so that

$$N\psi_n = n\psi_n. \tag{4.4.3.13}$$

We do not assume that *n* is an integer at this stage. This property is established later. Consider the effect of operating on  $a\psi_n$  with *N*.

$$Na\psi_{n} = a^{+}aa\psi_{n} = (aa^{+}-1)a\psi_{n} = a(a^{+}a-1)\psi_{n}$$
$$= a(n-1)\psi_{n} = (n-1)a\psi_{n}.$$
(4.4.3.14)

Eq. (4.4.3.14) tells us that  $a\psi_n$  is the eigenfunction of N which corresponds to the eigenvalue (n-1). Apart from the normalization factor,

$$a\psi_n = \psi_{n-1}.$$
 (4.4.3.15)

Similarly,

$$a\psi_{n-1} = \psi_{n-2}, \tag{4.4.3.16}$$

and so forth. Because of this property, a is called an annihilation or stepdown or destruction or demotion or lowering operator.

In similar manner, if we consider the operation  $Na^+\psi_n$ , there results

$$Na^{+}\psi_{n} = (n+1)a^{+}\psi_{n}. \tag{4.4.3.17}$$

Similarly,

$$a^+ \psi_{n+1} = \psi_{n+2}, \tag{4.4.3.18}$$

and so forth. The operator  $a^+$  is called creation or promotion or raising operator.

Considering that x and p are Hermitian operators, it is easy to show that  $\langle H \rangle \ge 0$ .

$$\langle H \rangle = \frac{1}{2m} \int_{-\infty}^{+\infty} dx \Psi^* p^2 \Psi + \frac{1}{2} m \omega^2 \int_{-\infty}^{+\infty} dx \Psi^* x^2 \Psi = \frac{1}{2m} \int_{-\infty}^{+\infty} dx (p\Psi)^* p\Psi + \frac{1}{2} m \omega^2 \int_{-\infty}^{+\infty} dx (x\Psi)^* x\Psi = \frac{1}{2m} \int_{-\infty}^{+\infty} dx |p\Psi|^2 + \frac{1}{2} m \omega^2 \int_{-\infty}^{+\infty} dx |x\Psi|^2 \ge 0.$$
 (4.4.3.19)

In the eigenstate  $\psi_n$ 

$$H\psi_n = \hbar\omega\left(N + \frac{1}{2}\right)\psi_n = \hbar\omega\left(n + \frac{1}{2}\right)\psi_n.$$
(4.4.3.20)

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$$\langle H \rangle = \hbar \omega \left( n + \frac{1}{2} \right) \ge 0.$$
 (4.4.3.21)

This implies that the eigenvalues n must obey the condition

$$n \ge -\frac{1}{2}.\tag{4.4.3.22}$$

That is, all eigenvalues of N, corresponding to eigenvalues n < -1/2 must vanish identically. This condition is guaranteed if we set

$$a\psi_0 = 0. \tag{4.4.3.23}$$

With Eq. (4.4.3.14) we obtain

$$a\psi_0 = \psi_{-1} = 0$$
 and  $a\psi_{-1} = \psi_{-2} = 0$ . (4.4.3.24)

As will be shown, Eq. (4.4.3.23) has a nontrivial (i. e., other than zero) solution for  $\psi_0$ . Furthermore,

$$N\psi_0 = a^+ a \psi_0 = 0 = 0 \psi_0, \qquad (4.4.3.25)$$

and we may conclude that the eigevalue of N corresponding to the eigenfunction  $\psi_0$  is zero. It follows that

$$Na^{+}\psi_{0} = a^{+}aa^{+}\psi_{0} = a^{+}(a^{+}a+1)\psi_{0} = a^{+}\psi_{0} = 1a^{+}\psi_{0} = \psi_{1}.$$
 (4.4.3.26)

This construction allows one to conclude that the index *n*, which labels the eigenfunction  $\psi_n$ , is indeed an integer.

Repeating Eq. (4.4.3.20),

$$H\psi_n = \hbar\omega\left(n + \frac{1}{2}\right)\psi_n \tag{4.4.3.27}$$

one finds that the energy eigenvalues of the simple harmonic oscillator are

$$E_n = \hbar \omega \left( n + \frac{1}{2} \right), \quad (n = 0, 1, 2, \cdots)$$
 (4.4.3.28)

Eq. (4.4.3.26) shows that the *n*, which labels the eigenfunction  $\psi_n$ , is indeed an integer. Now let us consider the effect of creation and annihilation operator on  $\psi_n = |n\rangle$ . Assume

$$a^{+}|n\rangle = c_{n}|n+1\rangle, \quad and \quad a|n\rangle = d_{n}|n-1\rangle.$$
 (4.4.3.29)

The Hermitian conjugate of Eq. (4.4.3.29) is

$$< n|a = c_n|n+1>, and < n|a^+ = d_n^* < n-1|.$$
 (4.4.3.30)

From Eqs. (4.4.3.29-30)

<

$$< n|aa^{+}|n> = |c_{n}|^{2} < n+1|n+1> = |c_{n}|^{2}.$$
 (4.4.3.31)

From Eqs. (4.4.3.6) and (4.4.3.13)

$$< n|aa^+|n> = < n|a^+a + 1|n> = (n+1) < n|n> = n+1.$$
 (4.4.3.32)

From Eqs. (4.4.3.31-32) we have

$$c_n = c_n^* = \sqrt{n+1}.$$
 (4.4.3.33)

From similar derivation we obtain

$$d_n = d_n^* = \sqrt{n}.$$
 (4.4.3.34)

## 4.5. Particle in Gravitational Field

#### 4.5.1. Unbound (Dissociated) Particle

Here the term "unbound" means that although the wavepacket is in a gravitational attractive potential field, the particle can move to infinity. Unbound particle can be called dissociated particle.

Assume that the mass of a particle is *m*, and the gravitation potential is -mgx (g = 9.81 m/sec<sup>2</sup>.). This potential is called linear potential, which can be generally expressed as Fx, due to that it is proportional to *x*. The particle falls from x = 0. Schrödinger equation is

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - mgx\right)\Psi = E\Psi,$$
(4.5.1.1)

where  $x \ge 0$ , g is the gravitation acceleration, and  $E \ge 0$ . If an electron is emitted from a metal surface x = 0, is accelerated by an electric fields along direction x > 0, and the potential energy of the electron is V(x) = -e|E|x, then the electron satisfies Eq. (4.5.1.1) as well.

Taking natural units ( $\hbar = m = mg = 1$ ), Eq. (4.5.1.1) becomes

$$\frac{d^2\Psi}{dx^2} + 2(E+x)\Psi = 0, \qquad (4.5.1.2)$$

where  $x \ge 0$ . Set

$$\xi = 2^{1/2}(x+E) \ge 0, \tag{4.5.1.3}$$

then Eq. (4.5.1.2) becomes

$$\frac{d^2}{d\xi^2} + \xi \Psi = 0. \tag{4.5.1.4}$$

Set

$$z = \frac{2}{3}\xi^{3/2} \quad \Psi = \sqrt{\xi}u \quad , \tag{4.5.1.5}$$

then

$$\frac{d^2u}{dz^2} + \frac{1}{z}\frac{du}{dz}\left[1 - \frac{(1/3)^2}{z^2}\right]u = 0.$$
(4.5.1.6)

Eq. (4.5.1.6) is Bessel equation with order of v = 1/3. Its general solution can be obtained by linear superposition of any two functions from  $J_{1/3}$ ,  $N_{1/3}$ ,  $H_{1/3}^{(1)}$ , and  $H_{1/3}^{(2)}$ . In physics, an unbound particle can move to infinity. Therefore, we need that the solution (wavefunction) of Eq. (4.5.1.6) is a traveling wave along the positive direction of *x*. Traveling wave means that the wave can go to  $\infty$ . Therefore, we have to take the first kind Hankel function  $H_{1/3}^{(1)}(z)$ , i. e.,

$$\Psi(\xi) = C\xi^{1/2} H_{1/3}^{(1)} \left(\frac{2}{3}\xi^{3/2}\right).$$
(4.5.1.7)

Eq. (4.5.1.7) tells us that the *E* is continuous. Let us at first introduce a wrong method to discuss the problem on the energy conservation (This wrong method can be found in many textbooks). Discuss the case  $\xi \gg 1$ . Using the expression of asymptotic expansion of Hankel function

$$H_{1/3}^{(1)}(z) = C_1 \sqrt{\frac{2}{\pi z}} \exp\left[i\left(z - \frac{5\pi}{12}\right)\right], \quad |z| \to \infty,$$
(4.5.1.8)

we have

$$\Psi(\xi) = CC_1 \xi^{-1/4} \exp\left(i\frac{2}{3}\xi^{3/2}\right), \quad \xi \to \infty.$$
(4.5.1.9)

The position probability current J and position probability density  $\rho$  are

$$J = \frac{\hbar}{2im} \left( \Psi^* \frac{d\Psi}{dx} - \Psi \frac{d\Psi^*}{dx} \right).$$
(4.5.1.10)

Using natural units (Note that  $dx = 2^{-1/3}d\xi$ ) and substituting Eq. (4.5.1.9) into Eq. (4.5.1.10) yield

$$J = \frac{1}{2i} 2^{1/3} \left( \Psi^* \frac{d\Psi}{d\xi} - \Psi \frac{d\Psi^*}{d\xi} \right) = 2^{1/3}.$$
 (4.5.1.11*a*)

$$\rho = \Psi^* \Psi = \xi^{-1/2}. \tag{4.5.1.11b}$$

The Eq. (3.5.6.13) in chapter 3 shows that *J* corresponds to product of the velocity and the position probability density taken by single particle. Therefore, the velocity of the particle *v* is

$$v = \frac{J}{\rho} = 2^{1/2} \sqrt{\xi} = \sqrt{2(x+E)}.$$
 (4.5.1.12)

In ordinary units, Eq. (4.5.1.12) becomes

$$v = \sqrt{2\left(gx + \frac{E}{m}\right)}.$$
(4.5.1.13)

Eq. (4.5.1.13) is the same as the result of classical mechanics. Because according to the energy conservation law in classical mechanics

$$\frac{1}{2}mv^2 - mgx = E. (4.5.1.14)$$

According to Eq. (4.5.1.13), the unbound falling neutron at  $x \to \infty$  will keep energy conservation. However, according to our exact derivations, we get Eq. (4.5.1.20) instead of Eq. (4.5.1.13). Eq. (4.5.1.20) indicates that the unbound falling neutron does not keep energy conservation although it is of energy continuous spectrum. The exercise (8) in the last section of chapter 4 requires the readers to point out the mistake in derivation of Eq. (4.5.1.11a).

Next we will see that the neutron falling processes do not obey the "energy conservation law". We do not assume  $\xi \to \infty$ . In this case we can still demonstrate the continuities of velocity *v* and energy spectrum *E* in case gravitational field. We have to use the exact expression of the first kind Hankel function  $H_{1/3}^{(1)}(z)$  ( $z \ge 0$ ) [78, 79]. Eq. (4.5.1.7) becomes

$$\Psi(\xi) = C\xi^{1/2} H_{1/3}^{(1)} \left(\frac{2}{3}\xi^{3/2}\right)$$
  
=  $\xi^{1/2} \frac{2e^{-i\pi/2 \times 3}}{i\pi} \int_0^\infty dt e^{i2\xi^{3/2} ch(t)/3} ch\left(\frac{t}{3}\right).$  (4.5.1.15)

In Eq. (4.5.1.15) the  $\xi$  and thus the *E* [See Eq. (4.5.1.3)] is continuous.

Substituting Eq. (4.5.1.15) into Eq. (4.5.1.11) yields

$$J = \frac{2 \times 2^{1/3} \xi}{2i\pi^2} \left[ \int_0^\infty dt e^{-i2\xi^{3/2} ch(t)/3} ch\left(\frac{t}{3}\right) \frac{d}{d\xi} \int_0^\infty dt e^{i2\xi^{3/2} ch(t)/3} ch\left(\frac{t}{3}\right) - \int_0^\infty dt e^{i2\xi^{3/2} ch(t)/3} ch\left(\frac{t}{3}\right) \frac{d}{d\xi} \int_0^\infty dt e^{-i2\xi^{3/2} ch(t)/3} ch\left(\frac{t}{3}\right) \right].$$
(4.5.1.16)

Substituting Eq. (4.5.1.15) into Eq. (4.5.1.11b) yields

$$\rho = \frac{4\xi}{\pi^2} \int_0^\infty dt e^{-i2\xi^{3/2} ch(t)/3} ch\left(\frac{t}{3}\right) \int_0^\infty dt e^{i2\xi^{3/2} ch(t)/3} ch\left(\frac{t}{3}\right).$$
(4.5.1.17)

From Eqs. (4.5.1.16) and (4.5.1.17) we have

$$v = \frac{J}{\rho} = \frac{2^{1/3}}{2} \sqrt{\xi} \left[ \frac{\int_0^\infty dt e^{i\frac{2}{3}\xi^{3/2}ch(t)}ch\left(\frac{t}{3}\right)ch(t)}{\int_0^\infty dt e^{i\frac{2}{3}\xi^{3/2}ch(t)}ch\left(\frac{t}{3}\right)} + \frac{\int_0^\infty dt e^{-i\frac{2}{3}\xi^{3/2}ch(t)}ch\left(\frac{t}{3}\right)ch(t)}{\int_0^\infty dt e^{-i\frac{2}{3}\xi^{3/2}ch(t)}ch\left(\frac{t}{3}\right)} \right]$$
$$\equiv \frac{2^{1/3}\sqrt{\xi}}{2} \times I = \frac{1}{2}\sqrt{2(x+E)} \times I = \frac{1}{2}\sqrt{\left[\frac{2(mgx+E)}{m}\right]} \times I.$$
(4.5.1.18)

Considering  $ch(t) \ge 1$  for any value of t in the first equality of Eq. (4.5.1.18) yields

$$v \ge \sqrt{\left[\frac{2(mgx+E)}{m}\right]}.$$
(4.5.1.19)

From Eq. (4.5.1.19) we have

$$\frac{mv^2}{2} - mgx > E. (4.5.1.20)$$

Eq. (4.5.1.20) indicates that even the particle can go to  $\infty$  (i. e., unbound or dissociated particle) and the *E* is continuous, but the movement of particle in gravitational field does not satisfy energy conservation law.

The COD experiments on the phase shift of gravitation for neutrons also clearly indicate that Shrödinger equation is correct for the unbound particle in gravitational field [41]-[81]. Therefore, the solution of Shrödinger equation Eq. (4.5.1.15), and thus Eq. (4.5.1.20) are correct.

#### 4.5.2. Bound Particle

If a particle (a wavepacket) suffers infinitely high potential barrier, then the guide-factor of wavepacket has discrete energy spectrum. In this case, the body-factor of wavepacket will take jumping motion from one energy level to another energy level according to the equiprobability symmetry and spontaneous equiprobability symmetry breaking law. Let us illustrate with the following example the jumping motion. Note that in section 4.5.2 we still use both actual and natural units, but the statements have some differences in comparison with the subsection 4.5.1.

A ultracold neutron is bounded above the horizontal plane z = 0 by using a reflecting mirror, i. e.,

$$V(z) = \begin{cases} \infty, & \text{if } z < 0\\ mgz, & \text{if } z \ge 0 \end{cases},$$
(4.5.2.1)

where m is the mass of neutron. The potential in Eq. (4.5.2.1) is called linear potential well. Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\Psi + (mgz - E)\Psi = 0 \quad (z \ge 0, \ E > 0).$$
(4.5.2.2)

Once again, we write the Eq. (4.5.2.2) in terms of dimensionless variables, based on appropriate scales for length and energy. In this case, the dimensionless length scale is  $z_{\circ} = [\hbar^2/(2mmg)]^{1/3}$  and dimensionless energy scale is  $\varepsilon_{\circ} = mgz_{\circ} = (\hbar^2 mg^2/2)^{1/3}$ . When we use dimensionless variables, we can say that we use natural units. Using dimensionless variables yields

$$\frac{d^2\Psi}{dz^2} + 2(E-z)\Psi = 0 \quad (z \ge 0, \quad E > 0).$$
(4.5.2.3)

Note that in Eq. (4.5.2.3) z and E are actually  $z/z_{\circ}$  and  $E/\varepsilon_{\circ}$ , respectively. The boundary conditions are

$$\Psi(0) = 0. \tag{4.5.2.4}$$

 $\Psi(\infty) = 0$  (boundary condition of bounding state). (4.5.2.4)'

Make variable transformation. Set

$$\xi = 2^{1/3}(z - E), \qquad (4.5.2.5)$$

Considering  $0 < z < \infty$ , we have

$$-2^{1/3}E < \xi < \infty, \tag{4.5.2.5}'$$

where  $-2^{1/3}E < \xi \le 0$  is the classical allowing region, and  $\xi > 0$  is the classical forbidden region. (Let us explain that the  $\xi > 0$  is in the classical forbidden region.  $\xi > 0$  means z > E. In dimensional units  $z/z_{\circ} > E/mgz_{\circ}$ , i. e., mgz > E. It is obvious that classical mechanics does not allow mgz > E.) Eqs. (4.5.2.3-5) become

$$\frac{d^2\Psi(\xi)}{d\xi^2} - \xi\Psi(\xi) = 0. \tag{4.5.2.6}$$

$$\Psi(-2^{1/3}E) = 0. \tag{4.5.2.6}'$$

$$\Psi(\infty) = 0$$
 (boundary condition of bounding state). (4.5.2.6)"

Eq. (4.5.2.6) is the Airy equation, which's solution is called Airy function, which is expressed by Ai. This function has a peculiar behavior, oscillatory for negative values of argument and decreasing rapidly towards zero for positive values. Of course, this is exactly the behavior we expect for the wavefunction, since  $\xi = 0$  is the classical turning point.

Note that the boundary condition at z = 0 [Eq. (4.5.2.4)] translate into zeros for  $Ai(\xi)$ , where  $\xi = -2^{1/3}E$  [Eq. (4.5.2.6)']. In other words, the zeros (roots) of the Airy function determines the quantized energies.

$$\Psi_n(-2^{1/3}E_n) = Ai(-2^{1/3}E_n) = Ai(-\lambda_n) = 0.$$
(4.5.2.7)

From the table 10.13 of Airy function in Ref. [82] we can find all the roots. For example,

$$\begin{array}{ll} \lambda_1 = 2.333, & \lambda_2 = 4.088, & \lambda_3 = 5.521, & \lambda_4 = 6.787, & \lambda_5 = 7.944 \\ \lambda_6 = 9.023, & \lambda_7 = 10.040, & \lambda_8 = 11.009, & \lambda_9 = 11.936, & \lambda_{10} = 12.829 \end{array} . \eqno(4.5.2.8)$$

It can be seen that the bound energy levels in linear potential well Eq. (4.5.2.1) are

$$E_n = 2^{-1/3} \lambda_n (natural unit) = \left(\frac{\hbar^2 m g^2}{2}\right)^{1/3} \lambda_n$$
  
=  $\varepsilon_0 \lambda_n = 0.602 \lambda_n (peV), n = 1, 2, 3, \cdots,$  (4.5.2.9)

where characteristic energy  $\varepsilon_{\circ} = mgz_{\circ}$ .

$$z_{\circ} = \left(\frac{\hbar^2}{2m^2g}\right)^{1/3} = 5.87 \quad (\mu m) \quad .$$
 (4.5.2.10)

. ...

From Eqs. (4.5.2.8) and (4.5.2.9) the bounding energy levels of ultracold neutron are  $(peV=10^{-12} eV)$ 

$$E_1 = 1.41, E_2 = 2.46, E_3 = 3.32, E_4 = 4.08, E_9 = 7.21, E_{10} = 7.75, \dots peV.$$
  
(4.5.2.11)

Eq. (4.5.2.11) indicates that the intervals between energy levels are not homogeneous. The larger the *n* are, the denser the energy levels are.

From Eq. (4.5.2.7) the eigenfunctions of bound ultracold neutron in gravitational field are

$$\Psi_n[\xi(z)] = \Psi_n(z) = C_n Ai[\xi(z)].$$
(4.5.2.12)

In quantum mechanics, the probability of observing a neutron with the energy  $E_n$  in the *n*-th quantum state at height *z* is equal to squared modulus of its wavefunction Eq. (4.5.2.12). We can see on left side in Fig. 4.2 that the squared modulus of the neutron wavefunction in the *n*-th pure quantum state has *n* maxima and n - 1 minima between them; the minimum values and the wavefunction at zero height are equal to zero, and the wavefunction tends asymptotically to zero at an infinitely large height. The squared modulus of the neutron wavefunction is greater than zero at any height z > 0; but it is exponentially small at height  $z > z_{n\circ} = E_n/mg$ . In physics, within the classical description, a neutron with the energy  $E_n$  can rise in the gravitational field up to the height  $z_{n\circ} = E_n/mg$ .  $z_{n\circ}$  is called classical turning height.  $z_{n\circ} = E_n/mg = 13.8$ , 24.0, 32.4, and 39.9  $\mu m$  for n = 1, 2, 3, and 4, respectively. For the four lowest quantum states. The square modules of eigenfunctions of lowest four energy levels, other data, and measurement equipments are given in Figs. 4.2-4. To see the original diagrams, please see Refs. [83, 36, 84].

The neutron wave functions  $\Psi_n(z)$  tend to the following asymptotic functions at large heights  $z >> z_n$  forbidden in classical mechanics:

$$\Psi_n[\xi_n(z)] = C_n \xi^{-1/4} e^{-\frac{2}{3}\xi^{3/2}}.$$
(4.5.2.13)



Figure 4.2. Wavefunctions of the quantum states of neutrons in the potential well formed by the Earth's gravitational field and the horizontal reflection mirror. The probability of finding neutrons at height z, corresponding to the *n*-th quantum state, is proportional to the square module of the neutron wavefunction  $|\Psi_n(z)|^2$ . The vertical axis z provides the length scale for this phenomenon.  $E_n$  is the energy of the *n*-th quantum state.

Here,  $\xi_n \rightarrow \infty$  and  $C_n$  are normalization constants.

Using the known eigenfunctions in Eq. (4.5.2.12), we can calculate their Fourier transform, thus obtaining the amplitudes  $\phi(v)$  measuring the velocity v of neutrons in the *n*-th quantum state (Refer to Refs. [83, 36, 84]):

$$\phi_n(v) = \sqrt{\frac{m}{2\pi\hbar}} \int_0^\infty dz \Psi_n(z) e^{i\frac{mvz}{\hbar}}.$$
(4.5.2.14)

 $v_{\circ} = \sqrt{2\epsilon/m}$  is the characteristic velocity in the problem. The probability  $|\phi_n(v)|^2$  of observing neutrons in the *n*-th quantum state as a function of velocity can be found in Ref. [36].

Using the asymptotic expansion of Airy function at  $z \rightarrow \infty$ , one obtains

$$\cos\left(\frac{2}{3}\lambda^{3/2} - \frac{\pi}{4}\right) = 0 \tag{4.5.2.15}$$

determines the eigenvalues, i. e.,

$$\frac{2}{3}\lambda_n^{3/2} - \frac{\pi}{4} = \left(n - \frac{1}{2}\pi\right), \text{ or } \lambda^{3/2} \frac{3}{2}\left(n - \frac{1}{4}\right)\pi.$$
(4.5.2.16)

$$\lambda_n = \left[\frac{3}{2}\left(n - \frac{1}{4}\right)\pi\right]^{2/3}, \ (\lambda_n, n >> 1).$$
(4.5.2.17)

$$E_n = 2^{-1/3} \lambda_n \ (natural \ unit) = \left(\frac{\hbar^2 m g^2}{2}\right)^{1/3} \left[\frac{3}{2} \left(n - \frac{1}{4}\right) \pi\right]^{2/3}, \ (n >> 1) \quad (4.5.2.18)$$

or

$$E_n = \left[\frac{9m}{8}(\pi\hbar g)^2 \left(n - \frac{1}{4}\right)^2\right]^{2/3}, \ (n >> 1).$$
(4.5.2.19)

The quantummechanical treatment of the linear potential such as gravitational potential may appear to have little to do with real world. It turns out, however, that a potential of type V = kz is actually of practical interest in studying the energy spectrum of a quark-antiquark bound system called quarkonium. In this case, the *z* represents the quark-antiquark separation distance. The constant *k* is empirically estimated to be in the neighborhood of

$$1\frac{GeV}{fm} \approx 1.6 \times 10^5 N, \qquad (4.5.2.20)$$

which corresponds to a gravitational force of about 16 tons.

Indeed, another real world example of linear potential is the "bouncing ball". In this case, the potential energy of a ball of mass m at a height z above the floor, and k = mg, where g is the local acceleration due to gravity. Of course, this is the potential energy only for  $z \ge 0$  as there is an infinite potential barrier that causes the ball to "bounce". In this case the quantummechanical calculations have been given by Eqs. (4.5.2.1-19), and have illustrated with neutron as an example.

The bouncing ball happens to be one of those rare cases where quantummechanical effects can be observed macroscopically. The trick is to have a very low mass "ball", which has been achieved with ultracold neutrons by the Nesvizhevsky' group working at the Institute Laue-Langevin in Grenoble, France [83, 36, 84]. These experiments verified clearly that the falling ultracold neutron makes a jump movement from high to low position due to quantization of energy (See, for example, the reports in Figs. 4.2-4 by Refs. [83, 36, 84].). It is the first time that this kind of jump movements is observed in human history. Let us introduce these experiments in details as follows.

The discrete quantum properties of matter are manifested in a variety of phenomena. Any particle that is trapped in a sufficiently deep and wide potential well is settled in quantum bound states. For example, the existence of quantum states of electrons in an electromagnetic field is responsible for the structure of atoms, and quantum states of nucleons in a strong nuclear field give rise to the structure of atomic nuclei. In an analogous way, the gravitational field should lead to the formation of quantum states. But the gravitational force is extremely weak compared to the electromagnetic and nuclear force, so the observation of quantum states of matter in a gravitational field is extremely challenging. Because of their charge neutrality, low mass, and long lifetime, neutrons are promising candidates with which to observe such an effect. Nesvizhevsky et al. report experimental evidence for gravitational quantum bound states of neutrons. The particles are allowed to fall towards a horizontal reflecting mirror which, together with the Earth's gravitational field, provides the necessary confining potential well. Under such conditions, the falling neutrons do not move continuously along the vertical direction, but rather jump from one height to another, as predicted by quantum theory. In order to allow for the experimental observation of gravitational bound states, all interactions of the massive particles with other fields must be so small that their interference with the gravitational quantum phenomena can be neglected. The choice of neutrons seemed the most favorable because (1). They are neutral; (2). They have a long lifetime; (3). They are elementary particles with low mass. The reasons why these properties are advantageous will become more evident from the following explanations.

We now consider how to demonstrate that bound states exist for neutrons trapped in the Earth's gravitational field. The gravitational field alone does not create a potential well, as it can only confine particles by forcing them to fall along gravity field lines. We need a second 'wall' to create the well. This can be obtained by introducing a reflecting mirror. Let us consider a neutron, which is lifted up by a few  $\mu m$  and is then dropped vertically onto the mirror. The neutron wave is reflected by the mirror and interferes with itself, as illustrated in Figs. 4.3 and 4.4. This self-interference creates a standing wave in the neutron position probability density distribution: the probability of finding a neutron at a given height exhibits maxima and minima along the vertical direction, the position of which depends on the quantum number of the bound states. The neutron that was dropped has gone through quantum 'steps'. The classical analogue, the vibrating musical string, gives a visualization of a particle in a rectangular potential well. In this case, strict boundary conditions must be met: both the wavefunction amplitudes of the particles and the displacement amplitudes of the string vanish at the boundaries. In contrast, the gravitational well described above is asymmetric: whereas the reflecting mirror (under total reflection condition) corresponds to an infinite sharp wall, the gravitational field is much softer; as a result, the gravitational well extends in the opposite direction to the gravity field with increasing quantum number.

Consequently, as can be seen from Fig. 4.2, the neutron wavefunctions are deformed upwards, and the energy differences between states with neighboring quantum numbers become smaller with increasing level number. More detailed discussions, precise analytical solutions and related publications can be found in the above equations of this subsection.

We will here simply summarize the results of these theoretical analyzes: the energies of the four lowest quantum states of a neutron in the Earth's gravitational field are  $E_1 = 1.41$  peV,  $E_2 = 2.46$  peV,  $E_3 = 3.32$  peV, and  $E_4 = 4.08$  peV, respectively (1 peV= $10^{-12}$  eV). It is worth keeping in mind that the classical energy that is needed to lift a neutron by 10  $\mu m$  against gravitation on Earth (given by mgz) is almost exactly 1 peV. (Here *m* is the neutron mass, *g* is the acceleration due to gravity, and *z* is the height.) Thus the energy  $E_1$  corresponds in the classical approximation to the height  $z_1 \approx 13.8 \,\mu m$ , at which the last level of the quantum phenomenon for neutrons should be observed.

This 'macroscopic' height is very advantageous, and helps people to design experiments to demonstrate the existence of gravitational levels for neutrons. In a realistic experiment it is not possible to just lift a neutron, let it drop, and then measure its position probability density distribution as a function of height. But we can take a beam of neutrons and let them fly horizontally above a reflecting mirror. If all forces can be eliminated except for gravitation and repulsion by the mirror (such as that due to magnetic field gradients, mechanical vibrations and so on), then the motion of the neutrons can be decoupled into independent vertical and horizontal components. The gravitational force acts on the verti-



Figure 4.3. Layout of the experiment. The limitation of the vertical velocity component depends on the relative position of the absorber and mirror. To limit the horizontal velocity component we use an additional entry collimator. The relative height and size of the entry collimator can be adjusted.

cal component only, and in this direction we then obtain the potential well that leads to the physical consequences described above. No forces act on the horizontal velocity component. A compromise has to be found between the length of the reflecting mirror and the horizontal velocity of neutrons. Refs. [83, 36, 84] used mirrors with a length of 10 cm, and neutrons with a horizontal velocity of 10 m/sec. The energy  $E_1$  corresponds in the classical approximation to the vertical velocity component  $v \approx 1.7$  cm/sec, which is significantly smaller than the horizontal velocity component. If we let the neutrons fly 'slightly upwards' (see Fig. 4.2), they will follow a parabolic trajectory due to gravity. At the maximum of the parabola their vertical velocity component will be zero in the classical approximation, and will then increase again. To limit the vertical velocity component, experimentalists use an absorber parallel to the bottom mirror and placed above it (see Fig. 4.3). The distance between absorber and mirror can be adjusted.

In experiments, neutrons flow between the mirror below and absorber above, and the neutron transmission N is measured as a function of the width z of the slit defined by the mirror and the absorber. This width z acts as a selector for the vertical velocity component. In order to keep the vertical and horizontal velocity components decoupled, severe restrictions concerning quality and adjustment of the different parts used in the set-up must be met. Ideally, from Fig. 4.3, we expect a stepwise dependence of N as a function of zat z = 14 - 15, 24, and 32  $\mu m$ . At sufficiently large slit width z, the classical dependence  $N \propto (z)^{1.5}$  should be approached, and the stepwise increase should be washed out. (Naively we might expect that classically  $N \propto (z)$ ; this is not the case because one can obtain an additional  $z^{0.5}$  due to the fact that an increase in z also allows for an increase in the accepted spread of velocities.) The identification of the lowest quantum state is easier than that of the higher states because in this case the relative change in the count rate N is maximal. The effects, that Nesvizhevsky et al observed (shown in Fig. 4.4) are consistent with the expectations described above theoretically. Careful analysis of the experiments has allowed us to rule out any systematic errors. In particular, tests have shown that the shape of the transmission curve (Fig. 4.4) does not depend on the value of the horizontal velocity component, but that it depends only on the vertical velocity component, as expected.

Fig. 4.4 shows on an extended scale the initial part of the transmission curve N as a



Figure 4.4. The neutron throughput *N* versus the absorber height at low height values. The data points are summed up in intervals of  $2\mu m$ . The dashed curve corresponds to a fit using the quantum-mechanical calculation, in which all level populations and the height resolution are fitted from the experimental data. The solid curve is again the full classical treatment. The dotted line is a truncated fit in which it is assumed that only the lowest quantum state-which leads to the lowest step-exists.

function of slit width z. The curve shows the results of a quantum fit, in which the level populations and the height resolution are free parameters. The solid line is the full classical treatment  $(N \propto z^{1.5})$ . The dotted line is a truncated fit to the assumption that only the lowest quantum level-which leads to the lowest-step exists. Then it continues at the absorber height of  $z_1 \propto 13.8 \,\mu m$  with a shifted classical treatment  $(N \propto (z - z_1)^{1.5})$  that is more like a 'guide to the eye' curve.

Here we want to give five comments for the Nesvizhevsky et al's ultracold neutron gravitational quantum state experiments.

(1). We argue that if the sensitivity of detector in Refs. [83, 36] can be raised, then the transparency number N(z) > 0 can be found at  $0 < z < 15 \ \mu m$ . Our reason is as follows. At z = 13.8 and  $z = 10 \ \mu m$ , the N(7.8) and N(10) are, respectively

$$N(13.8) = \sum_{n=1}^{4} |\Psi_n(13.8)|^2 = C(2+3.7+8.4+1) = C15.1.$$
(4.5.2.21)

$$N(10) = \sum_{n=1}^{4} |\Psi_n(10)|^2 = C(9.3 + 0.05 + 0 + 1.7) = C11.05.$$
(4.5.2.22)

From the comparison between Eqs. (4.5.2.21) and (4.5.2.22), it is obvious that  $N(13.8) \approx N(10)$ . Therefore, if N(13.8) can be observed, then N(10) can be observed as well. It might be wrong that the authors of Refs. [83, 36] concluded that if  $z < 13.8 \,\mu m$ , then N = 0.

(2). It is clear from Fig. 4.4 that besides the stepwise variation of N, there are also slow variations between two stepwise jumps such as between  $z \approx 13.8 - 15$ , between  $z \approx 24 - 26$ , and between  $z \approx 33 - 35$ . The theoretical origin is in that the square modules in these intervals are not zero although are small.

(3). Let us here make a theoretical comment. The gravitational potential belongs to a linear potential. The general treatment of linear potential can utilize Airy function. The linear function is

$$V(z) \equiv k|z|,$$
 (4.5.2.23)

where k is an arbitrary positive constant. Given a total energy E, this potential has a classical turning point at a value z = a, where E = ka. This point will be important for understanding the quantum behavior of a particle of mass m bound by this potential.

The Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi_E}{dz^2} + kx\Psi_E = E\Psi_E.$$
 (4.5.2.24)

It is easiest to deal with the absolute value by restricting our attention to  $z \ge 0$ . We can do this because V(-z) = V(z), so there are two types of solutions, namely  $\Psi_E(-z) = \pm \Psi_E(z)$ . In either case, we need  $\Psi_E(z)$  to tend towards zero as  $z \to \infty$ . If  $\Psi_E(-z) = -\Psi_E(z)$ , then we need  $\Psi_E(0) = 0$ . On the other hand, if  $\Psi_E(-z) = \Psi_E(z)$ , then we have  $\Psi'_E(0) = 0$ , because  $\Psi_E(\varepsilon) - \Psi_E(-\varepsilon) = 0$ , even for  $\varepsilon \to 0$ . We refer to these solutions as "odd" and "even" parity.

(4). For any states, the probability density distributions along the z axis cannot be always oscillatory. At the enough hight, it reaches the tuning point, above which the neutron goes into the gravitational battery domain, and the neutron will make barrier tunneling penetration, correspondingly, the probability density distribution becomes exponentially decreased.

(5). Fig. 4.2 clearly shows that when the cold neutron is, for example, the state  $\Psi_4(z)$  initially, and falls down to state  $\Psi_3$ , according to the spontaneous equiprobability symmetry breaking law the coldneutron is of a possibility to from hight 20  $\mu m$  to hight 30  $\mu m$ . This process violates momentum conservation, and is a prediction at this time.

## 4.6. Energy Quantization of Bound State

The definition of bound state is: a potential prevents the particle in this state from escaping to infinity. Bound states are thus characterized by

$$\begin{array}{ccc} \Psi(x) & \longrightarrow & 0 \\ & x \to \infty \end{array}$$

Bound states appear in quantum mechanics exactly where we expect them classically, namely, in situation where  $V(\pm \infty) > E$ .

The energy spectrum of bound state is always quantized (i. e., discrete). Many students might hear some about energy quantization, and feel that the quantum mechanics and microscopic world are strange and unimaginable. Now we prove that solutions of Schrödinger

equation for bound states have to be discrete energy spectrum, i. e., the energy quantization is an inevitable result solving Schrödinger equation under the boundary condition for bound states. To help readers to understand mathematical origin of the discrete spectrum vividly, we shell base our consideration on a qualitative, mostly graphical discussion on the solution of Schrödinger equation, in order to underscore the key elements. Actually, the oscillation theorem in this section was exactly proved by mathematicians, Sturm and Liuvile, in 1836. Oscillation theory was initiated by Jacques Charles Franois Sturm in his investigations of Sturm-Liouville problems (Sturm-Liouville problem was introduced is chapter 2.) from 1836. There Sturm showed that the *n*-th eigenfunction of SturmCLiouville problem has precisely n-1 nodes. For one dimensional Schrödinger equation the study about oscillation/non-oscillation answers the question whether the eigenvalues construct discrete/continuous spectrum. Readers can refer to Ref. [10, 5, 86], especially, to Ref. [10], for Theorem XIV.

For clarify, we rewrite the one dimensional Schrödinger equation:

$$\frac{d^2}{dx^2}\Psi(x) \equiv \Psi''(x) = -\frac{2m}{\hbar^2} [E - V(x)]\Psi(x) \equiv -k^2 \Psi(x).$$
(4.6.1)

If E - V(x) < 0, then the state is bound state. For reference, let us give the simplest one dimensional uniform potential

$$V(x) = \begin{cases} 0, & |x| < x_{\circ}/2 \\ U_{\circ} & |x| > x_{\circ}/2 \end{cases},$$
(4.6.2)

where  $x_{\circ}$  is the width of the potential well, and  $U_{\circ}$  is the hight of the well.

**Theorem XIV: Quantization of bound state.** For bound system, its ground state has no node. Its excited state is an oscillation function in space, has thus nodes. The *n*-th excited state has n nodes. The energy spectrum of excited states is discrete, i. e., energy quantization. (Note that the label of ground state is 0.)

**Proof.** Recall now that in analytic geometry,  $\Psi''(x)$  is related to the curvature of  $\Psi(x)$  at the point *x*.  $\Psi$  has the following properties.

(1) E > V(x) which correspond to classically permitted region. If  $\Psi$  is in upper halfplane  $\Psi > 0$ , then in classical permitted region  $\Psi'' < 0$ . Therefore, in upper half-plane  $\Psi$  is concave downward (See Fig. 4.5a.);

If  $\Psi$  is in lower half-plane  $\Psi < 0$ , then in classical region  $\Psi'' > 0$ . Therefore, in lower half-plane  $\Psi$  is concave upward. (See Fig. 4.5a.)

As shown in Fig. 4.5b, these conditions permit oscillation solutions.

(2) E < V(x) which correspond to classically forbidden region.  $\Psi$  has following properties.

If  $\Psi$  is in upper half-plane  $\Psi > 0$ , which is equivalent to negative kinetic energy, then  $\Psi'' < 0$ . Therefore, in upper half-plane  $\Psi$  is concave upward; (See Fig. 4.6a.)

If  $\Psi$  is in lower half-plane  $\Psi < 0$ , then  $\Psi'' < 0$ . Therefore, in lower half-plane  $\Psi$  is concave downward. (See Fig. 4.6a.)



Figure 4.5. The y axis represents  $\Psi$ .

These conditions permit monotonously rising (growing) or falling (decaying) solution, without oscillation phenomena with variation of *x*. The wavefunction can be of the form  $\exp(\pm\beta x)$ .  $\beta = \sqrt{2m(U_{\circ} - E)}/\hbar > 0$ . See Fig. 4.6b.

(3) Generally speaking, the solutions of Schrödinger equation have to be constructed from the elements in Figs. 5a and 6a in a continuous and continuously differentiable manner. On the above jointing conditions, the boundary conditions of bound state ( $\Psi \rightarrow 0$ at  $x \rightarrow \pm \infty$ ) will lead to the energy quantization of  $0 < E < U_{\circ}$ . Next, we give a detail qualitative explanations for this energy quantization.

According to Figs. 4.5 and 4.6, one can qualitatively analyze the possible energy (E) values corresponding to wavefunction, and node number of the wavefunction in region 0 < E < V.

At first we discuss ground state. For the ground state the possible energy is the smallest. In region  $x < -x_{\circ}/2$  (classical forbidden region), due to  $E < U_{\circ}$ , bound state  $\Psi \rightarrow 0$  at  $x \rightarrow -\infty$ . When x becomes larger,  $\Psi$  rises exponentially, and the curve of  $\Psi$  versus x is concave upward. When  $x > -x_{\circ}/2$  (classical permitted region), due to E > 0 = V(x), the curve of  $\Psi$  versus x is concave downward until  $x = x_{\circ}/2$ . However, when  $x > x_{\circ}/2$ , in this region  $x > x_{\circ}/2$  (classical forbidden region), due to  $E < U_{\circ} = V(x)$ , the curve of  $\Psi$  versus x is concave upward once again as in  $x < -x_{\circ}/2$ . (At the turning point we always has  $\Psi'' = 0$ .)

Due to two necessary requirements: (i). the requirement of the smoothing joint conditions (, i. e., the wavefunction and its first order derivative are continuous at boundary  $x = x_{\circ}/2$ , where is the turning point); (ii). the solution decaying or falling to zero at  $\pm \infty$ , it is only that when *E* takes an appropriate value, one can have  $\Psi \rightarrow 0$  at  $x \rightarrow \infty$ . If  $E_{\circ}$  satisfies the two requirements, then let us look at that what will happen for  $E = E_0 - |\varepsilon|$  or  $E = E_0 + |\varepsilon|$ .

Try if  $E = E_0 - |\varepsilon|$  can also satisfy the two requirements? At this small *E*, the turning point will have left shift. From Eq. (4.6.1) the small *E* corresponds to that the  $\Psi$  curve is weakly concave downward. After this left shifted turning point, the  $\Psi$  curve will be concave



Figure 4.6. The y axis represents  $\Psi$ .

upward, and cannot approach to zero as that case when  $E = E_0$ .

Try if  $E = E_0 + |\varepsilon|$  can also satisfy the two requirements? At this large *E*, the turning point will have right shift. From Eq. (4.6.1) the large *E* corresponds to that the  $\Psi$  curve is strongly concave downward. After this right shifted turning point, the  $\Psi$  curve will be concave upward, and cannot approach to zero as that case when  $E = E_0$ ; on the contrary, the  $\Psi$  curve will cross the *x* axis at some point, and after this cross point the  $\Psi$  curve goes into the plane where  $\Psi < 0$ , and thus the  $\Psi$  curve will continue to be concave downward, and will approach to  $-\infty$  instead of to  $+\infty$ . This appropriate value of *E* is the lowest energy eigenvalue of the particle. If the value of *E* is even a little departure from this appropriate value, then  $\Psi$  does not satisfy the boundary condition of bound state,  $\Psi = 0$  at  $x = +\infty$ .

When the energy of particle increases from the ground state energy, the curvatures of the curves of  $\Psi$  versus *x* will reduce at  $|x| > x_{\circ}/2$  (classical forbidden region). However, when the energy of particle increases from the ground state energy, the  $\Psi$  curve will be concave downward more strongly, and cross the *x* axis before arrive the turning point. The  $\Psi$  curve in the  $\Psi < 0$  region is concave upward, and will enter the classical forbidden region. Using the similar method as that when  $E = E_0$ , the wavefunction  $\Psi \rightarrow 0$  at  $x \rightarrow +\infty$ , one can know that the wavefunction  $\Psi_1$  at  $E = E_1 > E_0$  has one node in the classical permitted region. This appropriate value of  $E_1$  is the first exited energy level, the corresponding wavefunction is the first exited state, i. e., the second eigenstate of bound energy (odd parity state).

Continuing the similar analyses, one can obtain that: only when the particle energies in the well take some discrete values  $E_0, E_1, E_2, \cdots$ , the corresponding wavefunctions  $\Psi_0$ ,  $\Psi_1, \Psi_2, \cdots$  can satisfy the boundary conditions of bound states:  $\Psi \to 0$  at  $|x| \to \infty$ , and the smooth connecting conditions. These values of energy are the energy eigenvalues, and the corresponding wavefunctions are the energy eigenfunctions. The wavefunction of ground state is of no node point except the infinitely far points. The number of nodes of the *n*th exited state is *n*. The higher the energy of exited state is, the stronger the oscillation of the wavefunction in region |x| < a/2 is. This is the so called oscillation (or Sturm) theorem in the eigenvalue problem of differential equation (Refer to Ref. [10]). QED.

Let us make some discussions for the case of E > V.

In this region the kinetic energy E - V is everywhere positive. Classically, there are two independent states of motion: particle moves towards right and left. Quantummechanically, there are also two independent, if more complicated, states of motion which are just the two independent solutions of the second order differential equation Eq. (4.6.1). Since the kinetic energy is everywhere positive, we see from Eq. (4.6.1) that  $\Psi''$  and  $\Psi$  have opposite sign everywhere. Hence,  $\Psi$  is always concave towards the *x* axis, or in other words, oscillatory. Consequently  $\Psi$  is bounded but extends to infinity in both directions. These states occur for any energy *E*, and thus we conclude that the energy spectrum is continuous and doubly degenerate in this region.

Let us make some discussions for the case of 0 > E, where 0 is the minimum value of V(x).

In this region the kinetic energy is everywhere negative. No quantummechanical states exist either, because the solutions of Eq. (4.6.1) are everywhere convex with respect to the *x* axis (see Fig. 4.6a) and hence must increase without limit in one direction or the other.

If the well is, instead of that given by Eq. (4.6.2), as

$$V(x) = \begin{cases} 0, & |x| < a/2 \\ V_{\circ} & x > a/2/ \\ V_{1} & x < -a/2 & V_{\circ} > V_{1} \end{cases},$$
(4.6.3)

where *a* is the width of the non-symmetrical potential well.

Let us make some discussions for the case of  $V_1 < E < V_{\circ}$ .

In this region the kinetic energy is positive to the left of the intersection of E and  $V_{\circ}$ , negative to the right. The point of intersection, where  $E = V_{\circ}$  and the kinetic energy vanishes, is the classical turning point of the motion. Classically, a particle moving to the right is reflected at the turning point and returns to the left, which is the only general type of motion. Quantummechanically, there are still two independent solutions of Eq. (4.6.1), but only one is admissible (even as an idealized state), as we now show. To the left of the classical turning point, the solutions of Eq. (4.6.1) are oscillatory. To the right, however, where  $\Psi''$  has the same sign as  $\Psi$ , the solutions are convex with respect to the x axis and hence either increase without limit or decrease strongly to zero as x increases. The general solution to Eq. (4.6.1) contains an arbitrary superposition of these two types of terms, but only the particular solution which decreases to zero is permitted by the requirements of physical admissibility. We thus conclude that the energy spectrum is continuous and nondegenerate in this region. The solutions resemble the classical ones in the sense that a particle is always reflected.

The above method can, in principle, also be used to  $V(x) \neq V_{\circ}$ . For example, V(x) is the potential energy of the harmonic oscillator. It is clear how the above arguments generalize

to a particle bound by some arbitrary potential. If we try to keep  $\Psi$  exponentially damped as  $x \to -\infty$ , it blows up as  $x \to +\infty$  (and vise versa), except at some special energies.

### 4.7. Exercises and Solutions

(1) Referring to the derivation of Eq. (4.3.3.19) and Table 4.1b.down, under the condition that at the right side of the barrier there is a potential well,  $-V_{well} < 0$ , i. e.,  $V_{III} < 0$ , calculate the transmission coefficient *T*. Argue that the magnitude of *T* can be changed by the variation of the magnitude of  $-V_{well}$  due to that the wavenumber  $k_{xIII\circ}$  in region III will go up. Discuss the relation between transmission coefficient *T* and  $V_{III}$ . Then design a novel tunneling diode with high efficiency.

(2) According to our wavepacket-only theory, review the viewpoint and calculation method for the incident, reflecting, and transmitting wavepackets in the barrier problem in section 7.9 of Ref. [3].

Ref. [3] considers a chopped one dimensional pulse, L cm long, containing many particles moving with momentum  $p = \hbar k_{\circ}$  and the Fourier transform of any particle's "wavepacket" is

$$b(k) = \sqrt{\frac{2}{\pi L}} \frac{\sin(k - k_{\circ})L/2}{k - k_{\circ}}.$$
(7.159)

Suppose this "wavepacket" is at x = -X at t = 0, and the form of the "wavepacket" is

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk b(k) e^{ikX} e^{i(kx - \omega t)}, \qquad (7.158)$$

which is a superposition of plane waves. Each such incident *k*-component plane wave is reflected and transmitted. Every incident plane wave has its own reflected and transmitted plane wave. Reassembling all of these plane waves, Ref. [3] obtains three "wavepackets"

$$\begin{aligned} x &< -a \qquad & \Psi_{insident} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk b(k) e^{ikX} e^{i(kx - \omega t)}, \\ x &< -a \qquad & \Psi_{reflect} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \sqrt{R} e^{i\phi_R} b(k) e^{ikX} e^{-i(kx + \omega t)}, \\ x &> +a \qquad & \Psi_{tranmitted} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \sqrt{T} e^{i\phi_T} b(k) e^{ikX} e^{i(kx - \omega t)}. \end{aligned}$$

Then Ref. [3] obtains the following results. The trajectories of reflected, incident, and transmitted "wavepacket" are:

$$x = \frac{\hbar k_{x\circ}}{m} t + X + \left. \frac{\partial \phi_R}{\partial k_x} \right|_{k_{x\circ}}, \ x < -a.$$
(7.162)

$$x = \frac{\hbar k_{x\circ}}{m} t - X, \quad x < -a. \tag{7.163}$$

$$x = \frac{\hbar k_{x\circ}}{m} t - X - \left. \frac{\partial \phi_T}{\partial k_x} \right|_{k_{x\circ}}, \quad x > a.$$
(7.164)

In Eqs. (7.162-164), *X* represents the position of the incident "wavepacket" at t = 0. Do you agree with the above analyses and calculations? Why?

Solution:

We would like to remind readers to note that some references also use the above method in this kind of problems. Ref. [3] is just a typical, clearly writing, and representative one within some references. We do not agree the above analyses and calculations. Our opinions for the above method are listed by point by point as follows:

(A) We should remember that above method is to use Schrödinger equation to make calculation. Therefore, the first thing is to satisfy Schrödinger equation. A free Schrödinger equation can only have solution of plane wave. It is obvious that the so-called chopped pulse is very complex, and cannot be a solution of free Schrödinger equation.

(B) Actually, the chopped pulse can consist of many massive particles or photons. An correct calculation has, at least at the start step, to calculate one photon or one massive particle. As is well known, although one often says that a particle is a wavepacket, one has to remember in mind at the same time that the particle is rigid and thus cannot be separated. Therefore, the above "Reassembling all of these plane waves" is not physical.

(C) The barrier method of our wavepacket-only theory is that the wavefunction (=guide-factor) of a free particle, having complex structure, is a plane wave. It is that this plane wave makes scattering with the barrier, and the body-factor of wavepacket (wavepacket=particle) moves according to spontaneous equiprobability symmetry breaking law. We never consider the direct scattering between the particle (or the body-factor) and the potential barrier. We can consider the direct scattering between the wavefunction of particle and the potential barrier.

(3) Show that T + R = 1 [See Eq. (4.3.2.17).] for all one dimensional barrier problems.

#### Solution:

Since the scattering process is assumed to be steady-state, the continuity equation Eq. (3.5.6.12) becomes

$$\frac{\partial J_x}{\partial x} = 0$$

Integrating this equation yields

$$\int_{-\infty}^{\infty} dx \left(\frac{\partial J_x}{\partial x}\right) = J_x(\infty) - J_x(-\infty) = 0$$

But

$$J_x(-\infty) = J_{inc} - J_{ref}.$$
  
 $J_x(+\infty) = J_{trans}.$ 

So that the equation above becomes

$$J_{trans} + J_{ref} = J_{inc}$$
.

Dividing through by  $J_{inc}$  gives the desired result.

(4) Obtain the average value of  $x^2$  using the harmonic oscillator wavefunction

$$\Psi_n(x) = N_n e^{-\frac{\xi^2}{2}} H_n(\xi) = \left[ \left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \frac{1}{2^n n!} \right]^{\frac{1}{2}} e^{-\frac{\xi^2}{2}} H_n(\xi).$$
(4.1)

Solution:

=

The average value of  $x^2$  is

$$\langle x^{2} \rangle_{n,n} = \int_{-\infty}^{\infty} dx \Psi_{n}^{*}(x) x^{2} \Psi_{n}(x) = \frac{N_{n} N_{n}}{\alpha^{\frac{3}{2}}} \int_{-\infty}^{\infty} d\xi H_{n}(\xi) \xi^{2} H_{n}(\xi) e^{-\xi^{2}}.$$
 (4.2)

Let us at first calculate

$$\langle x^2 \rangle_{n,m} = \int_{-\infty}^{\infty} dx \Psi_n^*(x) \Psi_n(x) = \frac{N_n N_m}{\alpha^{\frac{3}{2}}} \int_{-\infty}^{\infty} d\xi H_n(\xi) \xi^2 H_m(\xi) e^{-\xi^2}.$$
 (4.3)

Using the recursion relations of Hermite polynomials

$$\xi^{2}H_{m}(\xi) = \xi \left[ mH_{m-1}(\xi) + \frac{1}{2}H_{m+1}(\xi) \right] = m\xi H_{m-1}(\xi) + \frac{1}{2}\xi H_{m+1}(\xi)$$

$$= (m-1)H_{m-2}(\xi) + \frac{1}{2}H_{m}(\xi) + \frac{1}{2}\left[ (m+1)H_{m}(\xi) + \frac{1}{2}H_{m+2}(\xi) \right]$$

$$= \left( m + \frac{1}{2} \right) H_{m}(\xi) + \frac{1}{4}H_{m+2}(\xi) + m(m-1)H_{m-2}(\xi). \quad (4.4)$$

Substituting Eq. (4.4) into Eq. (4.3) yields

$$\langle x^{2} \rangle_{n,m} = \int_{-\infty}^{\infty} dx \Psi_{n}^{*}(x) \Psi_{n}(x)$$
$$\frac{N_{n}N_{m}}{\alpha^{\frac{3}{2}}} \int_{-\infty}^{\infty} d\xi H_{n}(\xi) \left[ \left( m + \frac{1}{2} \right) H_{m}(\xi) + \frac{1}{4} H_{m+2}(\xi) + m(m-1)H_{m-2}(\xi) \right] e^{-\xi^{2}}.$$
 (4.5)

Substituting Eq. (4.5) into Eq. (4.2) yields

$$\begin{aligned} \langle x^{2} \rangle_{n,n} &= \int_{-\infty}^{\infty} dx \Psi_{n}^{*}(x) x^{2} \Psi_{n}(x) = \frac{N_{n} N_{n}}{\alpha^{\frac{3}{2}}} \left( n + \frac{1}{2} \right) \int_{-\infty}^{\infty} d\xi H_{n}(\xi) H_{n}(\xi) e^{-\xi^{2}} \\ &= \frac{N_{n}^{2}}{\alpha^{\frac{3}{2}}} \left( n + \frac{1}{2} \right) 2^{n} n! \sqrt{\pi} \\ &= \left[ \left( \frac{\alpha}{\pi} \right)^{\frac{1}{2}} \frac{1}{2^{n} n!} \right] \frac{1}{\alpha^{\frac{3}{2}}} \left( n + \frac{1}{2} \right) 2^{n} n! \sqrt{\pi} = \frac{2n+1}{2\alpha}. \end{aligned}$$
(4.6)

(5) Discuss the energy quantization in the following potential:

$$V(x) = \begin{cases} \infty, & x < 0 \\ -V_{\circ} & 0 < x < a \\ 0 & x > a. \end{cases}$$
(5.1)

Solution: Study  $-V_{\circ} < E < 0$ . (a) In the region I (x < 0).  $\Psi \equiv 0$ . (b) In the region II (0 < x < a).

$$\Psi = Asin(kx + \delta) \quad k = \frac{\sqrt{2m|E|}}{\hbar} \quad (5.2)$$

Utilizing the boundary condition  $\Psi(0) = 0$ , one knows

$$\Psi = Asin(kx). \tag{5.3}$$

(c) In the region III (x > a).

$$\Psi \propto e^{\pm \beta x} \quad \beta = \frac{\sqrt{2m(V_{\circ} - |E|)}}{\hbar} \quad .$$
(5.4)

Considering the boundary condition at  $x \to +\infty \Psi = 0$ , one can only take

$$\Psi = e^{-\beta x} \quad (x > a) \quad . \tag{5.5}$$

Then, according to the continuity condition of  $(ln\Psi)'$ , one can find

$$k \cot ka \Psi = -\beta. \tag{5.6}$$

Eq. (5.6) can be rewritten as

$$\cot ka = -\frac{\beta}{k} < 0. \tag{5.7}$$

Therefore, ka is in the II and IV quadrants. Eq. (5.7) can be rewritten as

$$\sin ka = \pm \frac{1}{\sqrt{1 + \cot^2 ka}} = \pm \frac{k}{\sqrt{k^2 + \beta^2}} = \pm \sqrt{\frac{|E|}{V_{\circ}}}.$$
 (5.8)

Utilizing the diagram method, one can find the roots of Eq. (4.8). For example, we can find out the initial five roots. These five roots are the intersection points of the line  $y = ka/k_{\circ}a$  and  $y = |\sin ka|$ .  $k_{\circ} = \sqrt{2mV_{\circ}}/\hbar$ .

When  $V_{\circ} \to +\infty$ , the problem becomes an infinitely deep well. The line  $y = ka/k_{\circ}a$  becomes y = 0. The intersection points of y = 0 and  $y = \sin ka$  are

$$ka = n\pi, \quad n = 1, 2, 3, \cdots,$$
 (5.9)

which is exactly same as we discussed before.

Note that the potential in Eq. (5.1) might be no bound state. The necessary and sufficient condition for, at least, existing one bound state is that at  $ka = \pi/2$ ,  $y = ka/k_{\circ}a \le 1$ , i. e.,  $k_{\circ}a \ge \pi/2$ . This condition can written as

$$V_{\circ}a^2 \ge \frac{\hbar^2 \pi^2}{8m}.\tag{5.10}$$

Eq. (5.10) is the limitation for the potential deep and width.

An application: estimate roughly the interaction between the proton and neutron in the deuteron. Experiment indicates that: the binding energy of the ground state of deuteron is  $B = V_{\circ} - |E| \approx 2.237$  MeV. The deuteron radius is  $a \approx 2.8 \times 10^{-13}$  cm,  $M_p \approx M_n = 1.67 \times 10^{-25}$  g, where  $M_p$  and  $M_n$  are the mass of proton and neutron, respectively. The reduced mass is  $m \approx M_p/2$ . Therefore, for the ground state of the deuteron, utilizing Eqs. (5.6) and (5.4) yields

$$ka \cot ka = -\beta = -\frac{\sqrt{2m\beta}a}{\hbar} \approx -0.650.$$
(5.11)

Numerical calculation gives ka = 1.90. From  $ka = \sqrt{2mBa/\hbar} = \sqrt{2m(V_{\circ} - B)a/\hbar}$ , one obtains  $V_{\circ} \approx 21.3$  MeV.

(6) Prove that the energy level of the neutron falling on the surface of Earth is equal to the average value of kinetic and potential energy on the corresponding state.

Solution:

This conclusion is just our guess. Readers can consult subsection 6.2.4 in chapter 6 to solve this problem.

(7) We have derived from Eqs. (4.4.3.4a-b)

$$a = \mathcal{N} \frac{1}{2m\hbar\omega} (m\omega x + ip) = \frac{1}{2m\hbar\omega} (m\omega x + ip)$$
$$a^{+} = \mathcal{N} \frac{1}{2m\hbar\omega} (m\omega x - ip) = \frac{1}{2m\hbar\omega} (m\omega x - ip)$$

the Eqs. (4.4.3.29)

$$a|n>=\sqrt{n-1}|n-1>$$
 and  $a^+|n>=\sqrt{n+1}|n+1>$ .

Now, would you please take Eq. (4.4.3.29) as starting point to prove Eqs. (4.4.3.4a-b).

Solution:

$$\begin{aligned} aa^{+}|n \rangle &= \sqrt{n+1}a|n \rangle = (n+1)|n \rangle \\ &= \mathcal{N}^{2}(p-im\omega)(p+im\omega)|n \rangle \\ &= \mathcal{N}^{2}\{2Hm+im\omega[p,x]\}|n \rangle \\ &= \mathcal{N}^{2}(n+1)2m\hbar\omega|n \rangle \end{aligned}$$

Solving the above equation yields

$$\mathcal{N}=\frac{1}{2m\hbar\omega}.$$

(8) Ref. [36] (2010) points out that: "Noncommutative extensions of quantum mechanics, in particular those following from quantum gravity theories, have been discussed for a long time, and most intensively recently. Noncommutative extensions are usually based on Heisenberg algebra in a D dimensional space. For gravitational quantum states, the problem reduces to the 2 dimensional space."

We give an exercise on the noncommutative extensions of quantum mechanics. If the readers want to know more about this exercise, please refer to Ref. [85].

Assume that

$$[x,y] = i\theta, \ [p_x, p_y] = i\eta, \ [x_i, p_j] = i\hbar\delta_{ij}, \ i = 1, 2,$$
 (8.1)

where, in the last commutation relation,  $x_1 = x$ ,  $x_2 = y$ ,  $p_1 = p_x$ , and  $p_2 = p_y$ , and the parameters  $\theta$  and  $\eta$  correspond to the noncommutative parameters.

The following Heisenberg uncertainty relations:

$$\Delta x \Delta y \ge \frac{\theta}{2}, \ \Delta p_x \Delta p_y \ge \frac{\eta}{2}, \ \Delta x \Delta p_y \ge \frac{\hbar}{2}.$$
 (8.2)

The first possible way of implementing algebra Eq. (8.1) is to construct the noncommutative variables  $x, y, p_x, p_y$  from the commutative variables  $x', y', p'_x, p'_y$  by means of linear transformations. Given the canonical commutation relations,

$$[x',y'] = 0, \ [p'_x,p'_y] = 0, \ [x'_i,p'_j] = i\hbar\delta_{ij}, \ i = 1,2,$$
(8.3)

Please prove that Eq. (7.1) can be obtained from Eq. (7.3) through the linear transformations:

$$x = x' - \frac{\theta}{\hbar} p'_y, \ y = y', \tag{8.4a}$$

$$p_x = p'_x = -i\hbar \frac{\partial}{\partial x'}, \ p_y = p'_y - \frac{\eta}{\hbar} x' = -i\hbar \frac{\partial}{\partial y'} - \frac{\eta}{\hbar} x'.$$
 (8.4b)

The second possible way of implementing algebra Eq. (8.1) is to construct the noncommutative variables  $x, y, p_x, p_y$  from the another commutative variables  $x'', y'', p''_x, p''_y$  by means of linear transformations. Given the canonical commutation relations,

$$[x'',y''] = 0, \ [p''_x,p''_y] = 0, \ [x''_i,p''_j] = i\hbar\delta_{ij}, \ i = 1,2,$$
(8.5)

Please prove that Eq. (7.1) can be obtained from Eq. (8.5) through the linear transformations:

$$x = x'', y = y'' + \frac{\theta}{\hbar} p_x'',$$
 (8.6*a*)

$$p_x = p''_x + \frac{\eta}{\hbar} y'' = -i\hbar \frac{\partial}{\partial x''} + \frac{\eta}{\hbar} y'', \ p_y = p''_y = -i\hbar \frac{\partial}{\partial y''}.$$
(8.6b)

The second possible way of implementing algebra Eq. (8.1) is to construct the noncommutative variables  $x, y, p_x, p_y$  from the another commutative variables  $x'', y'', p''_x, p''_y$  by means of linear transformations. Given the canonical commutation relations,

$$[x'', y''] = 0, \ [p''_x, p''_y] = 0, \ [x''_i, p''_j] = i\hbar\delta_{ij}, \ i = 1, 2,$$
(8.5)

Please prove that Eq. (8.1) can be obtained from Eq. (8.5) through the linear transformations:

$$x = x'', \ y = y'' + \frac{\theta}{\hbar} p_x'',$$
 (8.6*a*)

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$$p_x = p''_x + \frac{\eta}{\hbar} y'' = -i\hbar \frac{\partial}{\partial x''} + \frac{\eta}{\hbar} y'', \ p_y = p''_y = -i\hbar \frac{\partial}{\partial y''}.$$
(8.6b)

The third possible way of implementing algebra Eq. (8.1) is to construct the noncommutative variables  $x, y, p_x, p_y$  from the another commutative variables  $x''', y''', p'''_x, p'''_y$  by means of linear transformations. Given the canonical commutation relations,

$$[x''', y'''] = 0, \ [p_x''', p_y'''] = 0, \ [x_i''', p_j'''] = i\hbar\delta_{ij}, \ i = 1, 2,$$
(8.7)

Please prove that Eq. (8.1) can be obtained from Eq. (8.7) with a small modification through the linear transformations:

$$x = x''' - \frac{\theta}{2\hbar} p_y''', \ y = y'' + \frac{\theta}{2\hbar} p_x'',$$
 (8.8*a*)

$$p_x = p_x^{\prime\prime\prime} + \frac{\eta}{2\hbar} y^{\prime\prime\prime} = -i\hbar \frac{\partial}{\partial x^{\prime\prime\prime}} + \frac{\eta}{2\hbar} y^{\prime\prime\prime}, \ p_y = p_y^{\prime\prime\prime} - \frac{\eta}{2\hbar} x^{\prime\prime\prime} = -i\hbar \frac{\partial}{\partial y^{\prime\prime\prime}} - \frac{\eta}{2\hbar} x^{\prime\prime\prime}.$$
(8.8b)

The two first commutation relations in Eq. (8.1) are recovered. However, the last one is changed to:

$$[x_i, p_j] = i\hbar \left(1 + \frac{\theta \eta}{4\hbar^2}\right) \delta_{ij}.$$
(8.9)

(9) Eq. (4.5.1.13) indicates that at  $x \to \infty$  the unbound neutron in gravitational field (or electron in electric field) keeps energy conservation. However, our Eq. (4.5.1.20) indicates that for any value of x, including  $x \to \infty$ , the unbound falling neutron in gravitational field (or electron in electric field) does not keep energy conservation. Point out the mistake in derivation of Eq. (4.5.1.13) (Ref. [1] obtains Eq. (4.5.1.13) as well).

Solution: The Eq. (4.5.1.9) can be written as

$$\lim_{\xi \to \infty} \Psi(\xi) = CC_1 \xi^{-1/4} \exp\left(i\frac{2}{3}\xi^{3/2}\right).$$
(4.5.1.9)'

The position probability current J, Eq. (4.5.1.10), can be written as

$$\lim_{\xi \to \infty} J = \lim_{\xi \to \infty} \frac{\hbar}{2i\hbar m} \left( \Psi^* \frac{d\Psi}{dx} - \Psi \frac{d\Psi^*}{dx} \right).$$
(4.5.1.10)'

Because

$$\lim_{\xi \to \infty} J \neq \frac{\hbar}{2i\hbar m} \left( \Psi^* \frac{d}{dx} \lim_{\xi \to \infty} \Psi - \Psi \frac{d\Psi^*}{dx} \lim_{\xi \to \infty} \Psi^* \right), \tag{4.5.1.10}'$$

i. e., the exchange of order between derivative and limitation operations is illegible, one cannot substitute Eq. (4.5.1.9)' into Eq. (4.5.1.10)'. Therefore,

$$\lim_{\xi \to \infty} J \neq 2^{1/3}.$$
 (4.7.1.11)'

## Chapter 5

# **General Formalism**

## 5.1. Expansion in Eigenfunctions

We have defined the scalar product (inner product or dot product) in section 2.3 of chapter 2. If the scalar product of  $\Psi$  and  $\phi$  vanishes, that is,

$$(\Psi, \phi) = 0, \tag{5.1.1}$$

then  $\Psi$  and  $\phi$  are said to be orthogonal. Let  $\Psi_i$  are eigenfunctions of operator O and

$$(\Psi_i, \Psi_j) = 0, \quad for \quad i \neq j \quad . \tag{5.1.2}$$

The set of functions, which are both orthogonal to each other and normalized, is called orthonormal set.

Consider an orthonormal set of *n* (*n* can be equal to  $\infty$  as well as to finite number.) linearly independent functions:  $\Psi_1, \Psi_2, \dots, \Psi_n$ . Suppose that an arbitrary function (for example, state function or wavefunction)  $\Psi$  can be represented by the following linear combination (= expansion)

$$\Psi = \sum_{i=1}^{n} c_i \Psi_i, \text{ or in Dirac notation } |\Psi\rangle = \sum_{i=1}^{n} c_i |i\rangle, \qquad (5.1.3)$$

where  $c_i$  are a given set of complex number.

$$(\Psi_i, \Psi) = (\Psi_i, \sum_{j=1}^n c_j \Psi_j) = \sum_{j=1}^n c_j (\Psi_i, \Psi_j) = \sum_{j=1}^n c_j \delta_{ij} = c_i.$$
(5.1.4)

If Eq. (5.1.3) holds, then the set  $|i\rangle$  (in *x* representation  $\langle x|i\rangle = \Psi_i(x)$ ) is called complete set. For a complete set, we have the following completeness relation or closure relation of complete set  $|i\rangle$  (or  $\Psi_i(x)$ ).

$$\sum_{i} |i\rangle \langle i| = I, \text{ or in x representation } \sum_{i} \Psi_{i}^{*}(x')\Psi_{i}(x) = \delta(x - x').$$
(5.1.5)

where *I* is called identity operator or unit operator. In mathematics, the completeness problem is a very complex problem [1]. However, in case of quantum mechanics, the eigenfunction set of any Hermitian operator is definitely a complete set, and has completeness

relation [1]. General speaking, eigenfunction set of Hermitian operator,  $\Psi_i$ , constitute a complete basis of Hirbert space. Eq. (5.1.5) is invaluable to quantum mechanics. One often uses the completeness relation to expand any state function or to make decomposition of unity.

The scalar product  $\Psi$  and  $\Psi$  is

$$(\Psi, \Psi) = \left(\sum_{i=1}^{n} c_i \Psi_i, \sum_{j=1}^{n} c_j \Psi_j\right) = \sum_{i,j} c_i^* c_j (\Psi_i, \Psi_j) = \sum_{i=1}^{n} |c_i|^2 = 1,$$
(5.1.6)

in which  $c_i$  are the expansion coefficients in Eq. (5.1.3). The last equality in Eq. (5.1.6) comes from normalization of  $\Psi$ .

If an arbitrary wavefunction  $\Phi$  can be represented by a linear combination of  $\Psi_1$ ,  $\Psi_2, \dots, \Psi_n$  such that

$$\Phi = \sum_{i} o_i \Psi_i = o_1 \Psi_1 + o_2 \Psi_2 + \dots + o_n \Psi_n$$
(5.1.7)

where  $o_i$  are a given set of complex number. The scalar product of  $\Psi$  and  $\Phi$  is

$$(\Psi, \Phi) = \left(\sum_{i} c_i \Psi_i, \sum_{j} o_j \Psi_j\right) = \sum_{ij} c_i^* o_j (\Psi_i, \Psi_j) = \sum_{ij} c_i^* o_j \delta_{ij} = \sum_{i} c_i^* o_i.$$
(5.1.8)

Let  $\Psi_i$  be eigenfunctions of the operator *O* and, at the same time,  $\Psi_i$  is complete set of functions. The eigenvalue equation is

$$O\Psi_i = o_i \Psi_i, \tag{5.1.9}$$

where  $o_i$  is the eigenvalue of operator O. The average value of operator O is

$$= \int \Psi^* O \Psi dr = (\Psi, O \Psi) = \left(\sum_i c_i \Psi_i, O \sum_j c_j \Psi_j\right) = \left(\sum_i c_i \Psi_i, \sum_j o_j c_j \Psi_j\right),$$

$$= \sum_{ij} c_i^* c_j o_j \delta_{ij} = \sum_i |c_i|^2 o_i.$$
(5.1.10)
(5.1.10)

The average value of  $O^2$  is

$$< O^{2} > = \int \Psi^{*}O^{2}\Psi dr = (\Psi, O^{2}\Psi) = \left(\sum_{i}c_{i}\Psi_{i}, O^{2}\sum_{j}c_{j}\Psi_{j}\right)$$
$$= \left(\sum_{i}c_{i}\Psi_{i}, \sum_{j}o_{j}^{2}c_{j}\Psi_{j}\right), \qquad (5.1.11)$$
$$< O^{2} >= \sum_{ij}c_{i}^{*}c_{j}o_{j}^{2}\delta_{ij} = \sum_{i}|c_{i}|^{2}o_{i}^{2}. \qquad (5.1.11)'$$

In general

$$< O^n >= (\Psi, O^n \Psi) = \sum_i |c_i|^2 o_i^n.$$
 (5.1.12)

In some textbooks, the explanation for  $c_i$  is as follows: "The results of individual measurements of dynamical variable O for state  $\Psi$  are the eigenvalues  $o_i$ , the value of which depends on  $\Psi_i$ . Due to the normalization of  $\Psi$ ,  $|c_i|^2$  denotes the probability of the state  $\Psi_i$ in state  $\Psi$ , and therefore, denotes the probability that an individual measurement for the dynamical variable O yields the value  $o_i$ . In other words, the absolute square of the coefficient  $c_i$  in the expansion of  $\Psi$  in the eigenfunctions  $\Psi_1, \Psi_2, \dots, \Psi_n$  of operator O is the probability that a measurement of O will yield the eigenvalue  $o_i$ ."

This textbook thinks that it is better to do not connect quantum mechanics with measurements. This textbook prefers the following explanation: "According to the spontaneous equiprobability symmetry breaking law,  $|c_i|^2$  denotes the occupation probability of state  $\Psi_i$ in state  $\Psi$ , and therefore, denotes the probability that the dynamical variable O takes value  $o_i$ . In other words, the absolute square of the coefficient  $c_i$  in the expansion of  $\Psi$  in the eigenfunctions  $\Psi_1, \Psi_2, \dots, \Psi_n$  of operator O is the probability that O will take the eigenvalue  $o_i$ ." We think that the simpler the theory is, the better the theory is. Why we have to connect quantum mechanics with measurements? The probability is a property of any objects, and is, therefore, objective reality, and independent of any measurements absolutely. It is better to believe that objective law does not depend on subjective will certainly.

Consider that the  $\Psi$  is a function of continuous variable *x* only. Substituting Eq. (5.1.4) into Eq. (5.1.3) yields

$$\Psi(x) = \sum_{i} c_{i} \Psi_{i}(x) = \sum_{i} (\Psi_{i}, \Psi) \Psi_{i}(x) = \sum_{i} \left\{ \int dx' \Psi_{i}^{*}(x') \Psi(x') \right\} \Psi_{i}(x), \quad (5.1.13)$$

where x' is the dummy variable of integration. Interchanging the order of summation and integration yields

$$\Psi(x) = \int dx' \left\{ \sum_{i} \Psi_i^*(x') \Psi_i(x) \right\} \Psi(x').$$
(5.1.14)

If Eq. (5.1.14) holds water, then we have

$$\sum_{i} \Psi_{i}^{*}(x') \Psi_{i}(x) = \delta(x - x').$$
(5.1.15)

## 5.2. Hermitian Operators

A physical quantity *O* can be represented by a linear operator *O*. Readers note that, for brevity, in our book we always use *O* to represent both quantity (observable) and operator (of observable). Suppose we have the following scalar product.

$$\int_{-\infty}^{\infty} d\tau \Phi^* O \Psi = (\Phi, O \Psi), \qquad (5.2.1)$$

where O under the integral sign is operator.  $O^+$  is called the adjoint operator or conjugate operator to O if

$$(O^+\Phi,\Psi) = (\Phi, O\Psi), \tag{5.2.2}$$

that is,

$$\int_{-\infty}^{\infty} d\tau (O^+ \Phi)^* \Psi = \int_{-\infty}^{\infty} d\tau \Phi^* O \Psi.$$
 (5.2.3)

The operator O is called Hermitian or self adjoint or self conjugate operator if

$$O^+ = O,$$
 (5.2.4)

that is,

$$\int_{-\infty}^{\infty} d\tau (O\phi)^* \Psi = \int_{-\infty}^{\infty} d\tau \Phi^* O\Psi, \quad (O\Phi, \Psi) = (\Phi, O\Psi) \quad . \tag{5.2.5}$$

The operators representing position and momentum are Hermitian. The Hermitian operator has the following properties.

**Theorem XV: Eigenvalue of Hermitian operator.** The eigenvalue of Hermitian operator are real.

**Proof.** Let us consider the eigenvalues of the Hermitian operator O.

$$O\Psi_m = o_m \Psi_m. \tag{5.2.6}$$

$$\int d\tau \Psi_m^* O \Psi_m = \int d\tau \Psi_m^* o_m \Psi_m = o_m \int d\tau \Psi_m^* \Psi_m.$$
(5.2.7)

That is

$$(\Psi_m, O\Psi_m) = o_m(\Psi_m, \Psi_m) \tag{5.2.8}$$

and

$$\int d\tau (O\Psi_m)^* \Psi_m = \int d\tau (o_m \Psi_m)^* \Psi_m = o_m^* \int d\tau \Psi_m^* \Psi_m$$
$$= (O\Psi_m, \Psi_m) = o_m^* (\Psi_m, \Psi_m).$$
(5.2.9)

For O to be Hermitian (operator)

$$\int d\tau \Psi_m^* O \Psi_m = \int d\tau (O \Psi_m)^* \Psi_m = o_m \int d\tau \Psi_m^* \Psi_m$$
(5.2.10)

or

$$(o_m - o_m^*) \int d\tau \Psi_m^* \Psi_m = 0.$$
 (5.2.11)

$$o_m = o_m^*.$$
 (5.2.12)

Eq. (5.2.12) concludes the proof. QED.

**Theorem XVI: Orthogonality of eigenfunction.** The eigenfunctions of Hermitian operator are orthogonal to each other if the corresponding eigenvalues are unequal.

Proof. Consider the eigenvalue equation

$$O\Psi_m = o_m \Psi_m. \tag{5.2.13}$$

$$O\Psi_n = o_n \Psi_n. \tag{5.2.14}$$

Taking scalar product of Eq. (5.2.14) with  $\Psi_m$ 

$$(\Psi_m, O\Psi_n) = o_n(\Psi_m, \Psi_n). \tag{5.2.15}$$

From Eq. (5.2.13)

$$(O\Psi_m, \Psi_n) = o_m^*(\Psi_m, \Psi_n). \tag{5.2.16}$$

From Eqs. (5.2.15) and (5.2.14)

$$o_n(\Psi_m, \Psi_n) = o_m^*(\Psi_m, \Psi_n).$$
 (5.2.17)

$$(o_n - o_m^*)(\Psi_m, \Psi_n) = 0.$$
 (5.2.18)

Since the eigenvalue of Hermitian operator is real,

$$o_m = o_m^*.$$
 (5.2.19)

Eq. (5.2.18) is thus

$$(o_n - o_m)(\Psi_m, \Psi_n) = 0.$$
 (5.2.20)

If the eigenvalues are unequal

$$o_n \neq o_m, \tag{5.2.21}$$

then

$$(\Psi_m, \Psi_n) = 0.$$
 (5.2.22)

Eq. (5.2.22) concludes the proof. QED.

**Theorem XVII-1: Real average value.** The average value of Hermitian operator on any state is real.

**Proof.** According to the definition in Eq. (5.2.5)

$$=\int d\tau \Psi^* O \Psi = (\Psi, O \Psi) = (O \Psi, \Psi) = (\Psi, O \Psi)^* = ^*.$$
 (5.2.23)

Eq. (5.2.23) concludes the proof.

**Theorem XVII-2: Hermitian operator.** If for any state  $\Psi$  the average value of an operator is real, then the operator is Hermitian.

**Proof.** According to the assumption  $\langle O \rangle = \langle O \rangle^*$ , that is,

$$(\Psi, O\Psi) = (\Psi, O\Psi)^* = (O\Psi, \Psi).$$
(5.2.24)

Take

$$\Psi = \Psi_1 + c\Psi_2, \tag{5.2.25}$$

where  $\Psi_1$ ,  $\Psi_2$ , and c are arbitrary. Substituting Eq. (5.2.25) into Eq. (5.2.24) yields

$$c[(\Psi_1, O\Psi_2) - (O\Psi_1, \Psi_2)] = c^*[(O\Psi_2, \Psi_1) - (\Psi_2, O\Psi_1)].$$
(5.2.26)

Taking c = 1 and c = i in Eq. (5.2.26) yields two equations (1) and (2). Then from (1)+(2) and (1)-(2) we have

$$(\Psi_1, O\Psi_2) = (O\Psi_1, \Psi_2) \quad (\Psi_2, O\Psi_1) = (O\Psi_2, \Psi_1) .$$
 (5.2.27)

Eq. (5.2.27) satisfies the definition of Hermitian operator in Eq. (5.2.5). Thus Eq. (5.2.27) concludes the proof. QED.

Corollary XV: Average value of  $O^2$ . If O is Hermitian operator, then for any state

$$< O^2 >= (\Psi, O^2 \Psi) \ge 0.$$
 (5.2.28)

## **5.3.** Commutation Relations of Operators

The commutator or commutation relation,  $[O, P] \equiv OP - PO$ , of two operators plays a very important role in quantum mechanics. This commutation relation corresponds to Poison bracket in classical mechanics. If the commutation relation between canonical coordinates and canonical conjugate momenta are determined, then the dynamical equation of motion is determined as well. The evolution of commutation relation of operators O and P can be accomplished by allowing the operator to act on arbitrary function which is removed at the end of calculation. Let us consider the commutation relation of position and momentum.

The position and momentum in coordinate representation are represented by operator r and  $(\hbar/i) \bigtriangledown$ , respectively. Consider x component of position operator and  $p_x$  component of momentum operator. The corresponding operators are x and  $(\hbar/i)\partial/\partial x$  (Refer to theorem II in chapter 3). Actually, in coordinate representation, x is a special operator, i. e., it is a number.

$$[x, p_x]\Psi(x) = \left[x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right]\Psi(x) = \frac{\hbar}{i}\left(x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x\right)\Psi(x)$$
$$= \frac{\hbar}{i}x\frac{\partial\Psi}{\partial x} - \frac{\hbar}{i}\frac{\partial}{\partial x}(x\Psi(x)) = i\hbar\Psi(x).$$
(5.3.1)

From Eq. (5.3.1) one obtains

$$[x, p_x] = i\hbar. \tag{5.3.2}$$

The commutator between x and  $p_x$  plays a fundamental role in quantum mechanics. The appearance of  $\hbar$  in Eq. (5.3.2), which is much different from Poison bracket, signals that we are now in the regime of quantum mechanics.

Here, we remind readers to remember that the section 3.2 in chapter 3 has proved the operator property of  $p_x$  and the commutation relation Eq. (5.3.2). Due to the importance we repeat hear again.

In classical mechanics, Poisson bracket is given by

$$\{f,g\} = \frac{\partial f}{\partial x}\frac{\partial g}{\partial p_x} - \frac{\partial f}{\partial p_x}\frac{\partial g}{\partial x}, \qquad (5.3.3)$$

where  $f(x, p_x)$  and  $g(x, p_x)$  are functions of x coordinate and x component of momentum. In classical mechanics the x and  $p_x$  are called canonical variable or canonical conjugate variables or proper variables.

Consider Hamiltonian

$$H = \frac{p_x^2}{2m} + V(x).$$
 (5.3.4)

Poisson bracket of x and H is

$$\{x, H\} = \left\{x, \frac{p_x^2}{2m} + V(x)\right\} = \left\{x, \frac{p_x^2}{2m}\right\} + \left\{x, V(x)\right\}$$
$$= \frac{\partial x}{\partial x} \frac{\partial (p_x^2)}{\partial p_x} - \frac{\partial x}{\partial p_x} \frac{\partial (p_x^2)}{\partial x} + \frac{\partial x}{\partial x} \frac{\partial V}{\partial p_x} - \frac{\partial x}{\partial p_x} \frac{\partial V}{\partial x}$$
$$= \frac{p_x}{m} = \dot{x}.$$
(5.3.5)

Similarly,

$$\{p_x, H\} = \dot{p}_x. \tag{5.3.6}$$

$$\{x, p_x\} = 1. \tag{5.3.7}$$

From Eq. (5.3.2), the relation between Poisson bracket and commutator of x and  $p_x$  is

$$i\hbar\{x, p_x\} = [x, p_x].$$
 (5.3.8)

or, in general, commutator of f and g are related to Poisson bracket of f and g as

$$i\hbar\{f,g\} = [f,g].$$
 (5.3.9)

Consider the commutator of x and  $p_z$ .

$$[x, p_z]\Psi = \left[x, \frac{\hbar}{i}\frac{\partial}{\partial z}\right]\Psi = \frac{\hbar}{i}x\frac{\partial\Psi}{\partial z} - \frac{\hbar}{i}\frac{\partial}{\partial z}(x\Psi) = 0.$$
(5.3.10)

From Eq. (5.3.10) one obtains

$$[x, p_z] = 0. (5.3.11)$$

Thus x component of position vector and z component of momentum vector commutes. If two observables commute, then the two observables are called compatible because between these two observables there are no the limitation of Heisenberg uncertainty relation. If two observables do not commute, then the two observables are called incompatible because between these two observables there are the limitation of Heisenberg uncertainty relation.

Eqs. (5.3.7) and (5.3.11) can be generalized to

$$[x_i, p_i] = i\hbar \delta_{i,j}, \quad (i, j = 1, 2, 3) \quad , \tag{5.3.12}$$

where  $x_1 = x$ ,  $x_2 = y$ ,  $x_3 = z$  and  $p_1 = p_x$ ,  $p_2 = p_y$ ,  $p_3 = p_z$ .

**Theorem XVIII: Commutation.** If two linear and Hermitian operators, *O* and *P*, have the same eigenfunctions, then they commute, that is, [O, P] = 0.

**Proof.** Let O and P are the two operators and  $\Psi$  is their common eigenfunction, that is

$$O\Psi = o\Psi \tag{5.3.13}$$

and

$$P\Psi = p\Psi, \tag{5.3.14}$$

where o and p are eigenvalues. Operating on Eq. (5.3.13) with P from left and Eq. (5.3.14) with O from left

$$PO\Psi = oP\Psi = op\Psi. \tag{5.3.15}$$

$$OP\Psi = pO\Psi = po\Psi. \tag{5.3.16}$$

From Eqs. (5.3.15) and (5.3.16)

$$(OP - PO)\Psi = (op - po)\Psi = 0$$
  
$$(OP - PO)\Psi = 0,$$
 (5.3.17)

that is,

$$[O, P] = 0. \tag{5.3.18}$$

Eq. (5.3.18) concludes the proof. QED.

**Theorem XIX: Theorem of Common eigenfunction set.** If operators *O* and *P* commute, then a common set of eigenfunctions can be chosen for them.

**Proof.** Suppose  $\Psi$  is an eigenfunction of the operator O, i. e.,

$$O\Psi = o\Psi \tag{5.3.19}$$

Operating the Eq. (5.3.19) from the left by operator P

$$PO\Psi = OP\Psi \tag{5.3.20}$$

as O and P commute. The left of Eq. (5.3.19) becomes

$$PO\Psi = P(o\Psi) = o(P\Psi). \tag{5.3.21}$$

Therefore, from Eqs. (5.3.20) and (5.3.21)

$$O(P\Psi) = o(P\Psi). \tag{5.3.22}$$

Eq. (5.3.22) indicates that if  $P\Psi \neq 0$ , then  $P\Psi$  is also an eigenfunction of *O* corresponding to the same eigenvalue *o*. QED.

**Theorem XX: Inverse theorem.** If  $\Psi$  is common eigenfunction of O and P, then [O, P] = 0

**Proof.** Consider the case when o is non-degenerate, i. e., it correspond to one independent eigenfunction  $\Psi$ . The  $P\Psi$  can differ from  $\Psi$  by a constant multiplier, i. e.,

$$P\Psi = p\Psi, \tag{5.3.23}$$

where p is a constant. Eq. (5.3.20) becomes

$$(OP - PO)\Psi = 0 \quad , \tag{5.3.24}$$
i. e., [O, P] = 0. QED.

Let us consider the case when eigenvalue *o* is degenerate. Suppose *o* is doubly degenerate, i. e.,

$$O\Psi_1 = o\Psi_1, \quad O\Psi_2 = o\Psi_2$$
 . (5.3.25)

The linear composition of  $\Psi_1$  and  $\Psi_2$  is also an eigenfunction of O, i. e.,

$$\Psi = c_1 \Psi_1 + c_2 \Psi_2 \tag{5.3.26}$$

and

$$O\Psi = O(c_1\Psi_1 + c_2\Psi_2) = c_1O\Psi_1 + c_2\Psi_2 = o(c_1\Psi_1 + c_2\Psi_2)$$
(5.3.27)

Now  $c_1$  and  $c_2$  are to be determined.  $\Psi_1$  and  $\Psi_2$  do need not to be eigenfunction of *P* but  $\Psi$  is an eigenfunction of *P*, i. e.,

$$P\Psi = p\Psi = p(c_1\Psi_1 + c_2\Psi_2).$$
(5.3.28)

$$P\Psi = P(c_1\Psi_1 + c_2\Psi_2) = c_1P\Psi_1 + c_2P\Psi_2.$$
(5.3.29)

But

$$P\Psi_1 \neq p\Psi_1, \quad and \quad P\Psi_2 \neq p\Psi_2 \quad .$$
 (5.3.30)

Taking the scalar product of Eq. (5.3.29) with  $\Psi_1$  and  $\Psi_2$  yields

$$(\Psi_1, P\Psi) = (\Psi_1, c_1 P\Psi_1) + (\Psi_1, c_2 P\Psi_2) = c_1(\Psi_1, P\Psi_1) + c_2(\Psi_1, P\Psi_2), \quad (5.3.31)$$

$$(\Psi_2, P\Psi) = (\Psi_2, c_1 P\Psi_1) + (\Psi_2, c_2 P\Psi_2) = c_1(\Psi_2, P\Psi_1) + c_2(\Psi_2, P\Psi_2).$$
(5.3.31)

Taking the scalar product of Eq. (5.3.28) with  $\Psi_1$  yields

$$(\Psi_1, P\Psi) = p(\Psi_1, \Psi) = p(\Psi_1, c_1\Psi_1) + p(\Psi_1, c_2\Psi_2)$$
$$= pc_1(\Psi_1, \Psi_1) + pc_2(\Psi_1, \Psi_2) = pc_1.$$
(5.3.32)

Taking the scalar product of Eq. (5.3.28) with  $\Psi_2$  yields

$$(\Psi_2, P\Psi) = p(\Psi_2, \Psi) = p(\Psi_2, c_1\Psi_1) + p(\Psi_2, c_2\Psi_2)$$
$$= pc_1(\Psi_2, \Psi_1) + pc_2(\Psi_2, \Psi_2) = pc_1.$$
(5.3.33)

Comparing Eq. (5.3.31) and Eq. (5.3.32) and considering the orthogonality of eigenfunction yield

$$c_1(\Psi_1, P\Psi_1) + c_2(\Psi_1, P\Psi_2) = pc_1.$$
(5.3.34)

Comparing Eq. (5.3.31) and Eq. (5.3.33) and considering the orthogonality of eigenfunction yield

$$c_1(\Psi_2, P\Psi_1) + c_2(\Psi_2, P\Psi_2) = pc_2.$$
(5.3.35)

Let

$$(\Psi_1, P\Psi_1) = P_{11}, \quad (\Psi_1, P\Psi_2) = P_{12}, \quad (5.3.36)$$

$$(\Psi_2, P\Psi_1) = P_{21}, \quad (\Psi_2, P\Psi_2) = P_{22}$$
 (5.3.36)

From Eqs. (5.3.34), (5.3.35), and (5.3.36) one obtains

$$c_1 P_{11} + c_2 P_{12} = p c_1, \tag{5.3.37}$$

$$c_1 P_{21} + c_2 P_{22} = p c_2. \tag{5.3.37}'$$

The solution of Eqs. (5.3.37) is given by

$$\begin{vmatrix} P_{11} - p & P_{12} \\ P_{21} & P_{22} - p \end{vmatrix} = 0.$$
 (5.3.38)

From Eq. (5.3.38) one obtains the equation to determine the p.

$$p^{2} - p(P_{11} + P_{22}) + (P_{11}P_{22} - P_{12}P_{21}) = 0.$$
 (5.3.39)

The quadratic equation has two roots  $p^{(1)}$  and  $p^{(2)}$  which lead to two corresponding set of constants  $c_1^{(1)} c_2^{(1)}$  and  $c_1^{(2)} c_2^{(2)}$ . The two distinct functions are thus

$$\Psi^{(1)} = c_1^{(1)} \Psi_1 + c_2^{(1)} \Psi_2, \qquad (5.3.40)$$

$$\Psi^{(2)} = c_1^{(2)} \Psi_1 + c_2^{(2)} \Psi_2.$$
 (5.3.40)'

 $\Psi^{(1)}$  and  $\psi^{(2)}$  are common eigenfunctions of commuting operators *O* and *P*.

Operators *O* and *P* are defined to be compatible when [O, P] = 0, and to be incompatible when  $[O, P] \neq 0$ . QED.

Let us introduce concepts of the complete set of commuting observables, and the complete set of commuting conserved observables. We have already seen that for the particle in one dimension, the plane waves are possible eigenstates of H, and the eigenvalues are doubly degenerate. The two plane waves of H corresponding to the eigenvalue  $E = \hbar^2 k^2 / (2m)$ are exp(+ikx) and exp(-ikx). However, once we specify what p is (say,  $+\hbar k$ ), in addition to E, then one can say that the system is in one and only one state, exp(+ikx) (to within a multiplicative constant). Merely prescribing the energy of the particle does not uniquely determine the state of the particle. Further specifying the momentum removes this ambiguity and the state of the particle is uniquely determined.

Suppose that an operator *O* has degenerate eigenvalues. If *o* is one of these values, specifying *o* does not uniquely determine which state the system is in. Let *P* be another operator which is compatible with *O*. Consider all the eigenstates  $\{\phi_{op}\}$  which are common to *O* and *P*. Of the degenerate eigenstates of *O*, only a subset of these are also eigenfunctions of *P*. Under such conditions, if we specify the eigenvalue *p* and the eigenvalue *o*, then the state that the system can be in is a smaller set than that determined by specification of *o* alone. Suppose further that there is only one other operator *R* which is compatible with both *O* and *P*. Then they all share a set of common eigenstates. Call these states  $\phi_{opr}$ .

$$O\phi_{opr} = o\phi_{opr},\tag{5.3.41}$$

$$P\phi_{opr} = p\phi_{opr}, \tag{5.3.41}'$$

$$R\phi_{opr} = r\phi_{opr}.\tag{5.3.41}''$$

These wavefunctions are still a smaller set than the set  $\phi_o$  or  $\phi_{op}$ . Indeed, let us consider that  $\phi_{opr}$  is uniquely determined by the values o, p, and r. This means that having measured o, p, and r: (1). Since  $\phi_{opr}$  is a common eigenstate of O, P, and R, simultaneous measurement (or a succession of three immediately repeated "ideal" measurements) of O, P, and R will definitely find the values o, p, and r. (2). The state  $\phi_{opr}$  cannot be further resolved by more measurement. This state contains a maximum of information which is permitted by the laws of quantum mechanics. (3). There are no other operators independent of O, P, and R which are compatible with these. If there were, the state  $\phi_{opr}$  could be further resolved. An exhaustive set (in the sense that there are no other independent operators compatible with O, P, and R.) of communing operators such as O, P, and r and are a basis of Hilbert space, is called a complete set of communing operators.

If Hamiltonian of system does not explicitly contain time, i. e.,  $\partial H/\partial t = 0$ , then *H* is a conservative quantity. In this case, if the complete set of communing operators contains *H*, then every observable of the complete set of communing operators is a conservative quantity. This set is called complete set of communing conserved operators. If the eigenvalues *o*, *p*, *r*, and *E*, which may be so specified in the common eigenstate  $\phi_{oprE}$  of the complete set of communing conserved operators. Using  $\phi_{oprE}$  to expand stationary or non-stationary state the square of absolute value of the expanding coefficient does not change with time. The good quantum numbers are analogous to the generalized coordinates whose values determine the state of a system classically. Such classical coordinates are also labeled by good variables.

## 5.4. Normalization and Periodic Boundary Condition

We have addressed this problem in chapter 3. Now we address here in detail. For the eigenfunctions of continuum spectrum the normalization cannot be made in terms of the Kroneker delta function. For example, the momentum eigenfunction is a plane wave

$$\Psi_p(x) = Ce^{-ipx/\hbar}.$$
(5.4.1)

It is easy to see that

$$\int_{-\infty}^{\infty} dx |\Psi_p(x)|^2 = |C|^2 \int_{-\infty}^{\infty} dx = \infty,$$
(5.4.2)

i. e.,  $\Psi_p(x)$  cannot be normalized, is not square-integrable, and is, thus, outside Hilbert space. In this case, quantum mechanics loosens the square-integrable condition, and just requires the scalar product between any functions  $\in \mathcal{M}(\mathbb{R})$  and the eigenfunction of continuum spectrum is finite. According to this loosened condition one can also make Fourier expansion by using the eigenfunctions of continuum spectrum, and discuss the spontaneous equiprobability symmetry breaking [1, 53].

Under the above loosened condition, we solve the so-called "normalization" difficulty of continuous spectrum eigenfunction such as momentum eigenfunction (plane wave), by using two equivalent proofs, which are given in theorems XXI-1 and XXI-2.

First proof is to introduce Dirac  $\delta$  function. There are two methods to introduce Dirac

 $\delta$  function. The definition of  $\delta$  function is

$$\delta(x - x_{\circ}) = \begin{cases} 0, & x \neq x_{\circ} \\ \infty, & x = x_{\circ} \end{cases}$$
(5.4.3)

and 
$$\int_{x_\circ-\varepsilon}^{x_\circ+\varepsilon} dx \delta(x-x_\circ) = \int_{-\infty}^{\infty} dx \delta(x-x_\circ) = 1, \quad (\varepsilon \to o^+)$$
. (5.4.4)

From this definition of the  $\delta$  function, we know that it is not an ordinary function. The dimension of the  $\delta$  function is 1/x in this one dimensional case. Therefore, the  $\delta$  function is a distribution function, concerning the distribution theory in mathematics.

Or equivalently, we define the  $\delta$  function as: if f(x) is continuous in the vicinity of  $x_{\circ}$ , then

$$f(x_{\circ}) = \int_{-\infty}^{\infty} dx f(x) \delta(x - x_{\circ}).$$
(5.4.5)

We use the  $\delta$  function to express the "normalization" of continuum spectrum eigenfunction as follows.

**Theorem XXI-1:** Normalization of eigenfunction of continuous spectrum. The continuum spectrum eigenfunction is orthogonal and is normalized to Dirac  $\delta$  function.

**Proof.** From Fourier integration formula, a continuous function f(x) satisfies

$$f(x_{\circ}) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dk e^{ik(x-x_{\circ})}.$$
 (5.4.6)

Comparing of Eq. (5.4.6) with Eq. (5.4.5) yields

$$\delta(x - x_{\circ}) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ik(x - x_{\circ})}.$$
(5.4.7)

Therefore, for example, if we take momentum eigenfunction, i. e., plane wave, which is an eigenfunction of continuous spectrum,

$$\Psi_{p'}(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ip'x/\hbar},\tag{5.4.8}$$

then

$$(\Psi_{p'}, \Psi_{p''}) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx e^{i\frac{(p''-p')x}{\hbar}} = \delta(p'-p''), \qquad (5.4.9)$$

i. e., the continuum spectrum eigenfunction is orthogonal and normalized to Dirac  $\delta$  function. (Note that the discrete spectrum eigenfunction is orthogonal and is normalized to Kroneker  $\delta$  function.) QED.

The "normalization" of eigenfunctions of position operator can be treated similarly. According to the property of  $\delta$  function

$$(x - x')\delta(x - x') = 0, (5.4.10)$$

i. e.,

$$x\delta(x-x') = x'\delta(x-x').$$
 (5.4.11)

Eq. (5.4.11) tells us that  $\delta(x - x')$  is the eigenfunction of position *x*, its eigenvalue is *x'*, and can be written as

$$\Psi_{x'}(x) = \delta(x - x') = \delta(x' - x).$$
(5.4.12)

Using the property of  $\delta$  function, the normalization and orthogonality of position operator eigenfunction can be expressed as

$$(\Psi_{x'}, \Psi_{x''}) = \int dx \delta(x' - x) \delta(x'' - x) = \delta(x' - x'').$$
 (5.4.13)

Any function of position x can be expanded as

$$\Psi(x) = \int dx' \Psi(x') \delta(x' - x).$$
 (5.4.14)

The coefficient of expansion is

$$\Psi(x') = (\delta(x' - x), \Psi(x)). \tag{5.4.15}$$

 $|\Psi(x')|^2$  represents the position probability density distribution of a single particle.

Second method to introduce the normalization of continuous spectrum is to use box normalization. This method can be separated into two steps. First step, suppose that the particle is confined in a finite domain [-L/2, L/2]. Second step is to set  $L \rightarrow \infty$ .

At first, as a preparation to this second method, we demonstrate a theorem.

**Theorem XXII: Periodic boundary condition.** To ensure that the momentum operator  $p_x = -i\hbar\partial/\partial x$  in domain  $[-L/2 \le x \le L/2]$  is Hermitian operator,  $\Psi(x)$  has to satisfy periodicity boundary condition  $\Psi(-L/2) = \Psi(L/2)$ . (Refer to Ref. [1] for proof.)

**Proof.** According to the definition of Hermitian operator given by Eq. (5.2.1), for any two functions  $\phi$  and  $\Psi$ 

$$\int_{-\frac{L}{2}}^{\frac{L}{2}} dx \phi^* \frac{\hbar}{i} \frac{\partial}{\partial x} \Psi + \int_{-\frac{L}{2}}^{\frac{L}{2}} dx \left(\frac{\hbar}{i} \frac{\partial \phi^*}{\partial x}\right) \Psi = 0, \qquad (5.4.16)$$

i. e.,

$$\frac{\hbar}{i} \int_{-\frac{L}{2}}^{\frac{L}{2}} dx \frac{\partial}{\partial x} (\phi^* \Psi) = \frac{\hbar}{i} (\phi^* \Psi) \Big|_{-\frac{L}{2}}^{\frac{L}{2}} = 0.$$
(5.4.17)

Therefore,

$$\phi^*(L/2)\Psi(L/2) - \phi^*(-L/2)\Psi(-L/2) = 0, \qquad (5.4.18)$$

i. e., for any two functions

$$\frac{\phi^*(L/2)}{\phi^*(-L/2)} = \frac{\Psi(-L/2)}{\Psi(L/2)} = constant.$$
(5.4.19)

From Eq. (5.4.19) one deduces that for any function (or for all functions)  $\Psi$  has to be

$$\frac{\Psi(-L/2)}{\Psi(L/2)} = e^{i\alpha} \ (\alpha \ is \ real \ number).$$
(5.4.20)

The momentum eigenfunction

$$\Psi_{p'}(x) \propto e^{ip'x/\hbar}.$$
(5.4.21)

If p' = 0, then

$$\frac{e^{-i0L/2}}{e^{i0L/2}} = 1 = e^{i\alpha}.$$
(5.4.22)

Eq. (5.4.22) requires  $\alpha = 0$ . Therefore,

$$\Psi(-L/2) = \Psi(L/2)$$
 (periodicity boundary condition). (5.4.23)

Eq. (5.4.23) concludes the proof. QED

**Theorem XXI-2:** Normalization of eigenfunction of continuous spectrum. The continuum spectrum eigenfunction is orthogonal and is normalized to Dirac  $\delta$  function.

Proof. According to the periodicity boundary condition

$$\Psi_{p'}(-L/2) = \Psi_{p'}(L/2), \qquad (5.4.24)$$

i. e.,

$$e^{-ip'L/2\hbar} = e^{ip'L/2\hbar} \quad or \quad e^{ip'L/\hbar} = 1.$$
 (5.4.25)

Eq. (5.4.25) requires that

$$sin(p'L/\hbar) = 0, \quad cos(p'L/\hbar) = 1$$
. (5.4.26)

Therefore,  $p'L/\hbar = 2n\pi$  for  $n = 0, \pm 1, \pm 2, \cdots$ , i. e.,

$$p' = p_n = \frac{2n\pi\hbar}{L} = \frac{nh}{L}.$$
(5.4.27)

From Eq. (5.4.27) we see that the momentum eigenvalues are not continuous. The corresponding normalized eigenfunction is

$$\Psi_{p_n}(x) = \frac{1}{\sqrt{L}} e^{ip_n x/\hbar} = \frac{1}{\sqrt{L}} e^{i2n\pi x/L}.$$
(5.4.28)

Reader can verify that  $\Psi_{p_n}(x)$  satisfies orthogonal and normalized condition, i. e.,

$$\int_{\frac{-L}{2}}^{\frac{L}{2}} dx \Psi_{p_n}^*(x) \Psi_{p_m}(x) = \delta_{mn}.$$
 (5.4.29)

Using the set  $\Psi_{p_n}(x)$ ,  $\delta$  function can be expressed as

$$\delta(x - x') = \frac{1}{L} \sum_{n = -\infty}^{\infty} e^{i2n\pi(x - x')/L}.$$
(5.4.30)

When  $L \rightarrow \infty$ ,

$$\Delta p_n = p_{n+1} - p_n = \frac{2\pi\hbar}{L} \to 0, \qquad (5.4.31)$$

i. e., the momentum eigenvalue approaches continuous variation. Set

$$\frac{2\pi\hbar}{L} \to dp, \tag{5.4.32}$$

$$\sum_{n=-\infty}^{+\infty} \Delta p_n = \frac{2\pi\hbar}{L} \sum_{n=-\infty}^{+\infty} \to \int_{-\infty}^{+\infty} dp.$$
 (5.4.32)'

Or

$$\sum_{n=-\infty}^{+\infty} \to \frac{L}{2\pi\hbar} \int_{-\infty}^{+\infty} dp.$$
 (5.4.33)

Therefore, Eq.(5.4.30) approaches

$$\delta(x - x') = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp e^{ip(x - x')/\hbar} = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ik(x - x')}.$$
 (5.4.34)

Eq. (5.4.34) is same as the Eq. (5.4.10). When we treat particular problems, for avoidance of the normalization difficulty of plane wave, one can use the orthonormal wavefunction to make calculations, and at last set  $L \rightarrow \infty$ .

In three dimensional case, the normalized wavefunction is  $(V = L^3)$ 

$$\Psi_{p'}(r) = \frac{1}{\sqrt{V}} e^{i\frac{p'\cdot r}{\hbar}}$$
(5.4.35)

where

$$p'_{x} = \frac{2\pi\hbar}{L}n, \quad p'_{y} = \frac{2\pi\hbar}{L}l, \quad p'_{z} = \frac{2\pi\hbar}{L}m \quad ,$$
 (5.4.36)

and  $n, l, m = 0, \pm 1, \pm 2, \cdots, \Psi_{p'}(r)$  is of orthogonality and normalization

$$\int_{(V)} dx dy dz \Psi_{p'}^*(r) \Psi_{p''}(r) = \delta_{p'_x p''_x} \delta_{p'_y p''_y} \delta_{p'_z p''_z}.$$
(5.4.37)

The  $\delta$  function can be constructed as follows.

$$\delta(r - r') \equiv \delta(x - x')\delta(y - y')\delta(z - z') = \frac{1}{V} \sum_{n,l,m = -\infty}^{+\infty} e^{i\frac{2\pi[n(x - x') + l(y - y') + m(z - z')]}{L}},$$
(5.4.38)

When  $L \to \infty$ ,  $p'_x$ ,  $p'_y$ , and  $p'_z$  will become continuous, i. e.,  $(2\pi\hbar)^3/L^3 \to dp'_x dp'_y dp'_z$ ,

$$\sum_{n,l,m=-\infty}^{\infty} \to \frac{L^3}{(2\pi\hbar)^3} d^3 p'.$$
(5.4.39)

Eq. (5.4.39) indicates that the volume element in phase space,  $(2\pi\hbar)^3 = h^3$ , has one quantum state. Eq. (5.4.38) can be expressed as

$$\delta(r - r') = \frac{1}{(2\pi\hbar)^3} \int_{-\infty}^{\infty} d^3 p' e^{i\frac{p' \cdot (r - r')}{\hbar}}.$$
(5.4.40)

QED.

# 5.5. Motion Equation of Operator

**Theorem XXIII: Motion equation of operator.** An operator *O*, corresponding to an observable, satisfies

$$\frac{dO}{dt} = \frac{\partial O}{\partial t} + \frac{1}{i\hbar}[O, H]$$

**Proof.** The definition of average value is

$$\langle O \rangle = \int dr \Psi^* O \Psi. \tag{5.5.1}$$

If we assume that space  $\mathbf{r}$  and time t are independent, then

$$\frac{d < O >}{dt} = \int dr \left\{ \Psi^* \frac{\partial O}{\partial t} \Psi + \frac{\partial \Psi^*}{\partial t} O \Psi + \Psi^* O \frac{\partial \Psi}{\partial t} \right\}.$$
(5.5.2)

Using the Schrödinger equation

$$\frac{\partial \Psi}{\partial t} = \frac{1}{i\hbar} H \Psi, \quad \frac{\partial \Psi^*}{\partial t} = \frac{-1}{i\hbar} H \Psi$$
(5.5.3)

to find the values of the derivatives in Eq. (5.5.2), and bearing in mind that H is Hermitian, we can transform Eq. (5.5.2) as follows:

$$\frac{d < O >}{dt} = \int dr \Psi^* \left\{ \frac{\partial O}{\partial t} + \frac{1}{i\hbar} [O, H] \right\} \Psi.$$
(5.5.4)

Note that the Schrödinger equation in Eq. (5.5.3) also assumes that **r** and time *t* are independent. If we introduce the operator dO/dt by the relation

$$\frac{d < O >}{dt} = \langle \frac{dO}{dt} \rangle = \int dr \Psi^* \frac{dO}{dt} \Psi, \qquad (5.5.5)$$

then we get, using Eq. (5.5.4), the operator equation of motion

$$\frac{dO}{dt} = \frac{\partial O}{\partial t} + \frac{1}{i\hbar}[O, H].$$
(5.5.6)

In essence, Eq. (5.5.6) comes from Schrödinger equation Eq. (5.5.3). QED.

Note that motion equation of operator comes from both Schrödinger equation and the definition of average value of operator.

**Corollary XVI: Integral of motion**: If operator *O* does not explicitly depend on time and commutes with Hamilton operator, then the average value of the physical observable *O* does not change with time for any state. Such a observable is called a (quantummechanical) integral of motion. The proof for this corollary is easy.

# 5.6. Symmetries and Conservations of Average Values

## 5.6.1. Coordinate Transformations

We showed in section 5.5 that any physical quantity, the operator of which does not depend explicitly on time and commutes with Hamiltonian of system, is called integral of motion, i. e., its average value does not change in time. We remind ourselves that the integral of motion in classical mechanics is any function of the coordinates and momenta which remain constant whatever are the initial conditions. Once we know the integrals of motion, we can formulate the corresponding conservation laws which is very important for understanding physical properties of the phenomena we study. (Refer to Ref. [87] for section 5.6.)

Here, I would like to emphasize the following difference between quantum and classical mechanics and between quantum mechanics upon theorems and postulates: the quantummechanical conservation of a physical quantity just means the average value of corresponding operator on wavefunction. The contributions to this average value come from a large number of the still more microscopic processes, in which even very strong nonconservation can occur still. To point out this difference is a feature of section 5.6 of this textbook. In the following, I will emphasize this difference repeatedly.

We shell show that the presence of integral of motion and the corresponding conservation laws is closely connected with the symmetry properties of system of quantum mechanics, i. e., with the invariance of Hamiltonian operator under certain coordinate transformations.

Before considering different concrete examples we investigate how the wavefunction transforms under coordinate transformation. A coordinate transformation may be one of the two kinds:

(a) A transformation of coordinates, which determine position of points in the system; In this case, the basis vectors which determine the coordinate axes remain fixed;

(b) A transformation of coordinates of the basis vectors, which determine the coordinate axes. In the present section we consider coordinate transformation of the first kind.

Let S be an operation through which the coordinates of the vector  $\mathbf{r}$  determining the position the a point are transformed, i. e.,

$$r \to r' = Sr. \tag{5.6.1.1}$$

The inverse transformation of Eq. (5.6.1.1) is

$$r = S^{-1}r'. (5.6.1.2)$$

Let us consider how the wavefunction transforms under the coordinate transformation Eq. (5.6.1.1). The result of the coordinate transformation is that we find at the point  $\mathbf{r}$ ' the value of the function we found earlier at  $\mathbf{r}$ , i. e.,

$$\Psi'(r') = \Psi(r). \tag{5.6.1.3}$$

On the other hand, by definition the action of an operator upon the wavefunction  $\Psi(r')$  must give us a new wavefunction of the same argument

$$\Psi'(r') = R_S \Psi(r'). \tag{5.6.1.4}$$

Combining Eqs. (5.6.1.3) and (5.6.1.4) we find the rule defining the action of the operator  $R_S$  upon a wavefunction:  $R_S\Psi(r') = \Psi(r)$ . Substituting Eq. (5.6.1.2) into the right hand side of this equation, we have

$$R_S \Psi(r') = \Psi(S^{-1}r'), \qquad (5.6.1.5)$$

or, dropping the primes, we find finally the very important equation

$$R_S \Psi(r) = \Psi(S^{-1}r), \qquad (5.6.1.6)$$

which determines the rule for transforming wavefunction when the coordinates are transformed according to Eq. (5.6.1.1).

Let us now study the integrals of motion connected with the properties of space and time. Experimentally, one establishes that time is a uniform (i. e., homogeneity) quantity and that free space is uniform and isotropic. Which integrals of motion and conservation laws are connected with these properties of space and time?

#### 5.6.2. Uniformity of Time

**Theorem XXIV: Average energy conservation.** The uniformity of time leads to conservation of average value of Hamiltonian, i. e., average energy conservation.

**Proof.** As the time is a uniformity quantity, the Hamiltonian of any closed system, i. e., a system which is not subjected to the action of an external agent, or of a system that is acted upon by a constant external forces, will not depend explicitly on the time. If the Hamiltonian does not depend explicitly on the time (i. e.,  $\partial H/\partial t = 0$ ) we have from Eq. (5.5.6)

$$\frac{dH}{dt} = \frac{1}{i\hbar}[H,H] = 0.$$
(5.6.2.1)

Hence, we find from Eq. (5.5.5) that d < E > /dt = 0. If the average energy of system initially had a well-defined value, then this value is retained at a later time. Thus QED.

Let us make the following four discussions on the energy conservation and so on:

(1) The invariance of the operator H under certain transformation, defined by the operator F, means that the action of the operator F on the wavefunction  $H\Psi$  is equivalent to the action of H on the wavefunction  $F\Psi$ , i. e.

$$FH\Psi = HF\Psi. \tag{5.6.2.2}$$

In other wards, the invariance of H with respect to the transformation realized by the operator F reduces to the condition that F commutes with the Hamiltonian:

$$FH = HF. \tag{5.6.2.3}$$

Let us introduce a time-shift operator  $T_{\tau}$  which shifts the time by an amount  $\tau$ . By definition  $T_{\tau} = t + \tau$ , and we have from Eq. (5.6.1.6)

$$T_{\tau}\Psi(t) = \Psi(t-\tau). \tag{5.6.2.4}$$

The quantity  $\tau$  is a parameter of the operator  $T_{\tau}$ . The fact that the time is uniform for the system considered by us can mathematically be expressed by the commutation relation (i. e., commutator)

$$[T_{\tau}, H] = 0. \tag{5.6.2.5}$$

Instead of the time-shift operator it is convenient to use a generating function for the transformation or the infinitesimal time-shift operator I(t). which is defined as a limit as  $\tau \to 0$ of the derivative of the time-shift operator with respect to the parameter  $\tau$ .

We have thus

$$I(t) = \frac{\partial}{\partial \tau} T_{\tau} \Big|_{\tau=0}.$$
 (5.6.2.6)

We can easily find that the explicit form of the operator I(t), if we bear in mind that

$$I(t)\Psi(t) = \frac{\partial}{\partial\tau}T_{\tau}\Psi(t)\Big|_{\tau=0} = \frac{\partial}{\partial\tau}\Psi(t-\tau)\Big|_{t=0} = -\frac{\partial}{\partial t}\Psi.$$
 (5.6.2.7)

We have thus

$$I(t) = -\frac{\partial}{\partial t}.$$
 (5.6.2.8)

The energy conservation law is connected with the fact that the operator H commutes with the infinitesimal time-shift operator I(t). The operator

$$-i\hbar I(t) = i\hbar \frac{\partial}{\partial t}, \qquad (5.6.2.9)$$

which has the dimension of energy is in this connection sometimes called the energy operator.

(2) Many authors such as Ref. [87] at this stage will point out that: "One should, however, bear in mind the conditions under which one can use this terminology, i. e., the above energy operator. The energy in quantummechanical system in a stationary state is determined by the eigenvalues of Hamiltonian operator. Hamiltonian, i. e., a function of the operators of coordinates and momenta, is thus the operator of energy of system. In contrast to the spatial coordinates, the time coordinate is not an operator, and is only a parameter."

To this viewpoint, we have different viewpoint. We have proved in theorem II of chapter 3 that in time t representation the energy has to be an operator; on the other hand, in energy representation the time has to be an operator as well.

(3) The exact meaning of the energy in the quantummechanical energy conservation is average value of Hamiltonian. An average value of Hamiltonian comes from contributions of infinitely still more microscopic processes. Therefore, the energies in some still more microscopic processes might violate this classical energy conservation law.

(4) The necessary condition of theorem XXIV is uniformity of time. In chapter 10 we will introduce quantum transition theory under external perturbation. The existence of external perturbation will destroy the time uniformity, and thus the average energy nonconservation can occur in transition processes in principle.

## 5.6.3. Uniformity of Position Space

The uniformity of position space means that the properties of system do not change under any parallel displacement of the system as a whole. As in quantum mechanics the properties of a system are determined its Hamiltonian, uniformity of position space must imply that Hamiltonian is unchanged (invariant) when the system suffers a parallel displacement over any distance. Any finite displacement can be constructed out of infinitesimal displacements; it is thus sufficient to consider the invariance of the Hamiltonian under an infinitesimal displacement  $\delta a$ .

**Theorem XXV: Average momentum conservation.** The uniformity of position space leads to conservation of average value of momentum operator, i. e., average momentum conservation.

**Proof.** If the wavefunction depends only on the coordinate of a single particle, then according to Eq. (5.6.1.6) the wavefunction  $\Psi$  will change to the wavefunction

$$\Psi(r - \delta a) = \Psi(r) - (\delta a \cdot \nabla)\Psi(r) = [1 - (\delta a \cdot \nabla)]\Psi(r)$$
(5.6.3.1)

under the infinitesimal displacement  $r' = r + \delta a$ . It follows from Eq. (5.6.3.1) that the factor

$$T_{\delta a} = [1 - (\delta a \cdot \nabla)] \tag{5.6.3.2}$$

can be called the infinitesimal displacement operator as its action upon a wavefunction is equivalent to a displacement of the radius vector  $\mathbf{r}$  over a distance  $\delta a$ .

If we now use Eq. (5.6.3.2), then we can say that the condition that the operator *H* be invariant under an infinitesimally small displacement reduces to the equation

$$\nabla H = H\nabla, \tag{5.6.3.3}$$

since both the unit vector and the constant vector  $\delta a$  commute with any operator. As the operator *p* differs from  $\nabla$  only by a constant factor  $-i\hbar$ , this last equation can be written in the form

$$pH = Hp. \tag{5.6.3.4}$$

by using Eq. (5.5.6), Eq. (5.6.3.4) reduces to the statement that the momentum of a free particle is an integral of motion is thus a consequence of the uniformity of position space. Here we accomplish the proof. QED.

Expressing  $\nabla$  in terms of the momentum operator, we can rewrite the infinitesimal displacement operator as follows

$$T_{\delta a} = 1 - \frac{i}{\hbar} (p \cdot \delta a). \tag{5.6.3.5}$$

The operator for a displacement over a finite distance **a** can be obtained by successive application of Eq. (5.6.3.5). We find thus

$$T_a = e^{\left[-\frac{i}{\hbar}(p \cdot a)\right]}.$$
 (5.6.3.6)

The three components  $a_l$  (l = 1, 2, 3) of the displacement vector **a** are parameters of the displacement operator Eq. (5.6.3.6). Some books define

$$T_a = e^{\left[\frac{i}{\hbar}(p \cdot a)\right]} \tag{5.6.3.7}$$

as translation operator. We call the derivative of the displacement operator Eq. (5.6.3.6) with respect to the parameter  $a_l$  in the limit as all  $a_l \rightarrow 0$  the generating operator for the transformation of a spatial displacement, or the infinitesimal spatial displacement operator  $I(x_l)$ . The operator of an infinitesimal displacement along the *x* axis,

$$I(x_l) = -\frac{i}{\hbar} p_l \tag{5.6.3.8}$$

is thus directly connected with the corresponding momentum component operator.

If the wavefunction  $\Psi$  refers to a system of particles, the operator of an infinitesimal displacement of the system as a whole can also be expressed by Eq. (5.6.3.5) if we understand by the momentum operator **p** the sum-operator of the momenta of all particles of the system, i. e., if

$$p = \sum_{i} p_i. \tag{5.6.3.9}$$

In that case, the invariance with respect to spatial displacements reduces to the conservation of the total momentum of the system.

Our two comments for theorem XXV.

(1) The exact meaning of the momentum in the above quantummechanical momentum conservation is average value of momentum operator. An average value of momentum operator comes from contributions of infinitely still more microscopic processes. Therefore, the momentum in some still more microscopic processes might violate the classical momentum conservation law.

(2) The necessary condition of theorem XXV is uniformity of position space. If an external perturbation destroys the position space uniformity, and then the average momentum nonconservation can occur in principle.

#### 5.6.4. Isotropy of Position Space

**Theorem XXVI: Average angular momentum conservation.** The isotropy of position space leads to conservation of average value of angular momentum operator, i. e., average angular momentum conservation.

**Proof.** The isotropy of position space, i. e., the equivalence of all directions, consists in the invariance of the properties of closed systems under arbitrary rotations. Such an invariance also occurs for systems in centrally symmetrical fields if the rotation takes place with respect to the center of the field.

We shell determine the operator of an infinitesimal rotation. We shell consider a infinitesimal rotation. It is characterized by a vector  $\delta \vec{\phi}$ , the length of which is equal to the

angle  $\delta \phi$  over which we rotate, and the direction of which is along the axis of rotation. Under such a rotation the change in the radius vector **r** is determined by the expression

$$r \to r + [\delta \vec{\phi} \times r].$$
 (5.6.4.1)

Let us evaluate the corresponding change in the wavefunction retaining only the first order terms:

$$\Psi(r - [\delta \vec{\varphi} \times r]) = \{1 - [\delta \vec{\varphi} \cdot (r \times \nabla)]\}\Psi(r).$$
(5.6.4.2)

It follows from Eq. (5.6.4.2) that

$$R_{\delta\vec{\varphi}} = 1 - [\delta\vec{\varphi} \cdot (r \times \nabla)]$$
(5.6.4.3)

is the operator of an infinitesimal rotation over an angle  $\delta \vec{\phi}$ . It is easy to be verified that Eq. (5.6.4.3) can be expressed as

$$-i\hbar[r \times \nabla] = L, \tag{5.6.4.4}$$

where *L* is called angular momentum operator (or operator of moment of momentum). Eq. (5.6.4.4) gives

$$L_x = L_1 = -i\hbar \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) = y p_z - z p_y, \qquad (5.6.4.5)$$

$$L_{y} = L_{2} = -i\hbar \left( z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) = zp_{x} - xp_{z}, \qquad (5.6.4.5)'$$

$$L_z = L_3 = -i\hbar \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) = x p_y - y p_x.$$
(5.6.4.5)"

The operator of an infinitesimal rotation over an angle  $\delta \phi$  can thus be expressed in terms of the angular momentum operator:

$$R_{\delta\vec{\varphi}} = \left[1 - \frac{i}{\hbar}\delta\vec{\varphi} \cdot L\right]$$
(5.6.4.6)

That the Hamiltonian operator is invariant under arbitrary infinitesimal rotations is expressed by the fact that the Hamiltonian commutes with the operator  $R_{\delta \phi}$  or with the component along any rotational axis of the angular momentum operator:

$$(n \cdot L)H = H(n \cdot L), \tag{5.6.4.7}$$

where **n** is the unit vector in the direction of the rotational axis. It follows from Eq. (5.6.4.7) that in isotropic position space or in an arbitrary centrally symmetrical field the component of the angular momentum along an arbitrary direction will be an integral of motion. If the external field is axially symmetry, the Hamiltonian is invariant only under a rotation along the axis of axial symmetry and only the angular momentum component along that direction is conserved. Here we conclude the proof.

We can construct from the operators of an infinitesimal rotation around an axis, defined by the unit vector **n**, the operator of the rotation around the same axis over a finite angle  $\alpha$ :

$$R^n_{\alpha} = e^{-i\alpha(L \cdot n)/\hbar}.$$
(5.6.4.8)

Here, we define  $R_{\alpha}^{n}$  as rotational operator. However, some books define

$$R^n_{\alpha} = e^{i\alpha(L\cdot n)/\hbar}.$$
 (5.6.4.9)

as rotational operator.

It follows from Eq. (5.6.4.8) that the generator of the transformation of a rotation or the operator of an infinitesimal rotation or the operator of an infinitesimal rotation around an axis **n** is determined by the angular momentum component along that axis:

$$I(n) = -\frac{i}{\hbar}(L \cdot n).$$
 (5.6.4.10)

The connection between the angular momentum component operator and the infinitesimal rotation operator can be used to determine the angular momentum components and the commutation relations for them. Let  $\alpha$  be the angle of rotation around the axis 1. In a Cartesian system of coordinates the operator of rotation over an angle  $\alpha$  can then be written in the form of a matrix

$$R_{\alpha} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{pmatrix}.$$
 (5.6.4.11)

Hence, the operator of the infinitesimal rotation around the axis 1 can be expressed by the matrix (0, 0, 0, 0)

$$I_{1} = \frac{\partial R_{\alpha}}{\partial \alpha} \Big|_{\alpha=0} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}.$$
 (5.6.4.12)

In the same way, we find for rotations around the two other axes

$$I_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad I_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$
(5.6.4.13)

Using the expressions obtained here and the rules for matrix multiplication, we can evaluate the commutation relations for the operators of infinitesimal rotations

$$I_1 I_2 - I_2 I_1 = I_3. \tag{5.6.4.14}$$

We obtain two other relations from this one by a cyclic commutation of the indices. Since  $I_1 = -iL_1/\hbar$ , we get from these commutation relations for the  $I_1$  the commutation relations for the angular components:

$$L_1 L_2 - L_2 L_1 = i\hbar L_3. \tag{5.6.4.15}$$

We can also use the relation Eq. (5.6.4.10) to define the operator for the intrinsic angular momentum, i. e., the spin operator, although this operator does not have a classical counterpart, i. e., it cannot be reduced to a function of the coordinates and momenta (se chapter 8).

Our two comments for theorem XXVI.

(1) The exact meaning of the angular momentum in the above quantummechanical angular momentum conservation is average value of angular momentum operator. An average value of angular momentum operator comes from contributions of infinitely still more microscopic processes. Therefore, the angular momentum in some still more microscopic processes might violate the classical angular momentum conservation law.

(2) The necessary condition of theorem XXVI is isotropy of position space. If an external perturbation destroys the position space isotropy, and then the average angular momentum nonconservation can occur in principle.

#### 5.6.5. Inversion Invariance of Position Space

The above consideration of translations and rotations refers to a class of continuous translation since we can realize them through multiple consecutive applications of infinitesimal transformations. The invariance of the Hamiltonian under these transformations leads to the conservation laws for the average value of linear and angular momentum which correspond to the conservation laws of classical mechanics. Symmetry conditions may lead not only to continuous transformations, but also to discrete transformations which cannot be reduced to infinitesimal transformations. Invariance under such transformations does not lead to a conservation laws in classical mechanics. In quantum mechanics, however, there is no essential difference between continuous and discrete transformations. Therefore, discrete transformations will in quantum mechanics also lead to conservation laws.

Let us consider one such discrete transformation under which the Hamiltonian remain invariant: the so-called inversion. Inversion, or to be precise, spatial inversion, or spatial reflection consist in the simultaneous change in sign of all three spatial coordinates.

$$x \to -x, \quad y \to -y, \quad z \to -z.$$
 (5.6.5.1)

Under an inversion a right-handed system of coordinates goes over into a left-handed system.

The Hamiltonian of a closed system in which nuclear and electromagnetic forces operate is invariant under an inversion. This invariance, the symmetry between left-handed and right-handed systems of coordinates, remains true for systems in an external, central field, provided the center of the inversion is chosen to be the force center.

Let us denote the inversion operator by **P**. Many books call **P** also parity operator. Mathematically, we can express symmetry between left-handedness and right-handedness by the fact that **P** and the Hamiltonian commute, i. e.,

$$PH = HP. \tag{5.6.5.2}$$

**Theorem XXVII: Parity conservation.** The invariance of inversion leads to parity conservation.

**Proof.** By definition the action of the inversion operator upon the wavefunction  $\Psi$  reduces to the transformation Eq. (5.6.5.1), i. e.,

$$\Psi(-r) = P\Psi(r). \tag{5.6.5.3}$$

If we want to determine the eigenvalues of the inversion operator, then we must solve the equation

$$P\Psi(r) = P\Psi(r). \tag{5.6.5.4}$$

Applying to both sides of Eq. (5.6.5.4) the inversion operator and bearing in mind that applying the inversion operator twice reduces to the identical transformation, we get

$$\Psi(r) = P^2 \Psi(r). \tag{5.6.5.5}$$

From the condition  $P^2 = 1$  we get  $P = \pm 1$ . We can thus write Eq. (5.6.5.4) in the form

$$P\Psi(r) = \pm \Psi(r).$$
 (5.6.5.6)

We see thus from Eq. (5.6.5.6) that we can divide the wavefunctions of states with a well defined eigenvalue of the operator **P** into two classes:

(1) Wavefunctions which are not changed when acted upon by the inversion operator,

$$P\Psi_{+} = \Psi_{+}, \tag{5.6.5.7}$$

and the corresponding states are called even parity states;

(2) Wavefunctions which change sign when acted upon by the inversion operator,

$$P\Psi_{-} = -\Psi_{-}, \tag{5.6.5.8}$$

and the corresponding states are called odd parity states.

As the inversion operator commutes with the Hamiltonian, the parity of a state, i. e., the fact that a state is even or odd, is an integral of motion. The invariance of the Hamiltonian under an inversion leads thus to the conservation of parity.

Our two comments for theorem XXVII.

(1) The exact meaning of the parity in the above quantummechanical parity conservation is not average value of the parity operator, or, equivalently, the average value of the parity operator on a state is equal to the parity of this state, because we can prove that that the matrix element between different parity states is equal to zero as follows. (What does the matrix mean will be given in chapter 10. The matrix element represents the probability amplitude of transition from right state into the left state.)

$$<\Psi_{-}|P|\Psi_{+}>=<\Psi_{-}|(+)|\Psi_{+}>=<\Psi_{-}|(+)PP|\Psi_{+}>=<\Psi_{-}|P(+)P|\Psi_{+}>=-<\Psi_{-}|P|\Psi_{+}>,$$

therefore,  $\langle \Psi_- | P | \Psi_+ \rangle = 0$ .

(2) The necessary condition of theorem XXVII is invariance of inversion of position space. If an external perturbation destroys this invariance, then the parity nonconservation

can occur in principle.

The parity conservation is satisfied to a very high degree of accuracy in all phenomena determined by nuclear and electromagnetic interactions. Up to 1956, it was assumed that the parity conservation was a universal law of nature. However, it was established in 1956 by Yang and Lee and by Wu and co-workers that in the  $\beta$ -decay of atomic nuclei and in the decay of muon, pion, and hyperon an asymmetry was observed which made it possible to distinguish between left-handedness and right-handedness. These phenomena showed that for weak interactions which determine these decay processes, the symmetry between left and right is violated, that is, the invariance under a spatial inversion is violated. The parity conservation is thus violated. We shell in the present book consider only such processes for which there is a right-left symmetry.

## 5.7. Pictures of Quantum Mechanics

In addition to the representations in quantum mechanics stemming from transformation of bases in Hilbert space, one also speaks of different pictures of quantum mechanics. The different pictures give the different time evolutions of both state vectors and basic operators (like r, p, angular momentum, and spin). There are altogether three pictures: the Schrödinger, the Heisenberg, and interaction pictures. These alternative formulations stem from the fact that wavefunctions and operators cannot be observed directly, and the observable quantities are the average values coming from the combination of wavefunction and operator. We will find that some picture is convenient for some quantummechanical problems, and is not convenient for other quantummechanical problems. To introduce the three pictures we need the concept of unitary transformation.

## 5.7.1. Unitary Transformation

Let us give the definitions of unitary transformation and unitary (transformation) operator U. Suppose that  $|\Psi_i\rangle$  represents a set of orthogonal kets (i. e., bases).

$$\langle \Psi_i | \Psi_j \rangle = \delta_{ij}. \tag{5.7.1.1}$$

Consider a transformation

$$|\phi_i>=\sum_j U_{ij}|\Psi_j>.$$
 (5.7.1.2)

If the kets  $|\phi_i\rangle$  also form a set of orthogonal kets, i. e.,

$$\langle \phi_i | \phi_j \rangle = \delta_{ij}, \tag{5.7.1.3}$$

then the transformation is said to be unitary or unitary transformation and  $U_{ij}$  is said to be unitary matrix of unitary transformation operator. Thus, a unitary transformation correspond the a rotation of basis in  $\mathcal{H}$  space.

**Theorem XXVIII: Unitary transformation.** If U is a unitary transformation operator, then  $U^+ = U^{-1}$ .

**Proof.** Eq. (5.7.1.3) means that the unitary transformation connects the orthogonarmal basis. (Orthogonarmal basis represent orthogonalized and normalized basis.) Therefore, the coordinates of an arbitrary state in the two basis are related by unitary transformation. From Eq. (5.7.1.2)

$$<\phi_i| = \sum_j U_{ij}^* < \Psi_j|.$$
 (5.7.1.4)

From Eqs. (5.7.1.3) and (5.7.1.4)

$$<\phi_i|\phi_j>=\delta_{ij}=\sum_m\sum_n U_{im}^*U_{jn}<\phi_m|\phi_n>=\sum_n U_{in}^*U_{jn}.$$
 (5.7.1.5)

If i = j, then

$$U^+U = 1, (5.7.1.6)$$

where  $U^+$  is Hermitian adjoint of U. Applying  $U^{-1}$  ( $U^{-1}$  is the inverse operator of U,  $UU^{-1} = 1$ ) from the right on both sides of the Eq. (5.7.1.6) we have

$$U^+ U U^{-1} = U^{-1}, (5.7.1.7)$$

i. e.,

$$U^+ = U^{-1}. (5.7.1.8)$$

Eq. (5.7.1.8) concludes the proof. QED.

**Theorem XXIX: Three pictures of quantum mechanics.** If *H* does not depend on time explicitly, then define

$$U(t,t_{\circ}) = e^{-iH(t-t_{\circ})/\hbar}.$$
(5.7.1.9)

If *H* depends on time explicitly, then

$$U(t,t_{\circ}) = Te^{-i\int_{t_{\circ}}^{t} dt' H(t')/\hbar},$$
(5.7.1.9)'

where T is time-ordering operator.

If  $H = H_{\circ} + V(x,t)$  and  $H_{\circ}$  does not depend on time t explicitly, then we define

$$U_0(t,t_1) = e^{-iH_o(t-t_1)/\hbar},$$
(5.7.1.9)"

If  $H = H_{\circ}(t) + V(x,t)$  and  $H_{\circ}(t)$  depends on time t explicitly, then we define

$$U_0(t,t_1) = Te^{-i\int_{t_1}^{t} dt' H_o(t')/\hbar},$$
(5.7.1.9)'''

Schrödinger picture:

$$|\Psi_{S}(t)\rangle = U(t,t_{\circ})|\Psi_{S}(t_{\circ})\rangle.$$
 (5.7.1.10)

 $O_S$  is independent of time.

$$i\hbar \frac{\partial |\Psi_{S}(t)\rangle}{\partial t} = H |\Psi_{S}(t)\rangle. \qquad (5.7.1.11)$$

$$\frac{dO_S}{dt} = 0. (5.7.1.12)$$

Haisenberg picture:

$$|\Psi_H > \equiv |\Psi_S(t_\circ) > .$$
 (5.7.1.13)

$$O_H(t) = U^+(t, t_\circ) O_S U(t, t_\circ).$$
(5.7.1.14)

$$i\hbar \frac{\partial |\Psi_H\rangle}{\partial t} = 0. \tag{5.7.1.15}$$

$$i\hbar \frac{dO_H(t)}{dt} = [O_H(t), H].$$
 (5.7.1.16)

Interaction picture:

Assume that  $H = H_{\circ} + V(t)$ , where  $H_{\circ}$  represents kinetic energy operator, and is independent of time.

$$|\Psi_{I}(t)\rangle = U_{0}^{+}(t,t_{1})|\Psi_{S}(t)\rangle = U_{I}(t,t_{0})|\Psi_{I}(t_{0})\rangle.$$
(5.7.1.17)

$$O_I(t) = U_0^+(t, t_1) O_S U_0(t, t_1).$$
(5.7.1.18)

$$U_{I}(t,t_{\circ}) = U_{0}^{+}(t,t_{1})U(t,t_{\circ})U_{0}(t_{\circ},t_{1}) = T\exp\left(-\frac{i}{\hbar}\int_{t_{\circ}}^{t}dt'V_{I}(t)\right).$$
(5.7.1.19)

$$i\hbar \frac{\partial |\Psi_I(t)\rangle}{\partial t} = V_I |\Psi_I(t)\rangle.$$
(5.7.1.20)

$$V_I(t) = U_0^+(t,t_1)V(t)U_0(t,t_1).$$
(5.7.1.21)

$$i\hbar \frac{dO_I(t)}{dt} = [O_I(t), H_\circ].$$
 (5.7.1.22)

**Proof.** We would like to give a very detail proof for this theorem in the following three subsections. Refer to Ref. [10].

## 5.7.2. Schrödinger Picture

The so-called Schrödinger picture refers to the formulation which is based on the Schrödinger equation. In the description of the dynamical evolution of a physical system we used time-dependent wavefunction  $\Psi(r,t)$ . The physical quantities, at least the not explicitly time-dependent ones, are described by time-independent operator. Let us interpret these in detail as follows. For convenience we assume that the Hamiltonian *H* is time-independent. The time evolution of the state vector  $|\Psi(t)\rangle$  is then determined by the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi_{S}(t)\rangle = H|\Psi_{S}(t)\rangle. \qquad (5.7.2.1)$$

Since *H* is time-independent

$$\frac{\partial |\Psi_{\mathcal{S}}(t)\rangle}{|\Psi_{\mathcal{S}}(t)\rangle} = \frac{H}{i\hbar} dt = -\frac{iH}{\hbar} dt, \qquad (5.7.2.2)$$

$$|\Psi_{S}(t)\rangle = e^{-iH(t-t_{\circ})/\hbar} |\Psi_{S}(t_{\circ})\rangle \equiv U(t,t_{\circ}) |\Psi_{S}(t_{\circ})\rangle .$$
(5.7.2.3)

If the Hamiltonian contains time explicitly, then

$$U(t,t_{\circ}) = Te^{-\frac{1}{h}\int_{t_{\circ}}^{t} dt' H(t')},$$
(5.7.2.3)

where T is the so-called time-ordering operator. Here,  $U(t,t_{\circ})$  is called time evolution operator or time translation operator. It is easy to verify that  $U(t,t_{\circ})$  is a unitary operator.

In Schrödinger picture it is requires that the basic operators (like x or  $p_x$ ) are timeindependent, i. e.,

$$\frac{O_S}{dt} = 0, \tag{5.7.2.4}$$

and all the time evaluation from, the dynamics is from the states. Eqs. (5.7.2.3-4) are called Schrödinger picture.

## 5.7.3. Heisenberg Picture

In Schrödinger picture the state vectors evolve with time, while the operators are independent of time. In the Heisenberg picture the state vectors  $|\Psi_H\rangle$  are fixed in time, i. e.,

$$|\Psi_{H}\rangle = |\Psi_{S}(t_{\circ})\rangle = U^{+}(t,t_{\circ})|\Psi(t)\rangle.$$
(5.7.3.1)

One can derive the time evolution of the basic operators  $O_H$  from Schröinger picture and the physical requirement of the invariance of average values of operators in any pictures, i. e.,

$$<\Psi_{S}(t)|O_{S}|\Psi_{S}(t)>=<\Psi_{H}|O_{H}(t)|\Psi_{H}>.$$
 (5.7.3.2)

From Eqs. (5.7.4.3.1-2) we have the expression of  $O_H(t)$  as follows:

$$< \Psi_{S}(t)|O_{S}|\Psi_{S}(t) > = < \Psi_{S}(t_{\circ})|U^{+}(t,t_{\circ})O_{S}U(t,t_{\circ})|\Psi_{S}(t_{\circ}) >$$

$$= < \Psi_{H}|U^{+}(t,t_{\circ})O_{S}U(t,t_{\circ})|\Psi_{H} >$$

$$\equiv < \Psi_{H}|O_{H}(t)|\Psi_{H} > . \quad (5.7.3.3)$$

$$O_{H}(t) = U^{+}(t,t_{\circ})O_{S}U(t,t_{\circ}). \quad (5.7.3.4)$$

The time evolution of  $O_H(t)$  is

<

$$O_{H}(t) = U^{+}(t,t_{\circ})O_{S}U(t,t_{\circ}) = U^{+}(t,t_{\circ})O_{S}U^{+}(t_{\circ},t)$$
  
=  $U^{+}(t,t')U^{+}(t',t_{\circ})O_{S}U^{+}(t_{\circ},t')U^{+}(t',t)$   
=  $U^{+}(t,t')O_{H}(t')U(t,t').$  (5.7.3.5)

Taking the time derivatives on both sides of Eq. (5.7.3.4), we obtain

$$\frac{dO_{H}(t)}{dt} = \frac{iH}{\hbar} U^{+}(t,t_{\circ}) O_{S} U(t,t_{\circ}) + U^{+}(t,t_{\circ}) O_{S} U(t,t_{\circ}) \frac{-iH}{\hbar} \\ = \frac{-i}{\hbar} [O_{H},H].$$
(5.7.3.5)

Thus, in the Heisenberg picture the operator is time-dependent, and the time dependence of operator is governed by the commutator of the operator with the Hamiltonian. Eq. (5.7.3.5) is called Heisenberg equation.

In the following we will confine our attention entirely to the Heisenberg picture. The position and momentum operators,  $x_H$  and  $p_H$  respectively, satisfy

$$i\hbar \frac{dx_H}{dt} = [x_H, H].$$
 (5.7.3.6)

$$i\hbar \frac{dp_H}{dt} = [p_H, H].$$
 (5.7.3.7)

We see, at once, that if an operator commute with H, i. e.,

$$[O_S, H] = 0, \tag{5.7.3.8}$$

then  $O_S$  stays constant as a function of time and is called the constant of motion. In Heisenberg picture

$$\begin{bmatrix} O_H(t), H(t) \end{bmatrix} = \begin{bmatrix} U^+(t, t_\circ) O_S U(t, t_\circ), U^+(t, t_\circ) H U(t, t_\circ) \end{bmatrix} \\ = U^+(t, t_\circ) [O_S, H] U(t, t_\circ) = 0.$$
(5.7.3.9)

Therefore, in any picture a constant of motion still is a constant of motion.

For one dimensional free particle

$$H = \frac{p^2}{2m} + V(x). \tag{5.7.3.10}$$

The time evolution of the right hand side in Eq. (5.7.3.6) proceeds by the application of the fundamental commutation relation

$$[x, p] = [x_S, p_S] = i\hbar.$$
(5.7.3.11)

$$\frac{dx_{H}(t)}{dt} = \frac{1}{i\hbar} [x_{H}(t), H] = \frac{1}{i\hbar} U^{+}(t, t_{\circ}) [x, H] U(t, t_{\circ}) 
= U^{+}(t, t_{\circ}) \frac{p}{m} U(t, t_{\circ}) = \frac{p}{m}.$$
(5.7.3.12)

From Eq. (5.7.3.12) one obtains

$$x(t) = x(0) + \frac{p}{m}t,$$
(5.7.3.13)

which is same as a classical particle.

## 5.7.4. Interaction Picture

The interaction picture accommodates certain aspects of both the Schrödinger and Heisenberg pictures and is used must often when the interaction Hamiltonian, representing the potential, depends on time. Consider the following Hamiltonian

$$H = H_{\circ} + V(t), \tag{5.7.4.1}$$

where  $H_{\circ}(=p^2/(2m))$  represents the kinetic energy and is independent of time, while V(t) corresponds to the interaction potential, which can depend on time. Define

$$U_0(t,t_1) = e^{-iH_o(t-t_1)/\hbar},$$
(5.7.4.2)

where  $t_1$  is an arbitrary time parameter. If  $H_{\circ}$  depends on time t, then

$$U_0(t,t_1) = T e^{-i \int_{t_1}^t dt' H_o(t')/\hbar}, \qquad (5.7.4.2)'$$

where T is time-ordering operator. In our textbook we consider only the case that  $H_{\circ}$  does not depend on time.

Define the state vector in interaction picture as [88, 10]

$$|\Psi_I(t)\rangle = U_0^+(t,t_1)|\Psi_S(t)\rangle.$$
 (5.7.4.3)

From Eqs. (5.7.4.3) and (5.7.2.2)', we have

$$\begin{aligned} |\Psi_{I}(t) > &= U_{0}^{+}(t,t_{1})U(t,t_{\circ})|\Psi_{S}(t_{\circ}) > \\ &= U_{0}^{+}(t,t_{1})U(t,t_{\circ})U(t_{\circ},t_{1})|\Psi_{I}(t_{\circ}) > \equiv U_{I}(t,t_{\circ})|\Psi_{I}(t_{\circ}) >, \end{aligned}$$
(5.7.4.4)

where  $U_I(t, t_o)$  is called the time evolution operator in interaction picture.

Since the matrix elements of any operator *O* in different pictures must be the same in physics, we have

$$<\Psi_{S}(t)|O_{S}|\Psi_{S}(t)>=<\Psi_{I}(t)|O_{I}(t)|\Psi_{I}(t)>.$$
 (5.7.4.5)

Using Eq. (5.7.4.20), we have

$$<\Psi_{S}(t)|O_{S}|\Psi_{S}(t)>=<\Psi_{I}(t)|U_{0}^{+}(t,t_{1})O_{S}U_{0}(t,t_{1})|\Psi_{I}(t)>\equiv<\Psi_{I}(t)|O_{I}(t)|\Psi_{I}(t)>,$$
(5.7.4.6)

where  $O_I(t)$  represents the operator in interaction picture.

Taking the derivative of both sides of Eq. (5.7.4.3) yields

$$i\hbar \frac{\partial |\Psi_{I}(t)\rangle}{\partial t} = -U_{0}^{+}(t,t_{1})H_{\circ}|\Psi_{S}(t)\rangle + U_{0}(t,t_{1})i\hbar \frac{\partial}{\partial t}|\Psi_{S}(t)\rangle$$

$$= -U_{0}^{+}(t,t_{1})H_{\circ}|\Psi_{S}(t)\rangle + U_{0}^{+}(t,t_{1})(H_{\circ}+V(t))|\Psi_{S}(t)\rangle$$

$$= U_{0}^{+}(t,t_{1})V(t)|\Psi_{S}(t)\rangle = U_{0}^{+}(t,t_{1})V(t)U_{0}(t,t_{1})U_{0}^{+}(t,t_{\circ})|\Psi_{S}(t)\rangle$$

$$= V_{I}(t)|\Psi_{I}(t)\rangle.$$
(5.7.4.7)

The time derivative of  $O_I(t)$  can be calculated from its definition in Eq. (5.7.4.6). After certain mathematical steps similar to the case of  $O_H$  it is found that

$$i\hbar \frac{dO_I(t)}{dt} = [O_I(t), H_{\circ,I}] = [O_I(t), H_{\circ}].$$
 (5.7.4.8)

Eqs. (5.7.4.7-8) indicate, in the interaction picture, the time dependence of the state vectors is governed by the interaction Hamiltonian, while the time evolution of the operators is determined by the free Hamiltonian.

From Eqs. (5.7.4.4) and (5.7.4.7), we have that the time evolution operator  $U(t,t_{\circ})$  satisfies the equation

$$\frac{\partial U_I(t,t_\circ)}{\partial t} = -\frac{i}{\hbar} V_I(t) U_I(t,t_\circ).$$
(5.7.4.9)

From the definition of  $U_I(t,t_\circ)$  and  $U(t_\circ,t_\circ) = 1$ , we must have  $U_I(t_\circ,t_\circ) = 1$ . Integrating both sides of Eq. (5.7.4.9) yields

$$U_I(t,t_{\circ}) = 1 - \frac{i}{\hbar} \int_{t_{\circ}}^t dt_1 V_I(t_1) U_I(t_1,t_{\circ}).$$
 (5.7.4.10)

Through recursion of Eq. (5.7.4.10) we obtain the following series expansion.

$$U_I(t,t_{\circ}) = 1 - \frac{i}{\hbar} \int_{t_{\circ}}^t dt_1 V_I(t_1) + \left(-\frac{i}{\hbar}\right)^2 \int_{t_{\circ}}^t dt_1 V_I(t_1) \int_{t_{\circ}}^{t_1} dt_1 V_I(t_2) + \cdots$$
 (5.7.4.11)

Since the order of integration is unimportant, we can write

$$\int_{t_{\circ}}^{t} dt_1 V_I(t_1) \int_{t_{\circ}}^{t_1} dt_2 V_I(t_2) = \int_{t_{\circ}}^{t} dt_2 \int_{t_{\circ}}^{t_2} dt_1 V_I(t_2) V_I(t_1)$$
(5.7.4.12)

Hence

$$\int_{t_{o}}^{t_{i}} dt_{1} \int_{t_{o}}^{t_{1}} dt_{2} V_{I}(t_{1}) V_{I}(t_{2})$$

$$= \frac{1}{2} \left[ \int_{t_{o}}^{t} dt_{1} \int_{t_{o}}^{t_{1}} dt_{2} V_{I}(t_{1}) V_{I}(t_{2}) + \int_{t_{o}}^{t} dt_{2} \int_{t_{o}}^{t_{2}} dt_{1} V_{I}(t_{2}) V_{I}(t_{1}) \right]$$
(5.7.4.13)

To obtain a simple expression for  $U_I$ , let us define the "time-ordering product" of two operators  $A(t_1)$  and  $B(t_2)$  as

of.

$$T[A(t_1)B(t_2)] = \Theta(t_1 - t_2)A(t_1)B(t_2) + \Theta(t_2 - t_1)B(t_2)A(t_1), \qquad (5.7.4.14)$$

where the  $\theta$ -function is defined by

$$\boldsymbol{\theta}(t_1 - t_2) = \begin{cases} 0, & t_1 < t_2 \\ 1, & t_1 > t_2 \end{cases}$$
(5.7.4.15)

This function is also called a step function. The relation Eq. (5.7.4.12) can then be written as

$$\int_{t_{\circ}}^{t} dt_1 \int_{t_{\circ}}^{t_1} dt_2 V_I(t_1) V_I(t_2) = \frac{1}{2} \int_{t_{\circ}}^{t} dt_1 \int_{t_{\circ}}^{t} dt_2 T[V_I(t_1) V_I(t_2)], \qquad (5.7.4.16)$$

where according to the definition Eq. (5.7.4.14),

$$T[V_I(t_1)V_I(t_2)] = \Theta(t_1 - t_2)V_I(t_1)V_I(t_2) + \Theta(t_2 - t_1)V_I(t_2)V_I(t_1),$$
(5.7.4.17)

where T is called time-ordering operator. We note that the upper limits in the double integral are the same, and thus we can write the series form conveniently.

Even though it is somewhat complicated, one can define the time-ordering product when a product of more than two  $V_I$ 's is involved. We will not pursue this matter further. For now we note that Eq. (5.7.4.11) leads to

$$U_{I}(t,t_{\circ}) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^{n} \frac{1}{n!} \int_{t_{\circ}}^{t} dt_{1} \int_{t_{\circ}}^{t} dt_{2} \cdots \int_{t_{\circ}}^{t} dt_{n} T[V_{I}(t_{1})V(t_{2}) \cdots V_{I}(t_{n})].$$
(5.7.4.18)

Since the series in Eq. (5.7.4.18) is the same as the exponential series, one can write this more compactly as

$$U_I(t,t_{\circ}) = Te^{-i\int_{t_{\circ}}^t dt_1 V_I(t_1)/\hbar}.$$
(5.7.4.19)

# 5.8. Three Formulations of Quantum Mechanics

Just based on the canonical commutation relation, proved in chapter 3, between canonical coordinate x and canonical conjugate momentum p, this section will prove in mathematics all the formulations of quantum mechanics: Heisenberg matrix (operator) mechanics, Schrödinger wave mechanics, and Feynman path integral mechanics. Not exactly speaking, Schrödinger wave equation formulation of quantum mechanics looks like classical Jacobi-Hamiltonian equation, Heisenberg matrix formulation of quantum mechanics looks like classical Hamilton formulation, and Feynman path integral formulation of quantum mechanics looks like classical Lagrange formulation. For all the three formulations of quantum mechanics, we give the following theorem.

**Theorem XXX: Three formulations of quantum mechanics.** Just from the proved commutation relation  $[x, p] = i\hbar$ , all the three formulations of quantum mechanics can be derived exactly and without any assumptions, postulates, hypotheses, and axioms. The three formulations are:

(1) Heisenberg operator (matrix) formulation,

$$\frac{dO}{dt} = -\frac{i}{\hbar}[O,H] + \frac{\partial O}{\partial t},$$
(5.8.1)

(2) Schrödinger wave equation formulation,

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x,t),$$
(5.8.2)

(3-1) Propagator  $K(x_f, x_0; t_f, t_0)$  in phase space (=Feynman Hamiltonian path integral):

$$K(x_f, x_0; t_f, t_0) = \int_{x(t_0)=x_0}^{x(t_f)=x_f} \mathcal{D}p \mathcal{D}x \exp\left[\frac{i}{\hbar} \int_{t_0}^{t_f} dt [p\dot{x} - H(p, x)]\right],$$
(5.8.3)

where  $p = p(t), x = x(t), \dot{x} = dx(t)/dt$ ,

$$\mathcal{D}p\mathcal{D}x \equiv \lim_{N \to \infty} \left[ \prod_{k=1}^{N} \frac{dx_k dp_k}{2\pi\hbar} \right] \frac{dp_0}{2\pi\hbar},$$
(5.8.4)

$$\int_{x(t_0)=x_0}^{x(t_f)=x_f} \mathcal{D}p \mathcal{D}x = \lim_{N \to \infty} \left[ \prod_{k=1}^N \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dx_k dp_k}{2\pi\hbar} \right] \int_{-\infty}^{\infty} \frac{dp_0}{2\pi\hbar},$$
(5.8.5)

(3-2) Propagator in configuration space (=Feynman Lagrangian path integral)

$$K(x_f, x_0; t_f, t_0) = \int_{x(t_0)=x_0}^{x(t_f)=x_f} \mathcal{D}x \exp\left(\frac{iS}{\hbar}\right),$$
(5.8.6)

$$S = \lim_{\substack{N \to \infty \\ \epsilon \to 0}} \sum_{k=0}^{N} \left( m \frac{(x_{k+1} - x_k)^2}{2\epsilon^2} - V(x_k) \right) \epsilon = \int_{t_0}^{t_f} \left( \frac{m\dot{x}^2}{2} - V(x) \right) dt, \quad (5.8.7)$$

$$\mathcal{D}x = \lim_{\substack{N \to \infty \\ \epsilon \to 0}} \frac{1}{\sqrt{2\pi i\hbar m^{-1}\epsilon}} \prod_{k=0}^{N} \frac{dx_k}{\sqrt{2\pi i\hbar m^{-1}\epsilon}}.$$
(5.8.8)

**Proof.** We would like to make detail illustration for the notations, proofs and discussions in the following subsections. This proof is very long (It overs all the section 5.8).

#### 5.8.1. Heisenberg Matrix Mechanism Formulation

#### 5.8.1.1. Derivation of Matrix Mechanism

Here, the matrix is equivalent to an operator because an operator in a certain basis (representation) becomes a matrix. So, more general speaking, it is better to call Heisenberg operator mechanics formulation instead of matrix mechanics formulation. In this subsubsection we will show that just utilize the canonical commutation relation for canonical coordinate x and canonical conjugate momentum p, proved in chapter 3, we can derive the equation of motion of operator in Heisenberg picture.

We use the elementary identity:

$$[A, BC] = B[A, C] + [A, B]C.$$
(5.8.1.1.1)

Computing the commutator

$$[x, p2] = [x, p]p + p[x, p] = 2i\hbar p, \qquad (5.8.1.1.2)$$

we then obtain the result,

$$[x, p2]x = xp2x - p2x2 = 2i\hbar px.$$
(5.8.1.1.3)

Using Eq. (5.8.1.1.2), we obtain

$$[x, p^{n}] = i\hbar p^{n-1} + p[x, p^{n-1}].$$
(5.8.1.1.4)

Then we use induction to prove that

$$[x, p^n] = i\hbar n p^{n-1} \tag{5.8.1.1.5}$$

for  $n = 1, 2, \dots$ . Combining Eq. (5.8.1.1.5) and  $[x, x^m] = 0$ , we obtain

$$[x, x^m p^n] = i\hbar n x^m p^{n-1}$$
(5.8.1.1.6)

Eq. (5.8.1.1.6) can be symbolically be written as

$$[x, x^m p^n] = i\hbar \frac{\partial}{\partial p} (x^m p^n).$$
(5.8.1.1.7)

The analogous relation with p is obtained automatically if we interchange  $x \leftrightarrow p$  and change the sign of the commutator  $i\hbar$  to  $-i\hbar$ , i. e., we have also

$$[p, p^m x^n] = -i\hbar \frac{\partial}{\partial x} (p^m x^n).$$
(5.8.1.1.8)

By using Eq. (5.8.1.1.1) we can extend the Eq. (5.8.1.1.7-8) to the form  $x^a p^b x^c$ , and obtain

$$[x, x^{a}p^{b}x^{c}] = i\hbar bx^{a}p^{b-1}x^{c} = i\hbar \frac{\partial}{\partial p}(x^{a}p^{b}x^{c}).$$
(5.8.1.1.9)

Here it is implied that the derivative  $\partial/\partial p$  acts only on p where it appears in the expression. The operator (x and p) ordering should remain unchanged, i. g.,

$$\frac{\partial}{\partial p}(p^3 x p^2 x) = 3p^2 x p^2 x + 2p^3 x p x.$$
(5.8.1.1.10)

An analytic function f(x, p) is expanded into a sum of the terms of the form

 $\cdots x^a p^b x^c p^d \cdots$ 

and the Eq. (5.8.1.1.9) can be generalized to terms of this form. Each term of the expansion of f(x, p) satisfies the relation. Therefore, the sum will also satisfy the relation. So, we obtain

$$[x, f(x, p)] = i\hbar \frac{\partial}{\partial p} f(x, p), \quad [p, f(x, p)] = -i\hbar \frac{\partial}{\partial x} f(x, p). \tag{5.8.1.11}$$

Using Eq. (5.8.1.1.11), which comes from canonical commutation relation between x and p, the classical Hamilton equations Eqs. (2.2.3.5-6) become

$$\frac{dx}{dt} = -\frac{i}{\hbar}[x, H], \quad \frac{dp}{dt} = -\frac{i}{\hbar}[p, H].$$
(5.8.1.1.12)

The two equations in Eq. (5.8.1.1.12) are called quantum Hamilton equations, in which the Poison bracket is replaced by canonical commutation relations. Note that x does not commune with dx/dt because p = mdx/dt, where m is the mass of a particle, and is independent of t. So the time derivatives of, e. g.,  $x^3$  must be written as

$$\frac{d}{dt}x^3 = x^2\dot{x} + x\dot{x}x + \dot{x}x^2.$$
(5.8.1.1.13)

It is easy to show that for any operators A, B, H (A and B are not necessarily Hermitian) that satisfy

$$\frac{\partial}{\partial t}C = [C,H], \quad \frac{\partial}{\partial t}B = [B,H],$$
 (5.8.1.1.14)

the following properties hold:

$$\frac{\partial}{\partial t}(C+B) = [C+B,H], \quad \frac{\partial}{\partial t}(CB) = \frac{\partial C}{\partial t}B + C\frac{\partial B}{\partial t} = [CB,H]. \quad (5.8.1.1.15)$$

In terms of Eqs. (5.8.1.1.14-15) and quantum Hamilton equations Eq. (5.8.1.1.12) we can show that if A = f(p, x, t) is an analytical function, then A satisfies

$$\frac{dA}{dt} = -\frac{i}{\hbar}[A,H] + \frac{\partial A}{\partial t}, \qquad (5.8.1.1.16)$$

which is called Heisenberg equation of motion.

By induction, starting from x, p, and Eq. (5.8.1.1.12), we can prove the same property for arbitrary terms of the form  $\cdots x^a p^b x^c p^d \cdots$  and their linear combinations. Any analytical function A = f(x, p) that can be expressed by such a polynomial terms will satisfy Eq. (5.8.1.1.16).

Let us for simplicity take an operator which does not depend on time explicitly, i. e., A = f(x, p). The formal solution of Eq. (5.8.1.1.16) is

$$A(t) = e^{iH(t-t_{\circ})/\hbar} A(t_{\circ}) e^{-iH(t-t_{\circ})/\hbar}.$$
(5.8.1.1.17)

From the last equality of Eq. (5.7.3.3) we know that A(t) is just the operator  $O_H$  in Heisenberg picture. For any quantum state vector  $|\psi(t_\circ)\rangle = |\psi_H\rangle$  the time-dependent average value of A(t) is

$$< A(t) > = <\Psi_H |A(t)| \Psi_H > = <\Psi(t_{\circ}) |e^{iH(t-t_{\circ})/\hbar} A(t_{\circ}) e^{-iH(t-t_{\circ})/\hbar} |\Psi(t_{\circ}) > . \quad (5.8.1.1.18)$$

This relation can be rewritten using a time-dependent state vector

$$|\Psi(t)\rangle = e^{-\frac{i}{\hbar}H(t-t_{\circ})}|\Psi(t_{\circ})\rangle$$
 (5.8.1.1.19)

and time-independent operator  $A(t_{\circ})$  as

$$\langle A(t) \rangle = \langle \Psi(t) | A(t_{\circ}) | \Psi(t \rangle.$$
 (5.8.1.1.20)

Taking the time derivative of Eq. (5.8.1.1.19), we find that the state vector  $|\psi(t)\rangle$  satisfies the following equation:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle. \qquad (5.8.1.1.21)$$

We would like to reminder the readers that the basic starting point for all the derivations from Eq. (5.8.1.1.1) to Eq. (5.8.1.1.21) is the canonical commutation relation of operator x and p,  $[x, p] = i\hbar$ , and this canonical commutation relation has been proved by our wavepacket-only theory in a more general form of many degrees of freedom in chapter 3. So, the Heisenberg matrix (or say, operator) mechanics can be proved by our wavepacket-only theory.

Because the starting point of Heisenberg matrix mechanics is canonical commutation relations, we call the Heisenberg matrix mechanics formulation of quantum mechanics canonical quantization formulation of quantum mechanics.

#### 5.8.1.2. Application of Matrix Mechanism

We illustrate with two examples: (1). The a and  $a^+$  operators greatly facilitate the calculation of matrix elements of other operators between the oscillator eigenstate; (2). Seek the eigenstates of quantum harmonic oscillator.

(1) From Eqs. (4.4.4.29) and (4.4.4.33-34) we obtain

$$< n'|a|n> = n^{1/2} < n'|n-1> = n^{1/2}\delta_{n',n-1}.$$
 (5.8.1.2.1)

$$< n'|a^+|n> = (n+1)^{1/2} < n'|n+1> = (n+1)^{1/2}\delta_{n',n+1}.$$
 (5.8.1.2.2)

To find the matrix elements of x and p, we invert Eqs.(4.4.4.4a-b) to obtain

$$x = \left(\frac{\hbar}{2m\omega}\right)^{1/2} (a + a^{+}).$$
 (5.8.1.2.3)

$$p = i \left(\frac{m\omega\hbar}{2}\right)^{1/2} (a^+ - a).$$
 (5.8.1.2.4)

and then use Eqs. (5.8.1.2.1-2). The two basic matrices in this energy basis ( $|n\rangle$  is eigenstate of energy) are

$$a^{+} \leftrightarrow \begin{bmatrix} n = 0 & n = 1 & n = 2 & \cdots \\ n = 0 & 0 & 0 & 0 & \cdots \\ n = 1 & 1^{1/2} & 0 & 0 & \cdots \\ n = 2 & 0 & 2^{1/2} & 0 & \cdots \\ n = 3 & 0 & 0 & 3^{1/2} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}.$$
 (5.8.1.2.5)

and its adjoint operator

$$a \leftrightarrow \begin{bmatrix} n=0 & n=1 & n=2 & n=3 & \cdots \\ n=0 & 0 & 1^{1/2} & 0 & 0 & \cdots \\ n=1 & 0 & 0 & 2^{1/2} & 0 & \cdots \\ n=2 & 0 & 0 & 0 & 3^{1/2} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}.$$
 (5.8.1.2.6)

We get the matrices representing x and p by turning to Eqs. (5.8.1.2.3-4). The Hamiltonian is of course diagonal in its own basis:

$$H \leftrightarrow \begin{bmatrix} n=0 & n=1 & n=2 & n=3 & \cdots \\ n=0 & 1/2 & 0 & 0 & 0 & \cdots \\ n=1 & 0 & 3/2 & 0 & 0 & \cdots \\ n=2 & 0 & 0 & 5/2 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}.$$
 (5.8.1.2.7)

Eq. (4.4.4.4) also allows us to express all normalized eigenvectors  $|n\rangle$  in terms of the ground state  $|0\rangle$ :

$$|n\rangle = \frac{a^{+}}{n^{1/2}}|n-1\rangle = \frac{a^{+}}{n^{1/2}}\frac{a^{+}}{(n-1)^{1/2}}|n-2\rangle \dots = \frac{(a^{+})^{n}}{(n!)^{1/2}}|0\rangle.$$
(5.8.1.2.8)

The *a* and  $a^+$  operators greatly facilitate the calculation of matrix elements of other operators between the oscillator eigenstate. Consider, for example,  $< 3|x^3|2 >$ . In the *x* basis (coordinate representation) one would have to carry out the following integral (refer to section 4.4.2 in chapter 4):

$$<3|x^{3}|2> = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \left(\frac{1}{2^{3}3!}\frac{1}{2^{2}2!}\right)^{1/2} \int_{-\infty}^{\infty} \left\{e^{-m\omega x^{2}/2\hbar}\right\} \\ \times H_{3}\left[\left(\frac{m\omega}{\hbar}\right)^{1/2}x\right] x^{3}e^{-m\omega x^{2}/2\hbar}H_{2}\left[\left(\frac{m\omega}{\hbar}\right)^{1/2}x\right] dx$$

whereas in the  $|n\rangle$  basis (representation)

Since *a* lowers *n* by one unit and  $a^+$  raises it by one unit and we want to go up by one unit from n = 2 to n = 3, the only nonzero contribution comes from  $a^+a^+a$ ,  $aa^+a^+$ ,  $a^+aa^+$ . Therefore, we have the third equality in Eq. (5.8.1.2.9). From the above discussions we see that the  $|n\rangle$  basis is ideally suited for evaluating the matrix elements of operators between oscillator eigenstates.

(2) We illustrate with an example, the harmonic oscillator, to show that if one just uses the Heisenberg matrix mechanics (without using the Schrödinger equation), then we can also obtain the eigenvalue and eigenstates of a quantum harmonic oscillator. The eigenvalues of harmonic oscillation have been found by using the Heisenberg operator mechanics in subsection 4.4 of chapter 4. Therefore, here we just need to seek the eigenfunctions. There are three methods to solve this problem. First, to find the eigenvectors |x > of the matrix of operator x, which has been given by Eqs. (5.8.1.2.3) and (5.8.1.2.5-6); Second, to evaluate the inner product  $\langle x | n \rangle = \psi_n(x)$ ; Third, a more practical way is introduced in the next paragraph.

We start by projecting the equation defining the ground state of oscillator

$$a|0>=0 \tag{5.8.1.2.10}$$

on the *x* basis (representation):

$$|0\rangle \rightarrow \langle x|0\rangle = \Psi_0(x)$$

$$a = \left(\frac{m\omega}{2\hbar}\right)^{1/2} x + i \left(\frac{1}{2m\omega\hbar}\right)^{1/2} p$$

$$\rightarrow \left(\frac{m\omega}{2\hbar}\right)^{1/2} x + \left(\frac{\hbar}{2m\omega}\right)^{1/2} \frac{d}{dx}.$$
(5.8.1.2.11)

In terms of  $y = (m\omega/\hbar)^{1/2}x$  and Eq. (4.4.4.4a),

$$a = \frac{1}{\sqrt{2}} \left( y + \frac{d}{dy} \right).$$
 (5.8.1.2.12)

For later use we also note that (since d/dy is anty-Hermitian),

$$a^{+} = \frac{1}{\sqrt{2}} \left( y - \frac{d}{dy} \right).$$
 (5.8.1.2.13)

In the x basis Eq. (5.8.1.2.10) then becomes

$$\left(y + \frac{d}{dy}\right)\psi_0(y) = 0$$
 (5.8.1.2.14)

or

$$\frac{d\psi_0(y)}{\psi_0(y)} = -ydy$$
(5.8.1.2.15)

From Eq. (5.8.1.2.15) we obtain

$$\Psi_0(x) = C e^{-m\omega x^2/(2\hbar)}.$$
(5.8.1.2.16)

After normalization,

$$\Psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/(2\hbar)}.$$
(5.8.1.2.17)

By projecting the Eq. (5.8.1.2.8) on to the x basis, we get the normalized eigenfunction

$$< x|n> = \frac{1}{(n!)^{1/2}} \left[ \frac{1}{2^{1/2}} \left( y - \frac{d}{dy} \right) \right]^n \Psi_0(x)$$
  
=  $\frac{1}{(n!)^{1/2}} \left[ \frac{1}{2^{1/2}} \left( y - \frac{d}{dy} \right) \right]^n \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-y^2/2}.$  (5.8.1.2.18)

A comparison of the above result with the Eq. (4.4.2.27) shows that

$$H_n(y) = e^{y^2/2} \left( y - \frac{d}{dy} \right)^n e^{-y^2/2}.$$
 (5.8.1.2.19)

We would like to emphasize the following two points:

(1). The starting point or, say, the origin of the Heisenberg matrix or operator mechanics formulation of quantum mechanics is the theorem on the canonical commutation relation, proved by our wavepacket-only theory in chapter 3. Heisenberg matrix or operator mechanics formulation of quantum mechanics does not contain any assumptions or postulates;

(2). Although Heisenberg operator mechanics can give eigenvalues and eigenfunctions, but it is more trouble to do these in comparison with the Schrödinger wave mechanics formulation. Heisenberg operator mechanics starts from the canonical commutation relation, proved by our wavepacket-only theory. Therefore, Heisenberg operator mechanics can also be called canonical quantization formulation of quantum mechanics. This canonical quantization formulation formulation is easy to be extended to the systems with many or infinitely many degrees to freedom. We can call our living space a field. If we think that every point of this continuous position space is one degree of freedom, and use canonical quantization formulation of quantum mechanics formulation of quantum mechanics, then we obtain nonrelativistic and relativistic quantum field theory. We will derive in our coming textbook the nonrelativistic and relativistic quantum field theory.

## 5.8.2. Schrödinger Wave Mechanics Formulation

In this subsection we will derive the Schrödinger wave mechanics formulation of quantum mechanics from the canonical commutation relation between x and p. To do this, it is enough to continue the derivation of the Eq. (5.8.1.1.19).

Eq. (5.8.1.1.19) can be rewritten using a time-dependent state vector

$$|\Psi(t)\rangle = e^{-iH(t-t_{\circ})/\hbar}|\Psi(t_{\circ})\rangle$$
 (5.8.2.1)

and time-independent operator  $A(t_{\circ})$  as

$$\langle A(t) \rangle = \langle \Psi(t) | A(t_{\circ}) | \Psi(t \rangle.$$
 (5.8.2.2)

If we write the state vectors and operators in the manner in Eqs. (5.8.2.1-2), then this means that we consider problems in Schrödinger picture. Taking the time derivative of Eq. (5.8.2.1), we find that the state vector  $|\Psi(t)\rangle$  satisfies the following equation:

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H|\Psi(t)\rangle.$$
 (5.8.2.3)

Many textbooks call Eq. (5.8.2.3) Schrödinger equation, which does not depend a particular representation. We would like to reminder the readers that the basic starting point for all the derivations from Eq. (5.8.1.1.1) to Eq. (5.8.1.1.17) is the canonical commutation relation of operator x and p,  $[x, p] = i\hbar$ , and this canonical commutation relation has been proved by our wavepacket-only theory in a more general many degrees of freedom in chapter 3.

Next, we derive the form of Schrödinger wave equation, given by Eq. (5.8.2.3), in x representation. Eq. (5.8.2.3) can be expressed generally as

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \left[\frac{p^2}{2m} + V(x)\right]|\Psi(t)\rangle.$$
(5.8.2.4)

We express the state vector  $|\psi(t)\rangle$  in x representation. Eq. (5.8.2.4) gives directly the Schrödinger wave equation in x representation:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x,t).$$
(5.8.2.5)

#### 5.8.3. Feynman Path Integral Formulation

#### 5.8.3.1. Introduction

The Feynman path integral formulation of quantum mechanics is a description of quantum theory which generalizes the least action principle of classical mechanics. It replaces the classical notion of a single, unique trajectory for a system with a sum, or functional integral, over an infinity of possible trajectories to compute a probability amplitude.

The basic idea of the path integral formulation can be traced back to Wiener, who introduced the Wiener integral for solving problems in diffusion and Brownian motion. This idea was extended to the use of the Lagrangian in quantum mechanics by Dirac in his 1933 paper. The complete method was developed in 1948 by Feynman. Some preliminaries were worked out earlier, in the course of his doctoral thesis work with Wheeler. The original motivation stemmed from the desire to obtain a quantummechanical formulation for the Wheeler-Feynman absorber theory using a Lagrangian as a starting point rather than a Hamiltonian.

This formulation has proved to be crucial to the subsequent development of theoretical physics, because it is manifestly symmetric between time and space. Unlike previous formulation, the path integral allows a physicist to easily change coordinates between very different canonical descriptions of the same quantum system.

The path integral also relates quantum and stochastic processes, and this provided the basis for the grand synthesis of the 1970s which unified quantum field theory with the statistical field theory of a fluctuating field near a second-order phase transition. The Schrödinger equation is a diffusion equation with an imaginary diffusion constant, and the path integral is an analytic continuation of a method for summing up all possible random walks. For this reason path integrals were used in the study of Brownian motion and diffusion a while before they were introduced in quantum mechanics [89].

Recently path integrals have been expanded from Feynman paths to Lévy flights. The Lévy path integral formulation leads to fractional quantum mechanics and a fractional Schrödinger equation [90].

In subsubsection 5.8.3.2 we will derive the Feynman path integral formulation by just using the canonical communication relation between X and P. In subsection 5.8.3.2 we use X, P represent coordinates and momentum operators, respectively, and use x, p represent corresponding classical numbers. The summation over all possible pathes between initial point  $x_i$ ,  $t_0$  and final point  $x_f$ ,  $t_f$  is tied in mathematics to the existence of many decompositions of the unity, i. e., to the existence of many complete bases being of completeness.

Following this we will discuss in subsubsection 5.8.3.3 one simplest example: to seek the propagator of free particle. In subsubsection 5.8.3.4 we make the inverse derivations, i. e., we derive the canonical commutation relation from Feynman path integral formulation, i. e., from the result back to starting point. Because we can derive canonical commutation relation, we can say that from Feynman path integral formulation one can derive the Heisenberg matrix formulation. We can also demonstrate that the Feynman path integral formulation can derive Schrödinger equation. We will point out in subsubsection 5.8.3.5 that although the Feynman path integral has been applied successfully in many aspects, such as gauge field quantization, polymer, and so on. However, for the application in free particle, which, of course, should be the simplest application, some references made a conceptual mistake, and derived a fantastic conclusion.

#### 5.8.3.2. Derivations of the Path Integrals

**Propagator.** For convenience, we consider one spatial dimensional system, the Hamiltonian does not explicitly contain time. In Schrödinger picture the equation of motion of state vector is given by Eq. (5.8.2.3), which has a formal solution:

$$|\Psi(t_f)\rangle = U(t_f, t_0)|\Psi(t_0)\rangle,$$
 (5.8.3.2.1)

where the subscripts 0, f represent initial and final, and

$$U(t_f, t_0) = e^{-iH(t_f - t_0)/\hbar}$$
(5.8.3.2.2)

is called time evolution operator. In the coordinate representation, a quantum state is described by a wavefunction, which is

$$\begin{aligned} \Psi(x_f, t_f) &= \langle x_f | \Psi(t_f) \rangle = \langle x_f | U(t_f, t_0) \left( \int dx_0 | x_0 \rangle \langle x_0 | \right) | \Psi(t_0) \rangle \\ &\equiv \int dx_0 K(x_f, x_0; t_f, t_0) \Psi(x_0, t_0), \end{aligned}$$
(5.8.3.2.3)

where we used the decomposition of unit operator, and the matrix element

$$K(x_f, x_0; t_f, t_0) = \langle x_f | U(t_f, t_0) | x_0 \rangle$$
(5.8.3.2.4)

is called the propagator, which can give the final state wavefunction  $\psi(x_f, t_f)$  when the system is initially at the state  $\psi(x_0, t_0)$  in terms of Eq. (5.8.3.2.3). Note that the propagator is not an operator, it is just a number function.

**Expression of propagator as path integral.** The short time propagator is differential form of propagator. In any physical problems, one always begins from the derivation of short time propagator. The propagator can be expressed as an path integral over all trajectories connecting the initial state at  $x_0$ ,  $t_0$  and final state at  $x_f$ ,  $t_f$ . Note that in the following derivations we use a subscript index to distinguish different quantum states  $|x_0 >$ ,  $|x_1 >$ ,  $\cdots$  of the same system with one degree of freedom x. One should not confuse this subscript with an index enumerating the different degrees of freedom.

To express the propagator as a path integral, at first we need to divide the time interval from initial to final time,  $(t_0 \rightarrow t_f)$ , into N + 1 small equal intervals  $(t_0, t_1), \dots, (t_k, t_{k+1}), \dots, (t_N, t_f)$  with  $t_f = t_{N+1}$  and any small time interval =  $\varepsilon$ . This process is called time slicing. In this time slicing, there are N inner spatial points between  $x_0$  and  $x_f$ . Eventually, we shall pass to the limit  $N \rightarrow \infty$  and  $\Delta t_k \equiv t_{k+1} - t_k \rightarrow 0$ . The evolution operator  $U(t_f, t_0)$  is equal to the product of the evolution operators for the N + 1 intermediate ranges  $(t_k, t_{k+1})$ ,

$$U(t_f, t_0) = U(t_f, t_N) \cdots U(t_1, t_0) = \prod_{k=0}^N U(t_{k+1}, t_k), \quad (t_f = t_{N+1})$$
(5.8.3.2.5)

and therefore the propagator

$$K(x_f, x_0; t_f, t_0) = \langle x_f | U(t_f, t_0) | x_0 \rangle = \langle x_f | \prod_{k=0}^N U(t_{k+1}, t_k) | x_0 \rangle.$$
 (5.8.3.2.6)

Short time propagator. At first we express the propagator in Eq. (5.8.3.2.6) in terms of the N + 1 short time propagators. Inserting N decompositions of unity operator:

$$\int_{-\infty}^{\infty} dx_k |x_k| < x_k|$$

in Eq. (5.8.3.2.6) between any two nearest neighbor short time evolution operators, we have

$$K(x_{f} \equiv x_{N+1}, x_{0}; t_{f} \equiv t_{N+1}, t_{0})$$

$$= \langle x_{f} | U(t_{f} \equiv t_{N+1}, t_{N}) \int dx_{N} | x_{N} \rangle \langle x_{N} \rangle U(t_{N}, t_{N-1}) \cdots | x_{0} \rangle \cdots$$

$$\cdots \int dx_{k+1} | x_{k+1} \rangle \langle x_{k+1} \rangle U(t_{k+1}, t_{k}) \int dx_{k} | x_{k} \rangle \langle x_{k} \rangle U(t_{k}, t_{k-1}) \cdots$$

$$\times \int dx_{1} | x_{1} \rangle \langle x_{1} \rangle U(t_{1}, t_{0}) | x_{0} \rangle$$

$$= \int dx_{N} dx_{N-1} \cdots dx_{1} \left( \prod_{k=0}^{N} K(x_{k+1}, x_{k}; t_{k+1}, t_{k}) \right)$$

$$= \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dx_{N} dx_{N-1} \cdots dx_{1} \left( \prod_{k=0}^{N} K(x_{k+1}, x_{k}; \epsilon) \right), \qquad (5.8.3.2.7)$$

where the last equality comes from that the Hamiltonian does not explicitly contain time, and the  $x_0 x_1, x_2, \cdots$  label the different quantum states at the moments of  $t_0, t_1, t_2, \cdots$ , respectively. Thus, it follows that the propagator is the *N*-fold integrated product of the N+1 short time propagators of all the intermediate time intervals.

In Eq. (5.8.3.2.7) the product of (N+1) short time propagators,

$$K(x_{k+1}, x_k; \varepsilon) = \langle x_{k+1} | U(t_{k+1}, t_k) | x_k \rangle$$
(5.8.3.2.8)

is just equal to one special probability amplitude related with just the specially certain (or, more vividly speaking, constrained) chain of propagations  $|x_0 \rangle \rightarrow |x_1 \rangle \rightarrow |x_2 \rangle \rightarrow \cdots \rightarrow |x_f \rangle$ . This special probability amplitude just connects with that the particle propagates from fixed point  $x_0$  to fixed point  $x_f$  while visiting the special certain intermediate points  $x_k$  at time  $t_k$ . Actually, when a particle propagates from fixed point  $x_0$  at time  $t_0$  to fixed point  $x_f$  at time  $t_f$ , the particle should have many choices, because, e. g., the  $x_k$  can take different values. As is well known, the special probability amplitude is also a state vector in Hilbert space  $\mathcal{H}$ , and, therefore, satisfies superposition theorem. So, if we want to find the total probability amplitude at point  $x_f$  at time  $t_f$  and initially is at point  $x_0$  at time  $t_0$ , then we have to do the integrations in Eq. (5.8.3.2.7) (Please connect the integration with equiprobability symmetry and spontaneous equiprobability symmetry breaking.). At this stage of our derivations, the readers have understood the mathematical and physical origins of the path integral, and feel that the path integral formulation of quantum mechanics is so easier to be understood as that the other two formulations of the quantum mechanics.

At this stage of derivations, the readers will do not ask the question, such as, why we should do path integral. The readers will ask that how to continue the derivations? We will at first continue our derivation in phase space to connect the short time propagator with Hamiltonian of the system, and then do the derivation in configuration space to connect the propagator with Lagrangian of the system. (Here, phase space means (p,x) space, and configuration space means x space.)

Expanding the short time evolution operators as

$$U(t_{k+1}, t_k) = e^{-i(t_{k+1} - t_k)H/\hbar} = e^{-i\varepsilon H/\hbar} = 1 - \frac{i}{\hbar}\varepsilon H + 0(\varepsilon^2)$$
(5.8.3.2.9)

one obtains

$$K(x_{k+1}, x_k; \varepsilon) = \langle x_{k+1} | U(t_{k+1}, t_k) | x_k \rangle = \langle x_{k+1} | \left( 1 - \frac{i}{\hbar} H \varepsilon \right) | x_k \rangle + 0(\varepsilon^2). \quad (5.8.3.2.10)$$

The matrix element of Hamiltonian can be calculated by inserting the decomposition of unity operator in momentum representation,

$$I = \int_{-\infty}^{\infty} dp_k |p_k| > < p_k|, \qquad (5.8.3.2.11)$$

where we use  $p_k$  simply to distinguish the momentum eigenstates at  $t_k$ .

Considering

$$< x_{k+1}|H|x_k> = \int_{-\infty}^{+\infty} dp_k < x_{k+1}|p_k> < p_k|H|x_k>$$
 (5.8.3.2.11)

and the matrix element

$$\langle x_{k+1}|p_k \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ip_k x_{k+1}/\hbar},$$
 (5.8.3.2.11)"

one obtains

$$K(x_{k+1}, x_k; \varepsilon) = \int dp_k \langle x_{k+1} | p_k \rangle \langle p_k | x_k \rangle$$
  
- 
$$\int dp_k \frac{i\varepsilon}{\hbar} \langle x_{k+1} | p_k \rangle \langle p_k | H | x_k \rangle = \int \frac{dp_k}{2\pi\hbar} e^{ip_k (x_{k+1} - x_k)/\hbar}$$
  
- 
$$\int \frac{dp_k}{\sqrt{2\pi\hbar}} e^{ip_k x_{k+1}/\hbar} \frac{i\varepsilon}{\hbar} \langle p_k | H | x_k \rangle. \qquad (5.8.3.2.12)$$

To find  $\langle p_k | H | x_k \rangle$ , we must first reorder all the operators *P* in the Hamiltonian and move them to the left, so that H(X, P) is rewritten as

$$H = \sum_{j} f_{j}(P)g_{j}(X), \qquad (5.8.3.2.13)$$

which can be done by using the canonical communication relation  $[X, P] = i\hbar$ . For example, if

$$H = H(P,X) = XP^{2}X = P^{2}X^{2} + 2i\hbar PX, \qquad (5.8.3.2.14)$$

we have

$$H = H(P_k, X_k) = X_k P_k^2 X_k = P_k^2 X_k^2 + 2i\hbar P_k X_k.$$
(5.8.3.2.14)'

As a result, we find

$$< p_{k}|H|x_{k}> = \left[\sum_{j} f_{j}(p_{k})g_{j}(x_{k})\right] \times < p_{k}|x_{k}> \equiv H(p_{k}, x_{k}) < p_{k}|x_{k}>$$
  
 $= H(p_{k}, x_{k})\frac{1}{\sqrt{2\pi\hbar}}e^{-ip_{k}x_{x}/\hbar},$  (5.8.3.2.15)

where if H = H(P,X) is given by Eq. (5.8.3.2.14), then the  $H(p_k, x_k)$  in Eq. (5.8.3.2.15) is

$$H(p_k, x_k) = p_k^2 x_k^2 + 2i\hbar p_k x_k.$$
(5.8.3.2.16)
Note that the  $(p_k, x_k)$  in Eqs. (5.8.3.2.15-16) are numbers, other than operators. Substituting Eq. (5.8.3.2.15) into Eq. (5.8.3.2.12) yields

$$K(x_{k+1}, x_k; \varepsilon) = \int \frac{dp_k}{2\pi\hbar} \left[ 1 - \frac{i\varepsilon}{\hbar} H(p_k, x_k) + 0(\varepsilon^2) \right] e^{ip_k(x_{k+1} - x_k)/\hbar}$$
  
$$= \int_{-\infty}^{\infty} \frac{dp_k}{2\pi\hbar} \exp\left[ \frac{i\varepsilon}{\hbar} \left( p_k \frac{x_{k+1} - x_k}{\varepsilon} - H(p_k, x_k) \right) + 0(\varepsilon^2) \right].$$
(5.8.3.2.17)

**Propagator in phase space (Hamiltonian path integral).** Substituting Eq. (5.8.3.2.17) into Eq. (5.8.3.2.7) yields

$$K(x_f \equiv x_{N+1}, x_0; t_f \equiv t_{N+1}, t_0) = \int \left[\prod_{k=1}^N \frac{dx_k dp_k}{2\pi\hbar}\right] \frac{dp_0}{2\pi\hbar}$$
$$\exp\left[\sum_{k=0}^N \frac{i\epsilon}{\hbar} \left(p_k \frac{x_{k+1} - x_k}{\epsilon} - H(p_k, x_k)\right) + 0(\epsilon^2)\right].$$
(5.8.3.2.18)

We would like to point out that, since Eq. (5.8.3.2.7) contains N + 1 short time propagators, Eq. (5.8.3.2.18) contains (N + 1) integration over  $p_k$  but only N integration over  $x_k$ .

Now let us consider the limit  $N \to \infty \varepsilon \to 0$ . When the number of intermediate time points  $t_k$  becomes infinitely large, one can introduce the functions x(t), p(t) such that  $x_k = x(t_k)$ ,  $p_k = p(t_k)$ , and replace the sum replace the sum in Eq. (5.8.3.2.18) by an integral over *t*. In this limiting case Eq. (5.8.3.2.18) becomes

$$K(x_f, x_0; t_f, t_0) = \int_{x(t_0)=x_0}^{x(t_f)=x_f} \mathcal{D}p \mathcal{D}x \exp\left[\frac{i}{\hbar} \int_{t_0}^{t_f} dt [p\dot{x} - H(p, x)]\right], \qquad (5.8.3.2.19)$$

where  $p = p(t), x = x(t), \dot{x} = dx(t)/dt$ ,

$$\mathcal{D}p\mathcal{D}x \equiv \lim_{N \to \infty} \left[ \prod_{k=1}^{N} \frac{dx_k dp_k}{2\pi\hbar} \right] \frac{dp_0}{2\pi\hbar},$$
(5.8.3.2.20)

and note that

$$\int_{x(t_0)=x_0}^{x(t_f)=x_f} \mathcal{D}p \mathcal{D}x = \lim_{N \to \infty} \left[ \prod_{k=1}^N \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dx_k dp_k}{2\pi\hbar} \right] \int_{-\infty}^{\infty} \frac{dp_0}{2\pi\hbar}$$

Let us make the following five interpretations:

(1) The integration over infinitely many intermediate values of  $x_k$ ,  $p_k$  in Eq. (5.8.3.2.18) is naturally interpreted as the integration over all the functions x(t), p(t) such that  $x(t_0) = x_0$ ,  $x(t_f) = x_f$ . An integral of this kind is called a functional integral of path integral. In the limit  $N \to \infty$ , the (2N + 1)-fold integration over  $dp_k$  and  $dx_k$  becomes an infinite-dimensional integration measure, given by Eq. (5.8.3.2.20). This formal expression must be understood as the limit of the finite-dimensional integral in Eq. (5.8.3.2.18) as  $N \to \infty$ .

(2) The H(p,x) in Eq. (5.8.3.2.19) is no longer an operator, and it is a classical Hamiltonian. Correspondingly, according to classical mechanics, the phase factor  $\int_{t_0}^{t_f} dt[p\dot{x} - H(p,x)] = S_H[x(t), p(t)]$  is the Hamiltonian action, which is a functional of two functions x(t), p(t). According to the classical Hamiltonian action principle, i. e., x(t), p(t) must be varied independently to extremize  $S_H$ , and thus determine the trajectory of the particle in phase space. However, we should note that due to the uncertainty relation of canonical coordinate and canonical conjugate momentum we cannot use the classical Hamiltonian action principle in quantum mechanics.

(3) The generalization to the case of an arbitrary number of degrees of freedom, including an infinite number of degrees of freedom needed in field theory, is largely straightforward.

(4) So far we considered only systems with time independent Hamiltonian, but the path integral formulation also applies to time dependent Hamiltonian.

(5) At last we prove that the term in Eq. (5.8.3.2.18), containing  $0(\epsilon^2)$ , really can be neglected. The term is

$$\lim_{N \to \infty} \sum_{k=0}^{N} 0(\varepsilon^2) \sim N\varepsilon^2 = N \frac{(t_f - t_0)^2}{(N+1)^2} \to 0.$$
 (5.8.3.2.22)

**Propagator in configuration space (Lagrangian path integral).** If the Hamiltonian is a quadratic function of the momenta, then the integration over the momenta can be performed explicitly and the path integral is simplified. Let us consider, for example, a system with the Hamiltonian

$$H(P,X) = \frac{P^2}{2m} + V(X).$$
 (5.8.3.2.23)

In this case, the integral in Eq. (5.8.3.2.18) becomes

$$K(x_{k+1}, x_k; \varepsilon) = \int \frac{dp_k}{2\pi\hbar} \exp\left[\frac{i\varepsilon}{\hbar} \left(p_k \frac{x_{k+1} - x_k}{\varepsilon} - \frac{p_k^2}{2m} - V(x_k)\right) + O(\varepsilon^2)\right], \qquad (5.8.3.2.24)$$

where the integration over momentum belongs to Gaussian type, and can be finished in advance.

$$\int \frac{dp_{k}}{2\pi\hbar} \exp\left\{-\frac{i\varepsilon}{\hbar} \left(\frac{p_{k}^{2}}{2m} - \frac{p_{k}(x_{k+1} - x_{k})}{\varepsilon}\right)\right\}$$

$$= \int \frac{dp_{k}}{2\pi\hbar} \exp\left\{-\frac{i\varepsilon}{2m\hbar} \left[\left(p_{k} - \frac{m}{\varepsilon}(x_{k+1} - x_{k})\right)^{2} - \left(\frac{m}{\varepsilon}(x_{k+1} - x_{k})\right)^{2}\right]\right\}$$

$$= \left(\frac{m}{2\pi\hbar\epsilon}\right)^{1/2} \exp\left\{\frac{im\varepsilon}{2\hbar} \left(\frac{x_{k+1} - x_{k}}{\varepsilon}\right)^{2}\right\}.$$
(5.8.3.2.25)

In the last step of Eq. (5.8.3.2.25) we use the equality

$$\int_{-\infty}^{\infty} dp_k e^{-iap_k^2} = \sqrt{\frac{\pi}{ia}}.$$
 (5.8.3.2.26)

Substituting Eq. (5.8.3.2.25) into Eq. (5.8.3.2.24) yields

$$K(x_{k+1}, x_k; \varepsilon) = \sqrt{\frac{m}{2i\pi\hbar\varepsilon}} \exp\left[\frac{im}{\hbar 2} \frac{(x_{k+1} - x_k)^2}{\varepsilon} - \frac{i}{\hbar} \varepsilon V(x_k)\right] [1 + 0(\varepsilon^2)]. \quad (5.8.3.2.27)$$

Substituting the short time propagator in Eq. (5.8.3.2.27) into Eq. (5.8.3.2.7), taking  $N \rightarrow \infty$ ,  $\varepsilon \rightarrow 0$ , and finishing the  $N + 1 (\neq N)$  integration over momenta (due to the product  $k = 0, 1, 2, \dots, N$ ), we finally obtain

$$K(x_f, x_0; t_f, t_0) = \int_{x(t_0)=x_0}^{x(t_f)=x_f} \mathcal{D}x \exp\left(\frac{iS}{\hbar}\right),$$
 (5.8.3.2.28)

where

$$S = \lim_{\substack{N \to \infty \\ \epsilon \to 0}} \sum_{k=0}^{N} \left( m \frac{(x_{k+1} - x_k)^2}{2\epsilon^2} - V(x_k) \right) \epsilon = \int_{t_0}^{t_f} \left( \frac{m\dot{x}^2}{2} - V(x) \right) dt \quad (5.8.3.2.29)$$

is the Lagrangian action and the measure of the Lagrangian path integral is

$$\mathcal{D}x = \lim_{\substack{N \to \infty \\ \epsilon \to 0}} \frac{1}{\sqrt{2\pi i\hbar m^{-1}\epsilon}} \prod_{k=0}^{N} \frac{dx_k}{\sqrt{2\pi i\hbar m^{-1}\epsilon}}.$$
(5.8.3.2.30)

The dimension of  $\mathcal{D}x$  is the inverse of length.

From Eq. (5.8.3.2.28) we see that the contribution of every path between two points  $x(t_0) = x_0$  and  $x_{t_f} = x_f$  to the propagator is equal-probabilistic and the the weight is related to the Lagrangian action. Therefore, in practice, the main contributions to the propagator come from the pathes, along which the Lagrangian action is stable.

The propagator in Eq. (5.8.3.2.28) is not normalized. However, in practical applications when we seek the average value of a dynamic variable, the normalization factor is not important.

The Lagrangian path integral in Eq. (5.8.3.2.28) is the original form introduced by Feynman, and is called path integral. We should note that although the propagator for any system can be always written as the Hamiltonian path integral in Eq. (5.8.3.2.18), but the Lagrangian path integral exists only for the systems with Hamiltonians quadratic in momenta.

#### 5.8.3.3. Propagator of One Dimensional Free Particle

For seeking the propagator of one dimensional free particle, we need the Gaussian integration formulas:

$$\int_{-\infty}^{\infty} dx e^{i\alpha x^2} = \left(\frac{i\pi}{\alpha}\right)^{1/2}$$
$$\int_{-\infty}^{\infty} dx_k e^{i\alpha[(x_{k+1}-x_k)^2 + (x_k-x_{k-1})^2]} = \left(\frac{i\pi}{\alpha}\right)^{1/2} \frac{1}{\sqrt{2}} e^{i\alpha(x_{k+1}-x_{k-1})^2/2}.$$
(5.8.3.3.1)

Considering V(x) = 0 for free particle, neglecting terms  $0(\varepsilon)^2$  in Eq. (5.8.3.2.27), and utilizing Eq. (5.8.3.3.1), we have from Eqs. (5.8.3.2.27)

$$\int_{-\infty}^{\infty} dx_k K(x_{k+1}, x_k; t_{k+1}, t_k) K(x_k, x_{k-1}; t_k, t_{k-1})$$

$$= \frac{m}{2\pi i \hbar \sqrt{\epsilon^2}} \int_{-\infty}^{\infty} dx_k \exp\left\{\frac{im}{\hbar} \left[\frac{(x_{k+1} - x_k)^2}{2\epsilon} + \frac{(x_k - x_{k-1})^2}{2\epsilon}\right]\right\}$$

$$= \sqrt{\frac{m}{2\pi i \hbar 2\epsilon}} \exp\left[\frac{im}{\hbar} \frac{(x_{k+1} - x_{k-1})^2}{4\epsilon}\right]$$

$$= K(x_{k+1}, x_{k-1}; t_{k+1}, t_{k-1}). \qquad (5.8.3.3.2)$$

In this manner we can integrate over all the intermediate points  $x_k$  and obtain the propagator of free particle with mass m:

$$K(x_f, x_0; t_f, t_0) = \sqrt{\frac{m}{2\pi i \hbar(t_f - t_0)}} \exp\left[\frac{i}{\hbar} \frac{m(x_f - x_0)^2}{2(t_f - t_0)}\right].$$
 (5.8.3.3.3)

The characteristics of propagator of free particle are:

- (A) The expression depends only on the given boundary values of *x* and *t*;
- (B) The N and  $\varepsilon$  vanish automatically at the last step of the derivation;

(C) The factor  $m(x_f - x_0)^2/2(t_f - t_0)$  is equal to the classical action of free particle, because

$$S_{cl} = \int_{t_0}^{t_f} dt \frac{m\dot{x}}{2} = \frac{m}{2} \int_{t_0}^{t_f} dt \left(\frac{d(x\dot{x})}{dt} - x\ddot{x}\right) = \frac{m}{2} x\dot{x} \Big|_{t_0}^{t_f} = \frac{m}{2} \frac{(x_f - x_i)^2}{t_f - t_i}.$$
 (5.8.3.3.4)

(D) Noticing the expression of  $\delta$  function is

$$\delta(x_f - x_0) = \frac{1}{\sqrt{\pi}} \lim_{t_f \to t_0} \left\{ \frac{1}{\sqrt{t}} \exp\left[ -\frac{(x_f - x_0)^2}{t_f - t_0} \right] \right\},$$
(5.8.3.3.5)

one obtains

$$\lim_{t_f \to \infty} K(x_f, x_0; t_f, t_0) = \delta(x_f - x_0).$$
 (5.8.3.3.6)

It is easy to prove that  $K(x_f, x_0; t_f, t_0)$  satisfies the free particle Schrödinger equation

$$i\hbar\frac{\partial}{\partial t_f}K(x_f, x_0; t_f, t_0) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_f^2}K(x_f, x_0; t_f, t_0).$$
(5.8.3.3.7)

Schrödinger equation has infinite solutions, and the ordinary plane wave solution is only a solution with definite momentum. The propagator in Eq. (5.8.3.3.3) is the solution of free particle Scurödinger equation, satisfying the boundary condition of Eq. (5.8.3.3.6).

(E) For a free particle we can also use the matrix element of evolution operator  $U = \exp(-iHt/\hbar)$  to directly obtain

$$K(x_{f}, x_{0}; t_{f}, t_{0}) = \langle x_{f} | e^{-iHt/\hbar} | x_{0} \rangle$$
  
= 
$$\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \exp\left[-\frac{i}{\hbar} \frac{p^{2}}{2m}(t_{f} - t_{0}) + \frac{i}{\hbar}p(x_{f} - x_{0})\right]. \qquad (5.8.3.3.8)$$

After integration over p, we obtain the same expression as that of Eq. (5.8.3.3.3).

#### 5.8.3.4. Path Integral Formulation as Starting Point

**Derivation of Heisenberg matrix mechanics.** We assume that we have the Feynman formulation at first. We want to derive the Heisenberg matrix mechanics from Feynman path integral formulation. Of course, this thing is easy. We would like to remind the readers to remember that although the Feynman path integral is complex and useful, but the physical basis or origin is just the canonical commutation relation, which has been given as a theorem in chapter 3. Next, we make the inversive derivation, i. e., from path integral in Eq. (5.8.3.2.28) to canonical commutation relation, which is the starting point of Heisenberg matrix mechanism.

We take the variation over  $x_f$ ,  $\delta x_f \equiv \delta x(t_f) \neq 0$  and  $\delta x_0 \equiv \delta x(t_0) = 0$ , in Eq. (5.8.3.2.28). We can directly write

$$\delta K(x_f, x_0; t_f, t_0) = K(x_f + \delta x_f, x_0; t_f, t_0) - K(x_f, x_0; t_f, t_0) = \delta x_f \frac{\partial}{\partial x_f} K(x_f, x_0; t_f, t_0).$$
(5.8.3.4.1)

On the other hand,

$$\delta K(x_f, x_0; t_f, t_0) = \delta \int_{x_0}^{x(t_f) = x_f} \mathcal{D}x \exp\left(\frac{iS}{\hbar}\right)$$
$$= \int_{x(t_0) = x_0}^{x(t_f) = x_f} \mathcal{D}x \exp\left(\frac{iS}{\hbar}\right) \frac{i\delta S}{\hbar}.$$
(5.8.3.4.2)

The following steps are familiar from classical mechanics:

$$\begin{split} \delta S(x) &= \delta \int_{t_0}^{t_f} dt L(x, \dot{x}) = \int_{t_0}^{t_f} dt \left[ \frac{\partial L}{\partial x} \delta x + \frac{\partial L}{\partial \dot{x}} \delta \dot{x} \right] \\ &= \int_{t_0}^{t_f} dt \frac{\partial L}{\partial x} \delta x + \int_{t_0}^{t_f} dt \frac{\partial L}{\partial \dot{x}} \delta \dot{x} \\ &= \int_{t_0}^{t_f} dt \frac{\partial L}{\partial x} \delta x + \left[ \frac{\partial L}{\partial \dot{x}} \delta x \right]_{t_0}^{t_f} - \int_{t_0}^{t_f} dt \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) \delta x, \end{split}$$

and hence

$$\delta S(x) = \int_{t_0}^{t_f} dt \left[ \frac{\partial L}{\partial x} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) \delta x \right] \delta x + \left[ \frac{\partial L}{\partial \dot{x}} \delta x \right]_{t_0}^{t_f}.$$
 (5.8.3.4.3)

The classical equation of motion follows from the the least action principle for which  $\delta x = 0$  at  $t = t_f$ ,  $t_0$ . Thus in this case of classical mechanics

$$\frac{\partial L}{\partial x} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) = 0.$$
 (5.8.3.4.4)

However, in our case here  $\delta x_f \neq 0$  for  $t = t_f$  (although  $\delta x_0 = 0$  for  $t = t_0$ ), and we demand the validity of the equation of motion. Hence,

$$\delta S(x) = \left(\frac{\partial L}{\partial \dot{x}}\right)_{t_f} \delta x(t_f) = \left(\frac{\partial L}{\partial \dot{x}}\right)_{t_f} \delta x_f.$$
(5.8.3.4.5)

Substituting Eq. (5.8.3.4.5) into Eq. (5.8.3.4.2) yields

$$\delta K(x_f, x_0; t_f, t_0) = \delta x_f \int_{x(t_0)}^{x(t_f)} \mathcal{D} x \frac{i}{\hbar} \left(\frac{\partial L}{\partial \dot{x}}\right)_{t_f} \exp\left(\frac{iS}{\hbar}\right)$$
$$= \delta x_f \int_{x(t_0)}^{x(t_f)} \mathcal{D} x \frac{i}{\hbar} p(t_f) \exp\left(\frac{iS}{\hbar}\right).$$
(5.8.3.4.6)

Comparing Eq. (5.8.3.4.6) with Eq. (5.8.3.4.1) yields

$$\int_{x(t_0)}^{x(t_f)} \mathcal{D}x \frac{\partial}{\partial x_f} \exp\left(\frac{iS}{\hbar}\right) = \int_{x(t_0)}^{x(t_f)} \mathcal{D}x \frac{i}{\hbar} p(t_f) \exp\left(\frac{iS}{\hbar}\right).$$
(5.8.3.4.7)

From Eq. (5.8.3.4.7) we obtain

$$\frac{\partial}{\partial x_f} = \frac{i}{\hbar} p(t_f), \text{ or } p = -i\hbar \frac{\partial}{\partial x}.$$
 (5.8.3.4.8)

From Eq. (5.8.3.4.8) we obtain

$$[x, p] = i\hbar. \tag{5.8.3.4.9}$$

#### Derivation of Schrödinger equation. Eq. (5.8.3.2.3) is

$$\Psi(x,t) = \int dx_0 K(x,x_0;t,t_0) \Psi(x_0,t_0).$$
 (5.8.3.2.3)

The propagator  $K(x,x_0;t,t_0)$  is given by Eq. (5.8.3.2.28). Eq. (5.8.3.2.3)' shows that the propagator K is the kernel of the integral equation satisfied by the wavefunction. Next, let us demonstrate that the wavefunction  $\psi(x,t)$  satisfies Schrödinger wave equation.

To do this we need to seek the time partial derivative of  $\psi(x,t)$ . We expand the  $\psi(x,t+\varepsilon)$  in terms infinitesimal time  $\varepsilon$ ,

$$\Psi(x,t+\varepsilon) = \int dy K(x,y;t+\varepsilon,t)\Psi(y,t). \qquad (5.8.3.4.10)$$

From Eq. (5.8.3.2.27) we know

$$K(x,y;t+\varepsilon,t) = \sqrt{\frac{m}{2i\pi\hbar\varepsilon}} \exp\left\{\frac{i\varepsilon}{\hbar} \left[\frac{m}{2}\left(\frac{x-y}{\varepsilon}\right)^2 - V(y)\right]\right\} [1+0(\varepsilon^2)]. \quad (5.8.3.4.11)$$

Substituting Eq. (5.8.3.4.11) into Eq. (5.8.3.4.10) and making variable transformation  $y \rightarrow x + \eta$ , one obtains

$$\begin{aligned} \Psi(x,t+\varepsilon) &= \sqrt{\frac{m}{2i\pi\hbar\varepsilon}} \int_{-\infty}^{\infty} d\eta \exp\left\{\frac{im}{2\hbar\varepsilon}\eta^2\right\} \left[1 - \frac{i}{\hbar}\varepsilon V(x+\eta)\right] \\ &\times \quad \Psi(x+\eta,t)[1+0(\varepsilon^2)]. \end{aligned}$$
(5.8.3.4.12)

Due to that  $\varepsilon \to 0$  is very small, therefore, if  $\eta$  is large, then the exponential function oscillates strongly. Thus, we conclude that the main contribution to the integration comes from the region:  $0 \le |\eta| \le (2\pi\hbar\varepsilon/m)^{1/2}$ . Next steps are: Make Taylor expansions of the

functions  $\psi(x+\eta,t)$  and  $V(x+\eta)$  in the integrand, and keep the first order of  $\varepsilon$ ; Treat the expansion expression by using the following formulas:

$$\int_{-\infty}^{\infty} d\eta \exp\left\{\frac{im}{2\hbar\epsilon}\eta^2\right\} = \left(\frac{i2\pi\hbar\epsilon}{m}\right)^{1/2},$$
$$\int_{-\infty}^{\infty} d\eta\eta \exp\left\{\frac{im}{2\hbar\epsilon}\eta^2\right\} = 0,$$
$$\int_{-\infty}^{\infty} d\eta\eta^2 \exp\left\{\frac{im}{2\hbar\epsilon}\eta^2\right\} = \left(\frac{i2\pi\hbar\epsilon}{m}\right)^{1/2}\frac{i\hbar\epsilon}{m}$$

At last we obtain

$$\begin{aligned} \Psi(x,t+\varepsilon) &= \sqrt{\frac{m}{2i\pi\hbar\varepsilon}} \int_{-\infty}^{\infty} d\eta \exp\left\{\frac{im}{2\hbar\varepsilon}\eta^2\right\} \left[1 - \frac{i\varepsilon}{\hbar}V(x) + 0(\varepsilon^2)\right] \\ &\times \left[\Psi(x,t) + \eta\Psi'(x,t) + \frac{\eta^2}{2}\Psi''(x,t) + 0(\eta^3)\right] \\ &= \Psi(x,t) - \frac{i\varepsilon}{\hbar}V(x)\Psi(x,t) + \frac{i\hbar\varepsilon}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + 0(\varepsilon^2). \end{aligned}$$
(5.8.3.4.13)

Eq. (5.8.3.4.13) indicates that

$$\frac{\partial}{\partial t}\psi(x,t) = \lim_{\varepsilon \to 0} \frac{\psi(x,t+\varepsilon) - \psi(x,t)}{\varepsilon} = -\frac{i}{\hbar} \left( V(x) - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \psi(x,t).$$
(5.8.3.4.14)

Eq. (5.8.3.4.14) is the Schrödinger equation.

On the other hand, the Feynman propagator itself satisfies Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} K(x, x_0; t, t_0) = \langle x | He^{-iH(t-t_0)/\hbar} | x_0 \rangle$$
  
=  $\left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial t^2} + V(x) \right) K(x, x_0; t, t_0),$  (5.8.3.4.15)

and boundary condition

$$K(x, x_0; t, t_0) =_H < x, t | x_0, t >_H = \delta(x - x_0).$$
(5.8.3.4.16)

#### 5.8.3.5. One Wrong Application of Path Integral

Let us at first tell you that how to seek the free particle wavefunction  $\psi(x,t)$  by path integral in some references. Some references assumed that the initial free particle is a Gaussian wavepacket. The initial state is:

$$\Psi(x_0, t_0 = 0) = \frac{1}{\sqrt{a}\sqrt{2\pi}} e^{ik_0 x_0} e^{-x_0^2/(4a^2)},$$
(5.8.3.5.1)

which is normalized. Substituting the propagator in Eq. (5.8.3.3.3) and the initial wave-function in Eq. (5.8.3.5.1) into the Eq. (5.8.3.2.3) yields

$$\begin{split} \Psi(x,t) &= \frac{1}{\sqrt{a}\sqrt{2\pi}} \int_{-\infty}^{\infty} dx_0 \left[ \exp\left(ik_0 x_0 - \frac{x_0^2}{4a^2}\right) \right] \sqrt{\frac{m}{2\pi i \hbar t}} \exp\left[\frac{i}{\hbar} \frac{m(x-x_0)^2}{2t}\right] \\ &= \frac{1}{\sqrt{a}(2\pi)^{1/4} \sqrt{1+it/\tau}} \exp[ik_0 (x-\hbar k_0 t/(2m)]] \\ &\times \exp\left[-\frac{(x-\hbar k_0 t/m)^2}{4a^2(1+it/\tau)}\right], \end{split}$$
(5.8.3.5.2)

where  $\tau = 2ma^2/\hbar$ . In derivation the second equality in Eq. (5.8.3.5.2) we use the mathematical formula

$$\int_{-\infty}^{\infty} dy e^{uy^2} e^{vy} = \sqrt{\frac{\pi}{u}} e^{v^2/(4u)}, \quad (Re \ u > 0). \tag{5.8.3.5.3}$$

If Reu = 0, then to obtain a converge integral, first replace the *i* in the first equality of Eq.(5.8.3.5.2) by  $\alpha \equiv i + \varepsilon$ , where  $\varepsilon$  is a small positive number. After integrating, let  $\varepsilon \to 0$ .

The corresponding probability density is

$$P(x,t) = |\Psi(x,t)|^2 = \frac{1}{a(2\pi)^{1/2}\sqrt{1+t^2/\tau^2}} \exp\left[-\frac{(x-\hbar k_0 t/m)^2}{2a^2[1+(t/\tau)^2]}\right].$$
 (5.8.3.5.4)

If we compare this form with the initial probability density we see the generic shape of  $P(x_0,0) = |\Psi(x_0,0)|^2$ , i. e., that of a bell, has remained intact with the following three modification:

(a). It has became wider,  $a \rightarrow (1 + t^2/\tau^2)^{1/2}$ ;

- (b). The center of symmetry of the Gaussian wavepacket is now at  $x = \hbar k_0 t / m$ ;
- (c). The hight of the probability density function has diminished,

$$\frac{1}{a\sqrt{2\pi}} \rightarrow \frac{1}{a\sqrt{2\pi}(1+t^2/\tau^2)^{1/2}}.$$

(d). The area under the curve *P*, at any time, remains unity.

Let us give you a numerical estimation. If we represent a piece of chalk by a wavepacket, a = 1 cm, m = 1 g, there results

$$\tau \approx 10^{27} \ s \approx \ 10^{20} \ year.$$

It is quite clear that the wavepacket begins to distort significantly after a time  $\tau$ . But the universe is only about  $10^{10}$  year old. So some references think that the classical objects are never observed to suffer a quantummechanical spreading.

Let us make an estimation for proton or neutron.  $a \approx 10^{-13}$  cm,  $m \approx 10^{-24}$  g, and thus  $\tau = 2ma^2/\hbar \approx 10^{-23}$  second. Let us make an estimation for electron.  $a \approx 10^{-18}$  cm,  $m \approx 10^{-27}$  g, and thus  $\tau = 2ma^2/\hbar \approx 10^{-36}$  second. Therefore, according to the these estimations, all free electrons, protons, neutrons, and so on, cannot exist actually. However, the coldneutron experiment in 2010 mentioned in subsection 4.5 of chapter and the photoeffect experiment in 1916 mentioned in chapter 1 observed the stable (at leat more than 300 seconds) neutron and electron, separately. It is obvious that these theoretical derivations from Eq. (5.8.3.5.1) to Eq. (5.8.3.5.4) make mistake, violate the people's basic practice seriously. (At this stage, I hope that the readers to consider how to free from this predicament.)

Some authors also assumed that the initial free wavepacket is a delta function. The mathematical valid expression of the delta function is given by the limit

$$\delta(x) = \lim_{a \to 0} \frac{1}{a\sqrt{2\pi}} e^{-x^2/(2a^2)}.$$
 (5.8.3.5.5)

Of course, we can repeat the derivations from Eq. (5.8.3.5.1) to Eq. (5.8.3.5.4), and obtain the corresponding probability density. It is simple to take the limit  $a \rightarrow 0$  of Eq. (5.8.3.5.4) and obtain results from Eq. (5.8.3.5.4)

$$\lim_{a \to 0} P(x,t) = \lim_{a \to 0} \frac{2ma}{t\hbar(2\pi)^{1/2}} \exp\left[-\frac{2a^2(x-\hbar k_0 t/m)^2}{t^2\hbar^2/m^2}\right]$$
  
= 
$$\lim_{a \to 0} \frac{2ma}{t\hbar(2\pi)^{1/2}} [1+0(a^2)].$$
 (5.8.3.5.6)

The notation  $0(a^2)$  denotes "order" of  $a^2$ . It stands for a group of terms, the sum of which goes to zero like  $a^2$ , with decreasing a. From Eq. (5.8.3.5.6) we see that for all t > 0,  $\lim P(x,t)$  vanishes uniformly for all x, in the limit  $a \to 0$ . This instantaneous flattening of an infinitely peaked delta function initial state violates the special theory of relativity (the velocity of the propagation of perturbation is much larger than the light speed c).

Until now that, where is the mistake in, has not yet been pointed out by all until now references and textbooks. However, actually, this textbook thinks that the answer is simple. The answer is that the Feynman path integral formulation of quantum mechanics is correct, and the mistake in some references is in that the initial free state wavefunctions are not a reasonable assumption. The initial free wavefunctions has to satisfy the Schrödinger equation. Both the Gaussian and the delta function wavefunctions do not satisfy Schrödinger equation of free particle at all.

A free particle has to be described by a plane wave. Next, we prove that if the initial free state wavefunction is a plane wave, then path integral formulation will also give a plane wave final state wavefunction. Let us show you. Suppose that the initial state free particle wavefunction is a plane wave with momentum p:

$$\Psi(x_0, t_0) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx_0/\hbar} \frac{1}{\sqrt{2\pi\hbar}} e^{iE_0 t_0/\hbar}.$$
(5.8.3.5.7)

For simplicity, we take  $t_0 = 0$  in the following calculations. Substituting the propagator in Eq. (5.8.3.3.3) and the initial wavefunction in Eq. (5.8.3.5.7) into the Eq. (5.8.3.2.3) yields

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx_0 e^{ipx_0/\hbar} \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left[\frac{i}{\hbar} \frac{m(x-x_0)^2}{2t}\right]$$
  

$$\propto e^{ipx/\hbar} e^{-ip^2 t/(2\hbar m)}.$$
(5.8.3.5.8)

It is easy to verify that both the assumed initial state wavefunction and the final state wavefunction, obtained by path integral formulation, satisfy the following free particle Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t). \qquad (5.8.3.5.9)$$

The wavefunction in Eq. (5.8.3.5.8) is an oscillation function with time *t*, and thus it always does not decay.

# 5.9. Exercises and Solutions

(1) Find the eigenfunction of the z component,  $L_z = -i\hbar\partial/\partial\phi$ , of angular momentum.

Solution:

The eigenequation is

$$-i\hbar\frac{\partial\Phi}{\partial\phi} = l_z\Phi,\tag{1}$$

where  $l_z$  is the eigenvalue. Eq. (1) can be written as

$$\frac{\partial ln\Phi}{\partial \phi} = \frac{il'_z}{\hbar}.$$
(2)

The solution of Eq. (2) is

$$\Phi(\phi) = C e^{\frac{i l_z \phi}{\hbar}}.$$
(3)

The *C* is an integration constant, can be determined by the normalization condition. After rotating one circle around *z* axis,  $\phi \rightarrow \phi + 2\pi$ , the particle returns to the previous position. As an operator corresponding to an observable,  $L_z = -i\hbar\partial/\partial\phi$  must be a hermitian operator.

Let us demonstrate a theorem on the boundary condition of any eigenfunction of operator  $L_z$ .

**Theorem XXXI: Eigenfunction of**  $L_z$ . To ensure that  $L_z$  is a hermitian operator, any eigenfunction of  $L_z$  must satisfy periodic boundary condition (or, single value condition).

**Proof.** According to definition, if  $L_z$  is a hermitian operator, then  $(\Phi, L_z \Psi) = (L_z \Phi, \Psi)$ . Here  $\Phi$  and  $\Psi$  are any two states of the particle. In position representation

$$\begin{aligned} (\Phi, L_z \Psi) &= \int_0^{2\pi} d\phi \frac{\hbar}{i} \Phi^*(\Phi) \frac{\partial \Psi(\phi)}{\partial \phi} \\ &= \frac{\hbar}{i} \Phi^*(\phi) \Psi(\phi) \Big|_0^{2\pi} - \int_0^{2\pi} d\phi \frac{\hbar}{i} \left( \frac{\partial \Phi^*}{\partial \phi} \right) \Psi \\ &= \frac{\hbar}{i} \Phi^*(\phi) \Psi(\phi) \Big|_0^{2\pi} + (L_z \Phi, \Psi). \end{aligned}$$

Therefore,

$$\Phi^*(2\pi)\Psi(2\pi) - \Phi^*(0)\Psi(0) = 0, \tag{4}$$

that is,

$$\frac{\Psi(2\pi)}{\Psi(0)} = \frac{\Phi^*(0)}{\Phi^*(2\pi)}.$$
(5)

The ratio in Eq. (5) is the same for all wavefunctions  $\Psi$ ,  $\Phi$ ,  $\cdots$ . From Eq. (3) the eigenfunction corresponding to  $l'_z = 0$  is  $\Phi(\phi) = C$ . Thus  $\Phi^*(0)/\Phi^*(2\pi) = 1$ . From Eq. (5)  $\Psi(2\pi)/\Psi(0) = 1$ . Therefore, for any wavefunction  $\Psi(\phi)$ , we have  $\Psi(2\pi) = \Psi(0)$ , which is the so-called periodic boundary condition. Here we conclude the proof. QED.

Using the above theorem, we have

$$\Phi(\phi + 2\pi) = \Phi(\phi). \tag{6}$$

From Eq. (6) the eigenvalues of z component of angular moment operator  $L_z$  are

$$l'_{z} = m\hbar \quad (m = 0, \pm 1, \pm 2, \cdots) \quad .$$
 (7)

Eq. (7) indicates that  $l'_z$  is quantized. The corresponding eigenfunction is

$$\Phi_m(\phi) = C e^{im\phi}.$$
(8)

Using the normalization condition we can determine the C.

$$\int_{0}^{2\pi} d\phi |\Phi_m(\phi)|^2 = 2\pi |C|^2 = 1.$$
(9)

We often choose *C* is a positive real number,  $C = 1/\sqrt{2\pi}$ . Therefore, the normalized wave-function is

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}.$$
 (10)

It is to show that  $\Phi_m$  is orthogonal.

$$(\Phi_m, \Phi_n) = \int_0^{2\pi} d\phi \Phi^*(\phi) \Phi(\phi) = \delta_{mn}.$$
 (11)

(2) Find the energy eigenvalue of a rotor around z axis.

Solution:

The classical energy of a rotor around z axis is  $l_z^2/2I$ . I is rotation inertia.  $l_z$  is angular momentum. In quantum mechanics, the Hamilton operator of corresponding rotor is

$$H = \frac{l_z^2}{2I} = -\frac{\hbar^2}{2I} \frac{\partial^2}{\partial \phi^2}.$$
 (5.9.2.1)

The eigenequation is

$$-\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2}\Psi = E\Psi.$$
(5.9.2.2)

The wavefunction satisfying periodic boundary condition and orthonormal condition is

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \quad m = 0, \pm 1, \pm 2, \cdots .$$
 (5.9.2.3)

The corresponding energy is

$$E_m = \frac{m^2 \hbar^2}{2I} \ge 0. \tag{5.9.2.4}$$

Note that one energy eigenvalue corresponds to two eigenfunction (except m = 0), i. e.,  $\exp \pm i |m| \phi$ , where

$$|m| = \sqrt{\frac{2IE_m}{\hbar^2}}, \quad (|m| = 1, 2, \cdots) ,$$
 (5.9.2.5)

i. e., the energy level is two-fold degenerate.

(3) Find the eigenstate of x component of momentum,  $p_x = -i\hbar\partial/\partial x$ .

Solution:

The eigenequation is

$$-i\hbar\frac{\partial}{\partial x}\Psi = p'_{x}\Psi, \qquad (5.9.3.1)$$

where  $p'_x$  is eigenvalue of momentum. Obviously,

$$\frac{\partial ln\Psi}{\partial x} = \frac{ip'_x}{\hbar}.$$
(5.9.3.2)

Therefore,

$$\Psi_{p'_x} = C e^{\frac{i p'_x x}{\hbar}}, \tag{5.9.3.3}$$

where *C* is the integration constant. If the position of particle does not have limit, then  $p'_x$  can take any real number in  $-\infty < p'_x < \infty$ , and is continuous. Eq. (5.9.3.3) is a plane wave, and cannot be normalized. However, one often takes

$$\Psi_{p'_{x}}(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ip'_{x}x}{\hbar}}.$$
(5.9.3.4)

It is easy to show that

$$\int_{-\infty}^{+\infty} dx \Psi_{p_x'^*}(x) \Psi_{p_x''}(x) = \delta(p_x' - p_x'').$$
(5.9.3.5)

In this problem we have to note that it is that a wavepacket other than a plane wave represents the real particle.

(4) Find the energy eigenstate of one dimensional free particle.

Solution:

For one dimensional free particle, Hamiltonian is  $H = p_x^2/(2m) = -\hbar^2/(2m)\partial^2/\partial x^2$ . Eigenequation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi = E\Psi.$$
(5.9.4.1)

The solutions can be taken as

$$\Psi_E(x) \propto e^{\pm ik_x x}, \quad k_x = \sqrt{\frac{2mE}{\hbar^2}} \ge 0 \quad . \tag{5.9.4.2}$$

The corresponding energy is

$$E = \frac{\hbar^2 k_x^2}{2m} \ge 0. \tag{5.9.4.3}$$

Because  $k_x > 0$  and  $k_x < 0$  correspond to the same energy, the energy level is two-fold degenerate.

(5) Show the Hermiticity of the momentum operator  $p_x = -i\hbar\partial/\partial x$ .

Solution:

Let us look at the matrix elements of  $p_x$ .

$$(p_x)_{12} = (\Psi_1, p_x \Psi_2) = \int_{-\infty}^{\infty} dr \Psi_1^* \left( -i\hbar \frac{\partial}{\partial x} \right) \Psi_2$$
  
$$= -i\hbar \int_{-\infty}^{\infty} dr \Psi_1^* \left( \frac{\partial}{\partial x} \right) \Psi_2$$
  
$$= -i\hbar \Psi_2 \Psi_1^* \Big|_{-\infty}^{\infty} + i\hbar \int_{-\infty}^{\infty} dr \Psi_2 \left( \frac{\partial}{\partial x} \right) \Psi_1^*$$
  
$$= i\hbar \int_{-\infty}^{\infty} dr \Psi_2 \left( \frac{\partial}{\partial x} \right) \Psi_1^*$$
  
$$= ((p_x \Psi_1), \Psi_2),$$

where we consider that  $\Psi_1$  and  $\Psi_2$  are square-integrable functions, and thus

$$\Psi_2\Psi_1^*\big|_{-\infty}^{\infty}=0.$$

(6) Compute the commutator  $[p_x, x]$ .

Solution: Since

$$p_{x}x\Psi = -i\hbar\frac{\partial}{\partial x}(x\Psi) = -i\hbar\left(\Psi\frac{\partial x}{\partial x} + x\frac{\partial\Psi}{\partial x}\right) = -i\hbar\left(\Psi + x\frac{\partial\Psi}{\partial x}\right)$$

and

$$xp_x\Psi = x\left(i\hbar\frac{\partial\Psi}{\partial x}\right) = -i\hbar x\frac{\partial\Psi}{\partial x}$$

We easily obtain

$$[p_x, x] = p_x x - x p_x = -i\hbar.$$

(7) Let L,  $L_1$ ,  $L_2$ ,  $L_3$ , M be linear operators in a complex linear space. Show (with the help of the definition of a commutator) the some commutation rules for commutators.

Solution:

We use the definition [L,M]=LM-ML.

$$\begin{bmatrix} L_1 L_2, M \end{bmatrix} = L_1 L_2 M - M L_1 L_2 = L_1 M L_2 - M L_1 L_2 + L_1 L_2 M - L_1 M L_2 = [L_1, M] L_2 + L_1 [L_2, M]$$

$$\begin{split} [M,L_1L_2] &= -[L_1L_2,M] = -[L_1,M]L_2 - L_1[L_2,M] \\ &= L_1[M,L_2] + [M,L_1]L_2 \end{split}$$

$$\begin{aligned} [L_1, [L_2, L_3]] &= [L_1 L_2 L_3] - [L_1 L_2, L_3] \\ &= [L_1, L_2] L_3 + L_2 [L_1, L_2] - [L_1, L_3] L_2 - L_3 [L_1, L_2] \\ &= -[L_3, [L_1, L_2]] - [L_2, [L_3, L_1]] \end{aligned}$$

The last equation is also called Jacobi identity.

(8) Let A and B be Hermitian operators, C = -i[A,B], and  $D = \{AB + BA\}$ . Prove the following inequality of average values:

$$\geq \frac{1}{4}[+].$$

Solution:

Let  $\Phi(x,t)$  be an arbitrary state,  $\lambda = \alpha + i\beta$  be a complex number. We define

$$0 \le l(\lambda) = \int |(A+i\lambda B)\Phi|^2 dx$$
  
=  $\int \Phi^* (A-i\lambda^* B)(A+i\lambda B)\Phi dx$   
=  $\int \Phi^* A^2 \Phi dx + |\lambda|^2 \int \Phi^* B^2 \Phi dx + \int \Phi^* (ABi\lambda - BAi\lambda)\Phi dx$   
=  $\langle A^2 \rangle + \langle B^2 \rangle |\lambda|^2 - \alpha \langle C \rangle - \beta \langle D \rangle$ 

With

$$< B^{2} > \left[ \alpha - \frac{}{2 < B^{2} >} \right]^{2} = \alpha^{2} < B^{2} > -\alpha < C > + \frac{}{4 < B^{2} >}$$

and

$$< B^{2} > \left[\beta - \frac{}{2 < B^{2}>}\right]^{2} = \beta^{2} < B^{2} > -\beta < C > + \frac{}{4 < B^{2}>}$$

we now have

$$< A^{2} > + < B^{2} > \left[\alpha - \frac{}{2 < B^{2} >}\right]^{2}$$
$$+ < B^{2} > \left[\beta - \frac{}{2 < B^{2} >}\right]^{2} - \frac{}{4 < B^{2} >} - \frac{}{4 < B^{2} >} \ge 0$$

But  $\alpha$  and  $\beta$  can be chosen arbitrarily, i. e.,

$$< A^2 > < B^2 > \ge \frac{1}{4} (< C^2 > + < D^2 >)$$

must hold.

(9) Prove

$$T(a) = e^{ip \cdot a/\hbar}$$
 with  $p = -i\hbar \nabla$ .

Solution:

Let wavefunction can be expandable in its Taylor series. Then we have:

$$T(a)\Psi(r) = e^{i\frac{p\cdot a}{\hbar}}\Psi(r) = \sum_{n=0}^{\infty} \frac{1}{n!} \left[i\frac{(-i\hbar\nabla)\cdot a}{\hbar}\right]^n \Psi(r)$$
$$= \sum_{n=0}^{\infty} \frac{(a\cdot\nabla)^n}{n!}\Psi(r) = \Psi(r+a)$$

as the penultimate expression is simply the shorthand notation for the Taylor expansion of the function of [r+a] at the point **r**.

(10) If operator A is Hermitian, show

$$\langle A^2 \rangle \geq 0$$

Solution:

$$=\int_{-\infty}^{\infty}\Psi^{*}A^{2}\Psi dx=\int_{-\infty}^{\infty}(A\Psi)^{*}A\Psi dx$$
$$=\int_{-\infty}^{\infty}|A\Psi|^{2}dx\geq0.$$

(11) Prove that if

$$\int \Psi^* H \Psi dx$$

is minimum, then the normalized wavefunction is the ground state.

Solution:

It is easy to verify that the wavefunctions for a particle in a one dimensional box with walls at x = 0 and *a* satisfy the equality

$$\int_0^a \Psi^* \Psi_{xx} dx = -\int_0^a |\Psi_x|^2 dx, \qquad (5.9.11.1)$$

where the subscript x denotes differentiation. Apart from a constant factor and with the Eq. (5.9.11.1), we may write

$$< H > = -\int_{0}^{a} \Psi_{x}^{2} dx.$$
 (5.9.11.2)

Let  $\Psi$  minimize  $\langle H \rangle$ . Then infinitesimal variation of  $\Psi$  causes no change in  $\langle H \rangle$ . Let  $\Psi \rightarrow \Psi + \delta \Psi$ . The variation  $\delta \Psi$  is an arbitrary infinitesimal function of *x* that vanishes at x = 0 and *a*. Then

$$\langle H \rangle = \int \Psi_x^2 dx \to \int (\Psi_x + \delta \Psi_x)^2 dx = \langle H \rangle + \delta \langle H \rangle.$$
 (5.9.11.3)

$$\delta < H >= 2 \int \Psi_x \delta \Psi_x dx = 2 \int \Psi_x \frac{d}{dx} \delta \Psi dx = 0.$$
 (5.9.11.4)

Integrating the last term by parts and dropping the "surface" terms gives

$$\int \Psi_{xx} \delta \Psi dx = 0. \tag{5.9.11.5}$$

Variation of the normalization statement (both  $\Psi$  and  $\Psi + \delta \Psi$  are normalized) gives

$$\lambda \int \Psi \delta \Psi dx = 0, \qquad (5.9.11.6)$$

where  $\lambda$  is an arbitrary undetermined multiplier. Combining the last two equations yields

$$\int \delta \Psi (\Psi_{xx} - \lambda \Psi) dx = 0.$$
 (5.9.11.7)

If this equation is to be satisfied for an arbitrary variation of  $\Psi$  about the minimizing value, we may conclude

$$\Psi_{xx} = \lambda \Psi, \tag{5.9.11.8}$$

where  $\Psi$  is an eigenstate of *H*. It follows that, in any eigenstate,  $\langle H \rangle$  is stationary and is minimum in the ground state.

(12) Let  $O_{nl} \equiv \langle \Phi_n | O \Phi_l \rangle$ , show that  $(O^+)_{ln} = (O_{nl})^*$ .

Solution:

$$O_{nl} = \langle \Phi_n | O \Phi_l \rangle \ = \langle O \Phi_l | \Phi_n \rangle^*$$

Taking the complex conjugate of the last and first terms in this equality gives the desired result.

(13) Employing Hermitian property of H, show that, in general, extreme values of  $\langle H \rangle$  yield the eigenfunction of H, and that any eigenfunction of H makes  $\langle H \rangle$  an extremum. Your derivation should be independent of the specific boundary conditions.

Solution:

To incorporate the wavefunction normalization in the analysis we write

$$\langle H \rangle = \frac{\langle \Psi | H \Psi \rangle}{\langle \Psi | \Psi \rangle}.$$
 (5.9.13.1)

Taking the variation of Eq. (5.9.13.1) yields

$$\begin{aligned} (<\Psi|\Psi>)^2 \delta < H> &= -<\Psi|H\Psi>[<\delta\Psi|\Psi>+<\Psi\delta\Psi>] \\ &+ <\Psi|\Psi>[<\delta\Psi|H\Psi>+<\Psi|H\delta\Psi>]+0[(\delta\Psi)^2] \end{aligned}$$

Neglecting terms of  $0[(\delta\Psi)^2]$ , and recalling the Hermiticity of H, the preceding equation becomes

$$(\langle \Psi|\Psi\rangle)^2 \delta \langle H\rangle = -\langle \Psi|H\Psi\rangle [\langle \delta\Psi|\Psi\rangle + \langle \Psi\delta\Psi\rangle] + \langle \Psi|\Psi\rangle [\langle \delta\Psi|H\Psi\rangle + \langle \Psi|H\delta\Psi\rangle]$$

With  $\langle \Psi | H\Psi \rangle = \lambda$  and  $\langle \Psi | \Psi \rangle = 1$ , it follows that any wavefunction  $\Psi$  which makes  $\delta \langle H \rangle = 0$ , to first order in  $\delta \Psi$ , gives

$$0 = 2Re < \delta \Psi, (-\lambda + H)\Psi >$$

If we label  $< \delta \Psi$ ,  $(-\lambda + H)\Psi > \equiv z$ , where z is a complex number, then the preceding statement remain valid if  $\delta \Psi$  is multiplied by z, in which case the preceding gives

$$< \delta \Psi, (-\lambda + H)\Psi >= 0$$

If this relation is to be satisfied for any arbitrary variation  $\delta \Psi$ , then it must be the case that  $H\Psi = \lambda \Psi$ . Furthermore, it is clear from the equation above for  $\delta < H >$ , that any eigenfunction of *H* makes < H > an extremum.

(14) Give the forms of position and momentum operators of a free particle in Heisenberg picture.

Solution: For a free particle

$$H = \frac{p^2}{2m}.$$
 (5.9.14.1)

Substituting Eq. (5.9.14.1) into Eq. (5.7.3.10) yields

$$i\hbar \frac{dp_H}{dt} = [p_H, H] = 0.$$
 (5.9.14.2)

From Eq. (5.9.14.2) the momentum operator of free particle in Heisenberg picture is

$$p_H(t) = p_H(t_\circ) = p_H(0) = constant = p_S$$

Substituting Eqs. (5.9.14.1) and (5.7.3.7) into Eq. (5.7.3.10) yields

$$\frac{dx_{H}}{dt} = \frac{1}{i\hbar} [x_{H}, H] = \frac{1}{i\hbar} \left[ e^{\frac{i}{\hbar}H(t-t_{\circ})} x_{S} e^{-\frac{i}{\hbar}H(t-t_{\circ})}, H \right]$$
$$= \frac{1}{i\hbar} e^{\frac{i}{\hbar}H(t-t_{\circ})} \left[ x_{S}, \frac{p_{S}^{2}}{2m} \right] e^{-\frac{i}{\hbar}H(t-t_{\circ})} = e^{\frac{i}{\hbar}H(t-t_{\circ})} \frac{p_{S}}{m} e^{-\frac{i}{\hbar}H(t-t_{\circ})} = \frac{p_{H}}{m}.$$
(5.9.14.3)

From Eq. (5.9.14.3) we have the position operator of free particle in Heisenberg picture is

$$x_H(t) = x_H(t_\circ) + \frac{p_H}{m}t.$$
 (5.9.14.4)

(15) Discussion one dimensional oscillator in Heisenberg picture.

Solution:

$$H_S = H_H = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

$$x_H(t) = e^{i\frac{Ht}{\hbar}} x_S e^{-i\frac{Ht}{\hbar}}$$

$$p_{x,H}(t) = e^{i\frac{Ht}{\hbar}} p_{x,S} e^{-i\frac{Ht}{\hbar}}.$$
(5.9.15.1)

It is easy to find that

$$\frac{dx_H(t)}{dt} = \frac{1}{i\hbar} e^{i\frac{Ht}{\hbar}} [x_S, H] e^{-i\frac{Ht}{\hbar}} = \frac{p_{x,H}(t)}{m}$$
$$\frac{dp_{x,H}(t)}{dt} = \frac{1}{i\hbar} e^{i\frac{Ht}{\hbar}} [p_{x,S}, H] e^{-i\frac{Ht}{\hbar}} = -m\omega^2 x_H(t).$$
(5.9.15.2)

Therefore,

$$\frac{d^2}{dt^2}x_H(t) = \frac{1}{m}\frac{dp_{x,H}(t)}{dt} = -\omega^2 x_H(t),$$
(5.9.15.3)

which is similar to the Newton equation of one-dimensional harmonic oscillator. The solution of Eq. (5.9.15.3) is

$$x_H(t) = c_1 cos \omega t + c_2 sin \omega t$$
$$p_{x,H}(t) = m \frac{dx_H(t)}{dt} = -m \omega sin \omega t + m c_2 \omega cos \omega t.$$
(5.9.15.4)

If the initial condition is

$$x_H(0) = c_1 = x_o$$

$$p_{x,H}(0) = mc_2 \omega = p_o$$

$$c_2 = \frac{p_o}{m\omega},$$
(5.9.15.4)

then

$$x_{H}(t) = x_{\circ} cos \omega t + \frac{p_{\circ}}{m\omega} sin \omega t$$
$$p_{x,H}(t) = -m \omega x_{\circ} sin \omega t + p_{\circ} cos \omega.$$
(5.9.15.5)

(16) The project operator  $P_n$  is defined

$$P_n = |n|, \tag{5.9.16.1}$$

where  $|n\rangle$  is a normalized state. Applying  $P_n$  to an arbitrary state  $|\Psi\rangle$ 

$$P_n |\Psi\rangle = |n\rangle < n |\Psi\rangle = < n |\Psi\rangle |n\rangle.$$
(5.9.16.2)

Eq. (5.9.16.2) indicates that after acting of  $P_n$  on  $|\Psi\rangle$  we obtain a ket  $|n\rangle$  multiplied a constant  $\langle n|\Psi\rangle$ . We can say that the operator  $P_n$  projects  $|\Psi\rangle$  on to  $|n\rangle$ .

Prove

$$P_n^2 = P_n. (5.9.16.3)$$

Solution:

Consider

$$P_m P_n = |m| > < m|n| > < n| = \delta_{mn} |m| > < n| = P_n.$$
(5.9.16.3)

Eq. (5.9.16.4) gives Eq. (5.9.16.3). The Eq. (5.9.16.3) states that once a state is projected into a particular state, then a further projection on to that state does not change anything.

(17) Show that the matrix representation of  $P_n$  has eigenvalue zero and one.

Solution: From Eq. (5.9.16.3) we have

$$P_n(P_n-1) = 0. (5.9.46.1)$$

From Eq. (5.9.46.1) the projection operator has the value zero and one, i. e., the matrix representation of  $P_n$  has eigenvalue zero and one.

# Chapter 6

# Angular Momentum and Hydrogen-Like Atoms

# 6.1. Orbital Angular Momentum

# 6.1.1. Definition

Angular momentum is one of the fundamental constants of motion together with linear momentum and energy of an isolated system. In classical mechanics the angular momentum  $\mathbf{L}$  of a particle of mass *m* about the origin *O* is defined as

$$L = r \times p, \tag{6.1.1.1a}$$

where  $\mathbf{r}$  and  $\mathbf{p}$  represent the position and linear momentum of the particle.

Quantummechanically, we know  $p = -i\hbar\nabla$ . Thus Eq. (6.1.1.1a) can be rewritten as

$$L = -i\hbar r \times \nabla. \tag{6.1.1.1b}$$

The components of L are

$$L_x = yp_z - zp_y = -i\hbar \left( y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right).$$
(6.1.1.2*a*)

$$L_{y} = zp_{x} - xp_{z} = -i\hbar \left( z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right).$$
(6.1.1.2*b*)

$$L_z = xp_y - yp_x = -i\hbar \left( x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right).$$
(6.1.1.2c)

Utilizing the fundamental commutator

$$[x_{\alpha}, p_{\beta}] = i\hbar \delta_{\alpha\beta}, \qquad (6.1.1.3)$$

one can show the following commutation relations:

$$[L_x, x] = 0, \quad [L_x, y] = i\hbar z, \quad [L_x, z] = i\hbar y$$

$$\begin{split} [L_{y}, x] &= -i\hbar z, \quad [L_{y}, y] = 0, \quad [L_{y}, z] = i\hbar x \\ [L_{z}, x] &= i\hbar y, \quad [L_{z}, y] = -i\hbar z, \quad [L_{z}, z] = 0 . \end{split}$$
(6.1.1.4)  
$$[L_{x}, p_{x}] &= 0, \quad [L_{x}, p_{y}] = i\hbar p_{z}, \quad [L_{x}, z] = i\hbar p_{y} \\ [L_{y}, p_{x}] &= -i\hbar p_{z}, \quad [L_{y}, p_{y}] = 0, \quad [L_{y}, p_{z}] = i\hbar p_{x} \\ [L_{z}, p_{x}] &= i\hbar p_{y}, \quad [L_{z}, p_{y}] = -i\hbar p_{x}, \quad [L_{z}, p_{z}] = 0. \end{split}$$

If one writes x, y, z as  $x_1, x_2, x_3$  and  $L_x, L_y, L_z$  as  $L_1, L_2, L_3$ , then one can rewrite Eq. (6.1.1.4) as

$$[L_{\alpha}, x_{\beta}] = \varepsilon_{\alpha\beta\gamma} i\hbar x_{\gamma}, \qquad (6.1.1.5)$$

where  $\varepsilon_{\alpha\beta\gamma}$  is called Levi-Civita notation. It is a totally antisymmetric tensor in three dimensins, which's definition is:

$$\varepsilon_{\alpha\beta\gamma} = -\varepsilon_{\beta\alpha\gamma} = -\varepsilon_{\alpha\gamma\beta} \quad \varepsilon_{123} = 1 \quad , \tag{6.1.1.6a}$$

where  $\alpha, \beta, \gamma = (1, 2, 3)$ . For the permutation of subscripts in  $\varepsilon_{\alpha\beta\gamma}$ , its sign should be changed. Thus, if two subscripts are the same, then  $\varepsilon_{\alpha\beta\gamma}$  is zero, for example  $\varepsilon_{112} = \varepsilon_{121} = 0$ . The Eq. (6.1.1.6a) can be written in the following better form:

$$\varepsilon_{\alpha\beta\gamma} = \begin{cases} +1, & if \ \alpha, \beta, \gamma \ is \ an \ even \ permutation \ of \ 1, 2, 3 \\ -1, & if \ \alpha, \beta, \gamma \ is \ an \ odd \ permutation \ of \ 1, 2, 3 \\ 0 & if \ two \ or \ more \ subscripts \ are \ equal \end{cases}$$
(6.1.1.6b)

Similarly, one can show that

$$[L_{\alpha}, p_{\beta}] = \varepsilon_{\alpha\beta\gamma} i\hbar p_{\gamma}, \qquad (6.1.1.7)$$

$$[L_{\alpha}, L_{\beta}] = \varepsilon_{\alpha\beta\gamma} i\hbar L_{\gamma}, \qquad (6.1.1.8)$$

Eq. (6.1.1.8) can be written explicitly.

$$[L_x, L_y] = i\hbar L_z, \quad [L_y, L_z] = i\hbar L_x, \quad [L_z, L_x] = i\hbar L_y \quad . \tag{6.1.1.9a}$$

Eq. (6.1.1.9) tells us that the operators representing any two components of angular momentum do not commute and therefore the corresponding observable cannot be simultaneously measured. The commutator relations in Eq. (6.1.1.9a) are some times combined in the single vector equation

$$i\hbar L = L \times L, \tag{6.1.1.9b}$$

which in determinant form appears as

$$i\hbar(e_{x}L_{x}+e_{y}L_{y}+e_{z}L_{z}) = \begin{vmatrix} e_{x} & e_{y} & e_{z} \\ L_{x} & L_{y} & L_{z} \\ L_{x} & L_{y} & L_{z} \end{vmatrix}.$$
 (6.1.1.9c)

$$[L_x, L_x] = [L_y, L_y] = [L_z, L_z] = 0.$$
(6.1.1.10)

The Eqs. (6.1.1.9) and (6.1.1.10) can be written in an equivalent form as

$$L \times L = i\hbar L$$
 or also  $[L_{\alpha}, L_{\beta}] = i\hbar \epsilon_{\alpha\beta\gamma} L_{\gamma}$ . (6.1.1.1)



Figure 6.1. The spherical polar coordinates  $(r, \theta, \phi)$  of a space point P.

The square of angular momentum is

$$L^2 = L_x^2 + L_y^2 + L_z^2. (6.1.1.12)$$

The commutator of  $L^2$  with  $L_z$  is

$$[L^{2}, L_{z}] = [L_{x}^{2} + L_{y}^{2} + L_{z}^{2}, L_{z}] = [L_{x}^{2}, L_{z}] + [L_{y}^{2}, L_{z}] + [L_{z}^{2}, L_{z}]$$
  
$$= L_{x}[L_{x}, L_{z}] + [L_{x}, L_{z}]L_{x} + L_{y}[L_{y}, L_{z}] + [L_{y} - L_{z}]L_{y} + 0$$
  
$$= -i\hbar L_{x}L_{y} - i\hbar L_{y}L_{x} + i\hbar L_{x}L_{y} + i\hbar L_{y}L_{x} = 0. \quad (6.1.1.13)$$

Similarly,

$$[L^2, L_x] = [L^2, L_y] = 0 (6.1.1.14)$$

or

$$[L^2, L_{\alpha}] = 0 \quad (\alpha = x, y, z) \quad . \tag{6.1.1.15}$$

From Eq. (6.1.1.15) we see that  $L^2$  commutes with the three components of the angular momentum, therefore total angular momentum and one of its components can be simultaneously measured very precisely.

# 6.1.2. Angular Momentum Operator in Spherical Polar Coordinates

For determining the the eigenvalues and eigenfunctions of the operator  $L^2$ , it is more convenient to express  $L_x$ ,  $L_y$ , and  $L_z$  in spherical polar coordinates r,  $\theta$ , and  $\phi$  rather than in the Cartesian coordinates x, y, and z. The Cartesian coordinates and spherical polar coordinates are related as

$$x = y \sin\theta \cos\phi, \quad y = r \sin\theta \sin\phi, \quad z = r \cos\theta$$
. (6.1.2.1)

$$r = \sqrt{x^2 + y^2 + z^2}, \quad \theta = \arctan\frac{\sqrt{x^2 + y^2}}{z}, \quad \phi = \arctan\frac{y}{x}$$
 (6.1.2.2)

Differentiating r,  $\theta$ , and  $\phi$  with respect to x, y, and z, we have

$$\frac{\partial r}{\partial x} = \sin\theta\cos\phi, \quad \frac{\partial\theta}{\partial x} = \frac{\cos\theta\cos\phi}{r}, \quad \frac{\partial\phi}{\partial x} = \frac{-1}{r}\csc\theta\sin\phi.$$
 (6.1.2.3*a*)

$$\frac{\partial r}{\partial y} = \sin\theta \sin\phi, \quad \frac{\partial \theta}{\partial y} = \frac{\cos\theta \sin\phi}{r}, \quad \frac{\partial \phi}{\partial y} = \frac{1}{r}\csc\theta \cos\phi \quad .$$
 (6.1.2.3b)

$$\frac{\partial r}{\partial z} = \cos\theta, \quad \frac{\partial \theta}{\partial z} = -\frac{\sin\theta}{r}, \quad \frac{\partial \phi}{\partial z} = 0 \quad .$$
 (6.1.2.3c)

Operating  $L_z$  on wavefunction  $\Psi(r, \theta, \phi)$ , one has:

$$L_{z}\Psi(r,\theta,\phi) = -i\hbar \left[ x \frac{\partial\Psi}{\partial y} - y \frac{\partial\Psi}{\partial x} \right]$$
$$-i\hbar \left[ x \left( \frac{\partial\Psi}{\partial r} \frac{\partial r}{\partial y} + \frac{\partial\Psi}{\partial \theta} \frac{\partial \theta}{\partial y} + \frac{\partial\Psi}{\partial \phi} \frac{\partial \phi}{\partial y} \right) - y \left( \frac{\partial\Psi}{\partial r} \frac{\partial r}{\partial x} + \frac{\partial\Psi}{\partial \theta} \frac{\partial \theta}{\partial x} + \frac{\partial\Psi}{\partial \phi} \frac{\partial \phi}{\partial x} \right) \right]. \quad (6.1.2.4)$$

Substituting Eq. (6.1.2.3) into Eq. (6.1.2.4) yields

$$L_z \Psi(r, \theta, \phi) = -i\hbar \frac{\partial \Psi(r, \theta, \phi)}{\partial \phi}, \quad L_z = -i\hbar \frac{\partial}{\partial \phi} \quad .$$
 (6.1.2.5*a*)

Similarly,

=

$$L_x = i\hbar \left[ \sin\phi \frac{\partial}{\partial \theta} + \cot\theta \cos\phi \frac{\partial}{\partial \phi} \right].$$
 (6.1.2.5*b*)

$$L_{y} = i\hbar \left[ -\cos\phi \frac{\partial}{\partial \theta} + \cot\theta \sin\phi \frac{\partial}{\partial \phi} \right]. \qquad (6.1.2.5c)$$

Utilizing Eq. (6.1.2.5) yields

$$L_x^2 \Psi(r, \theta, \phi) = L_x L_x \Psi(r, \theta, \phi) = -\hbar^2 \left[ \sin \phi \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right]$$
$$\left[ \sin \phi \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right] \Psi(r, \theta, \phi). \tag{6.1.2.6}$$

We can also obtains the expressions of  $L_y^2 \Psi(r, \theta, \phi)$  and  $L_z^2 \Psi(r, \theta, \phi)$ . On adding these expressions one obtains

$$L^{2} = -\hbar^{2} \left[ \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left( \sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^{2}\theta} \frac{\partial^{2}}{\partial\phi^{2}} \right]$$
$$= -\frac{\hbar^{2}}{\sin\theta} \frac{\partial}{\partial\theta} \left( \sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^{2}\theta} L_{z}^{2}.$$
(6.1.2.7)

Since the variable *r* does not appear in any one of these operators, their eigenfunctions are independent of *r*. The operator  $L_z$  is also independent of  $\theta$  while  $L_x$ ,  $L_y$ , and  $L^2$  are functions of  $\theta$  and  $\phi$ .

# 6.1.3. Rising and Lowering Operators

In the next subsection we will derive the eigenvalues and eigenfunctions of  $L^2$  and  $L_z$  that follow from the commutation relations Eq. (6.1.1.9a). To facilitate the derivations we introduce the ladder operators  $L_+$  and  $L_-$ . The reader will find that these similar to the annihilation and creation operators (a and  $a^+$ ) introduced for the harmonic oscillator in chapter 4. The ladder operators are defined according to

$$L_{+} = L_{x} + iL_{y}, \quad L_{-} = L_{x} - iL_{y}$$
 (6.1.3.1)

Some immediate properties of these operators are

$$[L_z, L_+] = \hbar L_+, \quad [L_z, L_-] = -\hbar L_-$$
 (6.1.3.2)

$$[L^2, L_+] = 0, \quad [L^2, L_-] = 0$$
 (6.1.3.3)

The Eqs. (6.1.3.2) and (6.1.3.3) follow from Eq. (6.1.1.9a). To establish the two relations in Eq. (6.1.3.2) one merely inserts the definitions of  $L_+$  and  $L_-$ . For example,

$$[L_z, L_+] = [L_z, L_x + il_y] = [L_z, L_x] + i[L_z, L_y] = i\hbar L_y - i \cdot i\hbar L_x = \hbar L_+.$$
(6.1.3.4)

Other relations that  $L_+$  and  $L_-$  satisfy are

$$L^2 = L_- L_+ + L_z^2 + \hbar L_z. \tag{6.1.3.5a}$$

$$L^2 = L_+ L_- + L_z^2 - \hbar L_z. \tag{6.1.3.5b}$$

$$[L_+, L_-] = 2\hbar L_z. \tag{6.1.3.6}$$

$$2(L^2 - L_z^2) = L_+ L_- + L_- L_+.$$
(6.1.3.7)

The ladder operators can be written in spherical polar coordinates by using Eqs. (6.1.2.5b) and (6.1.2.5c).

$$L_{+}\Psi = (L_{x} + iL_{y})\Psi = i\hbar \left[\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right]\Psi$$
$$+i^{2}\hbar \left[-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right]\Psi.$$
(6.1.3.8)

From Eq. (6.1.3.8) one obtains

$$L_{+} = i\hbar e^{i\phi} \left[ -i\frac{\partial}{\partial\theta} + \cot\theta \frac{\partial}{\partial\phi} \right].$$
(6.1.3.9)

Similarly,

$$L_{-} = i\hbar e^{-i\phi} \left[ i\frac{\partial}{\partial\theta} + \cot\theta \frac{\partial}{\partial\phi} \right].$$
 (6.1.3.10)

# **6.1.4.** Eigenvalues and Eigenfunctions of $L^2$ and $L_z$

We have found the eigenvalues and eigenfunctions of the z component of angular momentum operator  $L_z$ . They are given by Eq. (5.8.1.10), and are depicted in the following:

$$L_{z}\Phi(\phi) = -i\hbar\frac{\partial}{\partial\phi}\Phi(\phi) = l_{z}\Phi(\phi). \qquad (6.1.4.1)$$

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}.$$
(6.1.4.2)

$$l_z = m\hbar, \quad m = 0, \pm 1, \pm 2, \cdots$$
 (6.1.4.3)

The commutation relation of operators  $L^2$  and  $L_z$  is zero [See Eq. (6.1.1.15)]. Therefore, the operator  $L^2$  and operator  $L_z$  have common eigenfunctions.

$$L^{2}\Psi(\theta,\phi) = \hbar^{2}\zeta\Psi(\theta,\phi) = \hbar^{2}\zeta\Theta(\theta)\Phi_{m}(\phi), \qquad (6.1.4.4)$$

where  $\zeta$  is proportional to the eigenvalue of operator  $L^2$ , is dimensionless and real.

Substituting Eqs. (6.1.2.7) and (6.1.4.1-3) into Eq. (6.1.4.4), and multiplying by  $\sin^2(\theta)/(\Theta(\theta)\Phi(\phi))$  yields

$$\frac{1}{\sin\theta} \frac{d}{d\theta} \left( \sin\theta \frac{d\Theta(\theta)}{d\theta} \right) + \left( \zeta - \frac{m^2}{\sin\theta^2} \right) \Theta(\theta) = 0.$$
 (6.1.4.5)

Putting  $\mu = \cos\theta$  in Eq. (6.1.4.5), writing  $\Theta(\theta) = P(\mu)$ , and noting that  $1 - \mu^2 = \sin^2\theta$  yield

$$\frac{d\Theta}{d\theta} = \frac{dP}{d\mu}\frac{d\mu}{d\theta} = -\sin\frac{dP}{d\mu} = -(1-\mu^2)^{1/2}\frac{dP}{d\mu},$$
(6.1.4.6)

or

$$-\frac{1}{\sin\frac{d}{d\theta}} = \frac{d}{d\mu}.$$
(6.1.4.7)

The Eq. (6.1.4.5) becomes

$$\frac{d}{d\mu} \left[ (1-\mu^2) \frac{dP(\mu)}{d\mu} \right] + \left[ \zeta - \frac{m^2}{1-\mu^2} \right] P(\mu) = 0.$$
 (6.1.4.8)

Eq. (6.1.4.8) is an eigenvalue equation that is a second order differential equation (associated Legendre equation) and therefore, has two solutions. The solutions are obtained in standard mathematical textbooks on special functions. One finds that for the solution that is regular in  $\theta$  in the interval  $(0,\pi)$ , i. e.,  $\cos\theta$  in the interval (-1,+1), is well known and is called the associated Legendre function, designated as

$$P_l^m(\cos\theta), \quad \zeta = l(l+1), \quad l = 0, 1, 2, \cdots, \quad |m| \le l \quad .$$
 (6.1.4.9)

In the section 6.2 we will show that the quantum number l is linked to the orbital angular momentum, while *m* is given by the *z* component of the orbital angular momentum. For fixed *m*,  $P_l^m$  and  $P_{l'}^m$  are mutually orthogonal

$$\int_{-1}^{1} d\mu P_{l}^{m}(\mu) P_{l'}^{m} = \frac{2}{2l+1} \frac{(l+|m|)!}{(l-|m|)!} \delta_{ll'}.$$
(6.1.4.10)

The function  $\Theta(\theta)$  can now written down as

$$\Theta(\theta) = P(\mu) = constant \times P_l^m(\cos). \tag{6.1.4.11}$$

Using the normalization constant,  $\Theta(\theta)$  becomes

$$\theta_{lm}(\theta) = \left[\frac{2l+1}{2} \frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2} P_l^m(\cos\theta)(-1)^m.$$
(6.1.4.12)

The complete eigenfunction of  $L^2$  corresponding to quantum l and m is thus

$$\Psi(\theta,\phi) = \Theta(\theta)\Phi(\phi) = \left[\frac{2l+1}{2}\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2} P_l^m(\cos\theta)e^{im\phi}(-1)^m \equiv Y_l^m(\theta,\phi) \quad (6.1.4.13)$$

for  $m \ge 0$ .

For m < 0, using the property

$$Y_l^m = (-1)^m Y_l^m, (6.1.4.14)$$

one obtains that the same expression holds but without the factor  $(-1)^m$ . The function  $Y_l^m$  is called a spherical harmonic function or simply a spherical harmonic.

The function  $Y_l^m(\theta, \phi)$  forms an orthogonal and normalized set or, for brevity, forms an orthonormal set:

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\Theta Y_l^m(\Theta, \phi) Y_{l'}^{m'}(\Theta, \phi) = \delta_{ll'} \delta_{mm'}.$$
(6.1.4.15)

Thus the eigenvalue equation takes the form:

$$L^{2}Y_{l}^{m}(\theta,\phi) = \hbar^{2}l(l+1)Y_{l}^{m}(\theta,\phi), \quad (l=0,1,2,\cdots) \quad .$$
(6.1.4.16)

where  $l(l+1)\hbar^2$  are the eigenvalues of operator  $L^2$ ,  $Y_l^m \equiv |lm\rangle$  being the corresponding eigenfunction. (Note that  $L^2$  represents both operator and the eigenvalue of operator  $L^2$ .) The eigenvalues  $l(l+1)\hbar^2$  is (2l+1) fold degenerate corresponding to a particular value of l there will be (2l+1) values of  $m (= -l, -l+1, \cdots l)$ . l is often referred to as the orbital quantum number.

We also have:

$$L_{z}Y_{l}^{m}(\theta,\phi) = -i\hbar\frac{\partial}{\partial\phi}\left[\Theta_{l}(\theta)\frac{1}{\sqrt{2\pi}}e^{im\phi}\right] = m\hbar Y_{l}^{m}(\theta,\phi), \qquad (6.1.4.17a)$$

i. e.,

$$L_{z}Y_{l}^{m}|lm\rangle = m\hbar|lm\rangle, \quad |m| \le l \quad m = -l, -l+1, \cdots, l-1, l \quad .$$
(6.1.4.17b)

Thus  $Y_l^m(\theta, \phi)$  are simultaneously the eigenfunction of  $L^2$  and  $L_z$ . But  $L^2$  and  $L_x$  ( $L_y$ ) do not have simultaneously eigenfunction except for l = m = 0 case. *m* is referred to as the azimuthal or magnetic quantum number.

The form of Eq. (6.1.4.16) indicates the following. Suppose that a system (e. g., a wheel) is rotating some where in space, far removed from other object. According to spontaneous equiprobability symmetry breaking law, what possible values can be taken by

the body-factor? The values are only the form  $L = \hbar \sqrt{l(l+1)}$ , where *l* is some integer. For example, one would never observe the value  $L = \hbar \sqrt{7}$ , since it is not the form  $L^2 = \hbar^2 l(l+1)$ . There is no integer for which l(l+1) = 7, and thus the body-factor cannot take l(l+1) = 7. This is similar to the fact that a particle in an one dimensional box is never found to have the energy  $E = 7E_1$ . This value does not fit the energy eigenvalue recipe  $E = n^2 E_1$ .

Suppose that the body-factor takes the magnitude of angular momentum of the wheel and find the value  $L^2 = 6\hbar^2$  according to the wavepacket law. This corresponds to the l = 2. Having taken  $L^2$ , the body-factor is left in an eigenstate of  $L^2$ . What value does the body-factor take for  $L_z$ ? The answer is given by the form of the eigenvalues of  $L_z$  in Eq. (6.1.4.17). Since l = 2,  $L_z$  can only be found to have one of the five values:

$$l_z = 2\hbar, \hbar, 0, -\hbar, -2\hbar$$

Suppose that the body-factor takes  $l_z = 2\hbar$ , which means that the result of the spontaneous equiprobability symmetry breaking is that the body-factor chooses the m = 2. Then the wheel as a body-factor is left in the state  $Y_2^2$ .

The form of Eq. (6.1.4.16) indicates that the eigenvalues of operator  $L^2$  are 2l + 1-fold degenerate. For the problem considered, all the five states  $Y_2^2(\theta, \phi), Y_2^1(\theta, \phi), \dots, Y_2^{-2}(\theta, \phi)$  correspond to the same eigenvalue of operator  $L^2$  (i. e.,  $L^2 = 6\hbar^2$ ). (See Fig. 6.2.)

Since the angular momenta are quantum operators, they cannot be drawn as vectors like in classical mechanics. Nevertheless, it is common to depict them heuristically in this way. Depicted on the Fig. 6.2 is a set of states with quantum numbers, l = 2 and m = -2, -1, 0, 1, 2 for the five cones from bottom to top. Since,  $|L| = \sqrt{L^2} = \hbar\sqrt{6}$ , the vectors are all shown with length  $\hbar\sqrt{6}$ . The rings represent the fact that  $L_z$  is known with certainty, but  $L_x$  and  $L_y$  are unknown; therefore every classical vector with the appropriate length and z-component is drawn, forming a cone. The true angular momentum for the particle (i. e., the body-factor of the wavepacket) would be somewher on this conee according to the spontaneous equiprobability symmetry breaking. Again, this visualization should not be taken too literally.

This quantization rules of orbital angular momentum are technically true even for macroscopic systems, like the angular momentum **L** of a spinning torque. However they have no observable effect of angular momentum quantization. For example, if  $L_z/\hbar$  is roughly 100000000, it makes essentially no difference whether the precise value is an integer like 100000000 or 100000001, or a non-integer like 100000000.2, because the discrete steps are too small to notice. The classical torque is shown in Fig. 6.3.

For l = 2,  $L^2 = 6\hbar^2$ . The only possible orientations of **L** onto the *z* axis are the five values shown in Fig. 6.2. The precessional motion depicted preserves  $L^2$  and  $L_z$ .  $\theta = \cos^{-1}2/\sqrt{6}$  is the smallest possible angle between **L** and *z* axis.

Next we discuss the Heisenberg uncertainty relation of angular momentum. We have derived this relation in Eq. (3.4.1), and is depicted as follows:

$$(\Delta L_y)(\Delta L_z) \ge \frac{\hbar |< L_x > |}{2}.$$
(6.1.4.18)

$$(\Delta L_x)(\Delta L_z) \ge \frac{\hbar| < L_y > |}{2}, \qquad (6.1.4.19)$$



Figure 6.2. The vector model of angular momentum. The eigenvalue of operator  $L^2 = \hbar^2 l(l+1)$  is (2l+1)-fold degenerate. For a fixed magnitude,  $L = \hbar \sqrt{l(l+1)}$ , there are only (2l+1) possible projection of **L** onto a given axis. The vector *L*, of length  $\sqrt{l(l+1)}\hbar$ , precesses about the axis of quantization, the (2l+1)l allowed projections of *L* on this axis given by  $m\hbar$ , with  $m = -l, -l+1, \dots, +l$ .

$$(\Delta L_x)(\Delta L_y) \ge \frac{\hbar| < L_z > |}{2}, \qquad (6.1.4.20)$$

$$(\Delta L^2)(\Delta L_i) = 0.$$
  $(i = x, y, z)$  (6.1.4.21)

The three components of angular momentum cannot be simultaneously measured very precisely because there are uncertainty relations between them, from which we deduce that if a system (such as a wheel, a particle, an atom, a rigid rod, etc.) is in an eigenstate of one of angular momentum say  $L_x$ , it will not be simultaneously in an eigenstate of either of the  $L_x$ or  $L_z$ . The operator  $L^2$  commute with components of **L**, therefore total angular momentum and one of its component can be simultaneously measured very precisely.

Angular momentum is a vector operator. The square magnitude of this vector is given by  $L^2$ . Having obtained  $L^2$ , Eq. (6.1.4.18-21) tells us clearly that the body-facor absolutely cannot take precisely simultaneously all the three Cartesian components of **L**, the reason of which comes from the characteristic of a mathematical function (See chapter 3.) other than



Figure 6.3. The torque caused by the two opposing forces Fg and -Fg causes a change in the angular momentum  $\mathbf{L}$  in the direction of that torque (since torque is the time derivative of angular momentum). This causes the top to precess.

comes from the destruction or perturbation of measurement processes on the corresponding states. In one word, uncertainty relations do not have any connection with measurement.

Consider a case of a wheel whose center is fixed in space. The body-factor of the wheel takes some values of  $L^2$  according to the wavepacket law. What motion of the wheel will preserve these values but not preserve  $L_x$  and  $L_y$ ? A very worthwhile model for such motion is given by a classical solution in which the angular momentum vector of constant magnitude precesses about the z axis at a constant inclination to that axis (See Fig. 6.3.), thereby maintaining  $L_z$ . Such motion is realized by a spinning top, with fixed vertex, in a gravity field.

In classical mechanics L is precisely determined as a function of time. At any instant L may be observed and completely specified. In quantum mechanics L is an operator. It is in principle possible that the eigenstate of  $L^2$  is dependent on time. In this case the observed value at any instant of L may be completely specified as well as that in classical mechanics. If at any instant time t, the system is in such a state with definite l and m values, then it is more consistent to view the related configuration as one in which the L vector is uniformly spread over a cone about the z axis with half apex angle  $\theta = \cos^{-1}m/\sqrt{l(l+1)}$  (See Fig. 6.3). However, we have to point out that magnitudes of both the value of l and the value of m can be a function of time, i. e., the cone about z axis can be varied with time.

For a given value of L [i. e.,  $\hbar\sqrt{l(l+1)}$ ] the maximum value of  $L_z$  is  $\hbar l$ . But  $l < \sqrt{l(l+1)}$ . It is follows that the angular momentum vector is never aligned with a given axis. Furthermore, there are only a distance, finite l(l+1) number of inclinations that L makes with any given axis. This extraordinary property (classical mechanics permits a continuum of inclinations) is sometimes called the quantization of space.

In order to know the properties of eigenfunction  $Y_l^m(\cos\theta) \equiv Y_l^m(\mu)$ , we give the following mathematical formulas:

If m = 0, then  $P_l^m(\mu)$  becomes a simple polynomial called the Legendre polynomial, written as  $P_l(\mu)$ . We summarize the properties of  $P_l(\mu)$  first and then those of  $P_l^m(\mu)$  before

discussing  $Y_l^m(\theta, \phi)$ .

$$P_l(\mu) = (-1)^l \frac{1}{2^l l!} \frac{d^l}{dx^l} (1-\mu)^l.$$
(6.1.4.22)

$$P_l^m(\mu) = (1 - \mu^2)^{|m|/2} \frac{d^{|m|}}{dx^{|m|}} P_l(\mu).$$
(6.1.4.23)

Some of the individual functions can be written as:  $P_0(\mu) = 1$ ,  $P_1(\mu) = x$ ,  $P_2 = (3\mu^2 - 1)/2$ . We also note:  $P_l(-\mu) = (-1)^l P_l(\mu)$  and  $P_l(0) = 1$ .

The normalization relation for the Legendre polynomial is found to be

$$\int_{-1}^{1} d\mu P_l(\mu) P_{l'} = \frac{2}{2l+1} \delta_{ll'}.$$
(6.1.4.24)

We also note that  $P_l(\mu)$  appears as a coefficient of expansion for the following function:

$$\frac{1}{\sqrt{1-2\mu s+s^2}} = \sum_{l=0}^{\infty} P_l(\mu) s^l.$$
(6.1.4.25)

For the associated Legendre function,  $P_l^m(\mu)$ , we have correspondingly the following:  $P_1^1(\mu) = \sqrt{1-\mu^2}$ ,  $P_2^1(\mu) = 3\mu\sqrt{1-\mu^2}$ ,  $P_2^2(\mu) = 3(1-\mu^2)$ , with the normalization condition

$$\int_{-1}^{1} d\mu P_{l}^{m}(\mu) P_{l'}^{m}(\mu) = \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \delta_{ll'}.$$
(6.1.4.26)

The spherical harmonic function  $Y_l^m(\theta, \phi)$  is already defined in Eq. (6.1.4.13). Some typical expressions of  $Y_l^m(\theta, \phi)$  are given by:

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}.$$
 (6.1.4.27)

$$Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta.$$
 (6.1.4.28)

$$Y_1^{\pm 1} = \mp \sqrt{\frac{3}{8\pi}} e^{\pm i\phi} \sin\theta.$$
 (6.1.4.29)

$$Y_2^0 = \sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1). \tag{6.1.4.30}$$

$$Y_2^{\pm 1} = \mp \sqrt{\frac{15}{8\pi}} e^{\pm i\phi} \sin\theta.$$
 (6.1.4.31)

$$Y_2^{\pm 2} = \sqrt{\frac{15}{32\pi}} e^{\pm i2\phi} \sin\theta.$$
 (6.1.4.32)

The spherical harmonics can also be written in real form by taking linear combinations of  $Y_l^m(\theta, \phi)$ . The real form of spherical harmonics for m = 0 are

$$Y_{l,\cos\theta}^{0} \equiv \sqrt{\frac{1}{2}} \left( Y_{l}^{0} + Y_{l}^{0*} \right) = Y_{l}^{0} \quad Y_{l,\cos\theta}^{0} \equiv -i\sqrt{\frac{1}{2}} \left( Y_{l}^{0} - Y_{l}^{0*} \right) \quad .$$
(6.1.4.33)

1			
l	т	notation	Spherical harmonics in real form
0	0	S	$\sqrt{1/(4\pi)}$
1	0	$p_z$	$\sqrt{3/(4\pi)}\cos\theta$
1	1	$p_x$	$\sqrt{3/(4\pi)}$ sin $\theta$ cos $\phi$
1	1	$p_y$	$\sqrt{3/(4\pi)}$ sin $\theta$ sin $\phi$
2	0	$d_{3z^2-r^2}$	$\sqrt{5/(16\pi)}(3\cos^2\theta - 1)$
2	1	$d_{xz}$	$\sqrt{15/(4\pi)}$ sin $\theta$ cos $\theta$ cos $\phi$
2	1	$d_{yz}$	$\sqrt{15/(4\pi)}$ sin $\theta$ cos $\theta$ sin $\phi$
2	2	$d_{x^2-y^2}$	$\sqrt{15/(4\pi)}$ sin <sup>2</sup> cos2 $\phi$
2	2	$d_{xy}$	$\sqrt{15/(4\pi)}\sin^2\theta\sin^2\phi$

Table 6.1. The first few spherical harmonics in real form

For m = 0,  $Y_{l,\cos\theta}^0$  is identical to  $Y_l^0$ . The first few spherical harmonics in real forms are listed in Table 6.1. The subscripts in Tab. 6.1 *z*, *x*, *y*, *xy*, *yz* etc. indicate the behavior of the real spherical harmonics in terms of Cartesian coordinates. The designation for example  $p_z$  or  $d_{xy}$  reflects the orientation of these atomic orbitals along the *z* axis for  $p_z$  or along the *xy* plane for  $d_{xy}$ . The necessity to introduce the real forms  $p_z$  or  $d_{xy}$  etc. will be explained latter.

# 6.2. Hydrogen Atom

### 6.2.1. Two Body Problem

A hydrogen atom is an atom of the chemical element hydrogen. This electrically neutral atom contains a single positively-charged proton in the center of the hydrogen atom and a single negatively-charged electron bound to the nucleus by the Coulomb force. Atomic hydrogen comprises about 75% of the elemental mass of the universe.

In the next calculations we assume that the proton number is  $Z \ge 1$ . So, we can discuss both the hydrogen and the hydrogen-like atom. We consider the hydrogen-like atom as a system of two interacting particles  $m_1$  and  $m_2$  being at  $r_1$  and  $r_2$ , respectively, the interaction being due to Coulomb attraction potential  $V(|r_1 - r_2|) = V(r)$  of their electrical charges. Let the charge on the nucleus is  $Q_1 = Ze$  and the charge on the electron is  $Q_2 = -e < 0$ .

The time-dependent Schrödinger equation is

$$i\hbar\frac{\partial}{\partial t}\Psi(r_1, r_2, t) = \left[-\left(\frac{\hbar^2}{2m_1}\nabla_1^2 + \frac{\hbar^2}{2m_2}\nabla_2^2\right) + V(r_1 - r_2)\right]\Psi(r_1, r_2, t), \quad (6.2.1.1)$$

where

$$\nabla_i^2 = \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2}, \quad for \quad i = 1, 2$$
(6.2.1.2)

The  $\nabla^2$  is called Laplacian operator or "del squared" in rectangular coordinates. Eq. (6.2.1.2) can be separated into two equations, one of which represents the translational motion of the hydrogen-like atom as a whole and the other, the relative motion of the two

particles. For this we consider new variables *X*, *Y*, *Z* which are Cartesian coordinates of the center of mass of the hydrogen-like atom and *r*,  $\theta$ ,  $\phi$  of the poler coordinates of the second particle (electron) relative to the first (nucleus). These coordinates are related to the two particle by the equations:

$$r = r_1 - r_2 = (x, y, z).$$
 (6.2.1.3)

$$R = (X, Y, Z) = \frac{m_1 r_1 + m_2 r_2}{M},$$
(6.2.1.4)

where

$$M = m_1 + m_2 = total mass$$
. (6.2.1.5)

$$x = x_1 - x_2 = rsin\theta cos\phi. \tag{6.2.1.6a}$$

$$y = y_1 - y_2 = rsin\theta sin\phi. \tag{6.2.1.6b}$$

$$z = z_1 - z_2 = rcos\theta.$$
 (6.2.1.6c)

We introduce the reduced mass

$$\mu = \frac{m_1 m_2}{m_1 + m_2}.\tag{6.2.1.7}$$

Let us show that

$$\frac{\hbar^2}{2m_1}\nabla_1^2 + \frac{\hbar^2}{2m_2}\nabla_2^2 = \frac{\hbar^2}{2M}\nabla_R^2 + \frac{\hbar^2}{2\mu}\nabla_r^2, \qquad (6.2.1.8)$$

where  $\nabla_R^2$  and  $\nabla_r^2$  have the same expression as given by Eq. (6.2.1.2) except in the former case we replace x, y, z by X, Y, Z while in the latter case x, y, z refer to the relative coordinates in Eq. (6.2.1.6).

$$\frac{\partial}{\partial x_1} = \frac{\partial}{\partial X}\frac{\partial X}{\partial x_1} + \frac{\partial}{\partial x}\frac{\partial x}{\partial x_1} + \frac{\partial}{\partial Y}\frac{\partial Y}{\partial x_1} + \frac{\partial}{\partial y}\frac{\partial y}{\partial x_1} + \frac{\partial}{\partial Z}\frac{\partial Z}{\partial x_1} + \frac{\partial}{\partial z}\frac{\partial z}{\partial x_1}.$$
(6.2.1.9)

Substituting Eqs. (6.2.1.6) and (6.2.1.4) into Eq. (6.2.1.9) yields

$$\frac{\partial}{\partial x_1} = \frac{m_1}{M} \frac{\partial}{\partial X} + \frac{\partial}{\partial x}.$$
(6.2.1.10)

$$\frac{\partial^2}{\partial x_1^2} = \frac{\partial}{\partial x_1} \frac{\partial}{\partial x_1} = \left(\frac{m_1}{M}\right)^2 \frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial x^2} + 2\frac{m_1}{M} \frac{\partial^2}{\partial X \partial x}.$$
 (6.2.1.11*a*)

Similarly,

$$\frac{\partial^2}{\partial y_1^2} = \frac{\partial}{\partial y_1} \frac{\partial}{\partial y_1} = \left(\frac{m_1}{M}\right)^2 \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial y^2} + 2\frac{m_1}{M} \frac{\partial^2}{\partial Y \partial y}.$$
(6.2.1.11*b*)

$$\frac{\partial^2}{\partial z_1^2} = \frac{\partial}{\partial z_1} \frac{\partial}{\partial z_1} = \left(\frac{m_1}{M}\right)^2 \frac{\partial^2}{\partial Z^2} + \frac{\partial^2}{\partial z^2} + 2\frac{m_1}{M} \frac{\partial^2}{\partial Z \partial z}.$$
(6.2.1.11c)

$$\frac{\partial^2}{\partial x_2^2} = \frac{\partial}{\partial x_2} \frac{\partial}{\partial x_2} = \left(\frac{m_2}{M}\right)^2 \frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial x^2} - 2\frac{m_2}{M} \frac{\partial^2}{\partial X \partial x}.$$
(6.2.1.11d)

$$\frac{\partial^2}{\partial y_2^2} = \frac{\partial}{\partial y_2} \frac{\partial}{\partial y_2} = \left(\frac{m_2}{M}\right)^2 \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial y^2} - 2\frac{m_2}{M} \frac{\partial^2}{\partial Y \partial y}.$$
(6.2.1.11*e*)

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$$\frac{\partial^2}{\partial z_2^2} = \frac{\partial}{\partial z_2} \frac{\partial}{\partial z_2} = \left(\frac{m_2}{M}\right)^2 \frac{\partial^2}{\partial Z^2} + \frac{\partial^2}{\partial z^2} - 2\frac{m_2}{M} \frac{\partial^2}{\partial Z \partial z}.$$
(6.2.1.11*f*)

Substituting Eqs. (6.2.1.11a-f) into the left hand side of Eq. (6.2.1.8), one knows that Eq. (6.2.1.8) is correct.

Substituting Eq. (6.2.1.8) into Eq. (6.2.1.1), one obtains that the time-dependent Schrödinger equation (6.2.1.1) becomes

$$i\hbar\frac{\partial}{\partial t}\Psi(r,R,t) = \left[-\left(\frac{\hbar^2}{2M}\nabla_R^2 + \frac{\hbar^2}{2\mu}\nabla_r^2\right) + V(r\right]\Psi(r,R,t), \qquad (6.2.1.12)$$

To solve the energy eigenvalue problem we use the separation method of variables, and write, replacing the energy term by  $E_R + E$ ,

$$\Psi(r, R, t) = \Psi(r)\phi(R)e^{-i(E_R + E)t/\hbar}.$$
(6.2.1.13)

Substituting Eq. (6.2.1.13) into Eq. (6.2.1.12), one obtains

$$-\frac{\hbar^2 \Psi(r)}{2M} \nabla_R^2 \phi(R) - \frac{\hbar^2 \phi(R)}{2\mu} \nabla_r^2 \Psi(r) + V(r) \Psi(r) \phi(R) = (E_R + E) \Psi(r) \phi(R). \quad (6.2.1.14)$$

Dividing Eq. (6.2.1.14) by  $\Psi(r)\Psi(R)$  and simplifying yield

$$-\frac{\hbar^2}{2M}\nabla_R^2\phi(R) = E_R\phi(R), \qquad (6.2.1.15)$$

which is equivalent to Schrödinger equation of free particle.

$$-\frac{\hbar^2}{2\mu}\nabla_r^2\psi(r) + V(r\psi(r) = E\psi(r).$$
(6.2.1.16)

The solution of Eq. (6.2.1.15) is

$$\phi(R) \sim e^{iP \cdot R/\hbar} \tag{6.2.1.17}$$

with

$$E_R = \frac{\hbar^2 P^2}{2M},$$
 (6.2.1.18)

where  $P = p_1 + p_2$  is the total momentum of the hydrogen-like atom.

Eq. (6.2.1.16) is a partial differential equation because it contains three independent variables. To solve this equation it is often to use the separation method of variables. The purpose of variable separation is to split the equation into terms each of which just involves one such coordinate. However, the Coulomb potential  $V(r) = V(\sqrt{x^2 + y^2 + z^2})$ , and thus the separation into *x*, *y*, *z* cannot be carried out. We can utilize the spherical polar coordinates  $r, \theta, \phi$  instead the rectangular coordinates. From sunsubsection 3.5.9 in chapter 3 we know that the form of Eq. (6.2.1.16) in spherical polar coordinates is

$$\frac{1}{r^{2}}\frac{\partial}{\partial r}\left(r^{2}\frac{\partial\psi(r,\theta,\phi)}{\partial r}\right) + \frac{1}{r^{2}sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial\psi(r,\theta,\phi)}{\partial\theta}\right) + \frac{1}{r^{2}sin^{2}\theta}\frac{\partial^{2}\psi(r,\theta,\phi)}{\partial\phi^{2}} + \frac{2\mu}{\hbar^{2}}[E - V(r)]\psi(r,\theta,\phi) = 0.$$
(6.2.1.19)

Eq. (6.2.1.19) tells us that

$$\Psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi) \equiv R(r)Y(\theta,\phi). \tag{6.2.1.20}$$

Substituting the  $\Psi$  in Eq. (6.2.1.20) into Eq. (6.2.1.19), then dividing the obtained equation by  $\Psi$ , one obtains

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^{2}\frac{\partial R}{\partial r}\right) + \frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^{2}\theta}\frac{\partial Y}{\partial\phi^{2}}\right] + \frac{2\mu}{\hbar^{2}}[E - V(r)] = 0. \quad (6.2.1.21)$$

Using Eq. (6.1.2.7), Eq. (6.2.1.21) becomes

$$\left[-\frac{\hbar^2}{2\mu r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{L^2}{2\mu r^2} + V(r)\right]\psi(r,\theta,\phi) = E\psi(r,\theta,\phi).$$
(6.2.1.22)

Eq. (6.1.4.16) is

$$L^{2}Y_{l}^{m}(\theta,\phi) = \hbar^{2}l(l+1)Y_{l}^{m}(\theta,\phi), \quad (l=0,1,2,\cdots) \quad .$$
(6.2.1.23)

Thus

$$\Psi(r, \theta, \phi) = R_l(r) Y_l^m(\theta, \phi). \tag{6.2.1.24}$$

Substituting Eqs. (6.2.1.23-24) into Eq. (6.2.1.22) yields

$$\frac{d^2 R_l}{dr^2} + \frac{2}{r} \frac{dR_l}{dr} + \left[ -\frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2} [E - V(r)] \right] R_l = 0.$$
(6.2.1.25)

Eq. (6.2.1.25) is called radial equation. Under certain boundary conditions solve it, and can obtain the eigenvalues E. For the unbound state E is continuous. For the bound state the E is quantized.

Sometimes, make the following substitution

$$\chi_l(r) = rR_l(r).$$
 (6.2.1.26)

is convenient. Substituting Eq. (6.2.1.26) into Eq. (6.2.1.25) we have

$$\chi_l'' + \left[ -\frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2} [E - V(r)] \right] \chi_l = 0.$$
(6.2.1.27)

For the hydrogen-like atom the charge of atomic nucleus is Ze, the radius is about  $10^{-13}$  cm, the electron which moves around the nucleus, the charge is -e, the electron trajectory radius around the nucleus is about  $10^{-8}$  cm. The Coulomb potential between the nucleus and electron is

$$V(r) = -\frac{Ze^2}{r}.$$
 (6.2.1.28)

$$V(r = \infty) = 0$$
. Writing  $\chi_l(\rho) = \chi_l(r)$  with

$$\rho = \left(-\frac{8\mu E}{\hbar^2}\right)^{1/2} r, \qquad (6.2.1.29)$$

letting

$$\beta = \frac{Ze^2}{\hbar} \left( -\frac{\mu}{2E} \right)^{1/2}, \tag{6.2.1.30}$$

and using Eq. (6.2.1.8), Eq. (6.2.1.27) becomes

$$\chi_l'' + \left[ -\frac{l(l+1)}{\rho^2} + \frac{\beta}{\rho} - \frac{1}{4} \right] \chi_l = 0.$$
 (6.2.1.31)

# 6.2.2. Asymptotic Behavior

When  $\rho \rightarrow 0$  (i. e.,  $r \rightarrow 0$ ), Eq. (6.2.1.31) can be expressed asymptotically as

$$\chi_l'' + \left[ -\frac{l(l+1)}{\rho^2} \right] \chi_l = 0.$$
 (6.2.2.1)

At the neighborhood of  $\rho = 0$ , assume  $\chi_l(\rho) \propto \rho^s$ , and substitute it into Eq. (6.2.2.1), we have

$$s(s-1) - l(l+1) = 0,$$
 (6.2.2.2)

which is called characteristic equation, which has two solutions:

$$s_1 = l + 1 \quad s_2 = -l \quad , \tag{6.2.2.3}$$

i. e., the radial function at the neighborhood of  $\rho \rightarrow 0$  is

$$\chi_l \propto \rho^{(l+1)} \quad or \quad \propto \rho^{-l} \quad .$$
 (6.2.2.4*a*)

$$R_l \propto \rho^l \quad or \quad \propto \rho^{(l+1)} \quad .$$
 (6.2.2.4*b*)

Next, let us argue that the solution of asymptotic behavior  $R_l = \chi_l/r \propto r^{-l-1}$  has to be abandoned. The reason is as follows. In physics, the square of the absolute value of  $|R_l|^2$  at the neighborhood of  $\rho \rightarrow 0$  represents the position probability density, and therefore is finite. We conclude that we only keep the solution  $R_l = \chi_l/r \propto \rho^l$ .

Next, let us consider the asymptotic behavior at  $\rho \rightarrow \infty$ . We confine to bound state E < 0. Eq. (6.2.1.31) becomes

$$\chi_l'' - \frac{1}{4}\chi_l = 0. \tag{6.2.2.5}$$

The solution of Eq. (6.2.2.5) is

$$\chi_l(\rho) \propto e^{\pm \frac{\rho}{2}}.\tag{6.2.2.6}$$

Considering the boundary condition of bound state, we can only take

$$\chi_l(\rho) \propto e^{-\rho/2} \tag{6.2.2.7}$$

as our solution.

Thus, the general solution of the radial equation Eq. (6.2.1.31) is

$$\chi_l(\rho) = \rho^{l+1} e^{-\frac{\rho}{2}} L(\rho). \tag{6.2.2.8}$$

Substituting Eq. (6.2.2.8) into Eq. (6.2.1.31) yields

$$\rho L''(\rho) + [2(l+1) - \rho]L'(\rho) + [\beta - l - 1]L(\rho) = 0.$$
(6.2.2.9)

Let us try a power series solution for Eq. (6.2.2.9) by putting

$$L(\rho) = \sum_{s=0}^{\infty} a_s \rho^s \tag{6.2.2.10}$$
in Eq. (6.2.2.9). One obtains

$$\sum \{s[(s-1)+2l+2]a_s \rho^{s-1} + (\beta - l - 1 - s)a_s \rho^s\} = 0.$$
(6.2.2.11)

For Eq. (6.2.2.11) to be true the coefficient of each term must vanish which leads to

$$\frac{a_{s+1}}{a_s} = \frac{l+s+1-\beta}{(s+1)(s+2l+2)}.$$
(6.2.2.12)

For large value of s, and fixed l, Eq.(6.2.2.12) is

$$\frac{a_{s+1}}{a_s} \to \frac{1}{s}.\tag{6.2.2.13}$$

The behavior of an exponential series is

$$e^{\rho} = 1 + \rho + \frac{\rho^2}{2!} + \dots + \frac{\rho^{s-1}}{(s-1)!} + \frac{\rho^s}{s!} + \frac{\rho^{s+1}}{(s+1)!} + \dots, \qquad (6.2.2.14)$$

in which the coefficient at large *s* is same as that in Eq. (6.2.2.13). Thus the solution of Eq. (6.2.2.8) is of the form

$$\chi_l(\mathbf{\rho}) = \mathbf{\rho}^{l+1} e^{-\mathbf{\rho}/2} e^{\mathbf{\rho}} = \mathbf{\rho}^{l+1} e^{\mathbf{\rho}/2}.$$
 (6.2.2.15)

If the true  $\chi_l$  takes the form in Eq. (6.2.2.15), then the boundary condition  $\chi_l \to 0$  as  $\rho \to \infty$  is violated. Therefore, the series has to be terminated and this is only possible if for some value of  $s = s_{max}$ , we have

$$s_{max} + l + 1 = \beta. \tag{6.2.2.16}$$

 $s_{max} = 0, 1, 2, \cdots$  is radial quantum number, and is often written as  $n_r$ . Since both  $s_{max}$  and l take only integer value, we can write Eq. (6.2.2.16) as

$$s_{max} + l + 1 = \beta = n, \tag{6.2.2.17}$$

where *n* is called principal quantum number. From Eq. (6.2.2.17) we know that if *n* and *l* are fixed, then the radial quantum is fixed as well.

For a fixed energy level n, Eq. (6.2.2.17) tells us that

$$l = 0, 1, 2, \dots, n-1 \\ n_r \equiv s_{max} = n-1, n-2, n-3, \dots, 0 . (6.2.2.18)$$

#### 6.2.3. Eigenvalues

Substituting Eq. (6.2.1.30) into Eq. (6.2.2.17) yields

$$\beta^2 = -\frac{\mu z^2 e^4}{2E\hbar^2 n^2} = n^2. \tag{6.2.3.1}$$

From Eq. (6.2.3.1) we obtain the eigenvalues are

$$E_n = -\frac{\mu Z^2 e^4}{2n^2 \hbar^2} = -\frac{Z^2 e^2}{2a_o} \frac{1}{n^2} = -\frac{R_{\infty} ch Z^2}{n^2}, \quad n = 1, 2, 3, \cdots$$
(6.2.3.2)

where  $R_{\infty}$  is Ryderberg constant, and  $a_{\circ} = [\hbar^2/(\mu e^2)] = 0.529 \times 10^{-8}$  cm is the Bohr radius, and *n* is principal quantum number.

Eqs. (6.2.1.24) tells us that the hydrogen-like atom wavefunction is  $\Psi(r, \theta, \phi) = R(r)Y_l^m(\theta, \phi)$ . Eq. (6.2.1.25) tells us that the R(r) is *l*-dependent. Eq. (6.2.3.2) tells us further that  $R_l(r)$  is  $n_r$ - or *n*-dependent. Therefore, the hydrogen-like atom wavefunction is

$$\Psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_l^m(\theta,\phi). \tag{6.2.3.3}$$

From above calculations we know that the  $\Psi_{nlm}(r, \theta, \phi)$  are the common eigenfunctions of  $H, L^2, L_z$ . The quantum number n, l, m themselves may be said to indicate the eigenstate of the hydrogen-like atom. The allowed values of these quantum numbers are

$$n = 1, 2, 3, \cdots$$

$$l = 0, 1, 2, \cdots, n-1$$

$$m = 0, \pm 1, \pm 2, \cdots, \pm l$$
(6.2.3.4)

The quantum numbers l and m are related to the magnitudes of the orbital angular momentum L and the z component of L, i. e.,  $L_z$ , respectively. Since  $L^2$  and  $L_z$  do not operate on the radial part of the wavefunction,  $\Psi_{nlm}$  itself is a simultaneous eigenfunction. The energy eigenvalue  $E_n$  in Eq. (6.2.3.2) depends only on n, whereas the the wavefunction  $\Psi_{nlm}$ depends on n, l, and m. From Eq. (6.2.3.4) for the n-th energy level, l can takes values  $0, 1, \dots, n-1$  and for each value of l, there are 2l + 1 possible values of m. The total n-th energy level degeneracy is therefore given by

$$f_n = \sum_{l=0}^{n-1} (2l+1) = \sum_{l=0}^{n-1} 2l + \sum_{l=0}^{n-1} 1 = 2\left[\frac{n}{2}(n-1)\right] + n = n^2,$$
(6.2.3.5)

i. e.,  $n^2$ -fold degenerate.

Now let us use the energy level formula given by Eq. (6.2.3.2) to explain the observed rule of hydrogen atomic line spectra. According to Eq. (6.2.3.2), when the electron makes transition from high level  $E_n$  to low level  $E_m$ , the wavenumber of emitted light k(=v/c) (v is frequency.) is

$$k_{mn} = \frac{E_n - E_m}{hc} = R_{\infty} \left(\frac{1}{m^2} - \frac{1}{n^2}\right) \quad (n > m)$$
(6.2.3.6)

For hydrogen atom Z = 1.

For m = 1, i. e., transition from every excited state to ground state,

$$k_{1n} = \frac{E_n - E_1}{hc} = R_{\infty} \left( 1 - \frac{1}{n^2} \right) \quad (n = 2, 3, 4, \cdots)$$
(6.2.3.7)

When  $n \to \infty$ ,  $k_{1\infty} = R_{\infty}$ . This is the Lyman line series in chapter 1. For m = 2,

$$k_{2n} = \frac{E_n - E_2}{hc} = R_{\infty} \left(\frac{1}{4} - \frac{1}{n^2}\right) \quad (n = 3, 4, 5\cdots)$$
(6.2.3.8)



Figure 6.4. The energy spectrum of hydrogen atom.

when  $n \to \infty$ ,  $k_{2\infty} = R_{\infty}/4$ . This is the Balmer line series in chapter 1. For m = 3,

$$k_{3n} = \frac{E_n - E_3}{hc} = R_{\infty} \left(\frac{1}{9} - \frac{1}{n^2}\right) \quad (n = 3, 4, 5\cdots)$$
(6.2.3.9)

when  $n \to \infty$ ,  $k_{2\infty} = R_{\infty}/9$ . This is the Paschen line series in chapter 1. See Fig. 6.4.

The calculations in Eq. (6.2.3.7-9) are for hydrogen atom Z = 1. The Eq. (6.2.3.2) can also be used to hydrogen-like atoms:  $He^+$ ,  $Li^{++}$ ,  $Be^{+++}$ , etc., for which Z > 1.

For the hydrogen-like atom  $He^+$ , Z = 2. According to Eq. (6.2.3.2), when the electron makes transition from high level  $E_n$  to low level  $E_m$ , the wavenumber of emitted light k(=v/c) (v is frequency.) is

$$k_{mn} = \frac{E_n - E_m}{hc} = 4R_{\infty} \left(\frac{1}{m^2} - \frac{1}{n^2}\right) \quad (n > m)$$
(6.2.3.10)

For m = 4, Z = 2, and n > 4, we have

$$k_{4n} = \frac{E_n - E_4}{hc} = R_\infty \left(\frac{1}{4} - \frac{4}{n^2}\right) \to \frac{R_\infty}{4}, \quad if \quad n \to \infty$$
(6.2.3.11)

One can see that Eq. (6.2.3.11) is similar to the Balmer line series in Eq. (6.2.3.8), especially, is nearly same at  $n \to \infty$ . Let us explain the little difference between  $R_{\infty}(\mu_H)$  and

 $R_{\infty}(\mu_{He^+}) R_{\infty} \propto \mu.$ 

$$\mu_H = \frac{m_e m_H}{m_e + m_H} \approx m_e \left( 1 - \frac{1}{1836} \right). \tag{6.2.3.12}$$

$$\mu_{He^+} = \frac{m_e m_{He^+}}{m_e + m_{He^+}} \approx m_e \left( 1 - \frac{1}{4 \times 1836} \right).$$
(6.2.3.13)

#### 6.2.4. Eigenfunction

The polynomial solution of Eq. (6.2.2.9) can be expressed in terms of the associated Laguerre polynomial  $L_{n+l}^{2l+1}(\rho)$  apart from an arbitrary constant factor  $N_{nl}$ . Therefore, from Eqs. (6.2.1.26), (6.2.3.2) and (6.2.2.8) we know that the radial function in Eq. (6.2.1.24) is labeled by two indices *n* and *l*, and after normalization is

$$R_{nl}(r) = -\left[\left(\frac{2Z}{na_{\circ}}\right)^{3} \frac{(n-l-1)!}{2n(n+1)!}\right]^{1/2} e^{-\rho/2} \rho^{l} L_{n+l}^{2l+1}(\rho).$$
(6.2.4.1)

From Eqs. (6.2.1.29) and (6.2.3.2) we know

$$\rho = \frac{2Zr}{na_{\circ}}.\tag{6.2.4.2}$$

$$L_{n+l}^{2l+1}(\rho) = \sum_{k=0}^{n-l-1} (-1)^{k+2l+1} \frac{(n+l)^2 \rho^k}{(n-l-1-k)!(2l+1+k)!k!}.$$
(6.2.4.3)

Thus, the wavefunction given by Eq. (6.2.1.24) is

$$\Psi_{nlm} = R_{nl}(r)Y_l^m(\theta, \phi), \qquad (6.2.4.4)$$

where the radial function is given by Eqs. (6.2.4.1-3), and  $Y_l^m$  is given by Eq. (6.1.4.13). Explicit forms of  $\Psi_{nlm}$  are shown in Table 6.2.

The normalized expressions of the angular wavefunctions (spherical harmonics) have been given by Eqs. (6.1.4.23-28). One often uses the following spectroscopic notations: n = 1,  $l = 0 \rightarrow 1S$ , n = 2,  $l = 0 \rightarrow 2S$ , n = 2,  $l = 1 \rightarrow 2P$ , n = 3,  $l = 0 \rightarrow 3S$ , n = 3,  $l = 1 \rightarrow 3P$ , n = 3,  $l = 2 \rightarrow 3D$ .

The stationary state wavefunctions of hydrogen-like ions in Table 6.4 are the complete set of conservative quantities  $H, L^2, L_z$ . Utilizing these wavefunctions, one can obtain the following information. Take the hydrogen atom as an example.

(A) Radial probability density distribution.

The position probability of the electron in sphere shell  $r \rightarrow r + dr$  is

$$r^{2}dr \int d\Omega |\Psi_{nlm}(r,\theta,\phi)|^{2} = [R_{nl}(r)]^{2}r^{2}dr = [\chi_{nl}(r)]^{2}dr \equiv Q_{n}dr.$$
(6.2.4.5)

The curve of  $Q_n$  versus  $r/a_{\circ}$  is shown in Fig. 6.5. From Fig. 6.5 we see that the node number of radial wavefunction (do not contain the points  $r = \infty$  and r = 0) is equal to  $n_r$ .

n	l	$n_r$	$\Psi_{nlm}(r, 0, \mathbf{\phi})$
1	0	0	$\Psi_{100} = 2 \left(rac{Z}{a_\circ} ight)^{3/2} e^{-Zr/a_\circ} Y_0^0$
2	0	1	$\Psi_{200} = 2\left(\frac{Z}{(2a_{\circ})}\right)^{3/2} (1 - Zr/2a_{\circ})e^{-Zr/2a_{\circ}}Y_0^0$
2	1	0	$\begin{pmatrix} \Psi_{211} \\ \Psi_{210} \\ \Psi_{21-1} \end{pmatrix} = \frac{1}{\sqrt{3}} \left( \frac{Z}{(2a_{\circ})} \right)^{3/2} \frac{Zr}{a_{\circ}} e^{-Zr/2a_{\circ}} \begin{pmatrix} Y_1^1 \\ Y_1^0 \\ Y_1^{-1} \end{pmatrix}$
3	0	2	$\Psi_{300} = 2\left(\frac{Z}{3a_{\circ}}\right)^{3/2} \left[1 - 2Zr/3a_{\circ} + 2/3(Zr/3a_{\circ})^{2}\right]e^{-Zr/3a_{\circ}}Y_{0}^{0}$
3	1	1	$\begin{pmatrix} \Psi_{311} \\ \Psi_{310} \\ \Psi_{31-1} \end{pmatrix} = \frac{4\sqrt{2}}{9} \left(\frac{Z}{3a_{\circ}}\right)^{3/2} \frac{Zr}{a_{\circ}} (1 - Zr/6a_{\circ}) e^{-Zr/3a_{\circ}} \begin{pmatrix} Y_1^1 \\ Y_1^0 \\ Y_1^{-1} \end{pmatrix}$
3	2	0	$\begin{pmatrix} \Psi_{322} \\ \Psi_{311} \\ \Psi_{310} \\ \Psi_{31-1} \\ \Psi_{32-2} \end{pmatrix} = \frac{2\sqrt{2}}{27\sqrt{5}} \left(\frac{Z}{3a_{\circ}}\right)^{3/2} \left(\frac{Zr}{a_{\circ}}\right)^2 e^{-Zr/3a_{\circ}} \begin{pmatrix} Y_2^2 \\ Y_2^1 \\ Y_2^0 \\ Y_2^{-1} \\ Y_2^{-2} \end{pmatrix}$

Table 6.2. The first few normalized eigenfunctions of hydrogen-like ions ( $Z \ge 1$ )

In quantum mechanics, the electron in hydrogen atom does not have exact orbital, and we can only study its position probability distribution. However,  $Q_n$  has a maximum value (See Fig. 6.5).

For example, let us look at the ground state.

$$Q_{\rm p}n = (R_{10})^2 r^2 = \frac{4}{a_{\circ}^3} r^2 e^{-2r/a_{\circ}}.$$
 (6.2.4.6)

The maximum value of  $Q_n$  is at

$$\frac{d}{dr}Q_n = 0. \tag{6.2.4.7}$$

From Eq. (6.2.4.7) one obtains

$$r_{mas} = a_{\circ}.$$
 (6.2.4.8)

 $a_{\circ}$  is the Bohr radius, which represents the most probable radius.

It is interesting to note that for a fixed n, l = n - 1 (i. e.,  $n_r = 0$ ), the most probable radiuses of the radial probability distributions ( $|\chi_{10}|^2$ ,  $|\chi_{21}|^2$ ,  $|\chi_{32}|^2$ , etc.) can be found as follows.

$$\Psi_{nn-1m} \propto e^{-r/na_{\circ}} r^{n-1} Y_{n-1}^{m}(\theta, \phi).$$
(6.2.4.9)

Let us ask the probability of finding the electron of the hydrogen atom in spherical shell of radius r and thickness dr:

$$\int_{\Omega} |\Psi_{nn-1m}|^2 r^2 dr d\Omega \propto e^{-2r/na_{\circ}} r^{2n} dr.$$
 (6.2.4.10)



Figure 6.5. The electronic radial probability density distribution function of 2s and 3s states of hydrogen atom.

The probability density reaches a maximum when

$$\frac{d}{dr}\left(e^{-2r/na_{\circ}}r^{2n}\right) = 0.$$
(6.2.4.11)

Solve the Eq. (6.2.4.11). We obtain that the probable position of the electron in state  $\Psi_{nlm}$  is at

$$r_{max} = n^2 a_{\circ}, \quad (n = 1, 2, 3, \cdots)$$
 (6.2.4.12)

The average values of various power of r are defined as

$$\langle r^{k} \rangle_{nl} = \langle nl | r^{k} | nl \rangle = \int dr r^{k} [R_{nl}(r)]^{2}.$$
 (6.2.4.13)

For example, [4]

$$< r^{-1} >_{nl} = \frac{Z}{n^2 a_\circ}.$$
 (6.2.4.14)

(B) The angular dependence of probability density.

The probability of the electron in hydrogen atom in solid angle  $d\Omega$ , which's direction is  $(\theta, \phi)$  is

$$|Y_l^m(\theta,\phi)|^2 d\Omega \propto |P_l^m(\theta)|^2 d\Omega, \qquad (6.2.4.15)$$

which is independent of  $\phi$ . Therefore, the angular probability distribution keeps the turning symmetry. See Fig. 6.6. Note that only the  $|Y_0^0(\theta, \phi)|^2$  has sphere symmetry.

Fig. 6.6 shows the first few hydrogen atom orbitals (energy eigenfunctions). These are cross-sections of the probability density that are color-coded (white represents zero probability density and black represents the highest probability density). The angular momentum



Figure 6.6. Visualizing the hydrogen electron orbitals, or, say, the probability distributions of the electron in hydrogen atom. Probability densities through the *xz*-plane for the electron at different quantum numbers (l = 0, 1, 2, corresponding to s, p, d, respectively. m = 0).

(orbital) quantum number l is denoted in each column, using the usual spectroscopic letter code (*s* means l = 0, p means l = 1, d means l = 2). The main (principal) quantum number n (= 1, 2, 3, ...) is marked to the right of each symbol. For example,  $3d_{\circ}$  represents n = 3, l = 2, m = 0. For all pictures the magnetic quantum number m has been set to 0, and the cross-sectional plane is the *xz*-plane (*z* is the vertical axis). The probability density in three-dimensional space is obtained by rotating the one shown here around the *z*-axis.

The "ground state", i.e. the state of lowest energy, in which the electron is usually found, is the first one, the 1s state (principal quantum level n = 1, l = 0).

An image with more orbitals is also available (up to higher numbers *n* and *l*).

Here, we make a simple explanations for the introducing the linear composition of spherical harmonics, such as  $p_x$ ,  $p_y$ , and  $p_z$ . See Tab. 6.1 in subsection 6.1.4.  $Y_1^0$  and  $Y_1^{\pm}$  are three independent states. However,  $p_x$ ,  $p_y$ , and  $p_z$  are also three independent states. The difference between  $Y_1^{\pm}$  and  $p_x$ ,  $p_y$  is the forms of the squares of absolute values.  $|p_x|^2$  is a spindle like the  $|Y_1^0|^2$  in Fig. 6.6, but the spindle is along the *x* axis.  $|p_y|^2$  is a spindle like the  $|Y_1^0|^2$  in Fig. 6.6, but the spindle is along the *y* axis. When several atoms construct a molecule, it is necessary to have a wavefunctions which's probability distribution concentrates in some direction.

(C) Probability current density of the electron in hydrogen atom and magnetic moment.

The probability current density of the electron in hydrogen atom is given by Eq. (2.5.3.7), and is depicted as follows. (The charge of electron is -e.)

$$J = \frac{ie\hbar}{2\mu} (\Psi_{nlm}^* \nabla \Psi_{nlm} - \Psi_{nlm} \nabla \Psi_{nlm}^*).$$
(6.2.4.16)

Utilizing the expression of  $\nabla$  in spherical polar coordinates

$$\nabla = e_r \frac{\partial}{\partial r} + e_{\theta} \frac{1}{r} \frac{\partial}{\partial \theta} + e_{\phi} \frac{1}{rsin\theta} \frac{\partial}{\partial \phi}, \qquad (6.2.4.17)$$

one can obtain the components of **J**. Due to that the radial wavefunction  $R_{nl}(r)$  and the  $\theta$ -dependent part  $P_l^m(\theta)$  are real, one can see that  $J_r = J_{\theta} = 0$ . Thus we just need to seek

$$J_{\phi} = \frac{ie\hbar}{2\mu} \frac{1}{rsin\theta} \left( \Psi_{nlm}^* \frac{\partial}{\partial \phi} \Psi_{nlm} - \Psi_{nlm} \frac{\partial}{\partial \phi} \Psi_{nlm}^* \right)$$
  
$$= \frac{ie\hbar}{2\mu} \frac{1}{rsin\theta} 2im|\Psi_{nlm}|^2 = -\frac{e\hbar m}{\mu} \frac{1}{rsin\theta} |\Psi_{nlm}|^2. \qquad (6.2.4.18)$$

 $J_{\phi}$  is the probability current density around the axis z.

Eery part of  $|\Psi_{nlm}|^2$  moves with certain velocity around the *z* axis instead of motionless. The motion of  $|\Psi_{nlm}|^2$  cause important effect. Because the electron has mass, this motion makes the electron to have an angular momentum around *z* axis. Because the electron has charge -e < 0, this motion makes the electron to have a magnetic moment around *z* axis. The probability current density element, through cross section  $d\sigma$ ,  $dI = J_{\phi}d\sigma$ . This current element has magnetic moment (Gauss unit) SdI/c,  $S = \pi (rsin\theta)^2$  is area of circle turning around the *z* axis. Therefore, the total magnetic moment along the *z* axis is

$$M_{z} = \frac{1}{c} \int dIS = \frac{1}{c} \int \pi r^{2} \sin^{2}\theta \cdot J_{z} d\sigma$$
  
$$= -\frac{e\hbar}{2\mu c} m \int |\Psi_{nlm}|^{2} 2\pi r \sin\theta d\sigma$$
  
$$= -\frac{e\hbar}{2\mu c} m \int |\Psi_{nlm}|^{2} d\tau, \qquad (6.2.4.19)$$

where volume element  $d\tau = 2\pi r sin\theta d\sigma$ . Considering the normalization of  $\Psi_{nlm}$ , from Eq. (6.2.4.19)

$$m_z = -\frac{e\hbar}{2\mu c}m = -\mu_B m, \qquad (6.2.4.20)$$

where Bohr magneton

$$\mu_B = \frac{e\hbar}{2\mu c} = 5.79 \times 10^9 (eV/G) \tag{6.2.4.21}$$

is a minimum unit of atomic magnetic moment. From Eq. (6.2.4.20) one sees that quantum number *m* determines the magnitude of magnetic moment, and is therefore called magnetic quantum number. For state with l = 0 the magnetic moment is zero, which's physical origin is the zero current.

From Eq. (6.2.4.20)

$$\frac{M_z}{m\hbar} = -\frac{e}{2\mu c} \equiv g, \qquad (6.2.4.22)$$

where  $m\hbar$  represents the z component of orbital angular momentum, g is called gyromagnetic ratio or g factor. If take  $e/2\mu c = 1$ , then g = -1, which is the characteristic of orbital angular momentum. In chapters 7 and 8 we will explain that for electron spin angular

momentum and electron inherent magnetic moment (i. e., spin magnetic moment), g = -2.

Let us prove that the  $|\Psi_{nlm}|^2$  makes rotational motion. Using the similar method, we can calculate the angular momentum of the electron. The mass element  $d\mu$  of the electron in volume element  $d\tau$  is

$$d\mu = \mu |\Psi nlm|^2 d\tau = \mu |\Psi_{nlm}|^2 dSrsin\theta d\phi.$$
(6.2.4.23)

$$d\mu = \mu J_{\phi} dS dt, \qquad (6.2.4.24)$$

where dS is the the side area element, which is

$$dS = rd\theta dr. \tag{6.2.4.25}$$

From Eqs. (6.2.4.23-25) and (6.2.4.18), one obtains the the velocity of the probability density  $|\Psi_{nlm}|^2$  at  $(\theta, \phi)$ , which is

$$v = \frac{rsin\theta d\phi}{dt} = \frac{\mu J_z/(-e)}{\mu |\Psi_{nlm}|^2}.$$
(6.2.4.26)

Substituting Eq. (6.2.4.18) into Eq. (6.2.4.26) yields

$$v = \frac{\hbar m}{\mu r \sin \theta}.$$
 (6.2.4.27)

The mass element  $d\mu$  in the volume element  $d\tau$  has angular momentum element

$$dL_z = d\mu vrsin\theta = \hbar m |\Psi_{nlm}|^2 r^2 sin\theta dr d\theta d\phi. \qquad (6.2.4.28)$$

Making the integration over all the position space and considering the normalization of wavefunction, one obtains

$$L_z = \hbar m. \tag{6.2.4.29}$$

This result is obtained directly from the basic definition of angular momentum. It is obvious that Eq. (6.2.4.29) has to be consistent with that  $\Psi_{nlm}$  is an eigenstate of operators  $L^2$  and  $L_z$ , and the eigenvalue of operator  $L_z$  is  $\hbar m$ . We have given in section 6.1 of this chapter the operator form of  $L_z$  in position space.

$$< nlm | L_z | nlm >= m\hbar. \tag{6.2.4.30}$$

This result,  $\langle nlm | L_z | nlm \rangle \geq 0$ , makes us to believe that the  $|\Psi_{nlm}|^2$  makes rotation motion really, i. e., the variable  $\phi$  itself is a function of time *t*.

Here, we would like to remind readers to note the following points:

(A) Some references always say that the solution of the Schrödinger equation of hydrogen-like atom is a wavefunction, refers to one electron wavefunction, is called atomic orbital, and is described by the quantum numbers (n, l, m).

However, we hope the readers to note that an orbital (i. e.,  $\Psi_{nlm}$ ) does not indicate the exact location of an electron in position space. The  $|\Psi_{nlm}|^2$  only gives the position

probability density of the body-factor of the electron wavepacket to occupy any point in position space. The wavefunction is a guide-factor of an electron wavepacket;

(B) If there are many electrons out the nucleus and the interactions between electrons can be neglected, then the electrons will occupy states (n, l, m) according to energy minimum, i. e., low energy state is more stable. However, the electron is a Fermion, and thus obeys the Pauli theorem proved in identical particle system.

(C) Now we propose a sharp question. Does the electron in  $\Psi_{nlm}$  eigenstate really like an electron "cloud" distributing around the nucleus according to  $|\Psi_{nlm}|^2$ ? Our answer is: "No. Absolutely not." Our reason is obvious. Because an electron is a very rigid sphere with radius  $< 10^{-18}$  cm under nonrelativistic approximation. The electron cannot transform from a rigid small sphere to a "cloud" under the very weal electromagnetic interaction.

Now we propose an even more sharp question. If the electron moves around the nucleus, then the picture of an atom should be like a star model (The planets move around the sun). However, according to the observations after 2010, the cloud model of an atom is more appropriate. The wavepacket-only theory gives the following explanations. If an electron is in  $\Psi_{nlm}(r, \theta, \phi)$  state, according to the law of wavepacket, the electron in state  $\Psi_{nlm}(r, \theta, \phi)$ still can take many locations allowed by  $\Psi_{nlm}$  state. Therefore, we feel that the cloud model is better. However, the cloud model of the atom does not mean that the very rigid electrons in the atom becomes really a drifting cloud. On the contrary, the electrons in a atom are still the rigid sphere, but the electrons as rigid spheres in state  $\Psi_{nlm}$  changes theirs positions allowed by the state  $\Psi_{nlm}$  according to the spontaneous equiprobability symmetry breaking. Therefore, our observation is that the electrons look like cloud.

(D) According to the law of characteristic of wavepacket in chapter 3,  $|\Psi_{nlm}|^2$  represents the position probability density. We consider the state  $\Psi_{nlm}$ . If the electron as a very rigid small sphere, then this electron in state  $\Psi_{nlm}$  can occupy any point  $(r, \theta, \phi)$  in spherical polar coordinates with position probability density  $|\Psi_{nlm}(r, \theta, \phi)|^2$ . What is *z* component of angular momentum  $L_{z,electron}$  of this electron as a small rigid sphere at point  $(r, \theta, \phi)$ ? In comparison with the average value calculations in Eqs. (6.2.4.29) and (6.2.4.30), now we will make a microscopic calculation, i. e., we just calculate the angular momentum *z* component at one point. Because the electron is too small, we look upon it as a point particle. The angular momentum *z* component of a point particle with mass  $\mu$  at point  $(r, \theta, \phi)$  is

$$L_{z,electron} = R_I \times \frac{v}{rsin\theta},\tag{6.2.4.31}$$

where  $R_I$  is the rotation inertia of the point electron.

$$R_I = \mu \times (rsin\theta)^2, \tag{6.2.4.32}$$

where  $\mu \approx m_e$  is the relative mass, and  $m_e$  is the static mass of one electron. Substituting Eqs. (6.2.4.32) and (6.2.4.27) into Eq. (6.2.4.31) yields

$$L_{z,electron} = m\hbar. \tag{6.2.4.33}$$

That is, even the electron is a point particle in state  $\Psi_{nlm}$ , its angular momentum z component is also  $m\hbar$ , which is same as given by Eqs. (6.2.4.29) and (6.2.4.30). The consistence between microscopic and average value comes from that  $\Psi_{nlm}$  is the eigenstate of a physical quantity (Here, it is the angular momentum z component).

(E) Now let show you an interesting paradox. Would you please from now begin to consider where do we make mistake? We make the average value calculation of the energy and then make comparison with the energy eigenvalue. We discuss the energy in the ground state of hydrogen atom. The wavefunction of the ground state is

$$\Psi_{100}(r,\theta,\phi) = \sqrt{\frac{4}{a_{\circ}^3}} e^{-r/a_{\circ}} Y_0^0(\theta,\phi) = R_{10}(r) Y_0^0(\theta,\phi).$$
(6.2.4.34)

From the definition of average energy in a quantummechanical state, we know that the average energy of the ground state is

$$E_{1} = \int r^{2} sin\theta dr d\theta d\phi \Psi_{100}^{*} H\Psi_{100}$$
$$= \int r^{2} sin\theta dr d\theta d\phi \Psi_{100}^{*} \left[ -\frac{\hbar^{2}}{2\mu} \nabla^{2} - \frac{e^{2}}{r} \right] \Psi_{100}$$
$$\equiv \int r^{2} sin\theta dr d\theta d\phi \Psi_{100}^{*} [T+V] \Psi_{100} = -\frac{e^{2}}{2a_{\circ}}.$$
 (6.2.4.35)

$$\Psi_{100} = \sqrt{\frac{1}{\pi a_{\circ}^3}} e^{-r/a_{\circ}}.$$
(6.2.4.36)

The average value of kinetic energy is

$$<100|T|100> = \frac{1}{\pi a_{\circ}^{3}} \int_{0}^{\infty} dr \int_{0}^{\pi} d\theta \int_{0}^{2\pi} d\phi r^{2} \sin\theta e^{-r/a_{\circ}} \left(-\frac{\hbar^{2}}{2\mu} \nabla^{2} e^{-r/a_{\circ}}\right)$$
$$= -\frac{2\hbar^{2}}{\mu a_{\circ}^{3}} \int_{0}^{\infty} dr r^{2} e^{-r/a_{\circ}} \left[\left(\frac{\partial^{2}}{\partial r^{2}} + \frac{2}{r}\frac{\partial}{\partial r}\right) e^{-r/a_{\circ}}\right]$$
$$= -\frac{4\hbar^{2}}{\mu a_{\circ}^{3}} \int_{0}^{\infty} dr r^{2} e^{-2r/a_{\circ}} + \frac{4\hbar^{2}}{\mu a_{\circ}^{4}} \int_{0}^{\infty} dr r e^{-2r/a_{\circ}}$$
$$= -\frac{4\hbar^{2}}{\mu a_{\circ}^{5}} \frac{2!}{(2/a_{\circ})^{3}} + \frac{4\hbar^{2}}{\mu a_{\circ}^{4}} \frac{1}{(2/a_{\circ})^{2}} = \frac{\hbar^{2}}{2\mu a_{\circ}^{2}}.$$
(6.2.4.37)

Using the expression of the ground state wavefunction in Eq. (6.2.4.35) or in the Table 6.2, one can obtain the average value of potential energy in the ground state, which is

$$<100|V|100> = \frac{1}{\pi a_{\circ}^{3}} \int_{0}^{\infty} dr \int_{0}^{\pi} d\theta \int_{0}^{2\pi} d\phi r^{2} \sin\theta e^{-r/a_{\circ}} \left(-\frac{e^{2}}{r} e^{-r/a_{\circ}}\right)$$
$$= -\frac{e^{2}}{a_{\circ}}.$$
(6.2.4.37)'

Therefore,

$$<100|H100> = <100|T+V|100> = -\frac{e^2}{2a_\circ}.$$
 (6.2.4.38)

The result of Eq. (6.2.4.38) comes from average value of energy, and is the same as the eigenvalue of eigenstate  $|100\rangle$ , given by Eq. (6.2.3.2).

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Now we use another average method, which will gives a paradox. The wavefunction is  $\Psi_{100}$  given by Eq. (6.2.4.35) and Table 6.2.

$$\Psi_{100} = \frac{2}{(a_{\circ})^{3/2}} e^{-r/a_{\circ}} \sqrt{\frac{1}{4\pi}}.$$
(6.2.4.39)

Eq. (6.2.4.39) tells us that in principle the electron in ground state can appear anywhere with corresponding probability. For example, the position probability density at  $r \rightarrow r + dr$  is

$$P_{100}(r) = \left|\frac{2}{(a_{\circ})^{3/2}}e^{-r/a_{\circ}}\right|^2 r^2.$$
(6.2.4.40)

Let us consider that the electron is a small individual rigid sphere, which's wavefunction (guide-factor) is in the ground state  $\Psi_{100}$ . This electron's potential energy is only a function of *r*.

$$V(r) = -\frac{e^2}{r}.$$
 (6.2.4.41)

If the electron takes  $r = 10^3 a_{\circ}$  with non-zero probability, then  $V(10^3 a_{\circ}) = -e^2/(10^3 a_{\circ})$ .

The ground wavefunction  $\Psi_{100}$  is not the eigenstate of kinetic energy or momentum operator. Therefore, the kinetic energy and the momentum is not definite. To seek the momentum probability density, we should make a Fourier transformation of the ground state wavefunction from position space to momentum space.

$$\Psi_{100} = \frac{1}{(2\pi)^{3/2}} \sqrt{\frac{1}{4\pi}} \frac{2}{(a_{\circ})^{3/2}} \int dk_x dk_y dk_z \overline{\Psi}(k_x, k_y, k_z) e^{-\sqrt{x^2 + y^2 + z^2}/a_{\circ}} e^{ik \cdot r}.$$
 (6.2.4.42)

$$\begin{split} \overline{\Psi}(k_x, k_y, k_z) &= \frac{1}{(2\pi)^{3/2}} \sqrt{\frac{1}{4\pi}} \frac{2}{(a_\circ)^{3/2}} \int dx dy dz e^{-\sqrt{x^2 + y^2 + z^2}/a_\circ} e^{-ik \cdot r} \\ &= \frac{1}{(2\pi)^{3/2}} \sqrt{\frac{1}{4\pi}} \frac{2}{(a_\circ)^{3/2}} \int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\phi r^2 \sin\theta e^{-r/a_\circ} e^{ik\cos\theta r} \\ &= \frac{\sqrt{2a_\circ} \sin[\operatorname{arctg}(ka_\circ)]}{\pi(1 + k^2 a_\circ^2)k} \equiv \overline{\Psi}(k). \end{split}$$
(6.2.4.43)

Eq. (6.2.4.43) indicates that  $\overline{\Psi}(k_x, k_y, k_z)$  is a function of k or momentum  $p = \hbar k$ . Therefore, the momentum probability density between  $k \to k + dk$  or  $p \to p + dp$  is

$$P_{100}(k) = |\overline{\Psi}(k)|^2 k^2 4\pi = \frac{8a_{\circ} sin^2 [arctg(ka_{\circ})]}{(1+k^2 a_{\circ}^2)^2}.$$
 (6.2.4.44)

From Eq. (6.2.4.44) we can see that the electron in the ground state  $\Psi_{100}$  can take, for example,  $k = 1000/a_{\circ}$  with non-zero probability. In this case the kinetic energy of the electron in the ground state is (Use  $\hbar^2/\mu = a_{\circ}e^2$ )

$$T(k = 1/1000a_{\circ}) = \frac{\hbar^2 k^2}{2\mu} = \frac{\hbar^2 (1000)^2}{2\mu} \frac{1}{a_{\circ}^2}.$$
 (6.2.4.45)

The total energy is

$$E_e = T(k = 1/1000a_\circ) + V(r = 1000a_\circ) = \frac{e^2}{a_\circ} \left(\frac{10^6}{2} - \frac{1}{1000}\right) >> -\frac{e^2}{2a_\circ} = E_1.$$
(6.2.4.46)

Eq. (6.2.4.46) indicates clearly that even the electron, which's wavefunction (guidefactor) is in the ground state  $\Psi_{100}$ , the electron's energy can be still possible equal to the  $10^6 \times$  (eigenvalue of the ground state). It is easy to see that if the electron, which's wavefunction (guide-factor) is in the eigenstate  $\Psi_{nlm} \neq \Psi_{100}$ , then the electron's energy can be still possible equal to the  $10^6 \times$  (eigenvalue of the eigenstate  $\Psi_{nlm}$ ). Therefore, if there is a transition of the electron from  $\Psi_{100}$  to  $\Psi_{nlm}$ , then, generally speaking, the energy is not conservative.

We see that the two differen methods of seeking the average values on energy give completely different conclusion. This is the paradox. Actually, the second method is wrong. In the first method to seek the average value uses the position space. In position space, the kinetic energy in Eq. (6.2.4.37) is a differential operator. The second method is to use the momentum space. In this space, the position coordinates should be a differential operator. However, the second method looks upon the *r* as a number. Therefore, the first method is correct. The second method is wrong.

Therefore, this paradox tells us that one cannot in calculations and derivations use both representations corresponding to the two non-commutative operators at the same problems. This is the so called "One cannot stand on two boats at the same time".

# 6.3. Hellmann-Feynman Theorems

Hellmann-Feynman (HF) theorem concerns the rules of the variations of the parameters in the average value expressions of energy. If the energy eigenvalue has been sought, then one can obtain in terms of HF theorem many informations about the average values of mechanical quantities without large number of calculations by using the wavefunction. One can derives the virial theorem by using the HF theorem as well. Now the HF theorem is used in molecular structure, quantum chemistry, and particle physics. More particularly speaking, HF theorem relates the derivative of the total energy with respect to a parameter, to the expectation value of the derivative of the Hamiltonian with respect to that same parameter. Its most common application is in the calculation of forces in molecules (with the parameters being the positions of the nuclei) where it states that once the spatial distribution of the electrons has been determined by solving the Schrödinger equation, all the forces in the system can be calculated using concepts of classical electrostatics (Refer to the problem 15 in the last section).

The theorem has been proved independently by many authors, including Güttinger (1932), Pauli (1933), Hellmann (1937) and Feynman (1939).

#### 6.3.1. HF Theorem of Time-Independent Wavefunctions

#### Theorem XXXII: HF theorem of time-independent wavefunctions.

$$\frac{\partial E_{n\lambda}}{\partial \lambda} = \int \Psi_{n\lambda} \frac{\partial H_{\lambda}}{\partial \lambda} \Psi_{n\lambda} dr, \qquad (6.3.1.1)$$

where  $H_{\lambda}$  is Hamiltonian operator depending upon a continuous parameter  $\lambda$ ,  $\Psi_{n\lambda}$  is a wavefunction (eigenfunction) of the Hamiltonian, depending implicitly upon  $\lambda$ ,  $E_{n\lambda}$  is the energy (eigenvalue) of the wavefunction, dr implies an integration over the domain of the wavefunction.

**Proof.** The proof of Hellmann-Feynman theorem requires that the wavefunction is an eigenfunction of the Hamiltonian under consideration. However, the wavefunction does not need to be exact. For instance in Hartree-Fock theory the wavefunction is a relatively poor approximation to the true wavefunction, but because it is variationally optimized with respect to the Hamiltonian, the Hellmann-Feynman theorem can be applied. The proof also employs an identity of normalized wavefunctions, which can set that the derivatives of the overlap of a wavefunction with itself must be zero. Using Dirac's bra-ket notation these two conditions are written as

$$H_{\lambda}|\Psi_{n\lambda}\rangle = E_{n\lambda}|\Psi_{n\lambda}\rangle. \tag{6.3.1.2}$$

$$1 = \langle \Psi_{n\lambda} | \Psi_{n\lambda} \rangle \implies 0 = \frac{\partial}{\partial \lambda} \langle \Psi_{n\lambda} | \Psi_{n\lambda} \rangle.$$
(6.3.1.3)

The proof then follows through an application of the derivative product rule to the average value of the Hamiltonian viewed as a function of  $\lambda$ :

$$\begin{aligned} \frac{\partial E_{n\lambda}}{\partial \lambda} &= \frac{\partial}{\partial \lambda} \left\langle \Psi_{n\lambda} \middle| H_{\lambda} \middle| \Psi_{n\lambda} \right\rangle \\ &= \left\langle \frac{\partial \Psi_{n\lambda}}{\partial \lambda} \middle| H_{\lambda} \middle| \Psi_{n\lambda} \right\rangle + \left\langle \Psi_{n\lambda} \middle| \frac{\partial H_{\lambda}}{\partial \lambda} \middle| \Psi_{n\lambda} \right\rangle + \left\langle \Psi_{n\lambda} \middle| \frac{\partial \Psi_{n\lambda}}{\partial \lambda} \right\rangle \\ &= E_{n\lambda} \left\langle \frac{\partial \Psi_{n\lambda}}{\partial \lambda} \middle| \Psi_{n\lambda} \right\rangle + \left\langle \Psi_{n\lambda} \middle| \frac{\partial H_{\lambda}}{\partial \lambda} \middle| \Psi_{n\lambda} \right\rangle + E_{n\lambda} \left\langle \Psi_{n\lambda} \middle| \frac{\partial \Psi_{n\lambda}}{\partial \lambda} \right\rangle \\ &= E_{n\lambda} \frac{\partial}{\partial \lambda} \langle \Psi_{n\lambda} \middle| \Psi_{n\lambda} \rangle + \left\langle \Psi_{n\lambda} \middle| \frac{\partial H_{\lambda}}{\partial \lambda} \middle| \Psi_{n\lambda} \right\rangle \\ &= 0 + \left\langle \Psi_{n\lambda} \middle| \frac{\partial H_{\lambda}}{\partial \lambda} \middle| \Psi_{n\lambda} \right\rangle \end{aligned}$$

Here, we finish the proof. QED.

The most common application of the Hellmann-Feynman theorem is to the calculation of intramolecular forces in molecules.

#### 6.3.2. HF Theorem for Time-Dependent Wavefunctions

**Theorem XXXIII: HF theorem for time-dependent wavefunctions.** For a general time-dependent wavefunction satisfying the time-dependent Schrödinger equation, the Hellmann-Feynman theorem is not valid. However, the following identity holds:

$$\left\langle \Psi_{n\lambda}(t) \middle| \frac{\partial H_{\lambda}}{\partial \lambda} \middle| \Psi_{n\lambda}(t) \right\rangle = i\hbar \frac{\partial}{\partial t} \left\langle \Psi_{n\lambda}(t) \middle| \frac{\partial \Psi_{n\lambda}(t)}{\partial \lambda} \right\rangle.$$
(6.3.2.1)

**Proof.** The proof only relies on the Schrödinger equation and the assumption that partial derivatives with respect to  $\lambda$  and *t* can be interchanged.

$$\begin{split} \left\langle \Psi_{n\lambda}(t) \left| \frac{\partial H_{\lambda}}{\partial \lambda} \right| \Psi_{n\lambda}(t) \right\rangle &= \frac{\partial}{\partial \lambda} \left\langle \Psi_{n\lambda}(t) \left| H_{\lambda} \right| \Psi_{n\lambda}(t) \right\rangle - \left\langle \frac{\partial \Psi_{n\lambda}(t)}{\partial \lambda} \right| H_{\lambda} \left| \Psi_{n\lambda}(t) \right\rangle \\ &- \left\langle \Psi_{n\lambda}(t) \right| H_{\lambda} \left| \frac{\partial \Psi_{n\lambda}(t)}{\partial \lambda} \right\rangle \\ &= i\hbar \frac{\partial}{\partial \lambda} \left\langle \Psi_{n\lambda}(t) \left| \frac{\partial}{\partial t} \Psi_{n\lambda}(t) \right\rangle - i\hbar \left\langle \frac{\partial \Psi_{n\lambda}(t)}{\partial \lambda} \right| \frac{\partial \Psi_{n\lambda}(t)}{\partial t} \right\rangle \\ &+ i\hbar \left\langle \frac{\partial \Psi_{n\lambda}(t)}{\partial t} \right| \frac{\partial \Psi_{n\lambda}(t)}{\partial \lambda} \right\rangle \\ &= i\hbar \left\langle \Psi_{n\lambda}(t) \right| \frac{\partial^2 \Psi_{n\lambda}(t)}{\partial t^2} \right\rangle + i\hbar \left\langle \frac{\partial \Psi_{n\lambda}(t)}{\partial t} \right| \frac{\partial \Psi_{n\lambda}(t)}{\partial \lambda} \right\rangle \\ &= i\hbar \frac{\partial}{\partial t} \left\langle \Psi_{n\lambda}(t) \right| \frac{\partial \Psi_{n\lambda}(t)}{\partial \lambda} \right\rangle \end{split}$$

Here, we finish the proof. QED.

## 6.4. General Properties of Central Field

In section 6.2 we addressed the hydrogen-like ions, which are only an example referring to the central field problems. Actually, in our nature there are many phenomena which refer to the central field problems. For example, the Earth moves around the sun under action of the gravitational field; the electron moves around the nucleus under action of the Coulomb field; harmonic fields; the important effect of the screen Coulomb field on nucleus structure; the spectroscopic analysis of heavy meson (quarkonium) indicates that there are some characteristics of logarithmic and linear central potential. In view of importance of the central field we address in this section some general properties of central force fields.

#### 6.4.1. Conservation of Angular Momentum and Radial Equation

The most important characteristic of motion in central force fields is the conservation of angular momentum  $L = r \times p$ .

For classical particle (mass  $\mu$ ) this conservation is obvious, because

$$\frac{d}{dt}L = \frac{dr}{dt} \times p + r \times \frac{dp}{dt} = v \times \mu v + r \times F = 0 + r \times \left(-\frac{r}{r}\frac{dV(r)}{dr}\right) = 0.$$
(6.4.1.1)

Eq. (6.4.1.1) implies the force moment of the particle is zero. Considering  $L \cdot r = L \cdot p = 0$ , the classical motion of a particle in central field is in plane surface. The normal line direction of the motion is just the direction of **L**. In an appropriate coordinate system the classical motion in central field can be reduced to a plane motion. (For the closure of trajectory Refer to [1].)

In quantum mechanics the *L* is also a conservative quantity. Eq. (5.6.4.6) tells us that *L* is an operator of infinitesimal rotation.  $p^2 = p \cdot p$  is a scalar quantity. A scalar quantity does not change under rotation. Thus  $[L, p^2] = 0$ . L depends only on the angular variables  $\theta, \phi$ , thus [L, V(r)] = 0. Therefore,

$$H = \frac{p^2}{2\mu} + V(r). \tag{6.4.1.2}$$

$$[L,H] = [L,p^2/2\mu] + [L,V(r)] = 0.$$
(6.4.1.3)

Eq. (6.4.1.3) indicates that L is also a conservative quantity.

The difference between classical and quantum mechanics is that the three components of  $\mathbf{L}$  do not commute. Therefore, the three components of  $\mathbf{L}$  do not have definite values simultaneously except zero angular momentum, and thus the motion cannot be reduced to a simple plane motion.

We have to seek a complete set of conservation quantities, and use this set to describe a stationery eigenstate. Considering  $[L^2, L_\alpha] = 0$ ,  $(\alpha = x, y, z)$ , and  $[H, L^2] = 0$ , one often takes  $H, L^2, L_z$  as the complete set. The energy eigenequation is

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right]\Psi = E\Psi.$$
(6.4.1.4)

Considering a spherical symmetry of central field, we take spherical polar coordinate. In spherical polar coordinates the kinetic energy operator T is

$$T = -\frac{\hbar^2}{2\mu} \nabla^2 = \frac{p_r^2}{2\mu} + \frac{L^2}{2\mu r^2},$$
(6.4.1.5)

where

$$p_r = -i\hbar \left(\frac{\partial}{\partial r} + \frac{1}{r}\right) = -i\hbar \left(\frac{1}{r}\frac{\partial}{\partial r}r\right), \qquad (6.4.1.6)$$

and  $p_r$  is called radial momentum and is a Hermitian operator, i. e.,

$$p_r = p_r^+. (6.4.1.7)$$

$$p_r^2 = -\hbar^2 \left(\frac{1}{r}\frac{\partial}{\partial r}r\right)^2. \tag{6.4.1.8}$$

Thus the stationary Schrödinger equation is

$$H\Psi = [T+V]\Psi = \left[-\frac{\hbar^2}{2\mu}\left(\frac{1}{r}\frac{\partial}{\partial r}r\right)^2 + \frac{L^2}{2\mu r^2} + V(r)\right]\Psi$$
$$= \left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{L^2}{2\mu r^2} + V(r)\right]\Psi$$
$$= \left[-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2} + \frac{L^2}{2\mu r^2} + V(r)\right]\Psi = E\Psi.$$
(6.4.1.9)

In Eq. (6.4.1.9) the first term is called radial kinetic energy, and the second term is called centrifugal potential. Note that the total kinetic energy T is equal to the sum of the two terms.

Take  $\Psi$  as the eigenfunction of operator complete set  $(H, L^2, L_z)$ , i. e.,

$$\Psi(r, \theta, \phi) = R_l(r) Y_l^m(\theta, \phi)$$
  
 $l = 0, 1, 2, \cdots, \qquad m = l, l - 1, \cdots, -l + 1, -l.$ 
(6.4.1.10)

The radial equation is

$$\frac{d^2 R_l}{dr^2} + \frac{2}{r} \frac{dR_l}{dr} + \left[ -\frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2} [E - V(r)] \right] R_l = 0.$$
(6.4.1.11)

Making transformation  $R_l(r) = \chi_l/r$ , one obtains the radial equation given by Eq. (6.2.1.27)

$$\chi_l'' + \left[ -\frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2} [E - V(r)] \right] \chi_l = 0.$$
(6.4.1.12)

Under certain boundary conditions solving the Eq. (6.4.1.12), one obtains the energy eigenvalues. For unbound state the *E* is continuous. For bound state the *E* is discrete, and is dependent on the radial quantum number  $n_r$ ,  $n_r = 0, 1, 2, \cdots$ .  $n_r$  represents the nodal number of radial wavefunction. *E* depends of  $n_r$ , *l* or *n*, *l*, and is independent on *m*. *E* is denoted by  $E_{nl}$ .

#### **6.4.2.** Behavior of Radial Wavefunction near r = 0

Suppose that V(r) satisfies

when 
$$r \to 0, r^2 V(r) \to 0$$
. (6.4.2.1)

Many central potentials, such as harmonic potential  $\propto r^2$ , liner center potential  $\propto r$ , Coulomb potential  $\propto 1/r$ , effective potential  $\propto exp(-\alpha r)/r$ , free particle, spherical square potential, logarithmic center potential etc. satisfy Eq. (6.4.2.1). When  $r \rightarrow 0$ , Eq. (6.4.1.11) becomes

$$\frac{d^2 R_l}{dr^2} + \frac{2}{r} \frac{dR_l}{dr} + \left[ -\frac{l(l+1)}{r^2} \right] R_l = 0.$$
(6.4.2.2)

In the neighborhood of the canonical singular point r = 0, supposing  $R_l \propto r^s$  yields

$$s(s+1) - l(l+1) = 0,$$
 (6.4.2.3)

which is called characteristic equation. From Eq. (6.4.2.3) we have

$$s_1 = l, \quad s_2 = -(l+1) \quad , \tag{6.4.2.4}$$

i. e.,

$$R_l(r) \propto r^l$$
 or  $r^{-(l+1)}$  at neighborhood of  $r = 0$ . (6.4.2.5)

Next, we argue that the solution  $r^{-(l+1)}$  has to be abandoned. The probability *P* of appearance of the particle in neighborhood around r = 0 should be finite.

$$P \propto \int_{0} dr r^{2} |r^{-(l+1)}|^{2} = \int_{0} dr r^{-2l} \propto \left. \frac{1}{-2l+1} r^{-2l+1} \right|_{r=0}.$$
 (6.4.2.6)

If  $l \ge 1$ , then  $|P| = \infty$ , i. e., the solution of  $r^{-(l+1)}$  is not reasonable. If l = 0, then is the solution  $r^{-(l+1)}$  reasonable? Our answer is that although Eq. (6.4.2.6) tells us that it is reasonable, but the solution  $\Psi_{l=0} = R_l Y_0^0 = R_0 / \sqrt{4\pi} \propto 1/r$  does not satisfy Schrödinger equation Eq. (6.4.1.4) if the point r = 0 is included, because

$$\nabla^2 \frac{1}{r} = -4\pi \delta(r). \tag{6.4.2.7}$$

Therefore,

$$[E - V(r)]\Psi_{l=0} = \frac{2\pi\hbar^2}{\mu}\delta(r).$$
(6.4.2.8)

Eq. (6.4.2.8) does not hold. Therefore, the  $\Psi_{l=0} \propto 1/r$  does not satisfy Schrödinger equation Eq. (6.4.1.4). Thus we conclude that the radial wavefunction in Eq. (6.4.1.11) can only take the solution  $R_l(r) \propto r^l$  and  $\chi_l(r) = rR_l(r) \propto r^{1+l}$  when  $r \to 0$ .

Discuss the case l = 0. In this case Eq. (6.4.1.12) becomes

$$\frac{d^2\chi_0}{dr^2} + \frac{2\mu}{\hbar^2} [E - V(r)]\chi_0 = 0.$$
(6.4.2.9)

Eq. (6.4.2.9) likes the one dimensional Schrödinger equation, and the differences between them are: (a).  $\chi_0 \to 0$  when  $r \to 0$ ; (b).  $r \ge 0$  instead of  $-\infty < r < \infty$ .

Let us take a free particle as an example. For a free particle, Eq. (6.4.1.9) becomes

$$\left[-\frac{p_r^2}{2\mu} + \frac{L^2}{2\mu r^2}\right]\Psi_{klm} = E\Psi_{klm}.$$
(6.4.2.10)

The quantum number k is defined below. The radial kinetic energy operator  $p_r^2/2\mu$ inferred from Eq. (6.4.2.10). Insofar as  $p_r^2$  is a function only of r, and  $L^2$  is a function only of the angle variables  $(\theta, \phi)$ , one may seek solution of Eq. (6.4.2.10) by separation of variables. Substituting the product form

$$\Psi_{klm}(r,\theta,\phi) = R_{kl}Y_l^m(\theta,\phi) \tag{6.4.2.11}$$

into Eq. (6.4.2.10) yields

$$\left[ -\left(\frac{1}{r}\frac{d^2}{dr^2}r\right) + \frac{l(l+1)}{r^2} \right] R_{kl} = \frac{2\mu E}{\hbar^2} R_{kl}.$$
 (6.4.2.12)

With the substitution

$$E = \frac{\hbar^2 k^2}{2\mu}, \quad x = kr \tag{6.4.2.13}$$

Eq. (6.4.2.13) becomes the spherical Bessel differential equation

$$\frac{d^2}{dx^2}R_{kl} + \frac{2}{x}\frac{d}{dx}R_{kl} + \left[1 - \frac{l(l+1)}{x^2}\right]R_{kl} = 0.$$
(6.4.2.14)

The ordinary linear equation Eq. (6.4.2.14) for the radial function  $R_{kl}(r)$  has two linearly independent solutions. They are called spherical Bessel and Neumann functions and are denoted conventionally by the symbols  $j_l(x)$  and  $n_l(x)$ , respectively. However, only the spherical Bessel functions  $\{j_l(x)\}$  satisfy the asymptotic behavior at  $r \rightarrow 0$ , and are regular at the origin. The spherical Neumann function is not regular at origin. Thus we only take the spherical Bessel function as solution.

In this manner we take that the eigenstates and eigenenergies of the free particle Hamiltonian in spherical polar coordinates are (Refer to Ref. [3].)

$$\Psi_{klm}(r,\theta,\phi) = j_l(kr)Y_l^m(\theta,\phi) \tag{6.4.2.15}$$

$$E_k = \frac{\hbar^2 k^2}{2\mu}.$$
 (6.4.2.16)

The orthonormality of this sequence  $\{\Psi_{klm}\}$  is given by the relation

$$< lmk | l'm'k' > = \int_{0}^{\pi} d\theta sin\theta \int_{0}^{2\pi} d\phi \int_{0}^{\infty} drr^{2} [Y_{l}^{m}(\theta, \phi)]^{*} \left[Y_{l'}^{m'}(\theta, \phi)\right] j_{l}(kr) j_{l'}(k'r) = \delta_{ll'} \delta_{mm'} \frac{\pi}{2k^{2}} \delta(k-k').$$
(6.4.2.17)

The allowed values of momentum  $\hbar k$  of a free particle comprises a continuum.

Once again we note that the projection

$$\langle r, \theta, \phi | lmk \rangle = j_l(kr)Y_l^m(\theta, \phi)$$
 (6.4.2.18)

gives the coordinate representation of the ket vector  $|lmk\rangle$ . In a similar manner, the coordinate representation of the free-particle ket vector  $|k\rangle$  is given by

$$< r|k> = rac{1}{(2\pi)^{3/2}} e^{ik \cdot r}.$$
 (6.4.2.19)

In the spherical polar coordinates  $(H, L^2, L_z)$  are specified. In Cartesian coordinates  $(E, p = p_x, p_y, p_z)$  are specified. In the latter coordinates, *E* is redundant  $(E = p^2/2\mu)$ , but in the former coordinates it is not, because *E* is not determined by  $L^2 = \hbar^2 l(l+1)$  and  $L_z = \hbar m$ . Thus we find that in either Cartesian or spherical polar coordinates, there are three good quantum numbers.

#### 6.4.3. Expansion of Plane Wave in Spherical Harmonics

Expansion of plane wave in spherical harmonics is also called partial wave expansion of plane wave. As we have known, both massy particle and photon are wavepacket. In the Cartesian coordinates the guide-factor (i. e., wavefunction) of a free wavepacket is a plane wave with average wavevector  $k_{\circ}$  and average momentum  $p_{\circ} = \hbar k_{\circ}$ . According to the law

of wavepacket in chapter 3, the motion of the body-factor of the free wavepacket is related to the guide-factor. Thus the plena wave problem is equivalent to the free wavepacket problem. The free wavepacket is often met in practice. For example a free wavepacket (electron, photon, phonon, etc.) is scatted by a barrier or by an another particle (electron, photon, phonon, etc.). The guide-factor is a plane wave, and is expressed as

$$\Psi_{k_{\circ}}(r) = Ae^{ik_{\circ}\cdot r}.$$
(6.4.3.1)

The plane wave is an eigenstate of free Hamiltonian and momentum operator. Therefore, the energy *E* of the wavepacket is certain to be  $\hbar^2 k_o^2/2\mu$ , and the momentum of the wavepacket is certain to be  $p_o = \hbar k_o$ . Note that these problems do not have any connection with measurement. Even you do not make the energy measurement, the energy of the free wavepacket is still  $E = \hbar^2 k_o^2/2\mu$ . For brevity, in following calculations we use **k** instead of  $k_o$ .

The plane wave is not an eigenstate of operator  $L_z$  and  $L^2$ . We can ask that to what the probability of the free wavepacket in the eigenstate  $\Psi_{klm}$  of operators  $L^2, L_z$  is equal? Note that this question does not any connection with measurements.

As we know that  $\Psi_{klm}$  form a complete set, regular at the origin, of solutions of the Schrödiger equation. The energy of state  $\Psi_{nlm}$  is  $E = \hbar^2 k^2 / 2\mu$ . Any other regular solution can be expanded using this complete set. In particular, this can be applied to the pane wave that has no singularity at the origin,

$$e^{ik \cdot r} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} a_{lm}(k) j_l(kr) Y_l^m(\theta, \phi).$$
 (6.4.3.2)

To find the amplitudes  $a_{lm}$  in the expansion Eq. (6.4.3.2), we use the freedom of choice of the quantization axis z for the spherical functions  $Y_l^m$ . We combine the z axis with the direction of the wavevector **k**, so that

$$k \cdot r = k_z r cor \theta. \tag{6.4.3.3}$$

The plane wave in Eq. (6.4.3.2) has axial symmetry around the *z* axis and does not depend on the polar angle  $\phi$ . Therefore, the expansion contains only  $Y_l^0 = \sqrt{((2l+1)/4\pi P_l(\cos\theta))}$ so that

$$e^{ikrcos\theta} = \sum_{l=0}^{\infty} a_l P_l(\theta) j_l(kr), \quad a_l = \sqrt{\frac{2l+1}{4\pi}} a_{lo}.$$
(6.4.3.4)

Because the orthogonality of the Legendre polynomials,

$$\int_{-1}^{+1} d\cos\theta e^{ikr\cos\theta} p_l(\cos\theta) = \frac{2}{2l+1} a_l j_l(kr).$$
 (6.4.3.5)

This relation must be correct identically in kr, so that it is sufficient to calculate the left hand side for some value of kr. The integral by parts gives

$$\int_{-1}^{+1} d\cos\theta e^{ikr\cos\theta} p_l(\cos\theta) = \frac{i}{kr} \int_{-1}^{+1} d\cos\theta e^{ikr\cos\theta} p_l'(\cos\theta) + \frac{1}{kr} [e^{ikr} - (-1)^l e^{-ikr}],$$
(6.4.3.6)

for the boundary values of the Legendre polynomials we used the formulas:

$$P_l(\cos\theta) = \frac{1}{2^l l!} \frac{d^l}{d(\cos\theta)^l} (\cos^2\theta - 1)^l$$
(6.4.3.7)

and

$$P_l(-1) = (-1)^l. (6.4.3.8)$$

The integrated term of the left hand side of Eq. (6.4.3.6) equals  $(2/kr)i^l sin(kr - l\pi/2)$ , while, as can be seen by further integrations by parts, the remaining integral has order of magnitude  $1/(kr)^2$  at large kr. By equating the asymptotic  $j_l(kr) \rightarrow sin(kr - l\pi/2)/kr$  at  $(kr) \rightarrow \infty$  of the right hand side of Eq. (6.4.3.5), we come to

$$\frac{2}{kr}i^{l}\sin(kr - l\pi/2) = \frac{2}{2l+1}a_{l}\frac{\sin(kr - l\pi/2)}{kr} \to a_{l} = i^{l}(2l+1) \quad .$$
(6.4.3.9)

Eqs. (6.4.3.5) and (6.4.3.9) define a useful integral relation,

$$j_l(kr) = \frac{1}{2i^l} \int_{-1}^{+1} d\cos\theta e^{ikr\cos\theta} P_l(\cos\theta).$$
 (6.4.3.10)

Thus, the required expansion Eq. (6.4.3.2) of the plane wave over spherical waves is

$$e^{ik \cdot r} = e^{ikrcos\theta} = \sum_{l=0}^{\infty} i^{l} (2l+1) j_{l}(kr) P_{l}(\theta)$$
  
= 
$$\sum_{l=0}^{\infty} i^{l} (2l+1) j_{l}(kr) P_{l}(\theta_{k \cdot r}).$$
 (6.4.3.11)

Using normalized spherical harmonics,

$$Y_l^0 = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta), \qquad (6.4.3.12)$$

the Eq. (6.4.3.11) can be rewritten as

$$e^{ikrcos\theta} = \sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)} j_l(kr) Y_l^0(\theta).$$
 (6.4.3.13)

Eqs. (6.4.3.11) and (6.4.3.13) may both be used to advantage. Remind that the definition of  $\theta$  is the angle between **k** and **r**.

Let the plane wave propagate not in z direction, not in any other direction **k** defined by polar angles  $\Theta$ ,  $\Phi$  in Cartesian coordinates (x, y, z). Remind that the direction of **r** is determined by polar angles  $\theta$ ,  $\phi$  in the same Cartesian coordinates (x, y, z). If  $\theta'$  denotes the angle between the vector **k** and **r**, we have according to Eq. (6.4.3.13),

$$e^{ikrcos\theta} = e^{k \cdot r} = \sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)} j_l(kr) Y_l^0(\theta').$$
(6.4.3.14)

We then make use of the addition theorem of spherical harmonics,

$$\sqrt{\frac{2l+1}{4\pi}}Y_l^0(\theta') = \sum_{m=-l}^{m=l}Y_l^{m*}(\Theta, \Phi)Y_l^m(\theta, \phi)$$

yielding the generalized formula

$$e^{k \cdot r} = \sum_{l=0}^{\infty} 4\pi i^{l} j_{l}(kr) Y_{l}^{m*}(\Theta, \Phi) Y_{l}^{m}(\Theta, \phi).$$
 (6.4.3.15)

# 6.5. Exercises and Solutions

### 6.5.1. Angular Momentum

(1) Define

$$J_{\pm} = J_x \pm i J_y. \tag{6.5.1.1.1}$$

Prove that:

$$J_x = \frac{1}{2}(J_+ + J_-), \quad J_y = \frac{1}{2}(J_+ - J_-) ;$$
 (6.5.1.1.2)

$$[J_z, J_{\pm}] = \pm \hbar J_{\pm}; \tag{6.5.1.1.3}$$

$$J_{\pm}J_{\mp} = J^2 - J_z^2 \pm \hbar J_z. \tag{6.5.1.1.4}$$

$$[J_+, J_-] = J_+ J_- - J_- J_+ = 2\hbar J_z; \qquad (6.5.1.1.5)$$

$$[J_+, J_-]_+ = J_+ J_- + J_- J_+ = 2(J^2 - J_z^2);$$
(6.5.1.1.6)

Solution:

Let us prove Eq. (6.5.1.1.3).

$$\begin{split} [J_z, J_+] &= [j_z, J_x + iJ_y] = [j_z, J_x] + i[J_z, J_y] = i\hbar J_y + i(-i\hbar J_x) \\ &= i\hbar J_y + \hbar J_x = \hbar (J_x + iJ_y) = \hbar J_+. \\ [J_z, J_-] &= [j_z, J_x - iJ_y] = [j_z, J_x] - i[J_z, J_y] = i\hbar J_y - i(-i\hbar J_x) \\ &= i\hbar J_y - \hbar J_x = -\hbar (J_x - iJ_y) = -\hbar J_-. \end{split}$$

Let us demonstrate Eq. (6.5.1.1.4).

$$J_{+}J_{-} = (J_{x} + iJ_{y})(J_{x} - iJ_{y}) = J_{x}^{2} - iJ_{x}J_{y} + iJ_{y}J_{x} + J_{y}^{2}$$
  

$$= J_{x}^{2} - i(J_{x}J_{y} - J_{y}J_{x}) + J_{y}^{2} = J_{x}^{2} - i[J_{x}, J_{y}] + J_{y}^{2}$$
  

$$= J_{x}^{2} - i(i\hbar J_{z}) + J_{y}^{2} = J_{x}^{2} + J_{y}^{2} + \hbar J_{z} = J^{2} - j_{z}^{2} + \hbar J_{z}.$$
  

$$J_{-}J_{+} = (J_{x} - iJ_{y})(J_{x} + iJ_{y}) = J_{x}^{2} + iJ_{x}J_{y} - iJ_{y}J_{x} + J_{y}^{2}$$
  

$$= J_{x}^{2} + i(J_{x}J_{y} - J_{y}J_{x}) + J_{y}^{2} = J_{x}^{2} + i[J_{x}, J_{y}] + J_{y}^{2}$$
  

$$= J_{x}^{2} + i(i\hbar J_{z}) + J_{y}^{2} = J_{x}^{2} + J_{y}^{2} - \hbar J_{z} = J^{2} - j_{z}^{2} - \hbar J_{z}.$$

Let us demonstrate Eq. (6.5.1.1.5).

$$[J_+, J_-] = J_+ J_- - J_- J_+. \tag{6.5.1.1.7}$$

Substituting Eq. (6.5.1.1.4) into Eq. (6.5.1.1.7) yields

$$[J_+, J_-] = J_x^2 + J_y^2 + \hbar J_z - J_x^2 - J_y^2 + \hbar J_z = 2\hbar J_z.$$

(2) We can define quasi-angular momentum (Refer to chapter 3), which are

$$L'_{x} = yk_{z} - zk_{y} = -i\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right). \qquad (6.5.1.2.4a)$$

$$L'_{y} = zk_{x} - xk_{z} = -i\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right). \qquad (6.5.1.2.4b)$$

$$L'_{z} = xk_{y} - yk_{x} = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right).$$
(6.5.1.2.4c)

Prove that the quasi-angular momentums are quantized as well as the angular momentum in quantum mechanics.

Solution:

In Eq. (6.5.1.2.4) **k** represents wavevector. Using the exactly same procedures as in section 6.1.4 of this chapter and assuming  $k = \bar{k}k$  (thus "**k**" is a quantity without dimension), we obtain a similar following equations like the Eqs. (6.1.4.16) and (6.1.4.17):

$$L^{2}Y_{l}^{m}(\theta,\phi) = \bar{k}^{2}l(l+1)Y_{l}^{m}(\theta,\phi), \quad (l=0,1,2,\cdots) \quad .$$
(6.5.1.2.5)

where  $l(l+1)\hbar^2$  are the eigenvalues of operator  $L'^2$ ,  $Y_l^m \equiv |lm\rangle$  being the corresponding eigenfunction. (Note that  $L'^2$  represents both operator and the eigenvalue of operator  $L^2$ .) The eigenvalues  $l(l+1)\bar{k}^2$  is (2l+1) fold degenerate corresponding to a particular value of l there will be (2l+1) values of  $m (= -l, -l+1, \cdots l)$ .

$$L'_{z}Y_{l}^{m}|lm\rangle = m\bar{k}|lm\rangle, \quad |m| \le l \quad m = -l, -l+1, \cdots, l-1, l \quad .$$
(6.5.1.2.6)

Therefore, the quasi-angular momentum is also quantized, and this quantization is independent of quantum mechanics, although at present we do not know how to measure L' or  $L'^2$ .

(3) According to the formula given in section 6.4,  $\theta = \cos^{-1} m / \sqrt{l(l+1)}$ , calculate

$$\Delta \theta \equiv \theta_{l=10^4, m=l} - \theta_{l=10^4, m=l-1}.$$
(6.5.1.14.1)

Solution:

$$\Delta \theta = 0.0057^{\circ}$$
.

(4) Prove the Eq. (6.4.1.7).

Solution: Eq. (6.4.1.7) is

$$p_r = \frac{\hbar}{i} \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) = p_r^+.$$
(6.5.1.4.1)

The Hermitian character of the radial momentum operator can easily be checked by showing it to be self-adjoint, i. e., to satisfy the relation

$$< u|p_rv> = < p_ru|v>$$
 (6.5.1.4.2)

for any pair of complex functions u and v for which these integrals exist.

$$\langle u|p_rv \rangle = \int dr u^* \frac{\hbar}{i} \left(\frac{\partial v}{\partial r} + \frac{v}{r}\right).$$
 (6.5.1.4.3)

$$\langle p_{r}u|v \rangle = \int dr \left\{ \frac{\hbar}{i} \left( \frac{\partial u}{\partial r} + \frac{u}{r} \right) \right\}^{*} v$$

$$= \int dr \left\{ -\frac{\hbar}{i} \left( \frac{\partial u^{*}}{\partial r} + \frac{u^{*}}{r} \right) \right\} v.$$
(6.5.1.4.4)

The two integrals in Eqs. (6.5.1.4.3-4) become equal if expansion

$$\frac{\hbar}{i} \int dr \left\{ u^* \frac{\partial v}{\partial r} + u^* \frac{1}{r} v + \frac{\partial u^*}{\partial r} v + u^* \frac{1}{r} v \right\} = 0$$
(6.5.1.4.5)

or if

$$\oint d\theta d\phi \sin\theta \int_0^\infty dr r^2 \left\{ \frac{\partial}{\partial r} (u^* v) + \frac{2}{r} u^* v \right\} = 0.$$
(6.5.1.4.6)

The inner integral may be reshaped into

$$\int_0^\infty dr \frac{\partial}{\partial r} (u^* v r^2) = u^* v r^2 \big|_0^\infty, \qquad (6.5.1.4.7)$$

which indeed vanishes if  $u^*$  and v remain finite at r = 0 and vanish exponentially for  $r \to \infty$ . It should be noted, however, that the normalization integrals  $\langle u|u \rangle$  and  $\langle v|v \rangle$  will still exist if u and v become singular as 1/r at the origin. Normalization alone therefore does not always suffer to exclude solutions without physical significance, e. g., inside a spherical potential well for l = 0.

(5) Show that, if a state is a simultaneous eigenstate of  $L_x$  and  $L_y$ , then this state has the eigenvalue  $L_x = L_y = L_z = 0$ .

Solution: Let  $\Psi$  be the said state. Then

$$0\Psi = [L_x, L_y]\Psi = i\hbar L_z\Psi.$$
(6.5.1.5.1)

Eq. (6.5.1.5.1) follows that  $\Psi$  is an eigenstate of operator  $L_z$  corresponding to the eigenvalue  $L_z = 0$  (This eigenstate is called null eigenfunction of operator  $L_z$ .). From the uncertainty relation Eq. (3.3.2.1.6), and the fact that  $\Psi$  is an eigenstate of operators  $L_x$  and  $L_y$  we find that

$$0 = (\Delta L_x)(\Delta L_z) \ge \frac{\hbar}{2} |< L_y > | = \frac{\hbar}{2} |L_y|.$$
(6.5.1.5.2)

Because the absolute value of any quantity is  $\geq 0$ , thus Eq. (6.5.1.5.2) tells us the  $\langle L_y \rangle = L_y = 0$ . Similarly,  $\langle L_x \rangle = L_x = 0$ .

This exercise shows that a state of a system corresponding to finite angular momentum cannot be a simultaneous eigenstate of any Cartesian components of operator L. Furthermore, from the definitions of operators  $L_x, L_y, L_z$ , it follows that any constant is a simultaneous, null eigenfunction of operators  $L_x, L_y, L_z$ .

(6) Show that operators  $L_x$  and  $L^2$  are Hermitian.

Solution:

To prove the Hermit property of operator  $L_x$ , we must show that

$$L_x = L_x^+$$

or, equivalently, that

$$(yp_z - zp_y)^+ = (yp_z - zp_y)$$

Look at the  $yp_z$  term.

$$(yp_z)^+ = p_z^+ y^+ = p_z y = yp_z.$$

The last two equalities from (a). Operator  $p_z$  and y are Hermitian ; (b).  $[y, p_z] = 0$ .

#### 6.5.2. Hydrogen-Like Ions

(1) For the ground state of hydrogen atom verify the uncertainty relation between position and momentum.

Solution:

The wavefunction of ground state of hydrogen atom is

$$\Psi_{100} = \left(\frac{1}{\pi a_{\circ}^3}\right)^{1/2} e^{-r/a_{\circ}}$$

Its parity is even. Due to the the parities of operators x and  $p_x$  are odd, we have

$$\langle x \rangle = \langle p_x \rangle = 0$$

Due to that  $\Psi_{100}$  is isotropic, appears as spherical symmetry distribution, it is obvious that

$$< x^{2} > = < y^{2} > = < z^{2} > = \frac{1}{3} < r^{2} >$$

$$< p_{x}^{2} > = < p_{y}^{2} > = < p_{z}^{2} > = \frac{1}{3} < p^{2} >$$

$$< r^{2} > = \int dr r^{2} (\Psi_{100})^{2} = 3a_{\circ}$$

$$< p^{2} > = \int |p\Psi_{100}|^{2} dr = \hbar^{2} \int \left(\frac{\partial\Psi_{100}}{\partial r}\right)^{2} dr = \frac{\hbar^{2}}{a_{\circ}^{2}}$$

Therefore,

$$< x^2 >= a_{\circ}^2, \quad \Delta x = [< x^2 > - < x >^2]^{1/2} = a_{\circ}$$
  
 $< p_x^2 >= \hbar^2/3a_{\circ}^2, \quad \Delta p_x = [< p_x^2 > - < p_x >^2]^{1/2} = \hbar/\sqrt{3}a_{\circ}$ 

At last we have

$$\Delta x \cdot \Delta p_x = \frac{\hbar}{\sqrt{3}} > \frac{\hbar}{2}$$

The general uncertainty relation is

$$\Delta x \cdot \Delta p_x \ge \frac{\hbar}{2}$$

#### 6.5.3. HF Theorem

(1) In terms of HF theorem seek the force acting on the *X* component of a given nucleus in a molecule at  $R_{\gamma}$ .

Solution:

For a molecule with  $1 \le i \le N$  electrons with coordinates  $r_i$ , and  $1 \le \alpha \le M$  nuclei, each located at a specified point  $R_{\alpha} = (X_{\alpha}, Y_{\alpha}, Z_{\alpha})$  and with nuclear charge  $Z_{\alpha}$  the molecule Hamiltonian is

$$H = T - \sum_{i=1}^{N} \sum_{\alpha=1}^{M} \frac{e^2 Z_{\alpha}}{|r_i - R_{\alpha}|} + \sum_{\alpha=1}^{M} \sum_{\beta > \alpha}^{N} \frac{e^2 Z_{\alpha} Z_{\beta}}{|R_{\alpha} - R_{\beta}|}$$
(6.5.3.1.1)

where T is the kinetic energy operator of the molecule, the second and third terms represent the electron-nucleus and nucleus-nucleus interaction potentials in the molecule, respectively.

The force along the X direction, applied on the  $\gamma$ -th  $F_{X_{\gamma}}$ , is equal to the negative of the derivative of the total energy E with respect to that coordinate. Employing the Hellman-Feynman theorem this is equal to

$$F_{X_{\gamma}} = -\frac{\partial E}{\partial X_{\gamma}} = -\left\langle \Psi \middle| \frac{\partial H}{\partial X_{\gamma}} \middle| \Psi \right\rangle$$
(6.5.3.1.2)

The parameter  $\lambda$  in the HF theorem corresponds to the coordinates of the nuclei. Only two components of the Hamiltonian in Eq. (6.5.3.1.1) contribute to the required derivative. Differentiating the Hamiltonian in Eq. (6.5.3.1.1) yields

$$\frac{\partial H}{\partial X_{\gamma}} = \frac{\partial}{\partial X_{\gamma}} \left( -\sum_{\alpha=1}^{M} \sum_{\alpha=1}^{N} \frac{e^2 Z_{\alpha}}{|r_i - R_{\alpha}|} + \sum_{\alpha=1}^{M} \sum_{\beta > \alpha}^{N} \frac{e^2 Z_{\alpha} Z_{\beta}}{|R_{\alpha} - R_{\beta}|} \right) \\
= -e^2 Z_{\gamma} \sum_{i=1}^{N} \frac{x_i - X_{\gamma}}{|r_i - R_{\alpha}|^3} + e^2 Z_{\gamma} \sum_{\alpha \neq \gamma}^{M} Z_{\alpha} \frac{X_{\alpha} - X_{\gamma}}{|R_{\alpha} - R_{\gamma}|^3}.$$
(6.5.3.1.3)

Suppose that the average position density of electron in the molecule is the same for every electron

$$\rho(r) = \rho(r_1) = \rho(r_2) = \dots = \rho(r_N) = \Psi^* \Psi.$$
 (6.5.3.1.4)

Insertion of Eq. (6.5.3.1.3) into the Hellmann-Feynman theorem in Eq. (6.5.3.1.2) returns the force on the *X*-component of the given nucleus at  $R_{\gamma}$  in terms of the electronic density  $\rho(r)$  in Eq. (6.5.3.1.4) and the atomic coordinates and nuclear charges:

$$F_{X_{\gamma}} = -e^2 Z_{\gamma} \left( \int dr \rho(r) \frac{x - X_{\gamma}}{|r_i - R_{\alpha}|^3} - \sum_{\alpha \neq \gamma}^M Z_{\alpha} \frac{X_{\alpha} - X_{\gamma}}{|R_{\alpha} - R_{\gamma}|^3} \right).$$
(6.5.3.1.5)

#### 6.5.4. General Properties of Central Field of Force

(1) Discuss the *S* states of free particle.

Solution:

S means l = 0. In this case the Schrödinger equation is

$$\frac{p_r^2}{2\mu}\Psi_k = E_k\Psi_k.$$
 (6.5.4.1.1)

The radial kinetic energy operator  $p_r^2/2\mu$  commutes with the radial momentum operator  $p_r$  and they have common eigenstates. Due to the degeneracy, however (the eigenstates  $E_k$  are doubly degenerate), eigenfunctions of  $p_r^2$  are not necessarily eigenfunction of  $p_r$ . Owing to the inadmissibility of the eigenfunctions of  $p_r$ , it is the eigenstates of  $p_r^2$  alone which are physical relevant. Namely, these functions are

$$\Psi_k = j_0(kr) = \frac{sinkr}{kr}.$$
 (6.5.4.1.2)

Rewritten  $\Psi_k$  in the form

$$\Psi_{+k} + \Psi_{-k} = \frac{1}{2i} \left( \frac{e^{ikr}}{kr} - \frac{e^{-ikr}}{kr} \right)$$
(6.5.4.1.3)

reveals that it is a superposition of the outgoing spherical wave  $\Psi_{+k}$ , and the ingoing spherical wave  $\Psi_{-k}$ , which gives zero flux at the origin.

(2) Seek the eigenstates and the eigenenergies if a particle of mass M is confined to the interior r < a of a spherical well with impenetrable walls.

Solution:

The general solution is given by Eqs. (6.4.2.16) and (6.4.2.15). To impose the boundary condition  $\Psi_{klm}(r = a, \theta, \phi) = 0$  we set

$$j_l(ka) = 0. \tag{6.5.4.2.1}$$

Actually, from Eq. (6.5.4.2.1) we can find infinite number of solutions. To delineate these values we return to the notation x = kr in terms of which Eq. (6.5.4.1) becomes

$$j_l(x_{ln}) = 0, (6.5.4.2.2)$$

where  $x_{ln}$  is the *n*th zero point of  $j_l(x)$ . The energy spectrum becomes a discrete spectrum instead of the continuous spectrum of *k* values for the free particle.

Eigenfunctions and eigenenergies for the spherical well are then

$$\Psi_{nlm}(r,\theta,\phi) = j_l \left(\frac{x_{ln}r}{a}\right) Y_l^m(\theta,\phi)$$
(6.5.4.2.3)

$$E_{nl} = \frac{\hbar^2 x_{ln}^2}{2Ma^2}.$$
 (6.5.4.2.4)

Orthogonality of the spherical Bessel functions is given by

$$\int_{0}^{a} dr r^{2} j_{l}\left(\frac{x_{ln}r}{a}\right) j_{l}\left(\frac{x_{ln'}r}{a}\right) = \frac{a^{3}}{2} [j_{l+1}(x_{ln})]^{2} \delta_{nn'}.$$
(6.5.4.2.5)

Using Eq. (6.5.4.2.5) one can normalize the wavefunction in Eq. (6.5.4.2.2).

The ground state wavefunction and eigenenergy for the spherical well are given by

$$\Psi_{l=0,n=1} = \sqrt{\frac{1}{2\pi a^3}} \frac{1}{j_1(\pi)} j_0\left(\frac{\pi r}{a}\right)$$
$$E_{l=0,n=1} = \frac{\hbar^2 \pi^2}{2Ma^2}$$

Note that this ground state is nondegenerate.

(3) Momentum space wavefunctions for central force potentials. To show that the splitting off a spherical harmonic in the wavefunction in ordinary space permits the same factorization in momentum space. (Refer to [94]. However, this book makes some modifications)

Solution: In the Fourier transform

$$\Psi(r) = \frac{1}{2\pi^{3/2}} \int dk e^{ik \cdot r} f(k)$$
(6.5.4.3.1)

and

$$f(k) = \frac{1}{2\pi^{3/2}} \int dr e^{-ik \cdot r} \Psi(r)$$
 (6.5.4.3.2)

it shell be supposed that  $\Psi$  is factorized:

$$\Psi(r) = \frac{1}{r} \chi_{nl} Y_l^m(\theta, \phi).$$
 (6.5.4.3.3)

In order to find its Fourier transform according to Eq. (6.5.4.3.2), let us expand the exponential into spherical harmonics of angle  $\gamma$  between the vectors **r** in direction  $\theta$ ,  $\phi$  and **k** in the direction  $\Theta$ ,  $\Phi$  [cf. Eq. (6.4.3.13)]

$$e^{-ikr\cos\gamma} = \sum_{\lambda=0}^{\infty} i^{-\lambda} \sqrt{4\pi(2\lambda+1)} j_{\lambda}(kr) Y_{\lambda}^{0*}(\cos\gamma).$$
(6.5.4.3.4)

Here  $Y_{\lambda}^{0}(\cos\gamma)$  may be expressed by the polar angles of **r** and **k** using the addition theorem of spherical harmonics [cf. Eq. (6.4.3.4)]

$$Y_{\lambda}^{0}(\cos\gamma) = \sqrt{\frac{4\pi}{2l+1}} \sum_{\mu=-\lambda}^{\mu=\lambda} Y_{\lambda}^{\mu*}(\Theta, \Phi) Y_{\lambda}^{\mu}(\Theta, \phi).$$
(6.5.4.3.5)

Substituting Eq. (6.5.4.3.5) into Eq. (6.5.4.3.4), and the result and Eq. (6.5.4.3.3) into Eq. (6.5.4.3.2), we get

$$f(k) = \frac{4\pi}{(2\pi)^{3/2}} \int_0^\infty dr r^2 \oint d\Omega_r \sum_{\lambda\mu} i^{-\lambda} j_\lambda(kr) Y_\lambda^\mu(\Theta, \Phi) Y_\lambda^{\mu*}(\Theta, \phi) \frac{\chi_{nl}}{r} Y_l^m(\Theta, \phi)$$

The integration over all the directions of the vector  $\mathbf{r}$  can be performed:

$$\oint d\Omega_r Y_{\lambda}^{\mu*}(\theta,\phi) Y_l^m(\theta,\phi) = \delta_{l\lambda} \delta_{\mu m}$$

so that only one term (l,m) remains of the double sum:

$$kf(k) = \sqrt{\frac{2}{\pi}} i^{-l} \int_0^\infty dr kr j_l(kr) \chi_{nl}(r) Y_l^m(\Theta, \Phi),$$

i. e., the momentum space function f(k) may be factorized in the form

$$f(k) = \frac{1}{k} g_{nl}(k) Y_l^m(\Theta, \Phi)$$
 (6.5.4.3.6)

with

$$g_{nl}(k) = \sqrt{\frac{2}{\pi}} i^{-l} \int_0^\infty dr kr j_l(kr) \chi_{nl}(r).$$
 (6.5.4.3.7)

The radial parts  $g_{nl}(k)$  and  $i^{-1}\chi_{nl}(r)$  therefore stand in the mutual relation of a Hankel integral transform. The inversion of Eq.(6.5.4.3.7) is

$$\chi_{nl}(r) = \sqrt{\frac{2}{\pi}} i^l \int_0^\infty dr kr j_l(kr) g_{nl}(k).$$
 (6.5.4.3.8)

If we normalize the position space function  $\Psi$  in the usual way to permit its probability density interpretation,

$$\int_0^\infty dr |\chi_{nl}(r)|^2 = 1, \qquad (6.5.4.3.9)$$

we find by putting Eq. (6.5.4.3.8) into Eq. (6.5.4.3.9):

$$\frac{2}{\pi} \int_0^\infty dr \int_0^\infty dk \int_0^\infty dk'' f(k') kr j_l(kr) g_{nl}(k) k' r j_l(k'r) g_{nl}^*(k') = 1.$$

Performing at first the integration over r,

$$\int_0^\infty kr j_l(kr)k'r j_l(k'r) = \frac{\pi}{2},$$
(65.4.3.10)

we get

$$\int_0^\infty dk |g_{nl}(k)|^2 = 1, \qquad (6.5.4.3.11)$$

i. e., the same probability density interpretation holds in momentum space: in the quantum state under consideration the particle will be found with the absolute value of momentum between k and k + dk with the probability  $|g_{nl}(k)|^2 dk$ .

(4) In the subsection 3.5.8 of chapter 3 we have derived a momentum space Schrödinger equation, which is a differential equation. This exercise is to derive a momentum space integral equation or, equivalently, momentum space Schrödinger integral equation for central force potentials. The Fourier transform f(k) of the wavefunction  $\Psi(r)$  describes the momentum distribution in a quantum state. An integral equation shell be derived for f(k) in which the Fourier transform of the potential plays the role of kernel. (Refer to [94]. However, this book makes some modifications)

Solution:

Between  $\Psi(r)$  and f(k) there hold the two reciprocal relations

$$\Psi(r) = \frac{1}{2\pi^{3/2}} \int dk e^{ik \cdot r} f(k).$$
(6.5.4.4.1)

$$f(k) = \frac{1}{2\pi^{3/2}} \int dr e^{-ik \cdot r} \Psi(r).$$
 (6.5.4.4.2)

The potential is

$$V(r) = \int dk e^{ik \cdot r} W(k).$$
 (6.5.4.4.3)

$$W(k) = \frac{1}{2\pi^3} \int dr e^{-ik \cdot r} V(r).$$
 (6.5.4.4.4)

The position space wavefunction satisfies the Schrödiger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V(r)\Psi = E\Psi.$$
 (6.5.4.4.5)

Substituting Eqs. (6.5.4.4.1) and (6.5.4.4.3) into Eq. (6.5.4.4.5) yields

$$\frac{1}{2\pi^{3/2}} \left\{ \frac{\hbar^2}{2m} \int dk e^{ik \cdot r} k^2 f(k) + \int dk \int dk' e^{i(k+k') \cdot r} W(k) f(k') -E \int dk e^{ik \cdot r} f(k) \right\} = 0.$$

In the double integral let us use k'' = k + k' as integration variable (and then again write **k** instead of k''). Then, as the integral will only vanish for any value of **r** if the integrand vanishes, we arrive at

$$\left(\frac{\hbar^2 k^2}{2m} - E\right) f(k) = -\int dk' W(k - k') f(k').$$
(6.5.4.4.6)

The integral equation Eq. (6.5.4.4.6) can be established only if the Fourier transform Eq. (6.5.4.4.4) of the potential exists, i. e., if V(r) at large values of r vanishes at least as  $r^{-1-\varepsilon}$  with infinitesimal  $\varepsilon > 0$ .

It should be noted that from the normalization

$$\int dr |\Psi(r)|^2 = 1$$
$$\int dk |f(k)|^2 = 1$$

one can obtains

just by direct substitution.

(5) Momentum space integral equation for central force potentials. We have shown in the problem (3) of this subsection that for a central force field the solution can be factorized in the form

$$f(k) = \frac{1}{k} g_{nl}(k) Y_l^m(\Theta, \Phi).$$
 (6.5.4.5.1)

The special integral equation for  $g_{nl}(k)$  shall be derived for the hydrogen atom.

Solution:

The integral equation Eq. (6.5.4.4.6), written in atomic units,

$$\left(\frac{k^2}{2} - E\right)f(k) = -\int dk' W(k - k')f(k')$$
(6.5.4.5.2)

with

$$W(k) = \frac{1}{2\pi^3} \int dr e^{-ik \cdot r} V(r)$$
 (6.5.4.5.3)

shall be reduced to a radial equation for  $g_{nl}(k)$  if V(r) depends on the absolute value r of the vector **r**. In that case, Eq. (6.5.4.5.3) may be integrated over the solid angle, the result depending only upon the absolute value of the vector **k**:

$$W(k) = \frac{4\pi}{8\pi^3} \int_0^\infty dr r^2 v(r) \frac{sinkr}{r}.$$
 (6.5.4.5.4)

The kernel of the integral equation then becomes a function of

$$(k-k')^2 = k^2 + k'^2 - 2kk'\cos\gamma, \qquad (6.5.4.5.5)$$

where  $\gamma$  is the angle between the vectors **k** and **k**'. The function *W* may be then expanded into a series of Legendre polynomials,

$$W(|k-k'|) = \sum_{i=0}^{\infty} a_i(k,k') P_i(\cos\gamma), \qquad (6.5.4.5.6)$$

whose coefficients  $a_i$  depend on the absolute values k and k' only. This is the essential point leading to possible factorization.

Using Eq. (6.5.4.5.1) for f(k), the integral equation Eq. (6.5.4.5.2) now becomes

$$\left(\frac{1}{2}k^2 - E\right)\frac{1}{k}g_{nl}(k)Y_l^m(\Theta, \Phi)$$
$$= -\sum_{i=0}^{\infty}\int_0^{\infty} dk'k'^2a_i(k,k')\frac{1}{k'}g_{nl}(k')\oint d\Omega'P_i(\cos\gamma)Y_l^m(\Theta', \Phi')$$

The angular integral can be evaluated using the addition theorem

$$P_i(\cos\gamma) = \frac{4\pi}{2i+1} \sum_{\mu=-i}^{i} Y_i^{\mu*}(\Theta', \Phi') Y_i^{\mu}(\Theta, \Phi)$$

which reduces the sums to one term only with  $i = l, \mu = m$ :

$$\frac{1}{k}g_{nl}(k)Y_l^m(\Theta,\Phi) = -\frac{4\pi}{2l+1}\int_0^\infty fk'k'a_l(k,k')g_{nl}(k')Y_l^m(\Theta,\Phi).$$

This is an identity in the polar angles thus showing that the factorization Eq. (6.5.4.5.1) is correct, and leaving us with the radial integral equation

$$\left(\frac{k^2}{2} - E\right)g_{nl}(k) = -\frac{4\pi k}{2l+1}\int_0^\infty dk' k' a_l(k,k')g_{nl}(k').$$
(6.5.4.5.7)

If the central force is Coulomb attraction of the hydrogen atom,

$$V(r) = -\frac{1}{r},\tag{6.5.4.5.8}$$

the integral Eq. (6.5.4.5.4) can solved using the limiting relation

$$\lim_{\varepsilon \to 0} \int_0^\infty dx e^{-\varepsilon x} \sin x = 1$$

So that we find

$$W(k) = -\frac{1}{2\pi^2 k^2},\tag{6.5.4.5.9}$$

and, according to Eq. (6.5.4.5.5),

$$W(k-k') = -\frac{1}{2\pi^2 |k-k'|^2} = -\frac{1}{4\pi^2 k k' (z - \cos\gamma)}$$

with

$$z = \frac{k^2 + k'^2}{2kk'}.$$
 (6.5.4.5.10)

Putting  $cos\gamma = t$ , Eq. (6.5.4.5.6) then is the well-known expansion of

$$\frac{1}{z-t} = \sum_{i=0}^{\infty} (2i+1)Q_i(z)P_i(t), \qquad (6.5.4.5.11)$$

where the coefficients

$$Q_i(z) = \frac{1}{2} \int_{-1}^{+1} dt \frac{P_i(t)}{z-t}$$
(6.5.4.5.12)

are the Legendre functions of the second kind. We therefore find

$$a_i(k,k') = -\frac{1}{4\pi^2 k k'} (2i+1) Q_i\left(\frac{k^2 + k'^2}{2kk'}\right) P_i(\cos\gamma), \qquad (6.5.4.5.13)$$

so that finally we arrive at the radial integral equation

$$\left(\frac{k^2}{2} - E\right)g_{nl}(k) = -\frac{1}{\pi} \int_0^\infty dk' Q_l\left(\frac{k^2 + k'^2}{2kk'}\right)g_{nl}(k'). \tag{6.5.4.5.14}$$

The integral equation Eq. (6.5.4.5.14) was solved by Ref. [95]. This way means determination of the momentum space eigenfunctions without any recourse to position space functions. The latter way, however, proves simpler for the Coulomb field field and shall be given in the following exercises.

(6) Momentum space wavefunctions for the hydrogen atom. To determine the momentum space wavefunctions for the lowest levels 1S, 2S, 2P of hydrogen atom. Refer to the Table 6.2. 1S means n = 1, l = 0, m = 0. 2S means n = 2, l = 0, m = 0. 2P means n = 2, l = 1, m = -l, 0, +1

Solution:

Since in exercise (3) of this subsection we have shown that, in a central field, a factorized coordinate wavefunction

$$\Psi_{nlm}(r,\theta,\phi) = \frac{1}{r} \chi_n(r) Y_l^m(\theta,\phi)$$
(6.5.4.6.1)

leads to a factorized momentum space wavefunction

$$f(k) = \frac{1}{k} g_n Y_l^m(\Theta, \Phi), \qquad (6.5.4.6.2)$$

we have only to determine the radial part  $g_n(k)$  which follows from a Hankel transform of  $\chi_n(r)$ , and is given in Eq. (6.5.4.3.7):

$$g_{nl}(k) = \sqrt{\frac{2}{\pi}} i^{-l} \int_0^\infty dr kr j_l(kr) \chi_{nl}(r).$$
 (6.5.4.6.3)

For the chosen states we have from Table 6.4, in atomic units,

1S:

$$\chi_{n=1,l=0} = 2re^{-r}.$$
$$j_0(kr) = \frac{sinkr}{kr}.$$

$$g_{n=1,l=0}(k) = \sqrt{\frac{2}{\pi}} 2 \int_0^\infty dr kr \frac{sinkr}{kr} 2r e^{-r}$$
  
=  $\sqrt{\frac{2}{\pi}} \frac{4k}{(1+k^2)^2}.$  (6.5.4.6.4*a*)

2S:

$$\chi_{n=2,l=0} = \frac{1}{\sqrt{2}} \left( r - \frac{1}{2} r^2 \right) e^{-r/2}.$$
  
 $j_0(kr) = \frac{sinkr}{kr}.$ 

$$g_{n=2,l=0}(k) = \sqrt{\frac{1}{\sqrt{\pi}} \int_0^\infty dr kr \frac{sinkr}{kr} \left(r - \frac{1}{2}r^2\right) e^{-r/2}}$$
  
=  $\frac{32}{\sqrt{\pi}} \frac{k(1 - 4k^2)}{(1 + 4k^2)^3}.$  (6.5.4.6.4b)

2P:

$$\chi_{n=2,l=1} = \frac{1}{24}r^2 e^{-r/2}.$$
  
$$j_1(kr) = \frac{sinkr}{(kr)^2} - \frac{coskr}{kr}.$$

$$g_{n=2,l=1}(k) = -i\frac{1}{\sqrt{12\pi}} \int_0^\infty dr kr \left(\frac{sinkr}{(kr)^2} - \frac{coskr}{kr}\right) r^2 e^{-r/2}$$
  
=  $-i\frac{128}{\sqrt{3\pi}} \frac{k^2}{(1+4k^2)^3}.$  (6.5.4.6.4c)

In all the cases there holds the normalization law

$$\int_0^\infty dk |g_{nl}(k)|^2 = 1, \qquad (6.5.4.6.5)$$

which can be checked directly for each of the functions in Eqs. (6.5.4.4a-4c).

# Chapter 7

# **Charged Particle in Electromagnetic Fields**

# 7.1. Electromagnetic Field in Classical Mechanics

Until now, we consider quantum problems with potential V(r). Magnetic fields, in contrast to the static electric field, cannot be included in this way. All the troubles come from including the magnetic field, when we treat the motion of charged particle in electromagnetic field. We must generalize the least action principle in classical Lagrange mechanics to include the magnetic field.

We introduce two approaches to include the electromagnetic field in classical mechanics. Both approaches can be used to the canonical quantization procedure in section 7.2.

(A) Lagrange function. The canonical quantization procedure, explained in section 7.2, is appropriate for any non-singular Lagrangian system (i. e., Hessian determinant is not equal to zero, and thus the Legendre transformation can be carried out). We treat the electromagnetic field as a classical external field, the Lagrangian is not singular, and thus the canonical quantization procedure can be carried out. The electromagnetic field is switched on for a non-relativistic charged particle of mass  $\mu$  and charge q through Lagrange function,

$$L(r,v) = \frac{\mu v^2}{2} - q\phi + \frac{q}{c} [A(r) \cdot v], \qquad (7.1.1)$$

where  $\phi$  is the electromagnetic scalar potential, and  $A(\mathbf{r})$  is the electromagnetic vector potential. The canonical momentum can be found from Lagrange function

$$p = \frac{\partial L}{\partial v} = \mu v + \frac{q}{c} A. \tag{7.1.2}$$

One can see from Eq. (7.1.2) that the canonical momentum does not equal to the mechanical kinetic momentum  $\mu v$ .

The Lagrangian equation of motion is given by

$$\frac{dp}{dt} = \frac{\partial L}{\partial r}.\tag{7.1.3}$$

The *i*-th component of Eq. (7.1.3) is

$$\mu \frac{dv_i}{dt} = -\frac{q}{c} \frac{\partial A_i}{\partial t} - q \frac{\partial \phi}{\partial r_i} + \frac{q}{c} v_j \left( \frac{\partial A_j}{\partial r_i} - \frac{\partial A_i}{\partial r_j} \right).$$
(7.1.4)

As always, the sum is implied over the twice repeated indices. At this point, one can introduce electric  $\mathbf{E}$  and magnetic  $\mathbf{B}$  fields though the derivatives of the potentials:

$$E = -\nabla\phi - \frac{1}{c}\frac{\partial A}{\partial t}.$$
(7.1.5)

$$B = \nabla \times A. \tag{7.1.6}$$

Substituting Eqs. (7.1.5-6) into Eq. (7.1.4) yields the equation of motion

$$\mu \frac{dv}{dt} = qE + \frac{q}{c}v \times B. \tag{7.1.7}$$

The second term in the Eq. (7.1.7) is called Lorentz force. In classical mechanics it is stressed that the **E** and **B** are contained in motion equation. On the other hand, the potential  $\phi$  and **A** are considered auxiliary quantities which are not observable because there is the gauge invariance which leads to some arbitrariness of the set of potentials  $\phi$  and **A**. To see the gauge invariance let us make a gauge transformation to a new set of potentials.

$$A \to A' = A + \nabla f(r, t),$$
  
$$\phi \to \phi' = \phi - \frac{1}{c} \frac{\partial f(r, t)}{\partial t},$$
 (7.1.8)

where f(r,t) is an arbitrary single-valued function, and is called gauge function. Under the gauge transformation in Eq. (7.1.8), the fields **E** and **B** and hence the equation of motion are invariant,

$$E' = -\nabla \phi' - \frac{1}{c} \frac{\partial A'}{\partial t} = E, \quad B' = \nabla A' = B.$$
(7.1.9)

One can determine the Hamilton function according to the rules of classical mechanics from Lagrange function in Eq. (7.1.1),

$$H = \frac{\partial L}{\partial v} \cdot v - L$$
  
=  $\frac{\mu v^2}{2} + q\phi$   
=  $\frac{(p - q/cA)^2}{2\mu} + q\phi.$  (7.1.10)

The second equality of Eq. (7.1.10) indicates that the velocity (or kinetic momentum)dependence of *Hamiltonian* does not change. The third equality of Eq. (7.1.10) indicates that the velocity (or kinetic momentum)-dependence of canonical momentum p does change.
(B) Hamilton function. In classical mechanics the Hamilton function is

$$H = \frac{\mu v^2}{2} + q\phi = \frac{(p - q/cA)^2}{2\mu} + q\phi.$$
(7.1.11)

Let us explain the reason to write the Hamiltonian in magnetic field as given by Eq. (7.1.11).

Substituting Eq. (7.1.11) into canonical equation

$$\dot{r} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial r},$$
 (7.1.12)

one obtains

$$\mu \ddot{r} = q \left( E + \frac{1}{c} v \times B \right), \qquad (7.1.13)$$

where electronic field **E** and **B** are given by Eqs. (7.1.5) and (7.1.6), respectively. Eq. (7.1.13) is the Newton equation of the charged particle in electromagnetic field. The second term in Eq. (7.1.13) is called Lorentz force. We take the *x* component of Eq. (7.1.13) as an example to show the Eq. (7.1.13).

$$\dot{x} = \frac{\partial H}{\partial p_x} = \frac{1}{\mu} \left( p_x - \frac{q}{c} A_x \right). \tag{7.1.14}$$

Therefore,

$$p_x = \mu \dot{x} + \frac{q}{c} A_x. \tag{7.1.15}$$

Eq. (7.1.15) is the same as Eq. (7.1.2).

Making derivative of Eq. (7.1.14) over t, and utilizing Eqs. (7.1.11) and (7.1.12), one obtains

$$\begin{split} \mu \ddot{x} &= \dot{p}_{x} - \frac{q}{c} \dot{A}_{x} = -\frac{\partial H}{\partial x} - \frac{q}{c} \dot{A}_{x} \\ &= \frac{1}{\mu} \sum_{i=1}^{3} \left( p_{i} - \frac{q}{c} A_{i} \right) \frac{q}{c} \frac{\partial A_{i}}{\partial x} - q \frac{\partial \phi}{\partial x} - \frac{q}{c} \dot{A}_{x} \\ &= \frac{q}{c} \sum_{i=1}^{3} \dot{x}_{i} \frac{\partial A_{x}}{\partial x} - q \frac{\partial \phi}{\partial x} - \frac{q}{c} \left( \frac{\partial A_{i}}{\partial t} + \sum_{i=1}^{3} \dot{x}_{i} \frac{\partial A_{x}}{\partial x_{i}} \right) \\ &= -q \left( \frac{\partial \phi}{\partial x} + \frac{1}{c} \frac{\partial A_{x}}{\partial t} \right) \\ &+ \frac{q}{c} \left( \dot{x} \frac{\partial A_{x}}{\partial x} + \dot{y} \frac{\partial A_{x}}{\partial x} + \dot{z} \frac{\partial A_{x}}{\partial x} - \dot{x} \frac{\partial A_{x}}{\partial x} - \dot{y} \frac{\partial A_{x}}{\partial y} - \dot{z} \frac{\partial A_{x}}{\partial z} \right) \\ &= -q \left( \nabla \phi + \frac{1}{c} \frac{\partial A}{\partial t} \right)_{x} + \frac{q}{c} [v \times (\nabla \times A)]_{x} = q \left( E + \frac{q}{c} v \times B \right)_{x}. \end{split}$$
(7.1.16)

### 7.2. Electromagnetic Field in Quantum Mechanics

Next we give you two statements on the transformation of the canonical momentum **p** into operator  $-i\hbar\nabla$  in position space (i. e., coordinate representation):

(a) In chapter 3 we have demonstrated generally that quasi-canonical momentum p' in position space is an operator:

$$p' = -i\nabla, \tag{7.2.1}'$$

and the relation between canonical and quasi-canonical momentum is  $p = \hbar p'$ , therefore,

$$p = -i\hbar\nabla, \tag{7.2.1}$$

(b) Some references take the following statement: according to the stipulation in quantum mechanics, which is called canonical quantization procedure, in coordinate representation we have Eq. (7.2.1).

This book prefers the statement (a), because it gives some reasons to take. Feynman gave a physical explanation for the Eq. (7.2.1) in Ref. [96]. Note that according to Eq. (7.2.1), the canonical momentum and canonical coordinate satisfie the normal commutation relation.

The Hamilton operator of the charged particle in electromagnetic field is thus

$$H = \frac{(p - q/cA)^2}{2\mu} + q\phi.$$
(7.2.2)

This book use **p** to represent both the operator and the quantity. The Schrödinger equation is

$$i\hbar\frac{\partial}{\partial t}\Psi = \left[\frac{(p-q/cA)^2}{2\mu} + q\phi\right]\Psi$$
$$= \left[\frac{1}{2\mu}\left(-i\hbar\nabla - \frac{q}{c}A\right) \cdot \left(-i\hbar\nabla - \frac{q}{c}A\right) + q\phi\right]\Psi.$$
(7.2.3)

General speaking, the operator  $\mathbf{p}$  and  $\mathbf{A}$  do not commute, and satisfies the commutation relation:

$$[p,A] = -i\hbar\nabla \cdot A. \tag{7.2.4}$$

If we use the transverse wave condition  $\nabla \cdot A = 0$ , then Eq. (7.2.3) can be written as:

$$i\hbar\frac{\partial}{\partial t}\Psi = \left[\frac{1}{2\mu}p^2 - \frac{q}{\mu c}A \cdot p + \frac{q^2}{2\mu c^2}A^2 + q\phi\right]\Psi$$
$$= \left[\frac{1}{2\mu}\left(p - \frac{q}{\mu c}A\right)^2 + q\phi\right]\Psi.$$
(7.2.5)

For the Schrödinger equation Eq. (7.2.5) we make the following three discussions:

(A) Gauge invariance of Schrödinger equation.

The canonical momentum operator and canonical coordinate operator do not change under the gauge transformation given by Eq. (7.1.8), because they do not relate to A and  $\phi$ . We show that if the wavefunction makes the following transformation:

$$\Psi \to \Psi' = e^{iqf/\hbar c} \Psi \tag{7.2.6}$$

under the gauge transformation, then the  $\Psi'$  satisfies the same equation as the  $\Psi$ , i. e.,

$$i\hbar\frac{\partial}{\partial t}\Psi' = \left[\frac{(p-q/cA')^2}{2\mu} + q\phi'\right]\Psi'.$$
(7.2.7)

The proof for the Eq. (7.2.7) is as follows:

Substituting the following equations

$$i\hbar\frac{\partial}{\partial t}\Psi' - q\phi'\Psi' = e^{iqf/\hbar c}\left(i\hbar\frac{\partial}{\partial t}\Psi + q\phi\Psi\right)$$
$$\left(-i\hbar\nabla - \frac{q}{c}A'\right)\Psi' = e^{iqf/\hbar c}\left(-i\hbar\nabla - \frac{q}{c}A\right)\Psi$$
$$\left(-i\hbar\nabla - \frac{q}{c}A'\right)^{2}\Psi' = e^{iqf/\hbar c}\left(-i\hbar\nabla - \frac{q}{c}A\right)^{2}\Psi$$

into Eq. (7.2.7), one obtains

$$i\hbar\frac{\partial}{\partial t}\Psi = \left[\frac{(p-q/cA)^2}{2\mu} + q\phi\right]\Psi.$$
(7.2.8)

This concludes the proof.

For the reader's convenience, we summarize the principal idea of gauge invariance in quantum mechanics, in relativistic notation. The gauge transformation in Eq. (7.1.8) for electromagnetic field  $A_{\mu}(x_n u)$  is

$$A'_{\mu} = A_{\mu} + \frac{\partial f}{\partial x_{\mu}}$$

with

$$A_{\mu} = \{A, i\phi\}, \quad and \quad x_{\mu} = \{x, ict\} \quad .$$
 (7.2.9)

This leaves the electromagnetic observables, i. e., the field strengths E and B, unchanged. The four momentum operator is given by

$$p_{\mu} = -i\hbar \left\{ \frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}, \frac{\partial}{\partial x_4} \right\} = \left\{ p, \frac{iH}{c} \right\},$$
(7.2.10)

and minimal coupling is achieved through the replacement

$$p_{\mu} \to p_{\mu} - \frac{q}{c} A_{\mu}. \tag{7.2.11}$$

Therefore, in quantum mechanics, to guarantee the the gauge invariance of Schrödinger equation, the gauge transformation Eq. (7.1.8) must be supplemented by the phase transformation Eq. (7.2.7) of the wavefunction.

(B) Gauge invariance of the continuity equation (i. e., the local probability conservation).

Take the complex conjugate of Eq. (7.2.5) (A and  $\phi$  are real function. In position space  $p^* = -p$ )

$$-i\hbar\frac{\partial}{\partial t}\Psi^* = \left[\frac{1}{2\mu}p^2 + \frac{q}{\mu c}A \cdot p + \frac{q^2}{2\mu c^2} + q\phi\right]\Psi^*.$$
 (7.2.12)

Making  $\Psi^* \times (7.2.5) - \Psi \times (7.2.12)$  and utilizing  $\nabla \cdot A = 0$ , one obtains

$$i\hbar\frac{\partial}{\partial t}(\Psi^{*}\Psi) = \frac{1}{2\mu}(\Psi^{*}p^{2}\Psi - \Psi p^{2}\Psi^{*}) - \frac{q}{\mu c}(\Psi^{*}A \cdot p\Psi + \Psi A \cdot P\Psi^{*})$$
$$= \frac{1}{2\mu}p \cdot (\Psi^{*}p\Psi - \Psi p\Psi^{*}) - \frac{q}{\mu c}p \cdot (\Psi^{*}A\Psi)$$
$$= -\frac{i\hbar}{2\mu}\nabla \cdot \left[(\Psi^{*}p\Psi - \Psi p\Psi^{*}) - \frac{2q}{\mu c}(\Psi^{*}A\Psi)\right].$$
(7.2.13)

Eq. (7.2.13) is

$$\frac{\partial}{\partial t}\rho + \nabla \cdot J = 0, \qquad (7.2.14)$$

where probability density is

$$\rho = \Psi^* \Psi, \tag{7.2.15}$$

and probability current density operator is

$$J = \frac{1}{2\mu} (\Psi^* p \Psi - \Psi p \Psi^*) - \frac{q}{\mu c} A \Psi^* \Psi$$
  

$$\equiv J_0 + J_d$$
  

$$= \frac{1}{2\mu} \left[ \Psi^* \left( p - \frac{q}{c} A \right) + \Psi \left( p - \frac{q}{c} A \right)^* \Psi^* \right]$$
  

$$= \frac{1}{2} (\Psi^* v \Psi + \Psi v^* \Psi^*) = Re(\Psi^* v \Psi), \qquad (7.2.16)$$

where  $\mathbf{v}$  is the velocity operator of the particle given in Eq. (7.1.2).

The first term in the first equality of Eq. (7.2.16) is the old expression for the probability current density,  $J_0$ , in a potential field, while the second term, the diamagnetic probability current density  $J_d$ , is directly proportional to the vector potential and the probability density at a given point,

$$J_d(r) = -\frac{q}{\mu c} |\Psi(r)|^2 A(r).$$
(7.2.17)

Note that the velocity field defined by  $J/\rho$  is no longer irrotational; its cul is proportional to the magnetic field.

$$\nabla \times \frac{J_d}{\rho} = -\frac{q}{\mu c} \nabla \times A = -\frac{q}{\mu c} B.$$
(7.2.18)

The Stokes theorem gives the circulation C of the velocity field along a closed contour pierced by the magnetic field line,

$$C = \oint dl \cdot v = -\frac{q}{\mu c} \oint dl A \cdot dl = -\frac{q}{\mu c} \int \nabla \times A \cdot dS$$
$$= -\frac{q}{\mu c} \int B \cdot dS = -\frac{q\Phi}{\mu c}, \qquad (7.2.19)$$

where  $\Phi$  is the magnetic flux through the surface subtended by the contour. This results is also gauge-invariant since the gradient of the single-valued gauge function f does not contribute to the contour integral Eq. (7.2.19). (C). Scully and Zubairy derived the Eq. (7.2.3) from free particle Schrödibger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(r,t) = H\Psi(r,t) = -\frac{\hbar^2}{2\mu}\nabla^2\Psi(r,t).$$
(7.2.20)

just in terms of gauge invariance under (local) gauge transformation given by Eq. (7.2.6). For detail see Ref. [97].

#### 7.3. Aharonov-Bohm Effect

The time-dependent Schrödinger equation is

$$i\hbar\frac{\partial}{\partial}\Psi(r,t) = -\frac{\hbar^2}{2\mu} \left(\nabla - \frac{iq}{c\hbar}A(r)\right)^2 \Psi(r,t), \qquad (7.3.1)$$

where we assume vector potential  $A(\mathbf{r})$  is time-independent. Consider Eq. (7.3.1) in a region where the magnetic field vanishes. That is, where

$$\nabla \times A = 0. \tag{7.3.2}$$

One can write the solution of Eq. (7.3.1) as

$$\Psi(r,t) = \kappa(r,t)e^{i\gamma(r)},\tag{7.3.3}$$

where

$$\gamma(r) = \int_0 \frac{q}{\hbar} A(r') \cdot dr', \qquad (7.3.4)$$

which is a function of **r** only.

To obtain the equation for  $\kappa(r,t)$  we note from Eqs. (7.3.3-4) that

$$\nabla \Psi = (\nabla \kappa) e^{i\gamma} + i\kappa \left(\frac{q}{\hbar}A\right) e^{i\gamma}.$$
(7.3.5)

Hence,

$$\left[\nabla - \frac{iq}{c\hbar}A(r)\right]\Psi = (\nabla\kappa)e^{i\gamma}.$$
(7.3.6)

Substituting Eq. (7.3.6) into Eq. (7.3.1) yields

$$i\hbar\frac{\partial\kappa}{\partial t} = -\frac{\hbar^2}{2\mu}\nabla^2\kappa. \tag{7.3.7}$$

Thus we have nicely separated out the function  $\kappa$ , which satisfies the Schrödinger equation without the presence of any interaction.

Consider a situation in which a solenoid carries the magnetic field  $B_0$  along its axis. The magnetic field is assumed to be uniform inside the solenoid but it vanishes outside. If the solenoid has radius R, then the magnetic flux through it is given by

$$\Phi = \pi R^2 B_0, \tag{7.3.8}$$



Figure 7.1. P is charged particle source. A and B are the two slits on screen  $S_1$ . The charged particle from source P is detected at, for example, D. If the magnetic field in solenoid (shaded area) does not equal zero, then the interference pattern on screen will change due to the phase shift given by Eq. (7.3.10).

and the vector potential at a point r > R from the axis of the solenoid is given by

$$A = \frac{\Phi}{2\pi r} \Phi \quad (r > R) \quad , \tag{7.3.9}$$

where  $\Phi$  is a unit vector in the direction of the azimuthal angle  $\phi$ . Note that the magnetic field vanishes in this region.

If a charge passes by the solenoid (See Fig. 7.1), then from the relation Eq. (7.3.4) the phase is given by

$$\gamma = \frac{q\Phi}{2\pi\hbar} \int \frac{\Phi}{r} \cdot rd\Phi = \pm \frac{q\Phi}{2\pi\hbar} \phi.$$
 (7.3.10)

The  $\pm$  sign depends on the whether the electrons are traveling in the same direction as the current in the solenoid (which is the same direction as **A**) or the opposite.

Suppose a beam of electrons directed at the solenoid splits in two and goes around either side of the solenoid. The phase difference between the two parts of the beam when they recombine on the other side causes interference between them. The azimuthal angle  $\phi$  covered by the beam in the direction of the current (which is in the same direction as **A**) will be  $\pi$ , and for the beam in the opposite direction will be  $-\pi$ . The difference between these two values is  $2\pi$ . Taking the positive sign for the difference we obtain the total phase difference is  $q\Phi/\hbar$ . This is the essence of the Aharonov-Bohm effect.

#### 7.4. Exercises and Solutions

(1) Prove that inherent in the Hamiltonian of Eq. (7.2.5) is a term that corresponds to the interaction of the magnetic field with the orbital angular momentum.

Solution:

Let us express the Hamiltonian of the Eq. (7.2.5) in the presence of a magnetic field as

$$H = \frac{1}{2\mu}p^2 - \frac{q}{2\mu c}(A \cdot p + p) \cdot A + \frac{q^2}{2\mu c^2}A^2.$$
 (1.1)

The second term on the right hand side gives, after substituting  $p = -i\hbar\nabla$  and introducing the wavefunction  $\Psi$ ,

$$(A \cdot p + p \cdot A)\Psi = -i\hbar [\nabla \cdot (A\Psi) + A \cdot (\nabla\Psi)]$$
  
=  $-i\hbar [(\nabla \cdot A)\Psi + 2A \cdot (\nabla\Psi)].$  (1.2)

We choose the transverse wave condition so that the condition

$$\nabla \cdot A = 0. \tag{1.3}$$

We then obtain

$$(A \cdot p + p \cdot A) = 2A \cdot p. \tag{1.4}$$

Let us now use symmetry gauge

$$A = \frac{1}{2}(B \times r), \tag{1.5}$$

where **r** is the radius vector. Eq. (1.5) satisfies the gauge condition for **A** and reproduces  $\nabla \times A = B$ , where **B** is the magnetic field. Hence

$$(A \cdot p + p \cdot A) = (B \times r) \cdot p. \tag{1.6}$$

Using the vector identity  $A \times B \cdot C = A \cdot (B \times C)$ , we obtain

$$(B \times r) \cdot p = B \cdot (r \times p) = B \cdot L, \tag{1.7}$$

where  $L = r \times p$  is the orbital angular momentum. Thus we have

$$\frac{(p-q/cA)^2}{2\mu} = \frac{1}{2\mu}p^2 - \frac{q}{2\mu c}B \cdot L + \frac{q^2}{2\mu c^2}A^2.$$
 (1.8)

Therefore, inherent in the Hamiltonian is a term that corresponds to the interaction of the magnetic field with the orbital angular momentum. The second term signifies an interaction of the type  $-M \cdot B$ , which corresponds to the interaction of the magnetic field with the magnetic moment due to the current generated through the particle's orbital motion, given by

$$M = \frac{q}{2\mu c}L.$$

(2) Would you please study on yours own the following content on Landau energy level and make discussions.

#### Landau Levels in Uniform Magnetic Field

(A) Classical mechanics.

Consider that an electron (Mass *M*, charge -e. e > 0) is in uniform magnetic field. Suppose that the magnetic direction is along the *z* axis. The equation of motion Eq. (7.1.7) becomes

$$\dot{v} = \frac{dv}{dt} = -\frac{e}{Mc}v \times B \equiv \vec{\omega} \times v,$$
 (1)

which describes circular motion of the particle in the plane perpendicular to the vector of angular velocity,

$$\stackrel{\rightarrow}{\omega} = \frac{e}{Mc}B.$$
 (2)

The rotation proceeds with the cyclotron angular frequency

$$\omega_c = |\vec{\omega}| = \frac{eB}{Mc}.$$
(3)

Integrating Eq. (1) over time yields

$$v = \overline{\mathbf{\omega}} \times (r - r_{\circ}) + v_{\circ}, \tag{4}$$

where we assume that the classical trajectory with the center at the point  $r_{\circ} = (x_{\circ}, y_{\circ})$  and longitudinal velocity  $v_{\circ} = (0, 0, v_z)$ . Written in coordinate representation, Eq. (4) becomes

$$v_x = -\frac{eB}{Mc}(y - y_\circ), \quad v_y = \frac{eB}{Mc}(x - x_\circ), \quad v_z = v_\circ.$$
 (5)

In order to express Eq. (5) in terms of canonical momentum Eq. (7.1.2), we need to select the gauge of the vector potential. Taking symmetry gauge  $A = B \times r/2$ , we have

$$Mv_x = p_x - \frac{eB}{c}y, \quad Mv_y = p_y, \quad Mv_z = p_z.$$
(6)

It is easy to verify that  $\nabla \times A = B$  and  $\nabla \cdot A = 0$  in the symmetry gauge. Substituting Eq. (5) into Eq. (6) yields

$$\frac{p_x}{M} - \frac{eB}{Mc}y = -\frac{eB}{Mc}(y - y_\circ), \quad \frac{p_y}{M} = \frac{eB}{Mc}(x - x_\circ), \tag{7}$$

where the fixed coordinates of the center of the orbit can now be linked to the running coordinates and components of the momentum,

$$x_{\circ} = x - \frac{cp_{y}}{eB},\tag{8a}$$

$$y_{\circ} = \frac{cp_x}{eB},\tag{8b}$$

Eq. (8) indicates that the center of the trajectory in (x, y) plane is a constant of motion in the symmetry gauge. [Note that in the exercise (5) in subsection 7.5.2, Eqs. (2.8-9)) shows this conclusion does not depend on the gauge. Eq. (2.13) shows that in quantum mechanics,  $(x_0, y_0)$  are non-compatible] (B) Quantum Mechanics.

Although in comparison with many other textbooks (such as Refs. [98, 1, 3], the following derivations are largely identical but with minor differences, we hope readers to note the differences in concepts. The wavefunctions of an object as a solution of Schrödinger equation has Landau levels, the object itself does not have any changes, and the object will move according to the guide of wavefunction with Landau energy levels. We have

$$(A_x, A_y, A_z) = \left(-\frac{1}{2}By, \frac{1}{2}Bx, 0\right).$$
 (9)

The electron's Hamilton is

$$H = \frac{1}{2M} \left[ \left( p_x - \frac{eB}{2c} y \right)^2 + \left( p_y + \frac{eB}{2c} x \right)^2 + p_z^2 \right]$$
  
=  $\frac{1}{2M} (p_x^2 + p_y^2) + \frac{e^2 B^2}{8Mc^2} (x^2 + y^2) + \frac{eB}{2Mc} (xp_y - yp_x) + \frac{1}{2M} p_z^2.$  (10)

We just discuss the motion on electron in the x, y plane. Therefore, we do not write the last term in Eq. (10). The Hamiltonian can be rewritten as

$$H = H_0 + \omega_L L_z, \tag{11a}$$

$$H_0 = \frac{1}{2M} (p_x^2 + p_y^2) + \frac{1}{2} \omega_L^2 M(x^2 + y^2), \qquad (11b)$$

where  $\omega_L = eB/2Mc = \omega_c/2$  is the Larmor frequency, *B* in  $\omega_L$  represents the interaction of the orbital magnetic moment of electron with the applied magnetic field, and the second term in Eq. (11b) is called anti-magnetic term.

$$L_z = xp_y - yp_x = -i\hbar \left( x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right) = -i\hbar \frac{\partial}{\partial \phi}.$$
 (11c)

The common eigenstates of the complete set of conservation quantities are the energy eigenstates of the electron. In cylindrical polar coordinates  $(r, \phi, z)$   $((r, \phi)$  is in the (x, y) plane)

$$\Psi(r,\phi) = R(r)e^{im\phi}, \quad m = 0, \pm 1, \pm 2, \cdots .$$
(12)

Substituting Eq. (12) into eigenequation  $H\Psi = E\Psi$ , one obtains the radial equation

$$\left[-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{|m|^2}{r^2}\right) + \frac{1}{2}M\omega_L^2 r^2\right]R(r) = (E - m\hbar\omega_L)R(r).$$
(13)

To determine the solution form of R(r), we try  $r \to 0$  and  $r \to \infty$ .

When  $r \rightarrow 0$ , Eq. (13) becomes

$$-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{|m|^2}{r^2}\right)R(r) = 0.$$
 (14)

The only non-singular solution of Eq. (14) at  $r \rightarrow 0$  is

$$R(r) \propto r^{|m|}.\tag{15}$$

When  $r \rightarrow \infty$ , Eq. (13) becomes

$$\left(-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial r^2} + \frac{1}{2}M\omega_L^2 r^2\right)R(r) = 0.$$
(16)

The solutions of Eq. (16) can be  $R(r) \propto exp(\pm \alpha^2 r^2/2)$  with  $\alpha = \sqrt{M\omega_L/\hbar}$ . However, the only the solution  $R(r) \propto exp(-\alpha^2 r^2/2)$  satisfies the boundary condition of bound state. Therefore, the general solution of Eq. (13) is

$$R(r) = r^{|m|} e^{-\alpha^2 r^2/2} u(r).$$
(17)

Substituting Eq. (17) into Eq. (13) and using natural unit ( $M = \hbar = \omega_L = 1$ . Thus  $\alpha = 1$ . We obtain

$$\frac{d^2u(r)}{dr^2} + \left(\frac{2|m|+1}{r} - 2r\right)\frac{du(r)}{dr} + [2(E-m) - 2(|m|+1)]u(r) = 0.$$
(18)

Set  $\xi = r^2$ . Eq. (18) becomes

$$\xi \frac{d^2 u(\xi)}{d\xi^2} + (|m| + 1 - \xi) \frac{du(\xi)}{d\xi} - \left(\frac{|m| + 1}{2} - \frac{E - m}{2}\right) u(\xi) = 0.$$
(19)

Eq. (19) is just the Kummer (i. e., confluent hypergeometric) equation [82]. Thus the radial part of the energy eigenfunction in Eq. (17) becomes

$$R(r) \sim r^{|m|} e^{-\alpha^2 r^2/2} F(-n_r, |m|+1, \alpha^2 r^2),$$
(20)

where *F* represents the confluent hypergeometric (or Kummer) function. The energy eigenvalues (Landau levels) are

$$E = E_N = (N+1)\hbar\omega_L = (N+1)\frac{\hbar eB}{2Mc},$$
(21a)

with

$$N = 2n_r + |m| + m = 0, 2, 4, \cdots, \quad n_r = 0, 1, 2, \cdots,$$
(21b)

where  $n_r$  represents the node number of the radial function except  $r = 0, \infty$ .

If we include the term  $p_z^2/2M$  in Eq. (10), and substitute Eq. (20) into Eq. (12), then the wavefunction of the electron in magnetic field becomes

$$\Psi_{nmk_z}(r,\phi,z) \sim r^{|m|} e^{-\alpha^2 r^2/2} F(-n_r,|m|+1,\alpha^2 r^2) e^{ip_z z/\hbar},$$
(20)'

where  $exp(im\phi)$  is the eigenfunction of angular momentum operator component  $L_z$ , and  $exp(ip_z z/\hbar)$  is the eigenfunction of canonical momentum operator component  $P_z$ .

If we include the term  $p_z^2/2M$  in Eq. (10), then the energy eigenvalues of the electron in magnetic field becomes

$$E = E_N = (N+1)\hbar\omega_L = (N+1)\frac{\hbar eB}{2Mc} + \frac{P_z^2}{2M},$$
 (21*a*)<sup>*t*</sup>

with

$$N = 2n_r + |m| + m = 0, 2, 4, \cdots, \quad n_r = 0, 1, 2, \cdots, \tag{21b}'$$

We make the following four discussions:

(A) Degeneracy of energy level.

For the electron in uniform magnetic field, the Hamiltonian Eq. (10) has the term  $\omega_L L_z$ . Although this term does not influence the form of energy eigenfunction, but the energy eigenvalues Eq. (21.a-b) has a term  $m\hbar\omega_L$ . Therefore, it is easy to see that all the terms of  $m \leq 0$  have the same energy. Thus the degeneracy of energy levels is  $\infty$ .

(B) The degeneracy of the energy levels is independent of the choice of the gauge.

For example, if we use the Landau gauge

$$A_x = -B_y, \quad A_y = A_z = 0$$
 . (22)

The Hamiltonian of the motion of the electron in (x, y) plane is

$$H = \frac{1}{2M} \left[ \left( p_x - \frac{eB}{c} y \right)^2 + p_y^2 \right].$$
(23)

The eigenstrates of the *H* can be the common eigenstates of the complete set  $(H, P_x)$  of conservative quantities, i. e.,

$$\Psi(x,y) = e^{ip_x x/\hbar} \chi(y).$$
(24)

In Eq. (24)  $p_x$  is the eigenvalue of operator  $p_x$ , and is real number.  $-\infty < p_x < +\infty$ .  $\chi(y)$  satisfies

$$\frac{1}{2M} \left[ \left( p_x - \frac{eB}{c} y \right)^2 - \hbar^2 \frac{d^2}{dy^2} \right] \chi(y) = E \chi(y).$$
(25)

Setting  $y_{\circ} = cp_x/eB$ , Eq. (25) becomes

$$-\frac{\hbar^2}{2M}\chi''(y) + \frac{1}{2}M\omega_c^2(y - y_\circ)^2\chi(y) = E\chi(y).$$
(26)

Remember that  $\omega_c = eB/Mc$  is called cyclotron angular frequency.

Eq. (26) is equivalent to an one dimensional harmonic, the equilibrium point is at  $y = y_{\circ} = cp_x/eB$ . Therefore, the energy eigenvalues are

$$E = E_n = \left(n + \frac{1}{2}\right) \hbar \omega_c, \quad n = 0, 1.2, \cdots$$
  
=  $(N+1)\hbar \omega_L, \quad N = 2n = 0, 2, 4, \cdots.$  (27)

Eq. (27) is same as the Eq. (21). The corresponding eigenfunctions are

$$\chi_{y_{\circ}n}(y) \propto e^{-\alpha^2 (y-y_{\circ})^2/2} H_n[\alpha(y-y_{\circ})], \quad \alpha = \sqrt{M\omega_c/\hbar}.$$
(28)

 $H_n$  represents Hermite polynomials. These eigenfunctions depend on n and  $y_\circ = cp_x/eB$ .  $-\infty < y_\circ < +\infty$ . However, the  $E_n$  do not depend on  $y_\circ$ . Therefore, energy levels are of infinitely large degeneracy. There is an interesting phenomenon, i. e., the electron in uniform magnetic field can appear at infinitely far location, which means that unbound state with discrete energy levels.

(C) The energy E > 0 shown in Eq. (21) can be understood as follows. When the electron moves in applied magnetic field B = (0, 0, B), it can has an induced magnetic moment  $\mu_z$ 

$$\mu_z = -(2n_r + 1 + |m| + m)\frac{e\hbar}{2Mc}.$$
(29)

The minus sign in Eq. (29) indicates that when the electron suffers the action of applied magnetic field, the electron is of anti-magnetism.

(D) The Landau energy levels are very helpful to understand the quantum Hall effect, which states that at low temperature and strong magnetic field the resistivity of two dimensional electron gas produces quantization phenomenon [98, 5].

## Chapter 8

# Particle of Spin 1/2

#### 8.1. General Concept

A large number of particles in nature have spin 1/2, such as electrons, neutrons, leptons, and quarks. We considered the angular momentum in chapter 6, which has a classical counterpart. The angular momentum is derived from the position coordinates and momentum of a particle and is akin to classical  $r \times p$  angular momentum. The dimension of spin is the same as angular momentum. Therefore, we call the spin spin angular momentum vividly. However, in contrast to the orbital angular momentum, the spin angular momentum does not relate to a particle's coordinates or momenta, nor are the eigenstates of spin dependent on boundary conditions imposed in the coordinate space. Spin is an inherent property of a particle, likes mass and charge. It is an extra degree of freedom attached to a quantummechanical particle and must be prescribed together with the values of all other compatible properties of a particle in order to designate the state of the particle. In particular, note that spin wavefunctions do not have a coordinate representation. The concept of particle of spin 1/2 is a uniquely quantummechanical. To understand the mathematical origin of spin one must go to relativistic quantum mechanics as outlined by Dirac's theory. This chapter considers the nonrelativistic, phenomenological aspect of the spin 1/2 concept. The spin 1/2 is treated as a new intrinsic (or internal) degree of freedom, and the corresponding magnetic moment is called intrinsic (or internal) magnetic moment.

The direct observation of the electron spin was by Stern and Gerlach in 1922, and concluded that the electron's spin just takes two values  $\pm \hbar/2$ . See Figs. 8.1 and 8.2. To explain the spectroscopic experiment data, Uhlenbeck and Goudsmit proposed the hypothesis of the existence of electron spin in 1925.

The Stern-Gerlach experiment involves sending a beam of particles through an inhomogeneous magnetic field and observing their deflection. The results in Fig. 8.1 show that particles possess an intrinsic angular momentum that is most closely analogous to the angular momentum of a classically spinning object, but that takes only two quantized values (Refer to Ref. [99].).

The experiment is normally conducted using electrically neutral particles or atoms. This avoids the large deflection to the orbit of a charged particle moving through a magnetic field and allows spin-dependent effects to dominate. If the particle is treated as a classical spinning dipole, it will precess in a magnetic field because of the torque that the magnetic



Figure 8.1. Basic elements of the Stern-Gerlach experiment.

field exerts on the dipole (torque-induced precession). If it moves through a homogeneous magnetic field, the forces exerted on opposite ends of the dipole cancel each other out and the trajectory of the particle is unaffected. However, if the magnetic field is inhomogeneous then the force on one end of the dipole will be slightly greater than the opposing force on the other end, so that there is a net force which deflects the particle's trajectory. If the particles were classical spinning objects, one would expect the distribution of their spin angular momentum vectors to be random and continuous. Each particle would be deflected by a different amount, producing some density distribution on the detector screen. Instead, the particles passing through the Stern-Gerlach apparatus are deflected either up or down by a specific amount. This was a measurement of the quantum observable now known as spin, which demonstrated possible outcomes of a measurement where the observable has discrete spectrum. Although some discrete quantum phenomena, such as atomic spectra, were observed much earlier, the Stern-Gerlach experiment allowed scientists to conduct measurements of deliberately superposed quantum states for the first time in the history of science.

By now it is known theoretically (See the next sections of this chapter 8.) that angular momentum of any kind has a discrete spectrum, which is sometimes imprecisely expressed as "angular momentum is quantized".

The present known spin values for some fermions are as follows.

Electrons are spin 1/2 particles. These have only two possible spin angular momentum values measured along any axis,  $+\hbar/2$  or  $-\hbar/2$ . Because its value is always the same, it is regarded as an intrinsic property of electrons, the spin angular momentum is a purely quantummechanical phenomenon, and is sometimes known as "intrinsic angular momentum" (to distinguish it from orbital angular momentum, which can vary and depends on the presence of other particles).

Many textbooks illustrate that the spin angular momentum is a purely quantummechanical phenomenon by using the following reasons: If the electron spin value arises as a result of the electron rotating the way a planet rotates, then the individual electron would have to



Figure 8.2. Spin values of electron.

be spinning impossibly fast. Even if the electron radius were as large as  $2.8 \text{ fm} (= 2.8 \times 10^{-15} \text{ m}$ =the classical electron radius), its surface would have to be rotating at  $2.3 \times 10^{11} \text{ m/s}$ . The speed of rotation at the surface would be in excess of the speed of light,  $2.998 \times 10^8 \text{ m/s}$ , and is thus impossible. This textbook would like to remind readers to note the fact that: The electron's radius is  $< 10^{-20}$  m, and thus the surface of electron would have to be rotating at  $2.3 \times 10^6$  m/swhich is much less than the light speed.

For electrons there are two possible values for spin angular momentum measured along an axis. The same is true for the proton and the neutron, which are composite particles made up of three quarks each (which are themselves spin-1/2 particles). Other particles have a different number of possible spin values. Delta baryons ( $\Delta^{++}$ ,  $\Delta^{+}$ ,  $\Delta^{0}$ ,  $\Delta^{-}$ ), for example, are spin-3/2 particles and have four possible values for spin angular momentum. Vector mesons, as well as photons, *W* and *Z* bosons and gluons are spin-1 particles and have three possible values for spin angular momentum.

#### 8.2. States of Spin 1/2

Because the spin 1/2 is a new degree of freedom, we have to describe an electron by the wavefunction  $\Psi(r, s_z)$ , where  $s_z$  represents the projection of spin 1/2 on the z axis.

Due to that  $s_z$  just takes two discrete values  $\pm \hbar/2$ , we use two component wavefunction to directly and explicitly write the two component values of the spin 1/2. We write

$$\Psi \equiv \Psi(r, s_z) = \begin{bmatrix} \Psi(r, \hbar/2) \\ \Psi(r, -\hbar/2) \end{bmatrix}, \qquad (8.2.1)$$

which is called spinor wavefunction. The physical meanings of the spinor wavefunction are as follows:

 $|\Psi(r,\hbar/2)|^2$  indicates probability density of the body-factor of electron with spin  $\hbar/2$  and at **r**.

 $|\Psi(r, -\hbar/2)|^2$  indicates probability density of the body-factor of the electron with spin  $-\hbar/2$  and at **r**.

 $\int |\Psi(r,\hbar/2)|^2 dr$  indicates probability of the electron with spin  $\hbar/2$ .

 $\int |\Psi(r, -\hbar/2)|^2 dr$  indicates probability of the electron with spin  $-\hbar/2$ .

Therefore, the normalization condition should be

$$\sum_{s_z = \pm \hbar/2} \int |\Psi(r, s_z)|^2 = \int \Psi^+ \Psi dr$$
  
=  $\int dr \left[ |\Psi(r, s_z = \hbar/2)|^2 + |\Psi(r, s_z = -\hbar/2)|^2 \right] = 1.$  (8.2.2)

If Hamiltonian does not include spin variables or can be expressed as a sum of spin space and position space part, then we write

$$\Psi(r, s_z) = \Psi(r)\Upsilon(s_z), \qquad (8.2.3)$$

where  $\Upsilon(s_z)$  is called wavefunction of spin state or, for brevity, spin function.

$$\Upsilon(s_z) = \begin{bmatrix} a \\ b \end{bmatrix}. \tag{8.2.4}$$

The spin 1/2 vector  $\Upsilon(s_z)$  is called spinor. The normalization condition of wavefunction of spin state is

$$\sum_{s_z = \pm \hbar/2} |\Upsilon(s_z)|^2 = \Upsilon^+ \Upsilon = (a, b) \begin{pmatrix} a \\ b \end{pmatrix} = |a|^2 + |b|^2 = 1.$$
(8.2.5)

Electrons, protons, and neutrons have spin 1/2 (spin of one-half). There are two values of  $m_s$ , 1/2 and -1/2. We use  $\Upsilon_{m_s}(s_z)$  to represent the spin state (or eignstate) with eigenvalue of  $s_z = m_s \hbar$ .  $m_s$  is called spin quantum number.  $s_z$  is the variable of the spin function. The spin function with quantum number  $m_s = 1/2$  is

$$\Upsilon_{1/2}(s_z) = \begin{bmatrix} 1\\0 \end{bmatrix}. \tag{8.2.6a}$$

The spin function with quantum number  $m_s = -1/2$  is

$$\Upsilon_{-1/2}(s_z) = \begin{bmatrix} 0\\1 \end{bmatrix}.$$
(8.2.6*b*)

Sometimes for brevity,

$$\alpha = \begin{bmatrix} 1\\0 \end{bmatrix}, \quad \beta = \begin{bmatrix} 0\\1 \end{bmatrix}. \tag{8.2.6.c}$$

 $\alpha$  and  $\beta$  construct an orthonormal complete basis vectors. Any spin state expressed by Eq. (8.2.4) can be expanded by  $\alpha$  and  $\beta$ :

$$\Upsilon(s_z) = a\alpha + b\beta. \tag{8.2.7}$$

Including position space coordinate r, Eq. (8.2.1) becomes

$$\Psi(r, s_z) = \Psi(r, \hbar/2)\alpha + \Psi(r, -\hbar/2)\beta.$$
(8.2.8)

Example 1. The wavefunction of electron with spin 1/2 (spinning free electron).

The coordinates of electron include the spin variables  $(s,m_s)$  and the position variables (x,y,z). The operators corresponding to these variables  $(S^2, S_z, x, y, z)$  are assumed to commute. Their eigenvalues may therefore be prescribed simultaneously because one may locate the electron without destroying its spin state. Another set of commuting operators for an electron is  $(S^2, S_z, P_x, P_y, P_z)$ ).

The Hamiltonian of an electron is

$$H = \frac{P^2}{2M} + H',$$
 (8.2.9)

where the first term is the Hamiltonian of free electron, and the second term is the interaction term, which can depend on time but is independent of the spin. The reason that operator S's do not enter in the Hamiltonian of a free electron is that the spin manifests itself only in the presence of an electromagnetic field. For relativistic electrons this is not the case. In this event, the free electron Hamiltonian includes spin-dependent term. It follows that H also commutes with  $S^2$  and  $S_z$ . These operators have simultaneous eigenstates. Let  $\Psi_k(r,t)$  be an eigenstate of H, and  $\Upsilon_{m_s}(s_z)$  is the eigenstate of  $S^2$  and  $S_z$ . The total wavefunction for the electron is

$$\Psi_{k,t,m_s}(r,t,s_z) = \Psi_k(r,t)\Upsilon_{m_s}(s_z).$$
(8.2.10)

If the electron is free, then

$$\Psi_{k,m_s}(r,s_z) = \frac{1}{(\sqrt{2\pi})^3} \Upsilon_{m_s}(s_z) e^{ik \cdot r}.$$
(8.2.11)

Due to that for the system of spin  $1/2 s = |s_z|$ , the *s* does not need to appear in Eq. (8.2.10-11).

Example 2. To describe the eigenstate of the electron in central field of force, neglecting the coupling between spin and orbital angular momentum, one can choose  $(H, L^2, L_z, s_z)$  as the complete set of conservative quantities, use notation  $\Psi_{nlmm_s}$ , which in  $(r, s_z)$  representation is

$$\Psi_{nlmm_s}(r,s_z) = \Psi_{nlm}(r,\theta,\phi)\Upsilon_{m_s} = R_{nl}Y_l^m(\theta,\phi)\Upsilon_{m_s}.$$
(8.2.12)

#### 8.3. Spin Operator

Considering that the spin has angular momentum dimension, we denote it by the symbol S. The Cartesian components of S, being angular momentum components, obey the commutation rules:

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x, \quad [S_z, S_x] = i\hbar S_y, \quad [S^2, S_i] = 0 \quad .$$
(8.3.1)

$$S^2 = S_x^2 + S_y^2 + S_z^2. aga{8.3.2}$$

Similarly to the orbital angular momentum operator **L**, we may conclude that a similar structure exists for the eigenstates of  $S^2$  and  $S_z$ :

$$S^{2}|sm_{s}\rangle = \hbar^{2}s(s+1)|sm_{s}\rangle, \quad S_{z}|sm_{s}\rangle = \hbar m_{s}|sm_{s}\rangle .$$
(8.3.3)

Unlike the quantum number, l, for the orbital angular momentum, which has values  $0, 1, 2, \cdots$  with z components  $m = -l, \cdots, +l$ , the quantum number s of the spin 1/2 is assumed to have a unique value s = 1/2 with z component  $m_s = -1/2, 1/2$ . The eigenstates are referred to as spin 1/2 states. They are characterized by the eigenvalues of two commuting operators,  $S^2$  and any one of the three  $S_i$  (Generally, take  $S_z$ .), and designated by the kets  $|1/2, m_s >$ .

A general eigenstate in spin 1/2 system is taken to be a column matrix of the type

$$\left[ \begin{array}{c} \# \\ \# \end{array} \right].$$

The spin operator  $S_i$  are then  $2 \times 2$  matrix,

$$\begin{bmatrix} \# & \# \\ \# & \# \end{bmatrix}$$

Introducing operator without dimension,  $\vec{\sigma} \equiv 2S/\hbar$ , which is called Pauli spin operator. If it is in the matrix form, then it is called Pauli matrix.

$$[\sigma_x, \sigma_y] = i2\sigma_z, \quad [\sigma_y, \sigma_z] = i2\sigma_x, \quad [\sigma_z, \sigma_x] = i2\sigma_y, \quad [\overrightarrow{\sigma}^2, \sigma_i] = 0 \quad (8.3.4)$$

$$\vec{\sigma}^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2. \tag{8.3.5}$$

Assume that  $\sigma_x, \sigma_y, \sigma_z$  are Hermitian operators same as the orbital angular momentum operator, i. e.,  $\sigma_x, \sigma_y, \sigma_z = \sigma_x^+, \sigma_y^+, \sigma_z^+$ , respectively. Eq. (8.3.4) can be rewritten as

$$[\mathbf{\sigma}_i, \mathbf{\sigma}_j] = 2i\boldsymbol{\varepsilon}_{ijk}\mathbf{\sigma}_k \tag{8.3.4}'$$

or

$$\vec{\sigma} \times \vec{\sigma} = 2i \vec{\sigma}$$
. (8.3.4)"

Due to that the projections of **S** on any direction can have only  $\pm\hbar/2$ , thus the projections of  $\vec{\sigma}$  on any direction can have only  $\pm 1$ . Therefore,

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1, \qquad (8.3.5)'$$

Utilizing the second equality of Eq. (8.3.4) and Eq. (8.3.5)'

$$\sigma_{y}(\sigma_{y}\sigma_{z}-\sigma_{z}\sigma_{y})=\sigma_{z}-\sigma_{y}\sigma_{z}\sigma_{y}=\sigma_{y}2i\sigma_{x}$$
(a)

Similarly,

$$\sigma_{y}(\sigma_{z}\sigma_{y}-\sigma_{y}\sigma_{z})=\sigma_{x}2i\sigma_{y}$$
 (b)

From (a) + (b) and similar method we have

$$\sigma_x \sigma_y + \sigma_y \sigma_x = 0$$
  

$$\sigma_y \sigma_z + \sigma_z \sigma_y = 0 .$$
  

$$\sigma_z \sigma_x + \sigma_x \sigma_z = 0$$
(8.3.6)

Eq. (8.3.6) indicates that the three components of  $\vec{\sigma}$  are anticommutative.

Combining Eqs. (8.3.6) and (8.3.4) yields

$$\sigma_{x}\sigma_{y} = -\sigma_{y}\sigma_{x} = i\sigma_{z}$$
  

$$\sigma_{y}\sigma_{z} = -\sigma_{z}\sigma_{y} = i\sigma_{x} \quad .$$
  

$$\sigma_{z}\sigma_{x} = -\sigma_{x}\sigma_{z} = i\sigma_{y}$$
  
(8.3.7)

Eqs. (8.3.5) and (8.3.7) and the requirement of Hermitian operator are the complete algebraic properties of Pauli spin operator.

Next, we choose a particular representation to express the Pauli spin operator as a matrix. We choose  $\sigma_z$  representation, i. e., in which representation  $\sigma_z$  is a diagonal matrix with +1 and -1 along the diagonal.

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{8.3.8}$$

Set the matrix of  $\sigma_x$  is

$$\mathbf{\sigma}_{x} = \begin{bmatrix} a & c \\ b & d \end{bmatrix}. \tag{8.3.9}$$

We will now try to determine the a, b, c, d.

Due to  $\sigma_z \sigma_x = -\sigma_x \sigma_z$  we have

$$\left[\begin{array}{cc} a & b \\ -c & -d \end{array}\right] = \left[\begin{array}{cc} -a & b \\ -c & d \end{array}\right]$$

Therefore, a = d = 0, and

$$\mathbf{\sigma}_{x} = \left[ \begin{array}{cc} 0 & c \\ b & 0 \end{array} \right]$$

According to the requirement of Hermitian operator,  $\sigma_x^+ = \sigma_x$ , one obtains  $c = b^*$ . Thus

$$\sigma_x = \begin{bmatrix} 0 & b \\ b^* & 0 \end{bmatrix}$$
$$\sigma_x^2 = \begin{bmatrix} 0 & b \\ b^* & 0 \end{bmatrix} \begin{bmatrix} 0 & b \\ b^* & 0 \end{bmatrix} = \begin{bmatrix} |b|^2 & 0 \\ 0 & |b|^2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Therefore,  $|b|^2 = 1$ , and  $b = exp(i\alpha)$  ( $\alpha$  is a real number).

$$\sigma_{x} = \begin{bmatrix} 0 & exp(i\alpha) \\ exp(-i\alpha) & 0 \end{bmatrix}.$$
 (8.3.10)

Utilizing the last equation in Eq. (8.3.7) yields

$$\sigma_{y} = -i\sigma_{z}\sigma_{x}$$

$$= -i\begin{bmatrix} 1 & 0\\ 0 & -1 \end{bmatrix}\begin{bmatrix} 0 & exp(i\alpha)\\ exp(-i\alpha) & 0 \end{bmatrix}$$

$$= -i\begin{bmatrix} 0 & exp(i\alpha)\\ -exp(-i\alpha) & 0 \end{bmatrix}.$$
(8.3.11)

As is well known, in quantum mechanics the matrix of a dynamical quantity in any representation has an uncertainty of the phase. We often take  $\alpha = 0$ . ( $\alpha = 0$  and diagonal  $\sigma_z$  are capped Pauli representation.) If  $\alpha = 0$ , then Eq. (8.3.11) becomes

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_x = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \quad (8.3.12)$$

Let us now define the following operators:

$$\sigma_{+} = \frac{\sigma_{x} + i\sigma_{y}}{2}, \quad \sigma_{-} = \frac{\sigma_{x} - i\sigma_{y}}{2}$$
(8.3.13)

These are the counterpart of the ladder operators  $L_{\pm}$  we consider in chapter 6. We note that  $\sigma_{-} = \sigma_{+}^{+}$ . One can derive the following commutation relations from Eq. (8.3.4)

$$[\sigma_z, \sigma_+] = 2\sigma_+, \quad [\sigma_z, \sigma_-] = -2\sigma_-, \quad [\sigma_+, \sigma_-] = 4\sigma_z \tag{8.3.14}$$

From Eq. (8.3.13) we obtain the matrix form of  $\sigma_{\pm}$ :

$$\boldsymbol{\sigma}_{+} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \boldsymbol{\sigma}_{-} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}.$$
(8.3.15)

#### 8.4. More about Eigenstates of Spin 1/2

We have thus far considered eigenstate of  $\sigma_z$ . Let us obtain, as a simple exercise, the eigenstates of the other Pauli matrixes. If we designate  $|x \pm \rangle$  as the spin-up and spin-down state in the *x* direction, then

$$\sigma_x | x + > = | x + >, \quad and \quad \sigma_x | x - > = -| x - > .$$
 (8.4.1)

Let us obtain  $|x+\rangle$  by writing it as a superposition of the eogenstates of  $\sigma_z$ ,

$$|x+\rangle = c_1 \begin{bmatrix} 1\\0 \end{bmatrix} + c_2 \begin{bmatrix} 0\\1 \end{bmatrix}, \qquad (8.4.2)$$

where

$$|c_1|^2 + |c_2|^2 = 1. (8.4.3)$$

From Eqs. (8.3.12), (8.4.1), and (8.4.2) we have

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \left\{ c_1 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + c_2 \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\} = c_1 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + c_2 \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad (8.4.4)$$

which gives, together with Eq. (8.4.3), the result

$$c_1 = c_2 = \frac{1}{\sqrt{2}},\tag{8.4.5}$$

where we have taken the positive square root. Thus,

$$|x+\rangle = \frac{1}{\sqrt{2}} \left\{ \begin{bmatrix} 1\\0 \end{bmatrix} + \begin{bmatrix} 0\\1 \end{bmatrix} \right\} = \frac{1}{\sqrt{2}} [|z+\rangle + |z-\rangle] = \frac{1}{\sqrt{2}} \begin{bmatrix} 1\\1 \end{bmatrix}.$$
(8.4.6)

Similarly, one can obtain the eigenstate of  $\sigma_{v}$ .

Let us now obtain eigenstates of  $\vec{\sigma}$  pointing in an arbitrary direction. We use  $\sigma_z$  representation. We designate a state corresponding to spin pointing in the direction of a unit vector **n** as

$$|\Upsilon_{n+}\rangle. \tag{8.4.7}$$

This state is then an eigenstate of the projection of the spin operator  $\vec{\sigma}$  in the **n** direction with eigenvalue +1, that is,

$$\vec{\sigma} \cdot n |\Upsilon_{n+}\rangle = |\Upsilon_{n+}\rangle.$$
 (8.4.8)

If the polar angle of **n** is  $\theta$  and the azimuthal angle is  $\phi$ , then in terms of its coordinates in the Cartesian system one can write

$$n = (sin\theta cos\phi, sin\theta sin\phi, cos\theta), \tag{8.4.9}$$

then

$$\vec{\sigma} \cdot n = \sigma_x \sin\theta \cos\phi + \sigma_y \sin\theta \sin\phi + \sigma_z \cos\theta = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \sin\theta \cos\phi + \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \sin\theta \sin\phi + \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \cos\theta = \begin{bmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{bmatrix}.$$
(8.4.10)

Let

$$|\Upsilon_{n+}\rangle = \begin{bmatrix} a\\b \end{bmatrix}, \qquad (8.4.11)$$

with  $|a|^2 + |b|^2 = 1$ , then according to Eq. (8.4.8) we have

$$\begin{bmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix}, \quad (8.4.12)$$

which gives rise the following two equations:

$$a\cos\theta + b\sin\theta e^{-i\phi} = a$$
,  $a\sin\theta e^{i\phi} - \cos\theta = b$ . (8.4.13)

The first equation gives

$$a(1 - \cos\theta) = b \sin\theta e^{-i\phi}.$$
 (8.4.14)

Since  $(1 - \cos\theta) = 2\sin^2(\theta/2)$  and  $\sin\theta = 2\sin(\theta/2)\cos(\theta/2)$ , we find a normalized solution as

$$a = \cos(\theta/2)$$
 and  $b = \sin(\theta/2)e^{i\phi}$ . (8.4.15)

Hence

$$|\Upsilon_{n+}\rangle = \cos(\theta/2) \begin{bmatrix} 1\\0 \end{bmatrix} + \sin(\theta/2)e^{i\phi} \begin{bmatrix} 0\\1 \end{bmatrix} = \begin{bmatrix} \cos(\theta/2)\\ \sin(\theta/2)e^{i\phi} \end{bmatrix}.$$
 (8.4.16)

Similarly,

$$|\Upsilon_{n-}\rangle = \begin{bmatrix} \sin(\theta/2) \\ -\cos(\theta/2)e^{i\phi} \end{bmatrix}.$$
 (8.4.17)

#### 8.5. Exercises and Solutions

(1) Would you please study on yours own the following content on the intrinsic magnetic moment of electron and make discussions.

#### **Intrinsic Magnetic Moment of Electron**

The systematic theory of inherent magnetic moment of electron will be interpreted in quantum field theory. For the method to introduce intrinsic magnetic moment of electron in this section please refer to Ref. [1].

A non-relativistic electron's Hamiltonian is often expressed as

$$H = \frac{P^2}{2M}.$$
 (1)

If we consider that the electron has spin 1/2, then we should assume that the free electron's Hamiltonian is

$$H = \frac{(\vec{\sigma} \cdot P)^2}{2M}.$$
 (2)

If there is no external magnetic field, then  $(\vec{\sigma} \cdot P)^2 = P^2$ , and Eq.(2) is same as the Eq. (1).

However, if we consider that the charge of electron is -e, and the external magnetic field is  $B = \nabla \times A$ , then according to the discussion in section 8.1, Eq. (2) becomes

$$H = \frac{\left[\vec{\sigma} \cdot (P + e/cA)\right]^2}{2M},\tag{3}$$

Using the equality  $(\vec{\sigma} \cdot V_1)(\vec{\sigma} \cdot V_2) = V_1 \cdot V_2 + i \vec{\sigma} \cdot (V_1 \times V_2)$ , Eq. (3) can be transformed into

$$H = \frac{\left(P + e/cA\right)^2}{2M} + \frac{i}{2M} \vec{\sigma} \cdot \left[\left(P + e/cA\right) \times \left(P + e/cA\right)\right],\tag{4}$$

where the first term on the right hand side includes the interaction between the electron's orbital magnetic moment and the external magnetic field, and the second can be transformed into

$$\frac{ie}{2Mc}\vec{\sigma}\cdot(P\times A + A\times P) = \frac{ie}{2Mc}\vec{\sigma}\cdot(-i\hbar\nabla\times A) = \frac{e\hbar}{2Mc}\vec{\sigma}\cdot B.$$
(5)

We define

$$\vec{\mu}_{s} = -\frac{e\hbar}{2Mc}\vec{\sigma} = -\frac{e}{Mc}S, \quad S = \frac{\hbar}{2}\vec{\sigma}.$$
(6)

From Eq. (5) we see that  $\vec{\mu}_s$  is equivalent to the magnetic moment corresponding to the electron's spin **S**, and is called intrinsic or internal magnetic moment. Eq. (5) denotes the interaction energy between the electron's intrinsic magnetic moment and external magnetic field. The absolute value of intrinsic magnetic moment is equal to the Bohr magneton  $\mu_B = e\hbar/2Mc$ . *M* is the static mass of electron.

If we define that the  $g \equiv$ (magnetic moment/angular moment), then the g factor of the intrinsic magnetic moment of the electron's spin is

For comparison, the magnetic moment,  $\overline{\mu}_L$ , of electron in external magnetic field satisfies

$$\vec{\mu}_L = -\frac{e}{2Mc}L.$$
(7)

Making comparison between Eqs. (6) and (7), we know that the g factor of intrinsic magnetic moment is equal to  $2 \times$  the g factor of the orbital magnetic moment.

## Chapter 9

# **Identical Particles**

### 9.1. Characteristics of Identical Particles

The definition of identity of particles: Particles (= Object = Wavepacket = Wavepacket-function  $\neq$  Wavefunction) are identical if they have the same intrinsic properties.

By "intrinsic" I mean properties inherent to the particles, such as static mass, charge, definite spin, magnetic moment, lifetime etc. The coordinate variables, momentum variables, and spin variables etc. do not belong to intrinsic properties of particles.

This chapter will use the wavepacket-only theory to analyze the identical particle system. Especially, note that any particle contains two factors: guide-factor and body-factor. At first we would like to point out that all the unique characteristics of identical particle system manifest in multiparticle guide-factor (i. e., multiparticle wavefunction) of identical wavepackets, other than the multiparticle body-factor of the identical wavepackets. In an identical multiparticle system the body-factor of a wavepacket still accepts the guide of the guide-factor according to the spontaneous equiprobability symmetry breaking law. However, the construction of multiparticle wavefunction (= multiparticle guide-factor) from all the single particle wavefunctions is of unique characteristic.

The following quantities in identical particle system are of obvious exchange symmetry:

(1) All observable quantities, i. e., operators;

(2) Average values of observable quantities.

Here, the "exchange" means the exchange of two particles, i. e., all the variables in all spaces, including position space, spin space, and so on, describing the two identical particles i and j.

Examples of exchange symmetry (symmetry=invariance) of observables in identical particles:

Example 1. The Hamiltonian H of identical particles. Hamiltonian is an operator corresponding to energy. In this aspect, the simplest example is helium atom. One helium atom has two electrons. These two electrons construct an identical particle system. The

Hamiltonian of this identical particle system is formally

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{|r_1 - r_2|}.$$
(9.1.1)

If we exchange the location variables of the two electrons 1 and 2, then it is obvious that the Hamiltonian in Eq. (9.1.1) does not change, i. e.,

$$[P_{12},H] = 0, (9.1.2)$$

where the  $P_{12}$  is called permutation operator, represents the exchange (of coordinate variables in this case) of two particles 1 and 2. Eq. (9.1.2) tells us that H and  $P_{12}$  commutes.

Example 2. Actually, any operators, corresponding to observables, such as the density at  $\mathbf{r}$  of the identical *N* particle system

$$\rho(r) = \sum_{i=1}^{N} \delta(r - r_i)$$

and the current density at **r** 

$$J(r) = \frac{1}{2} \sum_{i=1}^{N} \left[ \frac{p_i}{m} \delta(r - r_i) + \delta(r - r_i) \frac{p_i}{m} \right]$$

are invariant under the exchange of any two particles.

The above exchange symmetry does need the identity of the identical particles, and does not need the so called indistinguishability of identical particles. Although some references think that the identical particle system obeys the so called "indistinguishability principle", but this textbook still insists that if a terminology, i. e., indistinguishability in this case, is not necessary, we do not need to propose it. Or, more exactly speaking, this textbook thinks that the particles in a identical system are distinguishable.

At this stage, the quantum and classical mechanics do not have difference. As is well known, the exchange symmetry is trivial for classical mechanics. But quantum mechanics has the wavefunction besides the substance of a particle. For this identical multiparticle system there should be a multiparticle wavefunction if we use quantum mechanics to study the identical multiparticle system.

In quantum mechanics, the prominent character is the observed value of an object does not directly connect with substance of the object. The observed values of any observable quantities (= operators) are connected certainly with average values through the square(!) of absolute value of wavefunction.

Therefore, one cannot deduce from the two exchange symmetries of operators and average values that the wavefunction of an identical multiparticle system does not change under the particles' exchange. Let us make detail analyses.

Suppose that there are N identical particles, and the multiparticle wavefunction is

$$\Psi(q_1, q_2, \cdots, q_N), \tag{9.1.3}$$

where  $q_i$  denotes all the dynamical variables of the *i*-th particle, such as position space coordinates, spin coordinates etc.

The average value of Hamiltonian H is

$$< H > = \int \Psi^*(q_1, q_2, \cdots, q_N) H \Psi(q_1, q_2, \cdots, q_N) dq_1 \cdots dq_N.$$
 (9.1.4)

Besides the examples of the above mentioned exchange symmetries of identical particle system, we put a looking like trivial requirement, i. e., the exchange symmetry of average value.

$$P_{ij} < H > = P_{ij} \int \Psi^{*}(q_{1}, q_{2}, \dots, q_{N}) H \Psi(q_{1}, q_{2}, \dots, q_{N}) dq_{1} \dots dq_{N}$$

$$= \int P_{ij} P_{si}^{*}(q_{1}, q_{2}, \dots, q_{i}, \dots, q_{j}, \dots, q_{N}) P_{ij} H$$

$$P_{ij} \Psi(q_{1}, q_{2}, \dots, q_{i}, \dots, q_{j}, \dots, q_{N}) dq_{1} \dots dq_{N}$$

$$= \int P_{ij} \Psi^{*}(q_{1}, q_{2}, \dots, q_{i}, \dots, q_{j}, \dots, q_{N}) H$$

$$P_{ij} \Psi(q_{1}, q_{2}, \dots, q_{j}, \dots, q_{i}, \dots, q_{N})$$

$$= < H >$$

$$= \int \Psi^{*}(q_{1}, q_{2}, \dots, q_{i}, \dots, q_{j}, \dots, q_{N}) H$$

$$\Psi(q_{1}, q_{2}, \dots, q_{i}, \dots, q_{N}) dq_{1} \dots dq_{N}.$$
(9.1.5)

Making comparison between the third equality and the fifth equality yields

$$\begin{array}{l}
P_{ij}\Psi^*(q_1,q_2,\cdots,q_i,\cdots,q_j,\cdots,q_N)P_{ij}\Psi(q_1,q_2,\cdots,q_i,\cdots,q_j,\cdots,q_N)\\ \equiv \Psi^*(q_1,q_2,\cdots,q_i,\cdots,q_j,\cdots,q_N)\Psi(q_1,q_2,\cdots,q_i,\cdots,q_j,\cdots,q_N)\end{array}$$
(9.1.6)

From Eq. (9.1.6) we obtain if

$$P_{ij}\Psi(q_1,q_2,\cdots,q_i,\cdots,q_j,\cdots,q_N) = e^{i\Phi}\Psi(q_1,q_2,\cdots,q_i,\cdots,q_j,\cdots,q_N, \qquad (9.1.7)'$$

and

$$P_{ij}\Psi^*(q_1, q_2, \cdots, q_i, \cdots, q_j, \cdots, q_N) = e^{-i\Phi}\Psi^*(q_1, q_2, \cdots, q_i, \cdots, q_j, \cdots, q_N, \quad (9.1.7)''$$

where the  $\varphi$  can be an arbitrary real numbers, then Eq. (9.1.6) holds. From Eqs. (9.1.7)' and (9.1.7)'' and the definition of  $P_{ij}$ , we obtain two equations to determine  $\varphi$ 

$$P_{ij}P_{ij}\Psi(q_1, q_2, \cdots, q_i, \cdots, q_j, \cdots, q_N) = e^{i2\varphi}\Psi(q_1, q_2, \cdots, q_i, \cdots, q_j, \cdots, q_N) \\
 = \Psi(q_1, q_2, \cdots, q_i, \cdots, q_j, \cdots, q_N) , \quad (9.1.8)'$$

and

$$P_{ij}P_{ij}\Psi^{*}(q_{1},q_{2},\cdots,q_{i},\cdots,q_{j},\cdots,q_{N}) = e^{-i2\phi}\Psi^{*}(q_{1},q_{2},\cdots,q_{i},\cdots,q_{j},\cdots,q_{N})$$

$$= \Psi^{*}(q_{1},q_{2},\cdots,q_{i},\cdots,q_{j},\cdots,q_{N})$$
(9.1.8)"

Eqs. (9.1.8)' and (9.1.8)" require

$$e^{i2\varphi} = 1, \quad e^{-2i\varphi} = 1.$$
 (9.1.9)

The solution of Eq. (9.1.9) is

$$\varphi = 0, and \pi. \tag{9.1.10}$$

From Eq. (9.1.10) we deduce:

$$P_{ij}\Psi(q_1, q_2, \cdots, q_i, \cdots, q_j, \cdots, q_N) = e^{i\Phi}\Psi(q_1, q_2, \cdots, q_i, \cdots, q_j, \cdots, q_N)$$
  
$$\pm \Psi(q_1, q_2, \cdots, q_i, \cdots, q_j, \cdots, q_N).$$
(9.1.11)

Eq. (9.1.11) tells us that the eigenvalues of the permutation operator  $P_{ij}$  are +1 and -1. Because we have shown that  $P_{ij}$  is a constant of motion, the eigenvalues of  $P_{ij}$  and the energy eigenvalues can simultaneously describe the state of the identical particle system. Thus, the multiparticle wavefunction of identical particle system is proved to have to satisfy either

$$P_{ij}\Psi^{S} = +\Psi^{S} \tag{9.1.12}$$

or

$$P_{ij}\Psi^A = -\Psi^A \tag{9.1.13}$$

for  $i \neq j = 1, 2, \dots, N$ . We call the wavefunction  $\Psi^S$  with eigenvalue +1 the symmetric, and  $\Psi^A$  with the eigenvalue -1 the antisymmetric. We call the properties of the multiparticle wavefunction of identical multiparticle system in Eqs. (9.1.12) and (9.1.13) exchange symmetry of wavefunction of identical multiparticle system.

Eq. (9.1.2) tells us that  $P_{ij}$  is a constant of motion, and thus is a conservative quantity. Therefore the symmetry of multiparticle wavefunction does not change with time. This point can be explained as follows.

Suppose at initial state  $t = 0 \Psi(0)$  is of exchange symmetry.  $P_{ij}\Psi(0) = \lambda\Psi(0)$ . If H does not include time t explicitly, then  $\Psi(t) = exp(-iHt/\hbar)\Psi(0)$ . Considering  $[P_{ij}, H] = 0$ , one knows

$$P_{ij}\Psi(t) = P_{ij}e^{-iHt/\hbar}\Psi(0) = e^{-iHt/\hbar}P_{ij}\Psi(0) = e^{i\varphi}e^{-iHt/\hbar}\Psi(0) = e^{-iHt/\hbar}e^{i\varphi}\Psi(0).$$
(9.1.14)

Therefore,  $\Psi(0)$  and  $\Psi(t)$  are of the same exchange symmetry if *H* does not contain time *t* explicitly. If *H* depends on time explicitly, then

$$|\Psi(t)\rangle = Te^{-i\int_0^t dt' H(t')/\hbar} |\Psi(0)\rangle.$$
(9.1.15)

Using Eqs. (9.1.14-15), we can also obtain that  $\Psi(0)$  and  $\Psi(t)$  are of the same exchange symmetry if *H* contains time *t* explicitly.

We define that the particles described by an antisymmetrical wavefunction are called fermions, and the particles described by a symmetrical wavefunction are called bosons.

Note that the  $q_i$  in Eq. (9.1.5) can represents  $r_i$ ,  $t_i$  besides  $r_i$ , and all the above conclusions are correct also for the time-dependent case.

The quantum field theory proves a Pauli theorem, which states:

**Theorem XXXIV: Pauli theorem.** The criterion that distinguishes between the two kinds of particles is their spins: Fermions have half-integer spin, and obey Fermi-Dirac statistics;

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Bosons have integer and zero spin, and obey Bose-Einstein statistics.[6, 100]

Examples of fermions are electrons, protons, neutrons, neutrinos,  $C^{13}$  nuclei etc. (all spin 1/2). Examples of bosons are  $\pi$  mesons (spin 1),  $\alpha$  particles (spin 0), oxygen nuclei (spin 0). For particles that are consisted of several elementary particles, the total spin also determines the exchange symmetry of wavefunction. The  $\alpha$  particle that consists of 4 nucleons with spin 1/2 has spin zero and is boson. We get the same result when considering that the exchange of an  $\alpha$  particle requires the exchange of two protons and two neutrons; the signs that result from the two-fermion exchange compensate for each other in this state.

Next, we show that a transition between symmetric and antisymmetric states is impossible. This is because the interaction between particles is symmetric under their exchange; hence, e. g.,

$$V(r_1, r_2, \cdots, r_i, \cdots, r_j, \cdots, r_N) = V(r_1, r_2, \cdots, r_j, \cdots, r_i, \cdots, r_N).$$
(9.1.16)

For Eq. (9.1.16), the matrix elements between symmetric and antisymmetric states vanish:

$$\langle \Psi^{S} | V | \Psi^{A} \rangle = \langle \Psi^{S}(r_{1}, r_{2}, \cdots, r_{j}, \cdots, r_{j}, \cdots, r_{N}) | V(r_{1}, r_{2}, \cdots, r_{j}, \cdots, r_{i}, \cdots, r_{N}) \rangle$$

$$= \langle \Psi^{S}(r_{1}, r_{2}, \cdots, r_{j}, \cdots, r_{i}, \cdots, r_{N}) | V(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{j}, \cdots, r_{N}) \rangle$$

$$= \langle \Psi^{S}(r_{1}, r_{2}, \cdots, r_{j}, \cdots, r_{i}, \cdots, r_{N}) | V(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{j}, \cdots, r_{N}) \rangle$$

$$= \langle \Psi^{S}(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{j}, \cdots, r_{N}) | V(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{j}, \cdots, r_{N}) \rangle$$

$$= \langle \Psi^{S}(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{j}, \cdots, r_{N}) | V(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{j}, \cdots, r_{N}) \rangle$$

$$= \langle \Psi^{S}(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{j}, \cdots, r_{N}) \rangle$$

$$= \langle \Psi^{S}(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{j}, \cdots, r_{N}) \rangle$$

$$= \langle \Psi^{S}(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{j}, \cdots, r_{N}) \rangle$$

$$= \langle \Psi^{S}(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{j}, \cdots, r_{N}) \rangle$$

$$= \langle \Psi^{S}(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{j}, \cdots, r_{N}) \rangle$$

$$= \langle \Psi^{S}(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{j}, \cdots, r_{N}) \rangle$$

$$= \langle \Psi^{S}(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{j}, \cdots, r_{N}) \rangle$$

On the other hand,

$$<\Psi^{S}|V|\Psi^{A}> = <\Psi^{S}(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{i}, \cdots, r_{N})|V(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{j}, \cdots, r_{N})$$
$$|\Psi^{A}(r_{1}, r_{2}, \cdots, r_{i}, \cdots, r_{j}, \cdots, r_{N})>$$
(9.1.17)"

Making comparison between Eqs. (9.1.17)' and (9.1.17)'' yields  $\langle \Psi^{S} | V | \Psi^{A} \rangle = 0$ .

In summary, we give the following more general theorem, which contains the theorem XXXIV, for the identical multiparticle system:

**Theorem XXXV: Identity of identical multiparticle system.** The multiparticle wavefunction (which can depend on time) of identical particle systems are separated into two kinds: Symmetric if the eigenvalue of permutation operator is +1; Antisymmetric if the eigenvalue of permutation operator is -1. The particles in identical multiparticle system, described by an antisymmetric wavefunction, are of half-integer spin, are called fermions, and obey Fermi-Dirac statistics; The particles in identical particle system, described by a symmetric wavefunction, are of integer or zero spin, are called bosons, and obey Boson-Einstein statistics. The exchange symmetry of multiparticle wavefunction of the identical multiparticle system does not change with time, and the state transition between different symmetry states is impossible.

In some references our identity theorem is called "indistinguishability principle of identical multiparticle system". This textbook thinks: (1) The so called indistinguishability is not a necessary concept or even is a wrong concept. Because the particles in an identical multiparticle system are distinguishable. The identity defined in this textbook is enough to deduce all the properties of identical multipleparticle system;

(2) The unique characteristics of the identical multipleparticle system can be proved. Therefore, we use "identity theorem" other than "indistinguishable principle".

#### 9.2. System with two Identical Particles

Suppose that the Hamiltonian of two identical particles is

$$H = h(q_1) + h(q_2), (9.2.1)$$

where h(q) represents single particle's Hamiltonian, and can contain the external field potential, q represents the all coordinates of the single particle. Eq. (9.2.1) indicates that we neglect the interaction between the two particles. Obviously,  $[P_{12}, H] = 0$ .

Suppose that the operator h(q) is of eigenequation

$$h(q)\psi_k(q) = \varepsilon_k \psi_k(q), \qquad (9.2.2)$$

where  $\psi_k(q)$  is orthonormalized, and *k* represents a group of complete quantum number of the single particle. If one particle is in the state  $\psi_{k_1}$ , and another is in the state  $\psi_{k_2}$ , then  $\psi_{k_1}(q_1)\psi_{k_2}(q_2)$ ,  $\psi_{k_1}(q_2)\psi_{k_2}(q_1)$ , and their linear compositions are of energy  $\varepsilon_{k_1} + \varepsilon_{k_2}$ . The degeneracy which is connected with the exchange symmetry is called exchange degeneracy.

We need to use  $\psi_{k_1}(q_2)$ ,  $\psi_{k_2}(q_1)$ ,  $\psi_{k_1}(q_1)$ , and  $\psi_{k_2}(q_2)$  to construct the symmetric or antisymmetric multiparticle wavefunctuin for the two identical particles.

For bosons, we need a symmetric multiparticle wavefunction.

If  $k_1 \neq k_2$ , then the orthonormalized symmetric wavefunction is

$$\Psi_{k_1k_2}^{S}(q_1, q_2) = \frac{1}{\sqrt{2}} [\Psi_{k_1}(q_1)\Psi_{k_2}(q_2) + \Psi_{k_1}(q_2)\Psi_{k_2}(q_1)] \\ = \frac{1}{\sqrt{2}} (1 + P_{12})\Psi_{k_1}(q_1)\Psi_{k_2}(q_2), \qquad (9.2.3)$$

If  $k_1 = k_2 = k$ , then the orthonormalized symmetric wavefunction is

$$\Psi_{kk}^{S}(q_1, q_2) = \Psi_k(q_1)\Psi_k(q_2). \tag{9.2.4}$$

For fermions, we need antisymmetric multiparticle wavefunction. This wavefunction can be constructed as follows.

$$\begin{aligned} \Psi_{k_{1}k_{2}}^{A}(q_{1},q_{2}) &= \frac{1}{\sqrt{2}} [\Psi_{k_{1}}(q_{1})\Psi_{k_{2}}(q_{2}) - \Psi_{k_{1}}(q_{2})\Psi_{k_{2}}(q_{1})] \\ &= \frac{1}{\sqrt{2}} (1 - P_{12})\Psi_{k_{1}}(q_{1})\Psi_{k_{2}}(q_{2}) \\ &= \frac{1}{\sqrt{2}} \left| \begin{array}{c} \Psi_{k_{1}}(q_{1}) & \Psi_{k_{1}}(q_{2}) \\ \Psi_{k_{2}}(q_{1}) & \Psi_{k_{2}}(q_{2}) \end{array} \right|. \end{aligned}$$
(9.2.5)



Figure 9.1. Symmetric wavefunction given by Eq. (9.2.3) for a (bosonic) 2-particle state in an infinite 2-dimensional square well potential.

Eq. (9.2.5) clearly tells us that: it is not possible to exist a many fermion state in which there are two fermions in the same single particle states. Historically, this confirmation is called Pauli exclusion principle because Pauli proposed empirically this confirmation for the electrons of an atom in 1925. This textbook suggests to use the terminology "Pauli exclusion theorem" instead of "Pauli exclusion principle". For this suggestion we have two reasons: (a). The so called Pauli exclusion principle has been proved by the later quantum mechanics exactly; (b). For any theory, the less the principles, axioms, hypotheses, and postulates in the theory are, the better the theory is. Thus, we give:

**Theorem XXXVI: Pauli exclusion.** It is not possible to have a multiparticle fermion state in which there are two fermions in the same single particle states.

**Proof.** For general proof, see section 9.3.

Figs. 9.1 and 9.2 clearly show that the space distributions of wavefunctions of two identical bosons and fermions are completely different, respectively.

## 9.3. Wavefunctions of N Identical Particle System

#### 9.3.1. Three Identical Particles

(A) Consider a system consisting of three fermions. Due to the Pauli exclusion theorem, the three identical particles can only be in three different single particle states:  $\psi_{k_1}$ ,  $\psi_{k_2}$ , and  $\psi_{k_3}$ . For the convenience of normalization of the multiparticle wavefunction, we suppose that  $\psi_{k_1}$ ,  $\psi_{k_2}$ , and  $\psi_{k_3}$  are orthonormalized.  $k_i$  indicates the complete set of quantum



Figure 9.2. Antisymmetric wavefunction given by Eq. (9.2.5) for a (fermionic) 2-particle state in an infinite 2-dimensional square well potential.

numbers characterizing the quantum state of the single particle *i*. The antisymmetrical three particle wavefunction can be expressed as

$$\begin{split} \Psi^{A}_{k_{1}k_{2}k_{3}}(q_{1},q_{2},q_{3}) &= \frac{1}{\sqrt{3!}} \begin{vmatrix} \Psi_{k_{1}}(q_{1}) & \Psi_{k_{1}}(q_{2}) & \Psi_{k_{1}}(q_{3}) \\ \Psi_{k_{2}}(q_{1}) & \Psi_{k_{2}}(q_{2}) & \Psi_{k_{2}}(q_{3}) \\ \Psi_{k_{3}}(q_{1}) & \Psi_{k_{3}}(q_{2}) & \Psi_{k_{3}}(q_{3}) \end{vmatrix} \\ &= \frac{1}{\sqrt{3!}} [\Psi_{k_{1}}(q_{1})\Psi_{k_{2}}(q_{2})\Psi_{k_{3}}(q_{3}) + \Psi_{k_{1}}(q_{3})\Psi_{k_{2}}(q_{2})\Psi_{k_{3}}(q_{1}) \\ & +\Psi_{k_{1}}(q_{3})\Psi_{k_{2}}(q_{1})\Psi_{k_{3}}(q_{2}) - \Psi_{k_{1}}(q_{3})\Psi_{k_{2}}(q_{2})\Psi_{k_{3}}(q_{1}) \\ & -\Psi_{k_{1}}(q_{2})\Psi_{k_{2}}(q_{1})\Psi_{k_{3}}(q_{3}) - \Psi_{k_{1}}(q_{1})\Psi_{k_{2}}(q_{3})\Psi_{k_{3}}(q_{2})] \\ &= \frac{1}{\sqrt{3!}} (1 + P_{23} + P_{13} + P_{23}P_{12} - P_{13} - P_{12} - P_{23})\Psi_{k_{1}}(q_{1})\Psi_{k_{2}}(q_{2})\Psi_{k_{3}}(q_{3}) \\ &\equiv \widetilde{A} \Psi_{k_{1}}(q_{1})\Psi_{k_{2}}(q_{2})\Psi_{k_{3}}(q_{3}), \end{split}$$
(9.3.1.1)

where A is called antisymmetrizer.

(B) Consider a system consisting of three bosons. In Eqs. (9.2.3) and (9.2.4) we have considered the system consisting of two bosons. Similarly, we discuss the following three cases for the three identical particle system:

(1)  $k_1, k_2, k_3$  are different mutually. In this case every single particle is in different single

particle state. It is easy to verify that the symmetrical and normalized wavefunction is

$$\Psi_{k_{1}k_{2}k_{3}}^{S}(q_{1},q_{2},q_{3}) = \sqrt{\frac{1!1!1!}{3!}} [\Psi_{k_{1}}(q_{1})\Psi_{k_{2}}(q_{2})\Psi_{k_{3}}(q_{3}) + \Psi_{k_{1}}(q_{1})\Psi_{k_{2}}(q_{3})\Psi_{k_{3}}(q_{2}) \\
+ \Psi_{k_{1}}(q_{2})\Psi_{k_{2}}(q_{1})\Psi_{k_{3}}(q_{3}) + \Psi_{k_{1}}(q_{2})\Psi_{k_{2}}(q_{3})\Psi_{k_{3}}(q_{1}) \\
+ \Psi_{k_{1}}(q_{3})\Psi_{k_{2}}(q_{1})\Psi_{k_{3}}(q_{2}) + \Psi_{k_{1}}(q_{3})\Psi_{k_{2}}(q_{1})\Psi_{k_{3}}(q_{1})].$$
(9.3.1.2)

In Eq. (9.3.1.2) the number of terms is

$$\frac{3!}{1!1!1!} = 6, \tag{9.3.1.3}$$

and every term is orthogonal to all other terms.

(2) Two particles are in  $k_1$  state, and one particle is in  $k_2$  state. It is easy to verify that the symmetrical and normalized wavefunction is

$$\Psi_{k_1k_1k_2}^{S}(q_1, q_2, q_3) = \sqrt{\frac{2!1!0!}{3!}} [\Psi_{k_1}(q_1)\Psi_{k_1}(q_2)\Psi_{k_2}(q_3) + \Psi_{k_1}(q_1)\Psi_{k_1}(q_3)\Psi_{k_2}(q_2) + \Psi_{k_1}(q_3)\Psi_{k_1}(q_2)\Psi_{k_2}(q_1).$$
(9.3.1.4)

In Eq. (9.3.1.4) the number of terms is

$$\frac{3!}{2!1!0!} = 6, \tag{9.3.1.5}$$

and every term is orthogonal to all other terms.

(3) All the three particles are in state  $k_1$ . It is easy to verify that the symmetrical and normalized wavefunction is

$$\Psi_{k_1k_1k_1}^{\mathcal{S}}(q_1, q_2, q_3) = \sqrt{\frac{3!0!0!}{3!}} \left[ \psi_{k_1}(q_1)\psi_{k_1}(q_2)\psi_{k_1}(q_3) \right].$$
(9.3.1.6)

In Eq. (9.3.1.6) the number of terms is

$$\frac{3!}{3!0!0!} = 1. \tag{9.3.1.7}$$

#### 9.3.2. N Identical Particle System

(A) N fermions.

We can generalize the antisymmetrization property of the multiparticle wavefunctions for the two fermions in Eq. (9.2.5) and three fermions in Eq. (9.3.1.1) to the case of N fermions. In such a system there are N! possible different permutations of fermions. The function corresponding to one of these permutations can be obtained from the original standard function  $[\Psi_{k_1}(q_1)\Psi_{k_2}(q_2), \dots, \Psi_{k_N}(q_N)]$  by successive permutations of pair of fermions. Let  $P_V[\Psi_{k_1}(q_1)\Psi_{k_2}(q_2), \dots, \Psi_{k_N}(q_N)]$  denotes the function which can be obtained from  $[\psi_{k_1}(q_1)\psi_{k_2}(q_2), \dots, \psi_{k_N}(q_N)]$  by v consecutive permutations of fermion pairs. Then the antisymmetrical wavefunction of N fermion system is

$$\Psi^{A} = \sqrt{\frac{1}{N!}} \sum_{\mathbf{v}} (-1)^{\mathbf{v}} P_{\mathbf{v}}[\psi_{k_{1}}(q_{1})\psi_{k_{2}}(q_{2}), \cdots, \psi_{k_{N}}(q_{N})], \qquad (9.3.2.1)$$

where the summation is over all N! terms corresponding to the different possible permutations of the N fermions in the system, and every term is orthonormalized.

We can write the antisymmetrical wavefunction instead of the form Eq. (9.3.2.1) in the form of a determinant (the so-called Slater determinant)

$$\Psi^{A} = \Psi^{A}_{k_{1}k_{2}\cdots k_{N}} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \Psi_{k_{1}}(q_{1}) & \cdots & \Psi_{k_{1}}(q_{N}) \\ \Psi_{k_{2}}(q_{1}) & \cdots & \Psi_{k_{2}}(q_{N}) \\ \cdots & \cdots & \cdots \\ \Psi_{k_{N}}(q_{1}) & \cdots & \Psi_{k_{N}}(q_{N}) \end{vmatrix},$$
(9.3.2.2)

where the change in sign of the N! terms in Eq. (9.3.2.2) under a permutation of any two fermions follows immediately from the change of sign of a determinant when two of its columns are interchanged.

Here, we would like to mention once again the Pauli exclusion theorem in section 9.2. Eq. (9.3.2.2) is an antisymmetrical multiparticle wavefunction of an identical multiparticle system with particle number N. This N can be an infinitely large number. From the determinant property, we know that there cannot be two Fermions in a same single particle state. Therefore, from Eq. (9.3.2.2) we give a more general proof for the Pauli exclusion theorem.

(B) N bosons.

We can generalize the symmetrization of the wavefunction for the two bosons in Eq. (9.2.3) and three bosons in Eq. (9.3.1.2-7) also for the case of N bosons. In such a system there are  $N!/(\prod_{i=1}^{N} n_i!)$  possible different permutations of bosons. Here,  $n_i$  represents the number of bosons in  $k_i$  single particle state. The function corresponding to one of these permutations can be obtained from the original standard function  $[\Psi_{k_1}(q_1)\Psi_{k_2}(q_2), \cdots, \Psi_{k_N}(q_N)]$  by successive permutations of pair of bosons. Let  $P_v[\Psi_{k_1}(q_1)\Psi_{k_2}(q_2), \cdots, \Psi_{k_N}(q_N)]$  denote the function which can be obtained from  $[\Psi_{k_1}(q_1)\Psi_{k_2}(q_2), \cdots, \Psi_{k_N}(q_N)]$  by v consecutive permutations of boson pairs. Then the symmetrical wavefunction of N boson system is

$$\Psi^{S} = \Psi^{S}_{n_{1}n_{2}\cdots n_{N}} = \sqrt{\frac{\prod_{i=1}^{N} n_{i}!}{N!}} \sum_{v} P_{v}[\psi_{k_{1}}(q_{1})\psi_{k_{2}}(q_{2}), \cdots, \psi_{k_{N}}(q_{N})], \qquad (9.3.2.3)$$

where the summation is over all  $N!/\prod_{i=1}^{N} n_i!$  terms corresponding to the different possible permutations of the *N* bosons in the system, and every term is orthonormalized.

#### 9.4. Spin States of Two Electron System

Denote the spin operators of two electrons as  $S_1$  and  $S_2$ , respectively. Set

$$S = S_1 + S_2. \tag{9.4.1}$$

Due to that  $S_1$  and  $S_2$  belong to different electrons, and thus belong to different degrees of freedom. Therefore,  $[S_1, S_2] = 0$ . Utilizing this commutation relation, one can show that

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x, \quad [S_z, S_x] = i\hbar S_y \quad . \tag{9.4.2}$$

Set

$$S^2 = S_x^2 + S_y^2 + S_z^2. (9.4.3)$$

Using Eqs. (9.4.2) and (9.4.3), one can show

$$[S^2, S_i] = 0, \quad i = x, y, z \quad . \tag{9.4.4}$$

For the system consisting of two electrons, the spin degree of freedom is 2. We can choose operators  $(S_{1z}, S_{2z})$  or operators  $S^2, S_z$  as a complete set of spin dynamical variables. Suppose that the eigenstates of  $S_{1z}$  are  $\alpha(1)$  and  $\beta(1)$  and the eigenstates of  $S_{2z}$  are  $\alpha(2)$  and  $\beta(2)$ . We use notation  $\alpha(1)\alpha(2)$  to indicate a state where electron 1 has spin up and electron 2 has spin up. Similarly  $\beta(1)\beta(2)$  to indicate a state where electron 1 has spin down and electron 2 has spin down.

We choose operators  $(S_{1z}, S_{2z})$  as a complete set of spin dynamical variables. The common eigenstates of  $(S_{1z}, S_{2z})$  are 4, i. e.,

$$\alpha(1)\alpha(2), \ \beta(1)\beta(2), \ \alpha(1)\beta(2), \ \beta(1)\alpha(2)$$
. (9.4.5)

Let us apply the permutation operator  $P_{12}$  to the four spin wavefunctions in Eq. (9.4.5):

$$P_{12}\alpha(1)\alpha(2) = \alpha(2)\alpha(1). \tag{a}$$

$$P_{12}\beta(1)\beta(2) = \beta(2)\beta(1).$$
 (b)

$$P_{12}\alpha(1)\beta(2) = \alpha(2)\beta(1).$$
 (c)

$$P_{12}\alpha(2)\beta(1) = \alpha(1)\beta(2).$$
 (d)

From Eqs. (a)-(d), the spin wavefunction  $\alpha(1)\alpha(2)$  and  $\beta(1)\beta(2)$  are symmetric. However, the spin wavefunctions  $\alpha(1)\beta(2)$  and  $\alpha(2)\beta(1)$  are neither symmetric nor antisymmetric and so are not acceptable.

We try to choose operators  $S^2$ ,  $S_z$  as a complete set of spin dynamical variables. It is obvious that the four spin wavefunctions in Eq. (9.4.5) are also the eigenstates of  $S_z = S_{1z} + S_{2z}$ , the eigenvalues are  $\hbar, -\hbar, 0, 0$ , respectively. Therefore, the last two states are degenerate eigenstates of  $S_z$ . Let us demonstrate that they are the eienstates of  $S^2$  as well. The demonstrations are actually very simple. As is well known that  $S^2$  and  $S_z$  commute, i. e.,  $[S^2, S_z] = 0$ . Therefore,  $S^2$  and  $S_z$  have common eigenstates. Actually, we can also use the following method to demonstrate that  $\alpha(1)\alpha(2)$  and  $\beta(1)\beta(2)$  are the eigenstates of  $S^2$ , and to seek the eigenvalues:

$$S^{2} = (S_{1}^{2} + S_{2}^{2})^{2} = S_{1}^{2} + S_{1}^{2} + 2S_{1} \cdot S_{2}$$
  
=  $\frac{3}{2}\hbar^{2} + \frac{\hbar^{2}}{2}(\sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y} + \sigma_{1z}\sigma_{2z}).$  (9.4.6)

Utilizing the results in the exercise (1) of subsection 8.7.1 in chapter 8:

$$\sigma_x \alpha = \beta, \quad \sigma_x \beta = \alpha, \quad \sigma_y \alpha = i\beta, \quad \sigma_y \beta = -i\alpha$$
 (9.4.7)

and noting that  $\sigma_1$  and  $\sigma_2$  act on the spin wavefunctions of electron 1 and electron 2, respectively, it is easy to demonstrate that

$$S^{2}\Upsilon_{S=1,M_{s}=1}(S_{z1},S_{z2}) = S^{2}\alpha(1)\alpha(2) = 2\hbar^{2}\alpha(1)\alpha(2)$$
(9.4.8*a*)

and

$$S^{2}\Upsilon_{S=1,M_{s}=-1}(S_{z1},S_{z2}) = S^{2}\beta(1)\beta(2) = 2\hbar^{2}\beta(1)\beta(2)$$
(9.4.8*b*)

are the eigenstates of  $S^2$ , and the eigenvalues are  $2\hbar^2$ .

We use the linear superposition of the two degenerate eigenstatres of  $S_z$ ,  $\alpha(1)\beta(2)$  and  $\beta(1)\alpha(2)$ , to construct the another two eigenstates of  $S^2$ , which are of exchange symmetry of wavefunction of the system, and therefore satisfy the theorem of exchange symmetry. Set

$$\Upsilon = c_1 \alpha(1)\beta(2) + c_2 \beta(1)\alpha(2). \tag{9.4.9}$$

If  $\Upsilon$  is a eigenstate of  $S^2$ , then it satisfies the following eigenequation

$$S^2 \Upsilon = \lambda \hbar^2 \Upsilon, \tag{9.4.10}$$

where  $\lambda$  is a constant without dimension. Utilizing

$$S^{2}\Upsilon = \hbar^{2}(c_{1}+c_{2})\alpha(1)\beta(2) + \hbar^{2}(c_{1}+c_{2})\beta(1)\alpha(2) = \lambda\hbar^{2}[c_{1}\alpha(1)\beta(2) + c_{2}\beta(1)\alpha(2)],$$
(9.4.11)

one obtains

$$\begin{cases} (1-\lambda)c_1 + c_2 = 0\\ c_1 + (1-\lambda)c_2 = 0 \end{cases}$$
(9.4.12)

The sufficient and necessary condition for the nontrivial solution is

$$\begin{vmatrix} 1-\lambda & 1\\ 1 & 1-\lambda \end{vmatrix} = 0.$$
(9.4.13)

Solving the Eq. (9.4.13) yields two roots:

$$\lambda = 0, 2.$$
 (9.4.14)

Substituting  $\lambda = 0$  into Eq. (9.4.12) yields

$$\frac{c_1}{c_2} = -1. \tag{9.4.15}$$

Substituting  $\lambda = 2$  into Eq. (9.4.12) yields

$$\frac{c_1}{c_2} = +1.$$
 (9.4.16)
Utilizing the normalization condition and taking phase = 0 in the arbitrary phase factor, one obtains the two orthonormalized eigenfunctions, corresponding to Eqs. (9.4.15) and (9.4.16), of  $S^2$  are

$$\Upsilon_{S=0,M_s=0} = \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \beta(1)\alpha(2)], \quad \lambda = 0.$$
(9.4.17.*a*)

$$\Upsilon_{S=1,M_s=0} = \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) + \beta(1)\alpha(2)], \quad \lambda = 2.$$
(9.4.17.b)

Eqs. (9.4.17a-b) and (9.4.8.a-b) give the four normalized two electron spin common eigenstates of  $(S^2, S_z)$ , with correct exchange properties. They are:

$$\Upsilon_{S=1,M_s=1} = \alpha(1)\alpha(2)$$
 (9.4.18.*a*)

$$\Upsilon_{S=1,M_s=0} = \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) + \beta(1)\alpha(2)]$$
(9.4.18.b)

$$\Upsilon_{S=1,M_s=-1} = \beta(1)\beta(2) \tag{9.4.18.c}$$

$$\Upsilon_{S=0,M_s=0} = \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \beta(1)\alpha(2)]$$
(9.4.18.d)

The three states in Eqs. (9.4.18.a-c) are S = 1 = 1/2 + 1/2,  $M_s = 0, \pm 1$ , symmetrical for the exchange of the two spins in the system, and called spin triplet state. In physical picture, S = 1 = 1/2 + 1/2 means parallel coupling between the two spins of the two particle. The state in Eq. (9.4.18.d) is S = 0 = 1/2 - 1/2,  $M_s = 0$ , antisymmetrical for the exchange of the two spins, and called spin singlet state. In physical picture, S = 0 = 1/2 - 1/2,  $M_s = 0$ , antisymmetrical for the exchange of the two spins, and called spin singlet state. In physical picture, S = 0 = 1/2 - 1/2 means antiparallel coupling between the two spins of the two particle.

We can directly verify that  $\Upsilon_{S=1,M_s=0}$  and  $\Upsilon_{S=0,M_s=0}$  are symmetric and antisymmetric, respectively.

$$P_{12}\Upsilon_{S=1,M_s=0} = P_{12}\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) + \beta(1)\alpha(2)] = +\Upsilon_{S=1,M_s=0}.$$
$$P_{12}\Upsilon_{S=0,M_s=0} = P_{12}\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \beta(1)\alpha(2)] = -\Upsilon_{S=0,M_s=0}.$$

In the actual case, the electron's spin cannot exist individually. Because the electron's spin is an intrinsic property, therefore, we have to use both the spin and coordinate spaces to describe the electron's state.

For example, He atom where the two electrons are in *s* orbital we have the zeroth order ground state wavefunction 1s(1)1s(2) excluding the spin. ns(i) represents the quantum state n = 1, l = 0 of electron *i* in the hydrogen atom. This wavefunction in position space is symmetric with respect to the exchange of the two electrons. We now include the spin with the zeroth order ground state wavefunction. According to the Pauli exclusion theorem, the overall wavefunction including the spin must be antisymmetric with respect to the interchange of two electrons. Hence we must take the product of symmetric position space wavefunction 1s(1)1s(2) by an antisymmetric spin wavefunction. There is only one

antisymmetric two electron spin wavefunction given by Eq. (9.4.18.d). The ground ground state zeroth order wavefunction for the two electron system including the spin is therefore,

$$\Psi^{(\circ)} = 1s(1)1s(2)\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \beta(1)\alpha(2)] \text{ antisymmetric.}$$
(9.4.19)

 $\Psi^{(\circ)}$  is an eigenfunction of permutation operator  $P_{12}$  with eigenvalue -1 as pauli exclusion theorem requires.

Now consider the excited state of two electron system which is obtained by exciting one of the electron to the next *s* orbital. The wavefunction is 1s(1)2s(2) or 1s(2)2s(1). These wavefunctions are neither symmetric nor antisymmetric. However, their linear combinations can be symmetric or antisymmetric. The lowest excited states to have the zeroth order spatial wavefunction are

$$\frac{1}{\sqrt{2}}[1s(1)2s(2) - 2s(1)1s(2)] \quad antisymmetric. \tag{9.4.20.a}$$

$$\frac{1}{\sqrt{2}}[1s(1)2s(2) + 2s(1)1s(2)] \quad symmetric. \tag{9.4.20.b}$$

Since the spatial wavefunction according to Eq. (9.4.20.a) is antisymmetric, we must multiply it by a symmetric spin wavefunction. From Eqs. (9.4.18.a-c) and (9.4.20.a) we have the following three overall excited state wavefunctions:

$$\frac{1}{\sqrt{2}}[1s(1)2s(2) - 2s(1)1s(2)]\alpha(1)\alpha(2).$$
(9.4.21.*a*)

$$\frac{1}{\sqrt{2}}[1s(1)2s(2) - 2s(1)1s(2)]\beta(1)\beta(2).$$
(9.4.21.*b*)

$$\frac{1}{\sqrt{2}}[1s(1)2s(2) - 2s(1)1s(2)]\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) + \beta(1)\alpha(2)].$$
(9.4.21.c)

The first excited state is a triplet state (S = 1). For the next excited state the requirement of antisymmetric overall wavefunction leads to zeroth wavefunction by using Eqs. (9.4.20.b) and (9.4.18.d)

$$\frac{1}{\sqrt{2}}[1s(1)2s(2) + 2s(1)1s(2)]\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \beta(1)\alpha(2)].$$
(9.4.21.d)

The second excite state is a singlet state (S = 0). The same considerations apply to 1s2p, 1s3d etc. states.

Note that all states where the two electrons are assigned to the excited orbital turn out to have such a high energy that they cannot exist as a bound state. All the bound states of He atom therefore involve linear combination of products in which one of the electron's spatial wavefunction is in the 1s orbital, while the second electron is placed in atomic orbital, for example, 1s, 2p, 3s, 3p, 3d etc. Thus the excited states of He atom consist of one electron in 1s state (the hydrogen ground state) and the other in an excited states  $\Psi_{nlm}$ .

The requirement that the total wavefunction must be antisymmetric in the exchange of electrons leads a coupling between the spin and the spatial variables. They act as if they move under the influence of a force whose sign depends on the relative orientation of their spins. This is called exchange force. The force is zero for the two electrons which are far apart, for example, the two electrons of two hydrogen atoms. Although, in principle, these two electrons in the two hydrogen atoms are of exchange symmetry of the total wavefunction, but we do not need to consider this exchange symmetry of wavefunction in practice.

# 9.5. Bell Basis and Entangled States

From the discussions in section 9.4, we see that there are two approaches to construct the four spin states of two particles with spin  $\hbar/2$ . In this subsection we use another often used notations to express the spin state.  $\alpha = |\uparrow\rangle = |\frac{1}{2}\rangle$  and  $\beta = |\downarrow\rangle = |-\frac{1}{2}\rangle$ . For example,  $\alpha_{(1)}\beta_{(2)} = |\uparrow\rangle_1 |\downarrow\rangle_2 = |\frac{1}{2}, -\frac{1}{2}\rangle$ .

(A) The four spin states can be the common eigenstates of operators  $(S_{1z}, S_{2z})$ . Eq. (9.4.5) have given these four spin wavefunctions:

$$\alpha(1)\alpha(2), \ \beta(1)\beta(2), \ \alpha(1)\beta(2), \ \alpha(2)\beta(1)$$
. (9.5.1)

Using the arrow method, Eq. (9.5.1) can be rewritten as

$$|\uparrow>_1|\uparrow>_2, |\downarrow>_1|\downarrow>_2, |\uparrow>_1|\downarrow>_2, |\uparrow>_2|\downarrow>_1.$$
(9.5.2)

Using the four spin wavefunctions in Eq. (9.5.2), we can construct a vector space to express any spin states of two spin 1/2 particles. The two operators ( $S_{1z}$  and  $S_{2z}$ ) can be separated, belong to different particles, and both they are single body operators. We call this vector space, consisting of common eigenstate of single body operators, angular momentum noncoupling representation. We have pointed out that the two of the four spin wavefunctions in Eq. (9.5.2) do not satisfy the exchange symmetry of total.

(B) The four common eigenstates of operators  $(S^2, S_{2z})$ , given by Eqs. (9.4.18.a-d) can also construct a vector space. The two single body operators in operator  $S^2 = (S_1 + S_2)^2 = S_1^2 + S_2^2 + 2S_1 \cdot S_2 = 3\hbar^2/2 + 2S_1 \cdot S_2 = \hbar^2/2(3 + \vec{\sigma}_1 \cdot \vec{\sigma}_2)$  cannot be separated. The  $S^2$  is called two body operator. We call this vector space angular momentum coupling representation. Eqs. (9.4.18.a-d) is as follows:

$$\Upsilon_{S=1,M_s=1} = \alpha(1)\alpha(2)$$
 (9.5.3.*a*)

$$\Upsilon_{S=1,M_s=0} = \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) + \beta(1)\alpha(2)]$$
(9.5.3.b)

$$\Upsilon_{S=1,M_S=-1} = \beta(1)\beta(2) \tag{9.5.3.c}$$

$$\Upsilon_{S=0,M_s=0} = \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \beta(1)\alpha(2)]$$
(9.5.3.d)

Using the arrow method, Eq. (9.5.3) can be rewritten as

$$\Upsilon_{11} \equiv \Upsilon_{S=1,M_s=1} = |\uparrow\rangle_1 |\uparrow\rangle_2 \tag{9.5.4.a}$$

$$\Upsilon_{10} \equiv \Upsilon_{S=1,M_s=0} = \frac{1}{\sqrt{2}} [|\uparrow >_1 |\downarrow >_2 + |\downarrow >_1 |\uparrow >_2]$$

$$(9.5.4.b)$$

$$\Upsilon_{1-1} \equiv \Upsilon_{S=1,M_s=-1} = |\downarrow\rangle_1 |\downarrow\rangle_2 \tag{9.5.4.c}$$

$$\Upsilon_{00} \equiv \Upsilon_{S=0,M_s=0} = \frac{1}{\sqrt{2}} [|\uparrow>_1|\downarrow>_2-|\downarrow>_1|\uparrow>_2]$$
(9.5.4.d)

Using these four spin wavefunctions, we can also construct a vector space to express any spin states of two spin 1/2 particles.

If a quantum state of composite system consisting of more than one particle can be expressed as a product of single particle states, then it is called separable state, or in this simplest case it is called product state. If a quantum state of composite system consisting of more than one particle cannot be expressed as a product of single particle states, then it is called entangled state. For example, the four states in Eq. (9.5.2) and the two states,  $\Upsilon_{11}$  and  $\Upsilon_{1-1}$  in Eq. (9.5.4), are separable states, and the states  $\Upsilon_{00}$  and  $\Upsilon_{10}$  in Eq. (9.5.4) are entangled state.  $S_{1z}$ ,  $S_{2z}$ , and  $S_z = S_{1z} + S_{1z}$  are single body operators.  $S^2$  is two body operator because the two operators in  $\vec{\sigma}_1 \cdot \vec{\sigma}_2$  cannot be separated. If we take a complete set which contains even one two body operator, the the common eigenstates of the complete set contains entangled state.

If we take the two commuting two body operators  $(\sigma_{1z}\sigma_{2z}, \sigma_{1x}\sigma_{2x})$  as the complete set, then all the four common eigenstates are entangled states:

$$\frac{1}{\sqrt{2}}(\Upsilon_{11} + \Upsilon_{1-1}) = \frac{1}{\sqrt{2}}[|\uparrow >_1 |\uparrow >_2 + |\downarrow >_1 |\downarrow >_2].$$
(9.5.5.*a*)

$$\Upsilon_{10} = \frac{1}{\sqrt{2}} [|\uparrow >_1 |\downarrow >_2 + |\downarrow >_1 |\uparrow >_2].$$
(9.5.5.b)

$$\frac{1}{\sqrt{2}}(\Upsilon_{11} - \Upsilon_{1-1}) = \frac{1}{\sqrt{2}}[|\uparrow >_1 |\uparrow >_2 - |\downarrow >_1 |\downarrow >_2].$$
(9.5.5.c)

$$\Upsilon_{00} = \frac{1}{\sqrt{2}} [|\uparrow >_1 |\downarrow >_2 - |\downarrow >_1 |\uparrow >_2].$$

$$(9.5.5.d)$$

The four entangled states in Eq. (9.5.5) can also construct a complete basis as the basis in Eq. (9.5.4). The four entangled states in Eq. (9.5.5) are called Bell basis.

Now the entangled states have many applications, e. g., quantum computing, quantum communications, quantum state teleportation, information, and so on. This is an exciting and modern subject. Next we give a theorem, which is just to scratch the surface of the entangled state.

**Theorem XXXVII: Nonlocality of quantummechanical multibody states.** The quantummechanical multibody states such as entangled states have nonlocality (nonlocalty=distance-correlativity).

**Proof.** About the mathematical proofs for this theorem there are many references such as Refs. [102, 103, 104, 60, 105]. ([105] introduces representation of entangled states.) We do not want to repeat these purely mathematical proofs. If the readers do not have enough time, then it is OK that they do not read these proofs. We hope to note the origin of nonlocality, i. e., the aspect of physics, and ask why?.

We list some examples, and interpret the physical aspects of this theorem, especially, the origins of nonlocality, and the classical analogy if it has.

First example of nonlocality comes from the identity theorem XXXV. Considering the spin-singlet state (S = 0)

$$\Upsilon_{00} = \frac{1}{\sqrt{2}} [|\uparrow >_{1z} |\downarrow >_{2z} - |\downarrow >_{1z} |\uparrow >_{2z}], \qquad (9.5.5.d)'$$

which is a superposition of two product states  $|\uparrow >_{1z} \bigotimes |\downarrow >_{2z}$  and  $|\downarrow >_{1z} \bigotimes |\uparrow >_{2z}$ . Considering the invariance of space rotation of the  $\Upsilon_{00}$  [9], we can also take, equivalently,

$$\Upsilon_{00} = \frac{1}{\sqrt{2}} [|\uparrow >_{1x} |\downarrow >_{2x} - |\downarrow >_{1x} \uparrow >_{2x}].$$
(9.5.5.*d*)"

Let us explain what does the nonlocality of entangled states mean. Suppose that Alice is an observer for particle (system) 1, and Bob is an observer for particle (system) 2. If in the entangled state given in Eq. (9.5.5.d)' and Eq. (9.5.5.d)" Alice makes an observation in the eigenbasis of particle 1, there are two possible outcomes, occurring with equal probability:

(i) Alice observes  $\uparrow_z (\uparrow_x)$ , and the state of the particle 2 automatically (i. e., the probability is 1) is  $\downarrow_z (\downarrow_x)$ ;

(ii) Alice observes  $\downarrow_z (\downarrow_x)$ , and the state of the particle 2 automatically (i. e., the probability is 1) is  $\uparrow_z (\uparrow_x)$ ;

If the former (i) occurs, then any subsequent observation performed by Bob, in the same basis, will always return  $\downarrow$ . If the latter (ii) occurs, (Alice observes  $\uparrow_x$ ), then Bob's observation will return  $\uparrow$  with certainty. Thus, the particle 2 has been altered by Alice performing a local observation just on particle 1. This remains true even if the particles 1 and 2 are spatially separated very far. This is the so called nonlocality. Nonlocality has many manifestations.

The outcome of Alice's measurement is random, or more exactly speaking, has probability 50%. Alice cannot decide which state of the composite system (particles 1 and 2) will be, and therefore cannot transmit information to Bob by acting on her system. Causality is thus preserved, in this particular scheme.

To understand the origin of the entanglement of the above entangled states, we can even include more freedom degree besides spin. For example, Eq. (9.4.21.d) gives an expression of the many excited states of He atom, which is

$$\Psi(r_1, r_2) = \frac{1}{\sqrt{2}} [1s(1)2s(2) + 2s(1)1s(2)] \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \beta(1)\alpha(2)]. \quad (9.4.21.d)'(9.5.6)$$

Similarly to Eq. (9.5.6), if the two electrons are plane wave, then the wavefunction of these two electrons can be [4]

$$\Psi(r_{1}, r_{2}) = \frac{1}{\sqrt{2}} \left[ \frac{1}{\sqrt{2\pi\hbar}} e^{ip_{1} \cdot r_{1}/\hbar} \frac{1}{\sqrt{2\pi\hbar}} e^{ip_{2} \cdot r_{2}/\hbar} + \frac{1}{\sqrt{2\pi\hbar}} e^{ip_{2} \cdot r_{1}/\hbar} \frac{1}{\sqrt{2\pi\hbar}} e^{ip_{1} \cdot r_{2}/\hbar} \right] \\ \times \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \beta(1)\alpha(2)]$$
(9.5.7)

More vividly speaking, in Eq. (9.5.5.d)' there are two double particle states:  $|\uparrow\rangle_1|\downarrow\rangle_2$  and  $|\downarrow\rangle_1|\uparrow\rangle_2$ . Each state appears with probability 50%. We should always remember

that although the body-factor carries the substance of the particle, but the body-factor looks like a blend person, the body-factor's motion is always in terms of the guide of the guide-factor according to the spontaneous equiprobability symmetry breaking. Actually, if Alice observes that the particle 1 is in  $\uparrow$  state, which means that the body-factor of the particle 1 takes  $\uparrow$  due to the result of spontaneous equiprobability symmetry breaking. In this case the particle 2 has no other choice, and the sole choice of the particle 2 is  $\downarrow$ . Therefore, the entanglement and the nonlocality is a quantummechanically due and deserved effect.

We have the following physical analyses for the nonlocality.

(i) The two free electrons are identical particles (=wavepackets). The identity theorem XXXV of identical wavepackets requires that the wavefunction (=guide-factor) of this two electron system has to be antisymmetrical. Eq. (9.5.7) satisfies this requirement of antisymmetry.

(ii) This requirement of antisymmetry does not connect with the space distance of these two electrons (=wavepackets). The action of the guide-factor (=wavefunction) is to guide the motion of the body-factors of the two wavepackets. Actually, the electron's spin is carried by the body-factor. The  $[\alpha(1)\beta(2) - \beta(1)\alpha(2)]$  in Eq. (9.5.7) is only a mathematical function, and can guide the motion of the electron spins.

(iii) It is easy to see that the spacetime part of wavefunction (=guide-factor) of the two electrons has nonlocality as well. But until now the related experiments have not yet been reported, or even the two electron spacetime entanglement has yet not been noted by researchers.

Second example is two (or many) photon time-frequency entanglement [106, 104]. The single photon wavefunction (guide-factor) can be, generally, expressed as

$$\Phi_{one}(z/c-t) = \frac{1}{\sqrt{2\pi}} \int_0^\infty d\omega \overline{\Phi}_{one}(\omega) \mathcal{E}(\omega) e^{-i\omega(z/c-t)}, \qquad (9.5.8)$$

where  $\mathcal{E}(\hbar\omega/\epsilon_{o}V)^{1/2}$  is the electric field of one photon.  $\Phi_{one}(z/c-t)$  is the photon wavefunction (=guede-factor).  $|\Phi_{one}(z/c-t)|^2$  represents the spacetime distribution of field strength of one photon [104]. Note that some references think that  $\Phi_{one}(z/c-t)$  is a photon wavepacket other than a wavefunction. This textbook thinks that a photon wavepacket looks like an electron wavepacket, is a rigid sphere, and cannot be separated arbitrarily. One can only expand the wavefunction (=guide-factor), other than the substance of an object.

The general form of the two photon wavefunction is

$$\Phi_{two}(z_1/c - t_1, z_2/c - t_2) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2\pi}} \int_0^\infty d\omega_1 \int_0^\infty d\omega_2$$
  

$$\times \overline{\Phi}_{two}(\omega_1, \omega_2) \mathcal{E}(\omega_1) \mathcal{E}(\omega_2) e^{-i\omega[(z_1/c - t_1) + (z_2/c - t_2)]}$$
  

$$\neq \Phi_{one}(z_1/c - t_1) \times \Phi_{one}(z_2/c - t_2). \qquad (9.5.9)$$

There is two photon entanglement if

$$\overline{\Phi}_{two}(\omega_1, \omega_2) = \overline{\Phi}_{two}(\omega_2, \omega_1) \text{ or } \overline{\Phi}_{two}(\omega_1, \omega_2) = -\overline{\Phi}_{two}(\omega_2, \omega_1).$$
(9.5.10)

This two photon frequency entanglement has been observed by beam splitter experiments, and is called two photon interference [104, 107, 108].

Third example is the two photon coordinate-momentum entanglement, which is also called two photon interference [104].

Fourth example of nonlocality comes from the momentum-coordinate representation transformation for the entangled states. Let us use a very simple example to explain what does the momentum-coordinate representation transformation mean? We will address the paper of EPR (Einstein-Podolsky-Rosen) in 1935, because this paper propose a EPR paradox for the quantum mechanics, and EPR paradox is one kind of nonlocality [7, 103, 102, 109].

Suppose that we have two particles 1 and 2, and the wavefunction of this two particle's system is [109]

$$\Psi(x_{1}, x_{2}) = \frac{1}{\sqrt{2\pi\hbar}} \delta(x_{1} - x_{2} + x_{\circ}) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp' e^{ip'x_{\circ}/\hbar} \frac{1}{\sqrt{2\pi\hbar}} e^{ip'x_{1}/\hbar} \frac{1}{\sqrt{2\pi\hbar}} e^{-ip'x_{2}/\hbar}.$$
(9.5.11)

Now, the very important thing is to understand the physics of Eq. (9.5.11). The function in the right hand side of first equality is the eigenfunction of total momentum operator  $P = P_1 + P_2$  and relative coordinate operator  $X = X_1 - X_2$  (In the coordinate representation it is a number.)

$$X\Psi(x_1, x_2) = (X_1 - X_2)\Psi(x_1, x_2) = (x_1 - x_2)\frac{1}{\sqrt{2\pi\hbar}}\delta(x_1 - x_2 + x_0)$$
  
=  $-x_0\frac{1}{\sqrt{2\pi\hbar}}\delta(x_1 - x_2 + x_0).$  (9.5.12)

Therefore, the function in the right hand side of first equality in Eq. (9.5.11) is an eigenfunction of relative coordinate operator  $X = X_1 - X_2$  (In this coordinate representation it is a number.)

$$P\Psi(x_1, x_2) = (P_1 + P_2)\Psi(x_1, x_2)$$
  
=  $\left((-)i\hbar\frac{\partial}{\partial x_1} + (-)i\hbar\frac{\partial}{\partial x_2}\right)\frac{1}{\sqrt{2\pi\hbar}}\delta(x_1 - x_2 + x_\circ)$   
=  $\left((-)i\hbar\frac{\partial}{\partial x_1} - (-)i\hbar\frac{\partial}{\partial - x_2}\right)\frac{1}{\sqrt{2\pi\hbar}}\delta(x_1 - x_2 + x_\circ)$   
=  $0\frac{1}{\sqrt{2\pi\hbar}}\delta(x_1 - x_2 + x_\circ).$  (9.5.13)

Therefore, the function in the right hand side of first equality in Eq. (9.5.11) is a common eigenfunction of total momentum operator  $P = P_1 + P_2$  and relative coordinate  $X = X_1 - X_2$ .

Considering that  $[P_1, P] = 0$  and  $[P_2, P] = 0$ , but  $[P_1, X] \neq 0$  and  $[P_2, X] \neq 0$ , we know that the function in Eq. (9.5.11) as a common eigenstate of *X*, *P* cannot be the common

eigenstate of  $P_1$  and  $P_2$ , and only can be a superposition of common eigenstates of  $P_1, P_2$ , i. e., can have common eigenfunctions, such as

$$< x_1, x_2 | x = -x_{\circ}, P = 0 > = \frac{1}{\sqrt{2\pi\hbar}} \int dp' \frac{1}{\sqrt{2\pi\hbar}} e^{ip'x_1/\hbar} \frac{1}{\sqrt{2\pi\hbar}} e^{-ip'x_2/\hbar}.$$
 (9.5.14)

Eqs. (9.5.14) tells us that although the distance  $x_0$  of the two particles can be very large, but if you measure the momentum of particle 1, and obtain  $p_1 = p'$ , then the momentum of particle 2 is definitely  $p_2 = -p'$ . The two particles are in state given by Eq. (9.5.11). Why when the particle 1 is in a eigenstate p' of momentum of particle 1, then the particle 2 is automatically is in a eigenstate -p' of momentum of particle 2? This is the nonlocality. This kind of nonlocality can be understood by classical mechanics. The physical meaning of the  $\delta(x_1 - x_2 + x_0)$  in Eq. (9.5.11) is that two free particles 1 and 2 suffer an imposed constraint condition, i. e., always keep the distance  $x_1 - x_2 = x_0$ . For example, the two particles situate at the two ends of a rigid stick. The length of rigid stick is  $x_0$ . If you also require that the total momentum  $p = p_1 + p_2 = 0$  of the two particles, then from momentum conservation  $p = p_1 + p_2 \equiv 0$  and the measured  $p_1 = p'$ , you, of course, can say  $p_2 = -p'$ . So simple arithmetic! The  $p_2 = -p'$  is also independent of the distance between the two classical particles, because  $p = p_1 + p_2 \equiv 0$  does not depend on this distance.

According to our viewpoint that the historical experiences and lessens are worth notice, we introduce the discovery history of the nonlocality. From this history, you well understand that: (i). Science develops always, but the developing way might be tortuous sometimes; (ii). The discovery of nonlocality belongs to the so called "hit the mark by a fluke (like to point out the weak point of quantum mechanics), score a lucky hit (like to find a new effect of the nonlocality)"; (iii). The history of discovery of nonlocality tells us that even the wise are not always free from error.

The EPR paradox comes from the Einstein and et al.'s paper in 1935 [110]. The number citing by references is the largest in scientific history. This paper has two contents. This textbook will introduce the two contents, and in parentheses expresses our completely different opinions.

First content is to discuss one particle. EPR paper assumes that an one dimensional particle is in state, described by the wavefunction

$$\Psi_{p_{\circ}}(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ip_{\circ}x/\hbar}, \qquad EPR(2)(9.5.15)$$

in which EPR(2) represents that our Eq. (9.5.15) is same as the Eq. (2) of EPR paper. This wavefunction is an eigenfunction of momentum operator  $P = -i\hbar\partial/\partial x(EPR(3))$ , the eigenvalue is  $p_{\circ}(EPR(3))$ . EPR think that in this state given by Eq. (9.5.15), the momentum has a certain value and is thus a physical reality. Due to that in this state given by Eq. (9.5.15) the values of coordinate do not have the certain value, EPR think that in this state given by Eq. (9.5.15) the coordinate is not a physical reality.

#### Comment of this textbook for EPR paradox.

The wavefunction is only a mathematical function, does not carry any substances of a particle, acts just as a guider to guide the motion of the particle according to the spontaneous equiprobability symmetry breaking law. According to the spontaneous equiprobability symmetry breaking law, the wavefunction in Eq. (9.5.15) tells us that in position space

the particle will take any position with equiprobability. Of course, the particle's coordinates are still a truly physical quantity. The criterion of physical reality given by EPR is not correct.

Second content is just the above second example of nonlocality.

Schrödinger wrote a letter (in German) to Einstein in which he used the word Verschrünkung (translated by himself as entanglement) to describe the correlations between two particles that interact and then separate, as in the EPR thought experiment. Schrödinger shortly thereafter published a seminal paper defining and discussing the notion, and terming it "entanglement". In the paper he recognized the importance of the concept, and stated: "I would not call (entanglement) one but rather the characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought." [111, 112] Schrödinger (1935) proposed an another thought experiment, i. e., the so called Schrödinger cat. Schrödinger assumed that in a box there are one cat and one atom, and when the atom is in excited state with probability 50%, the cat is alive, and when the atom is in ground state with probability 50%, the cat is death. Schrödinger wrote the total wavefunction as follows:

$$\begin{split} |\Psi\rangle &= \alpha |alive\ cat\rangle |excited\ state\ of\ an\ atom\rangle \\ &+ \beta |death\ cat\rangle |ground\ state\ of\ an\ atom\rangle, \\ &\alpha^2 + \beta^2 = 1. \end{split} \tag{9.5.16}$$

This Schrödinger cat state  $|\Psi\rangle$  is a superposition of states and has nonlocality. If the "cat" is not a macroscopic system, then many experiments have alresady found the Schrödinger cat state.

Bohr thought that EPR prove a problem of quantum mechanics, and used his complementary principle to argue the completeness of quantum mechanics in 1935.

As with Einstein, Schrödinger was dissatisfied with the concept of entanglement because it seemed to violate the speed limit on the transmission of information implicit in the special theory of relativity. Einstein later famously derided entanglement as "spukhafte Fernwirkung" or "spooky action at a distance".

After the papers of Schrödinger and Bohr, the EPR paper generated significant interest among physicists and inspired much discussion about the foundations of quantum mechanics (perhaps most famously Bohm's quantum potential interpretation of quantum mechanics and hidden parameter), but relatively little other published work. Here we have to mention the important idea of Bohm [113]. Bohm is the first to explore the nonlocality by discussing a two spin system.

So, despite the interest, the flaw in EPR's argument was not discovered until 1964, when John Stewart Bell demonstrated precisely how one of their key assumptions, the principle of locality, conflicted with quantum mechanics. Specifically, he demonstrated an upper limit, known as Bell's inequality, regarding the strength of correlations that can be produced in any theory obeying local realism, and Bell showed that quantum mechanics predicts violations of this limit for certain entangled systems. Bell's inequality is experimentally testable, and there have been numerous relevant experiments, starting with the pioneering work of Freedman and Clauser in 1972 and Aspect's experiments in 1982. These experiments have shown agreement with the nonlocality of quantum mechanics rather than the principle of local realism. However, the issue is not finally settled, for each of these experimental tests has left open at least one loophole by which it is possible to question the validity of the results. The work of Bell raised the possibility of using these super strong correlations as a resource for communication.

At this stage, the readers have believed the quantum nonlocality without a wee bit of doubts. But, why is the nonlocality possible? Let us recall the super-light speed observation in the barrier tunneling experiments in chapter 4. In that subsection, we point out that due to the more microscopic process, mentioned in chapter 3, when the particle tunnels through a barrier, that the particle moves with super-light speed is possible. In the entanglement case, the propagation of information between two particles in entangled states or other quantummechanical multibody states is allowed to have super-light or even infinite speed. We think that the properties of more microscopic process is just the origin of nonlocality. It is obvious that even for a sole particle the transmission speed of information between the guide-factor and the body-factor can be infinitely large in principle, because for the more microscopic processes, which is stochastic processes, until now there are no any accepted theories.

# 9.6. Exercises and Solutions

# 9.6.1. Characteristics of Identical Particles

(1) Some references think that the symmetry of wavefunction of identical particle system is an effect which's cause is: "the overlapping of the single particle wavefunction. Originally the wavefunctions of massive particles, e. g., labeling 1 and labeling 2, are prepared separately. At the just beginning the single particle wavefunctions do not overlap. As time evolution, the single particle wavefunctions proceed, they overlap and it is no longer possible to distinguish the single particle wavefunctions, i. e., "who is who" cannot be distinguished because "you in me and I in you" [6].

Therefore, Ref. [6] thinks that the cause of the exchange symmetry of the multiparticle system is the indistinguishability of identical particles. please make comment.

Solution: We give the following five comments:

(A) There is misunderstanding on both the wavefunction and wavepacket in many textbooks. The wavepacket and particle are the same thing. For example, the electron is a rigid small sphere, and it cannot absolutely spread with time. According to wavepacket-only theory, one always has to remember that:

 $(wavepacket) \neq (wavefunction);$ (guide-factor of wavepacket) = (wavefunction); $(wavepacket) = (particle); (wavefunction) \neq (particle).$ 

(B) Even there is no any overlapping between the single particle wavefunctions, the identical particle system still has the exchange symmetry of multiparticle wavefunction. Just, if there is no any overlapping between single particle wavefunctions, then some properties such as exchange energy will be negligible. The basic origin of the exchange sym-

metry of multiparticle wavefunction comes from: The average value of operator and operator itself do not change when one exchanges two identical particle; This characteristic does not mean any thing for classical mechanics, and is just a trivial thing; However, for quantum mechanics, this characteristic can produce large effect because although the probability density does not change, but the multiparticle wavefunction can change its sign due to probability density  $|\pm wavefunction|^2$ .

(C) Theoretically, when one proves the theorem of exchange symmetry of multiparticle wavefunction, one does not need to consider the overlapping. In other word, the overlapping does not have a wee bit of connections with the exchange symmetry.

(D) Therefore, the following viewpoints are wrong:

(i) Ref. [4] thinks: "For the identical particle system there is a principle of indistinguishability."

(ii) Ref. [7] affirms: "In quantum mechanics, identical particles are truly indistinguishable, and are not even in principle."

(iii) Ref. [114] suggests: "The principle of indistinguishability of identical particle system refers to the fifth postulate of quantum mechanics."

(E) We would like to remend the readers to note a basic fact. In chapter 1 we introduce the double slit experiment. This experiment can be done in two approach, and get the same experimental interference pattern on the screen. One approach is to use just one particle (photon, electron, or the big  $C_{60}$  molecule) to go through the double slit at every time experiment, and do the same kind of experiments many times (for example, 1000 times). Another approach is to use just a beam of particles (photon, electron, or the big  $C_{60}$  molecule) to go through the double slit at one time experiment. Of course, the beam of identical particles constructs an identical multiparticle system. The two approaches in double slit experiments clearly tell us that the every particle in the beam still knows "who is who" or "which is which".

The aim of this exercise is to let the readers to believe that the particles in identical multiparticle system are distinguishable. This aim is meaningful, since some references accept the viewpoint that the particles in identical multiparticle system are indistinguishable.

(2) There were many different viewpoints on the identical particle system, for example,

(A) Ref. [4] thinks: "For the identical particle system there is a principle of indistinguishability."

(B) Ref. [7] affirms: "In quantum mechanics, identical particles are truly indistinguishable, and are not even in principle."

(C) Ref. [114] suggests: "The principle of indistinguishability of identical particle system refers to the fifth postulate of quantum mechanics."

Are the identical particles in quantum mechanics really indistinguishable as said in Refs. [4, 7, 114]? This exercise requires that readers give many arguments to negative the indistinguishability upon the bases of the exercise 1.

#### Solution:

No! The identical particles in quantum mechanics really distinguishable. Let us give you more reasons besides the reasons in the solution of exercise 1:

(A) Let us give you a very very simple example. Assume that there are two free electrons in an one dimensional box, i. e., in one dimensional infinite potential well. Every substance of the two electrons (=wavepackets) is still a small rigid sphere (non-relativistic approximation) in this one dimensional box. Every electron in the two electron has itself guide-factor (=wavefunction), which are simple triangle functions given by Eq. (4.2.1.22). If the two electrons are separated far from each other, then, of course, we know "who is who" obviously.

We think that the identical particles are distinguishable are a very obvious thing, and do not really understand that why some references do not consider the basic practice of mankind, and prefer the so called indistinguishability.

(B) That the two electrons in the box are distinguishable or indistinguishable does not have a wee bit of connections with that how to write the multiparticle wavefunction of the two electrons in the box. They refer to different things.

(C) Actually, to demonstrate that the eigenvalues of permutation operator are +1 or -1, we just need that the observables and the average value of observables is independent of the exchange of all coordinates of the identical particles. This is a trivial thing for classical mechanics. However, this is not a trivial thing for quantum mechanics, because in quantum mechanics the average value are determined by both  $\Psi^*$  and  $\Psi$ . Even we do not make any mathematical derivations, we can confirm that  $P_{ij}\Psi = \pm \Psi$  do not change the average value at all.

(D) We think that the permutation operator's existence itself means the distinguishable property of identical particles. Otherwise, how can you say the permutation of two particles?

(3) Do you prefer to name identity theorem or identity principle?

#### Solution:

The exchange symmetry of multiparticle wavefunction of identical particle system has been exactly demonstrated in subsection 9.1.1. Therefore, it is a theorem other than a principle or a postulate.

(4) Many textbooks write, for example Ref. [1]: " $\Psi$ " and  $P_{ij}\Psi$  can only have a difference of a constant? Does this statement exact?

#### Solution:

No, It is not exact. We should say that " $\Psi$ " and  $P_{ij}\Psi$  can only have a difference of a constant phase factor. For example, when  $|\Psi|^2$  represents probability density, it is needed to make the normalization of wavefunction. In this case we cannot give an arbitrary constant factor except an arbitrary constant phase factor.

(5) Ref. [54] makes a brief summary:

If the identical particles are distinguishable, then we obtain the Maxwell-Boltzmann distribution function (i. e., the average occupation number of identical particles at energy E)

$$n(E) = \frac{1}{e^{\alpha} e^{E/k_B T}}$$

If the identical particles with integer or zero intrinsic spin angular momentum are indistinguishable, namely bosons, then we obtain the Bose-Einstein distribution function (i. e., the average occupation number of identical particles at energy E)

$$n(E) = \frac{1}{e^{\alpha} e^{E/k_B T} + 1}$$

If the identical particles with half-integer intrinsic spin angular momentum, namely fermions, are indistinguishable, then we obtain the Fermi-Dirac distribution function (i. e., the average occupation number of identical particles at energy E)

$$n(E)=\frac{1}{e^{\alpha}e^{E/k_BT}-1}.$$

At high energy  $E >> k_B T$ , the Bose-Einstein distribution function and the Fermi-Dirac distribution function reduce to the Maxwell-Boltzmann distribution function.

After reading the above paragraph from Ref. [54] or any other textbooks on statistical physics, do you think that the identical bosons or fermions are indistinguishable?

Solution:

No. We still think that the identical bosons or fermions are distinguishable. "Indistinguishable property" is subjective. "Identity of intrinsic properties" is objective. The Maxwell-Boltzmann distribution function is historical thing [L. Boltzmann, Wier. Ber. 63, 397 (1871)]. Actually, today the Maxwell-Boltzmann distribution function is not necessary, it is just an approximations of the other two distributions.

We would like to introduce a paragraph from Ref. [61] for reference. "All particles which are known today obey the Bose-Einstein distribution function (or statistics) or Fermi-Dirac distribution function (or statistics). Because at high energy or high temperature the two types of statistics become the same, namely, the statistics play no role. Therefore, it is convenient to introduce a third type of distribution functions (or statistics), namely Maxwell-Boltzmann distribution function (or statistics), which gives the high temperature behavior of both the fermion and boson systems."

# 9.6.2. Two Identical Particles

(1) Suppose that a system contains three particles, every particle can be in any state of single states  $\psi_1, \psi_2, \psi_3$ . Seek the number of possible states of the three particle system.

Solution:

(A) The three particles are identical bosons. Because for bosons any state in  $\psi_1, \psi_2, \psi_3$  can contain infinitely many bosons, the possible number of multiparticle symmetrical wave-functions are 10

(B) The three particles are identical fermions. Because for fermions any state in  $\psi_1, \psi_2, \psi_3$  can contain only one fermions, the possible number of multiparticle antiferromagnetic wavefunctions are 1.

(C) The two particles are nonidentical particles. The number is  $3 \times 3 \times 3 = 27$ .

(2) Eq. (9.2.5) gives the wavefunction of two fermion system

$$\Psi^{A}_{k_{1}k_{2}}(q_{1},q_{2}) = \frac{1}{\sqrt{2}} [\Psi_{k_{1}}(q_{1})\Psi_{k_{2}}(q_{2}) - \Psi_{k_{1}}(q_{2})\Psi_{k_{2}}(q_{1})] \\ = \frac{1}{\sqrt{2}} \left| \begin{array}{c} \Psi_{k_{1}}(q_{1}) & \Psi_{k_{1}}(q_{2}) \\ \Psi_{k_{2}}(q_{1}) & \Psi_{k_{2}}(q_{2}) \end{array} \right|.$$
(2.1)

The second term in Eq. (2.1) comes from the antisymmetry of the wavefunction, and is called exchange term. Seek the probability density of the two fermion system.

Solution:

$$\begin{aligned} |\Psi_{k_1k_2}^A(q_1,q_2)|^2 &= \frac{1}{2} \left\{ |\psi_{k_1}(q_1)|^2 |\psi_{k_2}(q_2)|^2 + |\psi_{k_1}(q_2)|^2 |\psi_{k_2}(q_1)|^2 \\ &- 2Re[\psi_{k_1}(q_1)\psi_{k_2}^*(q_1)\cdot\psi_{k_2}(q_2)\psi_{k_1}^*(q_2)] \right\} \end{aligned}$$
(2.2)

The third term is exchange term. If the overlapping of the two states  $\psi_{k_1}(q_1)$  and  $\psi_{k_2}(q_1)$  is equal to zero, then the contribution of the exchange term is equal to zero as well.

(3) Suppose that a system contains three particles, every particle can be in any state of single states  $\psi_1, \psi_2, \psi_3$ . Seek the number of possible states of the three particle system.

Solution:

(A) The three particles are identical bosons. Because for bosons any state in  $\psi_1, \psi_2, \psi_3$  can contain infinitely many bosons, the possible number of multiparticle symmetrical wavefunctions are 10

(B) The three particles are identical fermions. Because for fermions any state in  $\psi_1, \psi_2, \psi_3$  can contain only one fermions, the possible number of multiparticle antiferromagnetic wavefunctions are 1.

(C) The two particles are nonidentical particles. The number is  $3 \times 3 \times 3 = 27$ .

(4) Define spin exchange operator

$$P_{12} = \frac{1}{2} (1 + \vec{\sigma}_1 \cdot \vec{\sigma}_2). \tag{a}$$

Prove

$$P_{12}\alpha(1)\beta(2) = \alpha(2)\beta(1).$$
 (b)

Solution:

$$P_{12}\alpha(1)\beta(2) = \frac{1}{2}(1+\vec{\sigma}_{1}\cdot\vec{\sigma}_{2})\alpha(1)\beta(2)$$

$$= \frac{1}{2}(1+\sigma_{1x}\sigma_{2x}+\sigma_{1y}\sigma_{2y}+\sigma_{1z}\sigma_{2z})\alpha(1)\beta(2)$$

$$= \frac{1}{2}(1+\sigma_{1x}\sigma_{2x}+\sigma_{1y}\sigma_{2y}+\sigma_{1z}\sigma_{2z})\begin{bmatrix}1\\0\end{bmatrix}_{1}\begin{bmatrix}0\\1\end{bmatrix}_{2}$$

$$= \frac{1}{2}\left\{\begin{bmatrix}1\\0\end{bmatrix}_{1}\begin{bmatrix}0\\1\end{bmatrix}_{2}+\begin{bmatrix}0\\1\end{bmatrix}_{1}\begin{bmatrix}1\\0\end{bmatrix}_{2}+i\begin{bmatrix}0\\1\end{bmatrix}_{1}(-i)\begin{bmatrix}1\\0\end{bmatrix}_{2}$$

$$-\begin{bmatrix}1\\0\end{bmatrix}_{1}\begin{bmatrix}0\\1\end{bmatrix}_{2}\right\}$$

$$= \begin{bmatrix}0\\1\end{bmatrix}_{1}\begin{bmatrix}\begin{bmatrix}0\\1\end{bmatrix}_{2}\\0\end{bmatrix}_{2}=\alpha(2)\beta(1).$$

(5) Prove

$$(\vec{\sigma}_1 \cdot \vec{\sigma}_2)^2 = 3 - 2(\vec{\sigma}_1 \cdot \vec{\sigma}_2). \tag{a}$$

Solution:

$$(\vec{\sigma}_{1} \cdot \vec{\sigma}_{2})^{2} = \sum_{ijk=x,y,z} \sigma_{1i}\sigma_{1j}\sigma_{2i}\sigma_{2j}$$
  
$$= \sum_{i=x,y,z} \sigma_{1i}^{2}\sigma_{2i}^{2} + \sum_{ijk=x,y,z} (i\varepsilon_{ijk})^{2}\sigma_{1k}\sigma_{2k}$$
  
$$= 3 - \sum_{\substack{ijk=x,y,z \\ i \neq j}} (\varepsilon_{ijk})^{2}\sigma_{1k}\sigma_{2k}$$
  
$$= 3 - 2 \vec{\sigma}_{1} \cdot \vec{\sigma}_{2}$$

(6) Sometimes one uses the spin exchange operator to calculate in spin noncoupling representation. For example, prove

$$<\alpha(1)\beta(2)|S_1\cdot S_2|\beta(1)\alpha(2)>=\frac{\hbar^2}{2}.$$
 (a)

Solution:

$$< \alpha(1)\beta(2)|S_1 \cdot S_2|\beta(1)\alpha(2) > = \frac{\hbar^2}{2} < \alpha(1)\beta(2)|P_{12} - \frac{1}{2}|\beta(1)\alpha(2) >$$
$$= \frac{\hbar^2}{2} < \alpha(1)\beta(2)|P_{12}|\beta(1)\alpha(2) > = \frac{\hbar^2}{2}.$$
(b)

# 9.6.3. Bell Basis and Entangled States

(1) Eqs. (9.6.3.a-d) have given the four common eigenfunctions of operators  $S^2, S_z$ . Prove:

$$i\sigma_{1y}\sigma_{2x}\Upsilon_{10} = \frac{1}{\sqrt{2}}(\sigma_{1z}\sigma_{2x} - \sigma_{1x}\sigma_{2z})\Upsilon_{1-1} = \frac{1}{\sqrt{2}}(\sigma_{1z}\sigma_{2x} - \sigma_{1x}\sigma_{2z})\Upsilon_{11} = \Upsilon_{00}$$

(2) The negatively charged pion  $\pi^-$  is a spin-zero particle roughly 280 times more massive than the electron. Suppose the two electrons in a helium atom are replaced with two  $\pi^-$ , generating a pionic atom. Assume that the ground state wavefunctions of the two  $\pi^-$ s are  $\Psi_{1g}$  and  $\Psi_{2g}$ . Which of the following four wavefunctions are correct for the pionic helium atom? (A).  $\Psi_{1g}(r_1)\Psi_{1g}(r_2)$ . (B).  $\Psi_{1g}(r_2)\Psi_{2g}(r_1)$ . (C).  $1/\sqrt{2}(\Psi_{1g}(r_1)\Psi_{2g}(r_2) + \Psi_{1g}(r_2)\Psi_{2g}(r_1))$ . (D).  $1/\sqrt{2}(\Psi_{1g}(r_1)\Psi_{2g}(r_2) - \Psi_{1g}(r_2)\Psi_{2g}(r_1))$ .

Solution:

Since the pion is a spin-zero particle, it is a boson. Consequently, the two pion's waveunction must be symmetric under particle exchange  $r_1 \leftrightarrow r_2$ . The wavefunctions (A) and (C) are symmetric under  $r_1 \leftrightarrow r_2$ , while (D) is antisymmetric under  $r_1 \leftrightarrow r_2$ . The wavefunction (B) does not have any definite symmetry under  $r_1 \leftrightarrow r_2$ . Thus only (A) and (C) are allowed wavefunctions for pionic helium atom.

(3) It is often stated that the Pauli exclusion theorem asserts that no two electrons can be in the same state in an atom. What then is wrong with the two electron waveunction:  $\Psi = \Psi_g(r_1)\Psi_g(r_2)\Upsilon_{\uparrow}(1)\Upsilon_{\downarrow}(2)$  in which one of the two electrons is in the single particle ground state with its spin up and the other is in the single particle ground state with its spin down?

Solution:

Because electrons are spin 1/2 particles, a two electron's wavefunction must be antisymmetric under exchange. The  $\Psi$  is symmetric under  $r_1 \leftrightarrow r_2$ , but if the spin states of the two electrons are exchanged  $\Upsilon_{\uparrow}(1)\Upsilon_{\downarrow}(2) \leftrightarrow \Upsilon_{\downarrow}(1)\Upsilon_{\uparrow}(2)$ . Thus the spin state is not antisymmetric under the combined operation of exchanging the positions nd spins of the two electrons. The correct  $\Psi$  is

$$\Psi = \Psi_g(r_1)\Psi_g(r_2)\frac{1}{\sqrt{2}}[\Upsilon_{\uparrow}(1)\Upsilon_{\downarrow}(2) - \Upsilon_{\downarrow}(1)\Upsilon_{\uparrow}](2)$$

# 9.6.4. Applications of Pauli Exclusion Theorem

(1) Basing on the energy level formula and eigenfunction notations of hydrogen atom in chapter 6, the electron spin in chapter 8, and Pauli exclusion theorem in this chapter, discuss the periodic table of elements.

Solution:

The quantum state of electron in atom can be described by four quantum numbers:  $n, l, m, m_z$  (The meaning of the notations n, l, m can be found in Eq. (6.2.3.4) of chapter 6.  $m_z$  is the quantum number of the z component of electron spin). According to Pauli exclusion theorem, we can assign different quantum state to the electron in a given atom, i. e., only one electron can have the certain values of  $n, l, m, m_z$ . The electrons that have the same principal quantum number n are said to be in the same shell. For a given n, the electrons having the same value of l are said to in the same sub shell. Now we can calculate the maximum number of electrons belonging to the same shell or sub shell.

(A) The case of a sub shell:

For electrons in a sub shell we have same value of quantum numbers n and l. These electrons must differ either by the value of quantum number m [which can be one of the 2l + 1 integer values between -l and +l. Please refer to Eq. (6.2.3.4)] or by quantum number  $m_z$  (which can take values -1/2 or 1/2). There exists, therefore, 2(2l + 1) distinct quantum states corresponding to the same value of n and l and therefore, there can be 2(2l + 1) electrons in a sub shell of quantum number l. According to the spectroscopic custom, we express  $l = 0, 1, 2, 3, 4, 5, 6, 7, \cdots$  as  $s, p, d, f, g, h, i, j, \cdots$ , and call s orbit (or sub shell) etc. The maximum number of electrons in s, p, d, and f sub shell are therefore 2, 6, 10, and 14, respectively. A sub shell containing 2(2l + 1) electrons is said to be complete.

(B) The case of a shell.

For electrons in a shell we have same values of principle quantum number n but different quantum numbers l, m, and  $m_s$ . The quantum number l can have all values from l to n-1. The maximum number of electrons in n-th shell,  $N_{n-\text{th},max}$ , can be obtained by adding the maximum number of electrons in each sub shell.

$$N_{n-\text{th},max} = \sum_{l=0}^{n-1} 2(2l+1) = 2 + 6 + 10 + 14 + \dots + 2(2n-1) = 2n^2.$$

For the above derivation refer to Eq. (6.2.3.5) in chapter 6. The maximum number of electrons of quantum *n* (*n*-th shell) is therefore  $2n^2$ . The shell notations corresponding to n = 1, 2, 3, 4, 5, 6 are K, L, M, N, O, P, respectively.

A shell containing the maximum number of electrons is called a complete shell. We may be tempted to say that the electron configuration of any atom follows the general rule, and thus the periodic table of elements obeys this rule:

$$1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}4f^{14}\cdots$$

But this is not true. The actual order in which the levels must be filled so that the resulting energy is minimum (corresponding to a stable atom) is as follows:

$$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^6 7s^2 6d^{10} \cdots$$

Let us explain the notations. For example,  $5p^6$  means n = 5, l = 2, and the maximum number of filled electrons is 6. s, p, d, f corresponding to l = 0, 1, 2, 3, respectively.

Let us explain the periodic table of elements.

The first period is the K shell. This period (or shell) contains two elements: H with atomic number Z = 1 and one electron; He with Z=2 and two electrons. Both the electrons are in the energy level 1s.

The second period is the L shell, atomic number  $3 \le Z \le 10$ , contains eight elements: *Li*, *Be*, *B*, *V*, *N*, *O*, *F*, *Ne*, and occupies two energy levels: 1*s* and 2*p*.

The third period is the M shell, atomic number  $11 \le Z \le 18$ , contains eight elements: Na, Mg, Al, Si, P, Cl, Ar, and occupies two energy levels: 3s and 3p.

The fourth period is the N shell, atomic number  $19 \le Z \le 36$ , contains 18 elements, and occupies three energy levels: 4s, 3d, 4p.

The fifth period is the O shell, atomic number  $37 \le Z \le 54$ , contains 18 elements, and occupies three energy levels: 5s, 4d, 5p.

The sixth period is the P shell, atomic number  $55 \le Z \le 86$ , contains 32 elements, and occupies three energy levels: 6s, 4f, 5d, 6p.

# Chapter 10

# **Time Dependent Perturbation Theory**

If a system is an isolated system, then this system is of time homogeneity, the related Shrödinger equation is time-independent, and the average energy conservation is proved in chapter 5. If a system is an open system, then it not is of time homogeneity, the related Shrödinger equation is time-dependent, and the energy in this system might be not conservative. The time dependent perturbation theory discusses an open system, but the external action is weak enough, such that we can make approximate perturbation calculations. Only a few problems of open system can be solved precisely [114, 118].

The quantum transition is caused by the time dependent perturbation. The development of time dependent perturbation was initiated by Dirac's work on the semi-classical description of atoms interacting with electromagnetic fields [119]. Dirac, Wheeler, Heisenberg, Feynman, and Dyson developed it into a powerful set of techniques for studying interactions and time evolution in quantummechanical systems which cannot be solved exactly. One often calls the quantum transition from continuous spectrum to continuous spectrum the scattering.

This chapter will prove some theorems of quantum transition, and give some examples to use the time dependent perturbation theory. Time dependent perturbation theory is an extremely important tool for calculating properties of any physical system.

Some references, such as Refs. [108, 10], conclude the energy conservation in quantum transition processes. Some references, such as Refs. [2, 103, 3], conclude the energy nonconservation more or less in quantum transition processes. This textbook hopes very much that readers especially notice:

(1) Is the energy nonconservation in quantum transition processes an exact result or an approximate result?

(2) What are the conditions of energy conservation or nonconservation in quantum transition processes?

(3) How many manifestations of energy nonconservations did we found, at least, theoretically?

(4) Continue the explorations on the possible energy nonconservation even after learning this textbook. (5) All until now textbooks and this textbook can prove the conditional correctness of the so-called Fermi golden rule. But, all until now textbooks require the energy conserbation; On the contrary, this textbook requires energy nonconservation.

(6) The mathematical treatment for transition processes, including scattering processes, in all until now references and textbooks exists one very seriously purely mathematical mistake in the treatment of limit *time*  $\rightarrow \infty$ .

# 10.1. The Problem

The studies on the quantum state in quantum mechanics before this section are separated into two kinds:

(A) The first kind is that under the condition that Hamiltonian does not explicitly contain time, to solve the energy eigenequation

$$H_{\circ}|n\rangle = E_n|n\rangle, \tag{10.1.1}$$

where  $|n\rangle$  is a complete set of quantum number including energy. For Eq. (10.1.1) we have many discussions before this chapter.

(B) Another main task for the study on the quantum state in quantum mechanics before this section is to calculate the state's time evolution. This time evolution of quantum state satisfies the time dependent Schrödinger equation, which was given by chapter 3,

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle.$$
 (10.1.2)

Eq. (10.1.2) includes a first order time derivative. If the system's Hamiltonian is given, then one can obtain  $|\Psi(t)\rangle$  at any time from initial state  $|\Psi(0)\rangle$ . It is deterministic [1].

If the Hamiltonian does not contains time explicitly (i. e.,  $\partial H/\partial t = 0$ ) and is expressed as  $H_{\circ}$ , then energy is an conservative quantity. In this case from Eq. (10.1.2) one obtains

$$|\Psi(t)\rangle = e^{-iH_{o}t/\hbar}|\Psi(0)\rangle \equiv U(t)|\Psi(0)\rangle, \qquad (10.1.1.3)$$

where operator U(t) called time evolution operator of quantum state. However, if H contains time t explicitly, then due to

$$[H(t_1), H(t_2)]] \neq 0, \quad for \ t_1 \neq t_2 \tag{10.1.3}'$$

$$|\Psi(t)\rangle = Te^{-i\int_0^t dt H(t)/\hbar} |\Psi(0)\rangle \neq e^{-i\int_0^t dt H(t)/\hbar} |\Psi(0)\rangle, \qquad (10.1.3)''$$

where T expresses the time-ordering operator. This textbook does not concerns the case H = H(t).

If we take the energy representation (the bases as the energy eigenstates of  $H_{\circ}$ ), then  $|\Psi(0)\rangle$  can be expanded as

$$|\Psi(0)\rangle = \sum_{n} a_n |n\rangle,$$
 (10.1.4)

and

$$a_n = < n | \Psi(0) >,$$
 (10.1.5)

where *n* represents a complete set of discrete quantum numbers, e. g. the bound energy states  $|n, l, m_l, m_s >$  of hydrogen atom or the states |n > of a harmonic oscillator are discrete.

Substituting Eq. (10.1.4) and  $H_{\circ}|n\rangle = E_n|n\rangle$  into Eq. (10.1.3) yields

$$|\Psi(t)\rangle = \sum_{n} a_{n} e^{-iE_{n}t/\hbar} |n\rangle.$$
(10.1.6)

If at t = 0 the system is in the state  $|k\rangle$ , is of energy  $E_k$ , then

$$|\Psi(0)\rangle = |k\rangle. \tag{10.1.7}$$

Substituting Eq. (10.1.7) into Eq. (10.1.5) yields  $a_n = \delta_{nk}$ . Therefore, Eq. (10.1.4) gives

$$|\Psi(t)\rangle_k = e^{-iE_k t/\hbar} |k\rangle.$$
 (10.1.8)

Eq. (10.1.8) means that the system still keeps the original energy eigenstate at t > 0, but in comparison with the original  $|\Psi(0)\rangle = |k\rangle$ ,  $|\Psi(t)\rangle$  has an additional factor

 $exp(-iE_kt/\hbar)$  (quantum beat), which does not alter its orthogonality to  $|\Psi(0)\rangle = |k\rangle$ .  $|\Psi(t)\rangle$  is called stationary state.

If at initial time t = 0 the system's state  $|\Psi(0)\rangle$  is in a superposition state of many energy eigenstates [Eq. (10.1.4)], then at t > 0 the system's state  $|\Psi(t)\rangle$  is still in a superposition state [Eq. (10.1.6)], which is a non stationary state. However, due to that His a conservative quantity,  $|a_n \exp(-iE_n t/\hbar)|^2 = |a_n|^2$  does not depend on time. Therefore, the proportionality of eigenstates in Eq. (10.1.6) do not change with time.

This chapter will introduce the third kind of studies on the quantum states in quantum mechanics. In many cases person does not interest in the time evolution of quantum state. Instead, person interests in the transition probability of a system between unperturbed bound stationary states under the influence of time dependent perturbation. We have proved in chapter 4 that the energy of bound state is discrete. The transition between bound states is called transition between discrete states, briefly, D-D transition. In section 10.6 we will study the transition between discrete and continuous states, briefly, D-C transition. Quantum transition as a new concept was proposed by Bohr in the early quantum theory before Dirac, but he did not give systematic method to solve this problem.

Let us explain the concept of quantum transition and transition probability in more detail.

Assume that at initial time t = 0 the system is in the state

$$|\Psi(0)\rangle = |k\rangle. \tag{10.1.9}$$

The state  $|\Psi(0) > \text{at } t > 0$  is [See Eq. (10.1.8)] is

$$|\Psi(t)\rangle_k = e^{-iE_k t/\hbar} |k\rangle.$$
 (10.1.9)'

If a system suffers an applied interaction H'(t), then the total Hamiltonian is

$$H = H_{\circ} + H'(t), \qquad (10.1.10)$$

and

$$\Psi_k(t) >= \sum_n < n |e^{iE_n t/\hbar}| \Psi_k > e^{-iE_n t/\hbar} |n| >= \sum_n a_{nk}(t) e^{-iE_n t/\hbar} |n| >.$$
(10.1.11)

From Eq. (10.1.11) we know that at time t the probability of the system in state  $|n\rangle$  is

$$P_{nk}(t) = |a_{nk}(t)|^2, \quad (a_{nk}(0) = \delta_{nk}).$$
 (10.1.12)

 $P_{nk}(t)$  is called transition probability. The average and instantaneous transition rate is defined as

$$w_{nk} = \frac{1}{t} P_{nk}(t) = \frac{1}{t} |a_{nk}(t)|^2, \text{ and } w_{ins \ nk} = \frac{d}{dt} P_{nk}(t), \quad (10.1.13)$$

respectively. To seek  $a_{nk}(t)$  we need to solve the time dependent Schrödinger equation, which has been given by chapter 3,

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle.$$
 (10.1.14)

Substituting Eq. (10.1.11) into Eq. (10.1.14) yields

$$i\hbar \sum_{n} \dot{a}_{nk}(t) e^{-iE_{n}t/\hbar} |n\rangle = \sum_{n} a_{nk}(t) e^{-iE_{n}t/\hbar} H'(t) |n\rangle.$$
(10.1.15)

Taking the inner product of the Eq. (10.1.15) with  $(|\Psi(t)\rangle_{k'})^* =_{k'} \langle \Psi(t)|e^{iE_{k'}t/\hbar}$ , defined in Eq. (10.1.9)', and utilizing the orthonormality of  $\langle k'|n\rangle = \delta_{k'n}$ , one obtains

$$i\hbar \dot{a}_{k'k}(t) = \sum_{n} e^{i(E_{k'} - E_n)t/\hbar} < k'|H'(t)|n > a_{nk}(t) \equiv \sum_{n} e^{i\omega_{k'n}t} < k'|H'(t)|n > a_{nk}(t).$$
(10.1.16)

 $a_{k'k}(t)$  is a probability amplitude of an object, initial in the eigenstate k of  $H_{\circ}$  and final at time  $t(H_{\circ} \rightarrow H)$  in the eigenstate k' of  $H_{\circ}$ . Actually, Eq. (10.1.16) is a matrix representation of Schrödinger equation in representation of  $H_{\circ}$ . The  $H_{\circ}$  refers to conservative system. But, H does not refer to conservative system. Therefore, the transition processes might be energy nonconservative.

If H'(t) is large, then the Eq. (10.1.16) is difficult to solve. If H'(t) is weak  $(H'(t) << H_{\circ})$ , then  $|a_{nk}(t)|^2 << 1$   $(n \neq k)$ , which means that  $|a_{nk}(t)|^2 << 1$  varies with time slowly, and the probability that the system still keeps in state  $|k\rangle$  is large. In the weak perturbation condition, we can use the time dependent perturbation theory to seek the transition probability.

# **10.2.** Basic Formulas

#### (A) Zero order approximation

Set H' = 0. Eq. (10.1.16) gives

$$\dot{a}_{k'k}^{(0)}(t) = 0, \ a_{k'k}^{(0)}(t) = a_{k'k}^{(0)}(0) = \delta_{k'k}.$$
 (10.2.1)

#### (B) First order approximation

Substituting the zeroth approximation into the right hand side of Eq. (10.1.16), one obtains first order approximation:

$$i\hbar \dot{a}_{k'k}^{(1)}(t) = e^{i\omega_{k'k}t}H'_{k'k}(t).$$
(10.2.2)

After integration over time t one obtains

$$a_{k'k}^{(1)}(t) = \frac{1}{i\hbar} \int_0^t e^{i\omega_{k'k}t'} H'_{k'k}(t') dt'.$$
 (10.2.3)

The *t* in Eq. (10.2.3) represents the duration time of perturbation. Therefore, from Eqs. (10.2.3) and (10.1.12) one obtains that in first order approximation

$$P_{k'k}(t) = P_{k'k}^{(1)}(t) = |a_{k'k}^{(1)}(t)|^2 = \frac{1}{\hbar^2} \left| \int_0^t e^{i\omega_{k'k}t} H_{k'k}'(t) dt \right|^2 \quad (k' \neq k).$$
(10.2.4)

In Eq. (10.2.4)  $P_{k'k}^{(1)} \ll 1$  to satisfy the perturbation conditions.

# 10.3. Periodic Perturbation Theory

### 10.3.1. Simple Case

Periodic perturbation

$$H'(t) = H'e^{-i\omega t}$$
(10.3.1.1)

can also be called harmonic perturbation.

The physical meaning of t in Eq. (10.2.3) is the duration time of H'(t).

According to Eq. (10.2.3), at time t the transition probability amplitude from initial state  $|k\rangle$  to final state  $|k'\rangle$  is

$$a_{k'k}^{(1)} = \frac{1}{i\hbar} \int_0^t e^{i(\omega_{k'k} - \omega)t} H_{k'k}' dt = \frac{1}{i\hbar} H_{k'k}' \frac{e^{i(\omega_{k'k} - \omega)t} - 1}{i(\omega_{k'k} - \omega)}.$$
 (10.3.1.2)

The corresponding transition probability is

$$P_{k'k}(t) = \left|a_{k'k}^{(1)}\right|^2 = \frac{4|H'_{k'k}|^2}{\hbar^2} \left[\frac{\sin[(\omega_{k'k} - \omega)t/2]}{(\omega_{k'k} - \omega)}\right]^2.$$
 (10.3.1.3)

Eq. (10.3.1.3) is an important basic formula of transition theory. If  $\omega = 0$ , then Eq. (10.3.1.3) is a formula for time independent perturbation in the time interval [0,t]. Let us make some discussions for this formula. If k' and k represent discrete energy states, then it is called D-D transition. If k' and k represent continuous and discrete energy state, respectively, then it is called D-C transition. If k' and k represent continuous energy states, then it is called C-C transition. In all textbooks entitled "Advanced Quantum Mechanics" there is a chapter, entitled "Scattering Theory", which is a general theory of C-C transition. Therefore, C-C transition and scattering theory have common theoretical basis.

For the convenience of statement, we use the method proposed in Ref. [1], i. e., we introduce formally the concept about the density of states for the discrete energy states,  $\overline{\rho(k')}$ , and set  $\overline{\rho(k')}dE_{k'}$  and  $\overline{\rho(k')}d\omega_{k'}$  are dimensionless.  $E_{k'} = \hbar\omega_{k'}$ . After introducing the  $\overline{\rho(k')}$  the summation over all states becomes integration, and after integration we set  $\overline{\rho(k')} = 1$ . Using the concept of density of states, if the final state is continuous energy states, then we put a factor,  $\rho(k')d\omega_{k'}$  or  $\rho(k')dE_{k'}$  to the Eq. (10.3.1.3), and if the initial state is continuous energy states, then we put a factor,  $\rho(k)d\omega_k$  or  $\rho(k)d\omega_k$  or  $\rho(k)dE_k$  to the Eq.

(10.3.1.3). Note that according to the definition,  $\rho(k')$  can represent state density of energy or angular frequency.

Make some discussions for Eq. (10.3.1.3).

(1) If we take the time *t* to be fixed, then the transition probability  $P_{k'k}(t)$  is an oscillation function of  $(\omega_{k'k} - \omega) = (E_{k'} - E_k - \hbar\omega)/\hbar$ , which means that  $P_{k'k}(t) > 0$  can occur at the case of  $|(\omega_{k'k} - \omega)| = |(E_{k'} - E_k - \hbar\omega)|/\hbar \ge 0$ . In physics,  $|(E_{k'} - E_k - \hbar\omega)| \ge 0$  means that the quantum transition process allows both energy conservation and nonconservation! For example,  $(E_{k'} - E_k - \hbar\omega) = 0$  means that the initial state energy  $E_k$  plus external energy  $\hbar\omega$  is equal to the final state energy  $E_{k'}$ . If we use photon language instead of electric field language, then  $(E_{k'} - E_k - \hbar\omega) = 0$  means the initial state energy  $E_k$  plus the absorbed photon energy  $\hbar\omega$  is equal to the final state energy  $E_{k'}$ .

(2) Further, the shorter the duration time *t* is, the more strong the energy nonconservation is. Let us explain this point. The first maximum value (first peak) of oscillation function in Eq. (10.3.1.3),  $sin[(\omega_{k'k} - \omega)t/2]/(\omega_{k'k} - \omega)^2$ , is  $t^2/4$  at  $(\omega_{k'k} - \omega) = 0$ . This latter expression means energy conservation. The second maximum value (second peak) of oscillation function in Eq. (10.3.1.3),  $sin[(\omega_{k'k} - \omega)t/2]/(\omega_{k'k} - \omega)^2$ , is  $t^2/(9\pi)^2$  at  $(\omega_{k'k} - \omega) = 3\pi/t \propto 1/t \neq 0$ . This latter expression means energy nonconservation. If we use the attosecond technology  $(10^{-18} \text{ second})$ , then  $(\omega_{k'k} - \omega)/(2\pi) = 3/(2t) = 1.5 \times 10^{18} Hz$ , which is equal to energy  $1.5 \times 10^{18} \times 4.1356 \times 10^{-15} eV = 6.2 \times 10^3 eV$ .

(3)  $\omega_{k'} = \omega_k + \omega$  means energy conservation. There is one question. If  $\omega_{k'} > \omega_k + \omega$  and such that  $(\omega_{k'} - \omega_k - \omega)t \ll 1$ , what is the time variation of  $P_{k'k}(t)$ ? In this case Eq. (10.3.1.3) may be expanded to yield

$$P_{k'k}(t) = \frac{t^2 |H'_{k'k}|^2}{\hbar^2}.$$
(10.3.1.4)

The related transition probability rate is

$$w_{k'k}(t) = \frac{1}{t} P_{k'k}(t) = \frac{t |H'_{k'k}|^2}{\hbar^2}.$$
 (10.3.1.5)

If the transition rate is independent of time, then persons call it Fermi golden rule. The cause of Fermi golden rule will be explained in the next. It is obvious that Eq. (10.3.1.5) violates Fermi golden rule.

(4) Of course, readers will ask a sharp question that if the energy nonconservation is possible, then why there is no any experimental report on the observed energy nonconservation in the quantum transition processes in the past 80 years? The author of this book would like to give four reasons:

(4.1) The attosecond technology is a newest thing. Until now this attosecond technology has not yet produced enough field intensity. Therefore, this kind of experiments has not yet been done;

(4.2) The large number of experiments of light pulse in the previous time is  $t > 10^{-13}$  second. In this case the scale of the quantity of the energy nonconservation at the second

peak  $(\omega_{k'k} - \omega) = 3\pi/t < 3.1 \times 10^{-2} eV$ . It is really a small quantity in comparison with the characteristic energy in the concerned problems. For example, the ground state energy of hydrogen atom is -13.6 eV. Therefore, the quantum transition corresponding to the second peak is neglected by experimentalists (Refer to Fig. 10.1);

(4.3) (The height of the first peak):(The height of the second)= $(t/2)^2$ :  $t^2 \times /(3\pi)^2 = 2.5\pi^2$ . Therefore, the first peak corresponding to the energy conservation is easy to be observed in comparison with the second peak corresponding to the energy nonconservation, because the transition probability corresponding to the first peak is much larger than that of the second peak.

From the above discussions, we see that under the periodic perturbation the system can transit to many final states including both energy conservative and energy non conservative. Therefore, if we seek the transition rate from the initial state  $|k\rangle$  to any final state under the periodic perturbation,  $w_{all \leftarrow k}$  ( $w_{all \leftarrow k}$  is called transition rate), we can use following two methods.

Method 1:

$$\begin{split} w_{all \leftarrow k} &\equiv \frac{1}{t} \sum_{k' \neq k} P_{k'k}(t) \\ &= \frac{1}{t} \int_{-\infty}^{+\infty} d\omega_{k'} \overline{\rho(\omega_{k'})} P_{k'k}(t) \\ &= \frac{1}{t} \int_{-\infty}^{+\infty} d\omega_{k'} \overline{\rho(\omega_{k'})} \frac{4|H'_{k'k}|^2}{\hbar^2} \left[ \frac{\sin[(\omega_{k'} - \omega_k - \omega)t/2]}{(\omega_{k'} - \omega_k - \omega)} \right]^2 \\ &= \frac{4|H'_{k'k}|^2}{\hbar^2} \overline{\rho(\omega_{k'})} \frac{1}{t} \int_{-\infty}^{+\infty} d\omega_{k'} \left[ \frac{\sin[(\omega_{k'} - \omega_k - \omega)t/2]}{(\omega_{k'} - \omega_k - \omega)} \right]^2 \\ &= \frac{2|H'_{k'k}|^2}{\hbar^2} \overline{\rho(\omega_{k'})} \frac{1}{t} t \int_{-\infty}^{+\infty} dx \frac{\sin^2 x}{x^2} \\ &= \frac{2\pi |H'_{k'k}|^2}{\hbar^2} \overline{\rho(\omega_{k'})} = \frac{2\pi |H'_{k'k}|^2}{\hbar} \overline{\rho(E_{k'})}. \end{split}$$
(10.3.1.6)

Method 2:

$$w_{ins,all \leftarrow k} \equiv \frac{d}{dt} \sum_{k' \neq k} P_{k'k}(t)$$
  
=  $\frac{d}{dt} \int_{-\infty}^{+\infty} d\omega_{k'} \overline{\rho(\omega_{k'})} P_{k'k}(t)$   
=  $\int_{-\infty}^{+\infty} d\omega_{k'} \overline{\rho(\omega_{k'})} \frac{4|H'_{k'k}|^2}{\hbar^2} \frac{d}{dt} \left[ \frac{sin[(\omega_{k'} - \omega_k - \omega)t/2]}{(\omega_{k'k} - \omega)} \right]^2$   
=  $\frac{4|H'_{k'k}|^2}{\hbar^2} \overline{\rho(\omega_{k'})} \int_{-\infty}^{+\infty} d\omega_{k'} \frac{d}{dt} \left[ \frac{sin[(\omega_{k'} - \omega_k - \omega)t/2]}{(\omega_{k'k} - \omega)} \right]^2$ 

$$= \frac{4|H'_{k'k}|^2}{\hbar^2} \overline{\rho(\omega_{k'})} \int_{-\infty}^{+\infty} d\omega_{k'} \frac{2sin[(\omega_{k'} - \omega_k - \omega)t/2]}{(\omega_{k'k} - \omega)^2} \\ \times \cos[(\omega_{k'} - \omega_k - \omega)t/2](\omega_{k'} - \omega_k - \omega)/2) \\ = \frac{4|H'_{k'k}|^2}{\hbar^2} \overline{\rho(\omega_{k'})} \int_{-\infty}^{+\infty} d\omega_{k'} \frac{sin[(\omega_{k'} - \omega_k - \omega)t]}{(\omega_{k'k} - \omega)} \\ = \frac{2|H'_{k'k}|^2}{\hbar^2} \overline{\rho(\omega_{k'})} \int_{-\infty}^{+\infty} d\omega_{k'} \frac{sin[(\omega_{k'} - \omega_k - \omega)t]}{(\omega_{k'k} - \omega)} \\ = \frac{2|H'_{k'k}|^2}{\hbar^2} \overline{\rho(\omega_{k'})} \int_{-\infty}^{+\infty} dx \frac{\sin x}{x} \\ = \frac{2\pi |H'_{k'k}|^2}{\hbar^2} \overline{\rho(\omega_{k'})} = \frac{2\pi |H'_{k'k}|^2}{\hbar} \overline{\rho(E_{k'})}.$$
(10.3.1.6)'

For D-C and C-C transitions, the  $\overline{\rho(k')}$  should be  $\rho(k')$ . In the fourth equality in Eqs. (10.3.1.6) and (10.3.1.6)', we make an approximation, i. e.,  $\overline{\rho(k')}|H'_{k'k}|^2$  does not depend of k'.

That the  $w_{all \leftarrow k}$  in the last equality of Eqs. (10.3.1.6) and (10.3.1.6)' is time independent is called Fermi golden rule.

We would like to tell the readers an interesting story on the Fermi golden rule. The formula similar to Eq. (10.3.1.6) was found to have such widespread application that Fermi dubbed it "Golden Rule No. 2" (E. Fermi, Nuclear Physics, University of Chicago, 1950). However, we should point out that the physics and method to derive Eq. (10.3.1.6) in this textbook are much different from some references. To derive the formula similar to Eq. (10.3.1.6), some references take the limit  $t \to \infty$ . In this limit some references obtain that the energy in the transition process from  $|k > \text{to } |k' > \text{is conservative}, P_{k'k}(t \to \infty) \propto t$ , and  $w_{k'k}(t \to \infty)$  is time independent. Based two conditions,  $t \to \infty$  and the k'-independence of  $|H'_{k'k}|^2 \rho(k')$ , some references obtain time-independence of  $w_{all \leftarrow k}(t \to \infty)$  Fermi golden rule. However, in our derivation, the time-independence of  $w_{all \leftarrow k}$  does not need the limit  $t \to \infty$ , but needs the k'-independence of  $|H'_{k'k}|^2 \rho(k')$ , and the calculations for  $w_{all \leftarrow k}$  consider essentially the contributions from all energy states. In the next we will mention Fermi golden rule once again.

Similarly to the derivation of Eq. (10.3.1.6), we can also obtain the transition probability from initial state  $|k\rangle$  to all possible final states,  $P_{all\leftarrow k}(t)$ .

$$P_{all \leftarrow k}(t) = \sum_{k'} P_{k'k}(t) = \sum_{k'} \left| a_{k'k}^{(1)} \right|^2$$
  
$$= \int_{-\infty}^{\infty} d\omega_{k'} \overline{\rho(\omega_{k'})} \frac{4|H'_{k'k}|^2}{\hbar^2} \left[ \frac{sin[(\omega_{k'k} - \omega)t/2]}{(\omega_{k'k} - \omega)} \right]^2$$
  
$$\equiv \int_{-\infty}^{\infty} d\omega_{k'} P_{k'k}$$
  
$$= \overline{\rho(\omega_{k'})} \frac{4|H'_{k'k}|^2}{\hbar^2} \int_{-\infty}^{\infty} d\omega_{k'} \left[ \frac{sin[(\omega_{k'k} - \omega)t/2]}{(\omega_{k'k} - \omega)} \right]^2$$

$$= \frac{2|H'_{k'k}|^2}{\hbar^2} \overline{\rho(\omega_{k'})} t \int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2}$$
  
=  $\frac{2\pi |H'_{k'k}|^2}{\hbar^2} \overline{\rho(\omega_{k'})} t.$  (10.3.1.3)'

In the fourth equality of Eq. (10.3.1.3)' we neglect the k'-dependence of  $|H'_{k'k}|^2$  and  $\rho(k')$ . In this condition, the oscillation function,  $sin^2[(\omega_{k'k} - \omega)t/2]/(\omega_{k'k} - \omega)^2$ , determines the magnitude of  $P_{all \leftarrow k}$ . Due to that the oscillation function has very large value at  $\omega_{k'k} - \omega = 0$  (energy conservation), we can say that, under the condition of k'-independence of  $|H'_{k'k}|^2 \rho(k')$ , the important transition process is energy conservative, i. e., the energy is approximately conservative.

(5) In Eq. (10.3.1.3)', if  $\omega = |\omega_k| = |\omega_b|$ , then we call it boundary transition.

#### Theorem XXXVIII: Boundary transition. For the boundary absorption, if

 $|H'_{k'k}|^2 \rho(k') = A \omega_{k'}^{\beta} \quad (\beta \ge 0) \text{ in Eq. (10.3.1.3)', then}$ 

(i) The transition probability (density)  $P_{k'k}(t)$  in Eq. (10.3.1.3)' has maximum value at  $\omega_{k'k} - \omega = \omega_{k'} \ge 0$ , which means that quantum transition of boundary absorption mainly occurs in the process being of energy nonconservation.

(ii) The time-dependence of transition probability  $P_{all \leftarrow k}(t)$  is  $t^{1-\beta}$ .

**Proof.** (i) In physics, this theorem means that, for example, if an electron of atom absorbs a photon with energy just equal to the binding energy of the electron in atom  $\omega = \omega_b$  and  $|H'_{k'k}|^2 \rho(k') \propto \omega_{k'}^{\beta}$  ( $\beta \ge 0$ ), then the transition is definitely energy non conservative.

Assume that  $\hbar \omega_k = -\hbar \omega_b$ , and  $|H'_{k'k}|^2 \rho(k') = A \omega_{k'}^{\beta}$ . Eq. (10.3.1.3) becomes

$$P_{k'k}(t) = \frac{1}{\hbar^2} A \omega_{k'}^{\beta} \frac{\sin^2[(\omega_{k'})t/2]}{[\omega_{k'})^2} \equiv \frac{1}{\hbar^2} A \times I$$
$$\equiv \frac{1}{\hbar^2} A \times \omega_{k'}^{\beta} \times II \equiv \frac{1}{\hbar^2} A \times III \times II.$$
(10.3.1.3)"

The factor *II* is called oscillation factor. If  $(\omega_{k'})t/2 = 0$ , then  $P_{k'k}(t) = 0$ . The largest value of *I* is called first peak of *I*. This first peak is at  $(\omega_{k'})t/2 > 0$  if  $\beta > 0$ . Let us seek the value of  $(\omega_{k'})t/2$ , at which is the first peak of *I*. Set  $(\omega_{k'})t/2 = x$ . Thus  $I = (t/2)^{2-\beta}x^{\beta-2}\sin^2 x$ . The maximum condition of *I* is

$$\tan x = \frac{2}{2-\beta}x, \quad x = \frac{\omega_{k'}t}{2}.$$
 (10.3.1.7)

(ii) From Eq. (10.3.1.3)' we have

$$P_{all \leftarrow k}(t) = \frac{1}{\hbar^2} \int_{-\infty}^{\infty} |H'_{k'k}|^2 \rho(E_{k'}) \frac{\sin^2[(E_{k'} - E_k - E)t_{\circ}]/(2\hbar)}{[(E_{k'} - Ek - E)/(2\hbar)]^2} dE_{k'}$$
  
=  $\frac{1}{\hbar^2} \int_{-\infty}^{\infty} |H'_{k'k}|^2 \rho(\omega_{k'}) \frac{\sin^2[(\omega_{k'} - \omega_k - \omega)t_{\circ}]/(2)}{[(\omega_{k'} - \omega_k - \omega)/(2)]^2} d\omega_{k'}$ 

$$= \frac{A}{\hbar^{2}} \int_{-\infty}^{\infty} \omega_{k'}^{\beta} \frac{\sin^{2}[(\omega_{k'} - \omega_{k} - \omega)t_{\circ}]/(2)}{[(\omega_{k'} - \omega_{k} - \omega)/(2)]^{2}} d\omega_{k'}$$

$$= \frac{A}{\hbar^{2}} \int_{-\infty}^{\infty} \omega_{k'}^{\beta} \frac{\sin^{2}[\omega_{k'}t_{\circ}/2]}{[\omega_{k'}/2]^{2}} d\omega_{k'}$$

$$= \frac{A2^{1+\beta}}{\hbar^{2}} \int_{-\infty}^{\infty} x_{k'}^{\beta} \frac{\sin^{2}x}{x^{2}} dxt^{1-\beta}$$

$$= \frac{A2^{1+\beta}\pi}{\hbar^{2}} t^{1-\beta}.$$
(10.3.1.7)'

Here we finish the proof for the theorem. QED.

Let us make many discussions for Eqs. (10.3.1.7) and (10.3.1.3)''.

To show the variation of  $P_{k'k}(t)$  with  $\omega_{k'}/(2\pi) = f$  clearly, we draw Figs. 10.1 and 10.2, which show the variations of  $P_{k'k}(t)$  with  $\omega_{k'}/(2\pi) = f$  when  $\beta = 0$  and  $\beta = 1.5$ , respectively. We use  $P_{k'k,n}$  to express the *n*-th maximum value of  $P_{k'k,n}$ .

If  $\beta = 0$ , then

$$\frac{P_{k'k,1}(t)}{P_{k'k,2}(t)} = \frac{1}{1/(1.5\pi)^2} >> 1.$$
(10.3.1.8)

The first peak is at  $\omega_{k'} = 0$ . (10.3.1.8) means that the main transition process is energy conservative (in case of boundary absorption,  $\omega_{k'} = 0$  means energy conservation).

If  $\beta = 2$ , then

$$\frac{P_{k'k,1}(t)}{P_{k'k,2}(t)} = \frac{P_{k'k,1}(t)}{P_{k'k,3}(t)} = \dots = 1.$$
(10.3.1.9)

Eq. (10.3.1.9) means that the transition probabilities of both energy conservation and energy nonconservation are exactly same.

If  $\beta > 2$ , then

$$\frac{P_{k'k,1}(t)}{P_{k'k,2}(t)} > \frac{P_{k'k,1}(t)}{P_{k'k,3}(t)} > \cdots .$$
(10.3.1.10)

Eq. (10.3.1.10) means that the more serious the energy nonconservation is, the more large the transition probability is. Considering the importance of  $|H_{k'k}|^2 \rho(k')$ , we name it vacuum energy support ability.

The solution of Eq. (10.3.1.7) can be found out approximately. For example if  $\beta = 1.5$ , the solution of Eq. (10.3.1.7) is

$$x = \frac{\omega_{k't}}{2} = \frac{3.113484}{2}.$$
 (10.3.1.11)

Eq. (10.3.1.11) indicates that the more shorter the duration time *t* is, the more larger, for example, the kinetic energy of the emitted electron in photoeffect is.

To show the variation of  $P_{k'k}(t)$  with  $2\pi\omega_{k'} = f$  clearly, we draw Figs. 10.1 and 10.2, which show the variation of  $P_{k'k}(t)$  with  $2\pi\omega_{k'} = f$  when  $\beta = 0$  and  $\beta = 1.5$ , respectively. Note that if the transition process is not boundary, then from Eq. (10.3.1.3)  $2\pi(\omega_{k'}\omega_k - \omega) = f$ .



Figure 10.1. Theoretical curve of II versus f. If there is no energy variation of *III*, i. e.,  $\beta = 0$ , then *II* is proportional to the transition probability  $P_{k'k}(t)$ .

# 10.3.2. General Case

In the following we do two things: (i). Consider a more general harmonic (or, periodic perturbation), which can be used to both absorption and emission. (ii). We express the duration time as  $t_{\circ}$  other than t. When  $t > t_{\circ}$ , the perturbation is zero, and the perturbed system will keep the state at  $t_{\circ}$  at any  $t \ge t_{\circ}$ . The perturbation is

$$H''(t) = \frac{H'}{2} \left( e^{i\omega t} + e^{-i\omega t} \right), \quad (H' = 0 \ if \ t \ge t_{\circ} \ or \ t < 0), \tag{10.3.2.1}$$

where the second and the first term correspond to processes of absorption and emission of photon, respectively. If  $\omega = 0$  in Eq. (10.3.2.1), then H'' represents a time-independent perturbation. From Eqs. (10.2.1.4), the transition probability from state  $\omega_k$  to interval



Figure 10.2. Theoretical curve of I versus f in case of  $\beta = 1.5$ . *I* is exactly proportional to the transition probability  $P_{k'k}(t)$ .

between  $\omega_{k'}$  and  $\omega_{k'} + d\omega_{k'}$  is

$$P_{k'k}(t \ge t_{\circ})d\omega_{k'} = |a_{k'k}^{(1)}(t)|^{2}d\omega_{k'} = \frac{1}{\hbar^{2}} \left| \int_{0}^{t_{\circ}} dt H_{k'k}^{"}(t)e^{i\omega_{k'k}}\rho(k')dE_{k'} \right|^{2}$$

$$= \frac{1}{\hbar^{2}} |H_{k'k}^{'}|^{2}\rho(k')d\omega_{k'} \left| \int_{0}^{t_{\circ}} dt [e^{i(\omega_{k'k}-\omega)} + e^{i(\omega_{k'k}+\omega)}] \right|^{2}$$

$$= \frac{1}{\hbar^{2}} |H_{k'k}^{'}|^{2}\rho(k')d\omega_{k'} \left| \frac{e^{i(\omega_{k'k}-\omega)t_{\circ}} - 1}{i(\omega_{k'k}-\omega)} + \frac{e^{i(\omega_{k'k}+\omega)t_{\circ}} - 1}{i(\omega_{k'k}+\omega)} \right|^{2}$$

$$\approx \frac{4|H'_{k'k}|^2}{\hbar^2}\rho(k')d\omega_{k'}\left\{\left[\frac{\sin[(\omega_{k'k}-\omega)t_{\circ}]/2}{(\omega_{k'k}-\omega)}\right]^2 + \left[\frac{\sin[(\omega_{k'k}+\omega)t_{\circ}]/2}{(\omega_{k'k}+\omega)}\right]^2\right\}.$$
(10.3.2.2)

If  $\omega = 0$ , then Eq. (10.3.2.2) becomes a formula of constant perturbation in finite time interval. The two terms in Eq. (10.3.2.2) have maximum values at  $\omega_{k'k} - \omega = \omega_{k'} - \omega_k - \omega =$ 

0 or  $\omega_{k'k} + \omega = \omega_{k'} - \omega_k + \omega = 0$ . The former and the latter correspond to absorb and emit one photon, respectively. The sizes of the two terms are equal each other. For brevity, we just consider the the term of absorbing a photon. Transform  $\omega$  to  $E/\hbar$ . In Eq. (10.3.2.2)  $P_{k'k}(t \ge t_{\circ})$  represents the transition probability from state  $|k\rangle$  to state  $|k'\rangle$ . The total transition probability from initial state  $|k\rangle$  with energy  $E_k$  to all possible final states  $|k'\rangle$ with energies  $E_{k'}$  is thus

$$P(t \ge t_{\circ}) \equiv \int P_{k'k}(t \ge t_{\circ}) dE_{k'} = \frac{1}{\hbar^2} \int |H'_{k'k}|^2 \rho(k') \frac{\sin^2[(E_{k'k} - E)t_{\circ}]/(2\hbar)}{[(E_{k'k} - E)/(2\hbar)]^2} dE_{k'}, \quad (10.3.2.3)$$

where  $E = \hbar \omega$  is the an energy of one photon. For the time-dependent transition ( $\omega \neq 0$ ), such as photoeffect (i. e., an atom absorbs a photon and emits an electron. See subsection 10.4.5,  $E_k = E_{(initial - electron)} - E_{(electron - binding - energy)} \equiv E_{(initial - electron)} - E_b$ , and  $E_{k'}$  is the kinetic energy of the ejected electron.

**Theorem XXXIX: Energy in transition processes.** If the energy-dependence of the integrand in the formula of  $P_{k'k}(t \ge t_{\circ})$  is

$$P_{k'k}(t \ge t_{\circ}) \propto E_{k'}^{\beta} \frac{\sin^{2} \frac{(E_{k'k} - E)t_{\circ}}{2\hbar}}{(E_{k'k} - E)^{2}} \equiv E_{k'}^{\beta} II, \qquad (10.3.2.4)$$

then the maximum values of  $P_{k'k}(t \ge t_{\circ})$ , which correspond to the <u>probable</u> transitions, satisfy the following relations

$$E_{k'} > E_k + E \quad \text{if} \quad \beta > 0,$$
  
 $E_{k'} = E_k + E \quad \text{if} \quad \beta = 0,$   
 $E_{k'} < E_k + E \quad \text{if} \quad -1 < \beta < 0,$ 

which means that the system energy in the most probable transition increases (i. e., nonconservation), maintains (i. e., conservation), and reduces (i. e., nonconservation) if  $\beta > 0$ ,  $\beta = 0$ , and  $-1 < \beta < 0$ , respectively.

**Proof.** This proof is easy. Note that  $E_{k'} = E_k + E$  at  $\beta = 0$  does not mean that all possible transitions are energy conservation because the transition processes of energy nonconservation still can occur with very small probability. The existence of transition process with energy nonconservation can see from the curve of  $P_{k'k}(t \ge t_o)$  versus  $E_{k'}$  under the condition of  $\beta = 0$ , i. e.,  $|H'_{k'k}|^2 \rho(k')$  is an energy constant. This curve has been shown in Fig. 10.1. In Fig. 10.1  $II = \sin^2[(E_{k'k} - E)t_o/(2\hbar)]/(E_{k'k} - E)^2 \propto P_{k'k}(t \ge t_o)$ , and f denotes frequency and  $f \propto (E_{k'} - E_k - E)$ . Note that in this case, the energy is still, generally speaking, not conservative. QED.

Next, let us consider the approximately conservative conditions of energy in, for example, the photoeffect. In photoeffect, an electron in atom or metal needs to overcome a barrier  $0 < E_b = \hbar \omega_b$ . Eq. (10.3.1.3)' is a transition formula of absorption of photon. We take the energy zero point is at the boundary of metal. Thus the initial energy of the

electron is  $E_k = -E_b = -\hbar\omega_b < 0$ . The following corollary XVII gives the condition of approximate energy conservation.

Corollary XVII: Condition of approximate energy conservation in transition processes. If the perturbation energy is vary large, and the k'-dependence of the vacuum support ability is weak enough.

**Proof.** The proof is easy. For example, we consider absorption process. If the incident photon (or phonon) frequency  $\omega >> |E_k|/\hbar = \omega_b$  and  $|\beta|$  is not too large, then the transition probability  $P_{k'k}(t)$  has maximum value at  $\hbar(\omega_{k'k} - \omega) = E_{k'k} - \hbar\omega = E_{k'} - E_k - \hbar\omega = E_{k'} + E_b - \hbar\omega = (\omega_{k'} + \omega_b - \omega)\hbar \approx 0$ , which means approximate energy conservation of the transition process.

In physics, this corollary means that, for example, if an electron of atom or metal absorbs a photon with very high energy much higher than the binding energy of the electron in the atom or metal, then the transition is energy conservation approximately even  $|H'_{k'k}|^2 \rho(k')$  is (k')-dependent but weakly.

**Theorem XXXX: Time-dependence of transition rate.** If  $|H'_{k'k}|^2 \rho(k') \propto \omega_{k'}^{\beta}$  ( $\beta \neq 0$ ) in Eq. (10.3.2.2), then the transition rates,  $w_{all \leftarrow k} \equiv \sum_{k' \neq k} P_{k'k}/t$  is time-dependent, i. e., the Fermi golden rule does not hold water. Fermi golden rule holds just in the case of  $\beta = 0$ .

**Proof.** Suppose  $|H'_{k'k}|^2 \rho(k') = A \omega_{k'}^{\beta}$ .

$$w_{all \leftarrow k} \equiv \frac{\sum_{k' \neq k} P_{k'k}(t)}{t}$$

$$= \frac{\int_{-\infty}^{+\infty} d\omega_{k'} \rho(\omega_{k'}) P_{k'k}(t)}{t}$$

$$= \frac{1}{t} \int_{-\infty}^{+\infty} d\omega_{k'} \rho(\omega_{k'}) \frac{4|H'_{k'k}|^2}{\hbar^2} \left[ \frac{\sin[(\omega_{k'} - \omega_k - \omega)t/2]}{(\omega_{k'} - \omega_k - \omega)} \right]^2$$

$$= \frac{4}{\hbar^2} A \frac{1}{t} \int_{-\infty}^{+\infty} d\omega_{k'} \omega_{k'}^{\beta} \left[ \frac{\sin[(\omega_{k'} - \omega_k - \omega)t/2]}{(\omega_{k'k} - \omega)} \right]^2$$

$$= t^{-\beta} \frac{4A}{\hbar^2 2^{1-\beta}} \int_{-\infty}^{+\infty} dx \left( x + \frac{(\omega_k - \omega)t}{2} \right)^{\beta} \frac{\sin^2 x}{x^2}. \quad (10.3.2.5)$$

Eq. (10.3.2.5) clearly shows theorem XXXX. QED.

Comments for theorem XXXX:

(1) If we define  $w_{all \leftarrow k} \equiv d \sum_{k' \neq k} P_{k'k}/dt$ , then  $w_{all \leftarrow k}$  is time-dependent for  $\beta \ge 0$ , and Fermi golden rule does not hold always.

(2) In some cases the time dependences of  $|H'_{k'k}|^2 \rho(k')$  are much more complex than  $|H'_{k'k}|^2 \rho(k') \propto \omega_{k'}^{\beta}$ . Let us illustrate with an example. The photoeffect in subsection 10.4.5

demonstrates that

$$|H'_{k'k}|^2 \rho(k') \propto \frac{\omega_{k'}^{1.5}}{(1+k'^2 a^2)^6}, \ k' = \sqrt{\frac{2\mu\omega_{k'}}{\hbar}}, \ a = 0.53 \times 10^{-8} cm, \ \mu = electron \ mass.$$
(10.3.2.6)

Substituting Eq. (10.3.2.6) into third equality of Eq. (10.3.2.5) and making numerical integration, we obtain a curve of  $w_{all \leftarrow k}$  versus *t*, which is shown in Fig. 10.3.



Figure 10.3. Theoretical curve of  $\log_{10} W \equiv \log_{10} w_{all \leftarrow k}$  versus  $\log_{10} t$  (t/second).

If Fermi golden rule holds water, then the curve in Fig. 10.3 should be a horizontal line.

(3) This textbook prove Fermi golden rule just under one condition, i. e.,  $|H_{k'k}|^2 \rho(k')$  is independent of k', and all other steps in our derivations are exact. However, all until now references and textbooks prove Fermi golden rule under two conditions: both the  $|H_{k'k}|^2 \rho(k')$  is independent of k' and the time limit condition  $t_o \rightarrow \infty$ . They use the following mathematical formula

$$\lim_{t_{\circ}\to+\infty}\frac{\sin^{2}\alpha t_{\circ}}{\pi t_{\circ}\alpha^{2}}=\delta(\alpha).$$
(10.3.2.7)

Substituting Eq. (10.3.2.7) into Eq. (10.3.2.5), the integrand has a delta function  $\delta(E_{k'} - E_k - E)$ , which is an energy conservation factor, and after integration the expression is

proportional to a factor  $t_{\circ}$ . From these, they think that both energy conservation and Fermi golden rule in transition processes are proved.

As is well known, the less the conditions in a theory are, the better the theory is. Therefore, the derivations for the Fermi golden rule in this textbook are certainly better than the method of until now all references and textbooks. Next we will point out the purely mathematical mistakes in all until now references and textbooks.

(4) The physical meaning of  $t_{\circ}$  is duration time of a time-dependent perturbation, the magnitude order of which should be the observed relaxation time. The magnitude orders of relaxation time are generally from  $10^{-6}$  to  $10^{-15}$  second. Therefore, the condition  $t_{\circ} \rightarrow \infty$  is not reasonable in physics, and is dangerous in mathematics (Every body knows the famous words on arbitrarily coming from taking infinite limit.).

(5) Based on the two conditions, all until now references and textbooks conclude that in the integrand of the total transition probability formula there is a delta function which can ensure energy conservation of transition processes. Some references think that energy conservation of transition processes is a matter of course, and in the past 80 years some references do not have a wee bit of doubts for this energy conservation in quantum transition processes. Even some authors found the possible energy nonconservation in transition processes, but still looked for some "reasons" to argue the energy conservation. For example, Schiff in Ref. [120] thought that the energy nonconservation comes from Heisenberg uncertainty relation and/or the Fourier expansion of a time-dependent perturbation function. However, in our above derivations the integrand in formula of total transition probability the energy conservation's delta function never appears. On the contrary, our proof for Fermi golden rule needs, exactly the inverse, the contributions of processes coming from even very strong energy nonconservation.

(6) We estimate that in the past 80 years (from 1930 to now) some references made probably  $10^3$  conclusions by using Fermi golden rule and the mathematical mistake taking infinite time limit, but 500 in the 1 000 are of clear mistakes. If readers check many calculations drawn from transition processes, including scattering processes, once again, then readers might modify the conclusions, and thus might have important new discoveries.

# **10.4.** Applications of Transition Theory

Many contents in this section come from Refs. [121]-[127].

## 10.4.1. Absorption and Stimulating Emission of Light

If an atom is in the energy level and absorbs the incident light wave or a photon (energy hv), then the atom can be excited to higher energy level  $E_{k'} = E_2$ . If the frequency, v, of the incident light  $v = v_{k'k} = (E_{k'} - E_k)/h$ , then the transition process will have larger probability. This process is called absorption of light or stimulated absorption.

If an atom is initially in the higher energy level  $E_k$ , and absorbs the incident light wave (a photon) with frequency  $v = v_{k'k} = (E_{k'} - E_k)/h$ , then this excited atom can also be stimulated, and transits to lower energy level  $E_{k'}$ , and emits a stimulated photon. This process is called stimulated or induced emission. If there are many electrons at higher energy level, which is called population inversion, then one incident photon can cause many high energy electrons to be stimulated emission, which's processes are the principle of laser.

In 1917, in an article titled "On the Quantum Theory of Radiation", Einstein laid out the basic principles of absorption and of spontaneous and stimulated emission of electromagnetic radiation in its interaction with atoms. Einstein's work established the basic principles responsible for laser action, although the first operational laser was not invented until 1960. Since then the laser has become such an invaluable and commonplace tool in science and technology that may be tempted to take its unusual quantum properties for granted.

We will use the periodic perturbation theory to the absorption of light in this subsection. Because in our calculations the electromagnetic field is classical, i. e., continuously variational field (not the photons), and the atom is a quantum system, the method in this subsection is semiclassical. In this method the electromagnetic field is treated as a time dependent periodic perturbation. This method cannot treat the spontaneous emission. The spontaneous emission will be treated in subsection 10.4.2.

For brevity, we assume that the incident light is monochromatic. The intensity of electromagnetic field is

$$E = E_{\circ} cos(\omega t - k \cdot r) \quad and \quad B = k \times E/|k|, \tag{10.4.1.1}$$

where **k** is a wave vector. The direction of **k** is the direction of light propagation.  $\omega$  is the angle frequency of light. For an atom, the electron speed  $v \ll c$ . Therefore, the action of magnetic field on electron is much less than that of electric field:

$$\left|\frac{e}{c}v \times B\right| / |eE| \sim \frac{v}{c} << 1.$$
(10.4.1.2)

Therefore, we can only consider the action of electric field in our physical problem. For the light wavelength  $\lambda$  is between  $(4000 \sim 7000) \times 10^{-10} m >> a$  (*Bohr radius*). In the atomic scale,  $k \cdot r \approx a/\lambda << 1$ , the variation of electric field is very small. Taking  $k \cdot r \approx a/\lambda = 1$  is called dipole approximation. In this approximation the field is uniform, and the field potential depends on **r**. We make dipole approximation, and the electric field becomes

$$E = E_{\circ} cos(\omega t). \tag{10.4.1.3}$$

The potential of the electric field is

$$\phi = -E \cdot r. \tag{10.4.1.4}$$

Substituting Eq. (10.4.1.3) into Eq. (10.4.1.4), one obtains the action of incident light on the atom is

$$H' = -e\phi = (E_{\circ}) \cdot (-er) cos\omega t \equiv E_{\circ} \cdot dcos\omega t \equiv U cos\omega t, \qquad (10.4.1.5)$$

where the vector d = -er is called electric dipole moment. Substituting H' in Eq. (10.4.1.5) into the Eq. (10.2.1.3), one obtains the first order transition amplitude

$$a_{k'k}^{(1)}(t) = \frac{1}{i\hbar} \int_0^t e^{i\omega_{k'k}t'} H_{k'k}'(t') dt' = \frac{U_{k'k}}{2i\hbar} \int_0^t e^{i\omega_{k'k}t'} \left(e^{i\omega t'} + e^{-i\omega t'}\right) dt'$$
  
$$= -\frac{U_{k'k}}{2\hbar} \left[\frac{e^{i(\omega_{k'k} + \omega)t} - 1}{\omega_{k'k} + \omega} + \frac{e^{i(\omega_{k'k} - \omega)t} - 1}{\omega_{k'k} - \omega}\right].$$
(10.4.1.6)

The second term of Eq. (10.4.1.6) will be much large, if  $\omega_{k'} = \omega_k + \omega$ . Therefore, the second term corresponds to transition of absorption of light. For the transition of absorption of light,

$$a_{k'k}^{(1)}(t) = -\frac{U_{k'k}}{2\hbar} \frac{e^{i(\omega_{k'k} - \omega)t} - 1}{\omega_{k'k} - \omega}.$$
(10.4.1.7)

Therefore, the transition probability from state  $|k\rangle$  to state  $|k'\rangle$  is

$$P_{k'k}(t) = |a_{k'k}^{(1)}(t)|^2 = \frac{|U_{k'k}|^2}{4\hbar^2} \frac{\sin^2[(\omega_{k'k} - \omega)t)/2]}{[(\omega_{k'k} - \omega)/2]^2}.$$
 (10.4.1.8)

To continue our derivations, we have to consider the physics of stimulated emission.

First. The photon energy of stimulated emission is  $\hbar \omega = \omega_{k'k}$ .

Second. The incident photon in the stimulated emission process cannot be precisely monochromatic, i. e., there is a natural dispersion, around  $\omega_{k'k}$ , coming from uncertainty relation.

Basing on the above physical considerations and supposing that the density of states of photon in free space is  $\rho(\omega)$ , Eq. (10.4.1.8) can be written as

$$P_{k'k}(t) = \int d\omega \rho(\omega) \frac{|U_{k'k}|^2}{4\hbar^2} \frac{\sin^2[(\omega_{k'k} - \omega)t)/2]}{[(\omega_{k'k} - \omega)/2]^2} \\ \approx \rho(\omega_{k'k}) \frac{|U_{k'k}|^2}{4\hbar^2} \int_{-\infty}^{\infty} d\omega \frac{\sin^2[(\omega_{k'k} - \omega)t)/2]}{[(\omega_{k'k} - \omega)/2]^2} \\ = \rho(\omega_{k'k}) \frac{|U_{k'k}|^2}{4\hbar^2} \int_{-\infty}^{\infty} d\omega \frac{\sin^2[(\omega_{k'k} - \omega)t)/2]}{[(\omega_{k'k} - \omega)/2]^2} \\ = \rho(\omega_{k'k}) \frac{|U_{k'k}|^2}{4\hbar^2} \frac{2t^2}{t} \int_{-\infty}^{\infty} dx \frac{\sin^2 x}{x^2} \\ = \frac{\pi |U_{k'k}|^2}{\hbar^2} \rho(\omega_{k'k})t. \quad (10.4.1.9)$$

The transition rate is

$$w_{k'k} = \frac{1}{t} P_{k'k} = \frac{\pi |U_{k'k}|^2}{\hbar^2} \rho(\omega_{k'k})$$
  
=  $\frac{\pi}{2\hbar^2} |d_{k'k} \cdot E_{\circ}|^2 \rho(\omega_{k'k}) = \frac{\pi}{2\hbar^2} |d_{k'k}|^2 E_{\circ}^2 \cos^2\theta \rho(\omega_{k'k}), \quad (10.4.1.10)$ 

where  $\theta$  is the angle between  $d_{k'k}$  and  $E_{\circ}$ . *E* is the intensity of electric field. If the light is not polarized, then we should seek the average value of  $\cos^2 \theta$  on all directions, i. e.,

$$\overline{\cos^2 \theta} = \frac{1}{4\pi} \int d\Omega \cos^2 \theta = \frac{1}{4\pi} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \cos^2 \theta = \frac{1}{3}$$

Therefore,

$$w_{k'k} = \frac{\pi}{6\hbar^2} \left| d_{k'k} \right|^2 E_{\circ}^2 \rho(\omega_{k'k}).$$
(10.4.1.11)

Eq. (10.4.1.11) is correct for monochromatic light with natural dispersion, such as laser light with angular frequency  $\omega$ .
From Eq. (10.4.1.11) we see that the transition rate is proportional to the light intensity, which is the feature of stimulated emission. Besides this, the transition rate is proportional to the matrix element  $r_{k'k}$ .  $r_{k'k} \neq 0$  concerns the property of initial and final states. Let us make discussions for this.

First, let us consider the parity of the initial and final states. Note that operator  $\mathbf{r}$  is an odd parity operator.

$$|k\rangle = |nlm\rangle \quad parity \Pi = (-1)^l, \quad |k'\rangle = |n'l'm'\rangle \quad parity \Pi' = (-1)^{-l'}.$$
 (10.4.1.12)

Because that **r** is an odd parity operator, only when  $\Pi' = -\Pi$ , the matrix element  $r_{k'k} \neq 0$ . Therefore, for the electric dipole radiation there is a parity selection rule: initial state and final state have to have different parity.

Second, let us study the angular momentum selection rule. Utilizing the following mathematical relations:

$$x = r\sin\theta\cos\phi = \frac{r}{2}\sin\theta(e^{i\phi} + e^{-i\phi})$$
$$y = r\sin\theta\sin\phi = \frac{r}{2i}\sin\theta(e^{i\phi} - e^{-i\phi}), \quad z = r\cos\theta$$
$$\cos\theta Y_l^m = \sqrt{\frac{(l+1)^2 - m^2}{(2l+1)(2l+3)}}Y_{l+1}^m + \sqrt{\frac{l^2 - m^3}{(2l-1)(2l+1)}}Y_{l-1}^m$$
$$e^{\pm\phi}\sin\theta Y_l^m = \pm\sqrt{\frac{(l\pm m+1)(l\pm m+2)}{(2l+1)(2l+3)}}Y_{l+1}^{m+1} + \sqrt{\frac{(l\mp m)(l\mp m+1)}{(2l-1)(2l+1)}}Y_{l-1}^{m\pm 1} \quad (10.4.1.13)$$

and considering the orthogonality of spherical harmonic function:

$$\int_{0}^{2\pi} d\phi \int_{0}^{\pi} d\theta \sin \theta Y_{l}^{m} Y_{l'}^{m'} = \delta_{ll'} \delta mm', \qquad (10.4.1.14)$$

one can see that the non zero conditions of  $d_{k'k} = -er_{k'k} \neq 0$  are  $l' = l \pm 1$  and m' = m,  $m \pm 1$ . Electromagnetic radiation caused by non-vanishing matrix element  $r_{k'k}$  is called electric dipole (quadrupole) radiation and is denoted simply by E1. Thus we obtain the angular momentum section rule of electric dipole radiation is:

$$\Delta l = l' - l = \pm 1$$
, and  $\Delta m = m' - m = 0, \pm 1.$  (10.4.1.15)

Generally, electric  $2^l$ -pole transitions are denoted by El-transition.

Correspondingly, magnetic  $2^l$ -pole transitions are denoted by Ml-transition.

In the above discussions we have not yet considered the electron spin-spin and spinorbital coupling. If we consider them, then the selection rules of transition processes have a bit of changes.

For the future reference, we give a formula of energy density of electromagnetic field for one photon with angular frequency  $\omega$  [3]. We consider the atom in interaction with a plane electromagnetic wave whose vector is of the form

$$A(r,t) = aA_{\circ}cos(k \cdot r - \omega t), \qquad (10.4.1.16)$$

where **a** is a unit polarization vector  $(|a|^2 = 1)$  which is normal to the propagation vector **k**. We wish to construct the amplitude  $A_{\circ}$  so that the corresponding wave carries one photon per unit volume. One time period-averaged energy density carried in a plane wave is

$$\overline{U} = \frac{1}{4\pi} \overline{E^2} = \frac{1}{4\pi} \overline{B^2}.$$
 (10.4.1.17)

As we know

$$B = \nabla \times A. \tag{10.4.1.18}$$

$$\overline{U} = \frac{1}{4\pi} \overline{B^2} = \frac{1}{8\pi} k^2 A_\circ^2.$$
(10.4.1.19)

For one photon per unit volume we set

$$\frac{k^2 A_{\circ}^2}{8\pi} = \frac{\hbar\omega}{V},$$
(10.4.1.20)

which, with  $\omega = ck$ , gives

$$A_{\circ}^{2} = \frac{8\pi\hbar c^{2}}{\omega V}.$$
 (10.4.1.21)

#### 10.4.2. Spontaneous Emission

The first term in Eq. (10.4.1.6) shows that if an external light applies on an atom, then the atom can transit from high energy level to low energy, and at the same time emits an photon, which is called stimulated emission. Besides stimulated emission, experimentalists also observed spontaneous emission or spontaneous decay, i. e., the excited atom can transit from high energy level to low energy level, and at the same time emits an photon. However, in our earlier description of hydrogen we found atomic states to be stationary if there is no external perturbation. So, in reality, spontaneous decay must have a triggering mechanism. What is this mechanism?

The answer to this question stems from the observation that an electromagnetic field may be represented as a collection of harmonic oscillators. We have found in chapter 4 that a harmonic oscillator always has a residual energy which is called its zero point energy. In like manner, no region of space is ever free of electromagnetic energy perturbation. It is such a perturbation is responsible for the spontaneous emission. Besides the zero point energy, there is also a term which is proportional to the number of quantum of harmonic oscillator. This later term corresponds to the stimulating emission [87]. In this subsection we just discuss the spontaneous emission.

Using the notations in Eq. (10.4.1.8), Eq. (10.3.2.2) gives the total transition probability of emission of photon is

$$P(t \ge t_{\circ}) \equiv \int P_{k'k}(t \ge t_{\circ})\rho(\hbar\omega)d\hbar\omega$$
  
=  $\int \rho(\hbar\omega)d\hbar\omega \frac{|U_{k'k}|^2}{4\hbar^2} \frac{\sin[(\omega_{k'k} + \omega)t_{\circ})/2]}{[(\omega_{k'k} + \omega)/2]^2}$   
=  $\frac{1}{4\hbar^2} \int \rho(\hbar\omega)d\hbar\omega |U_{k'k}|^2 \frac{\sin^2[(E_{k'k} + E)t_{\circ}]/(2\hbar)}{[(E_{k'k} + E)/(2\hbar)]^2}$   
=  $\frac{e^2}{4\hbar^2} \frac{\pi E_{\circ}^2}{3} \int \rho(E)dE |r_{k'k}|^2 \frac{\sin^2[(E_{k'k} + E)t_{\circ}]/(2\hbar)}{[(E_{k'k} + E)/(2\hbar)]^2},$  (10.4.2.1)

where the  $\rho(\hbar\omega)$  ( $\rho(E)$ ) represents the the density of states per unit frequency (per unit energy) in volume V and in solid angle of  $d\Omega$  of the light wave or the photon (The energy spectrum of photon in free space constructs a continuum). The number of states in volume V for light wave or photon with momentum between p and p + dp and within a solid angle  $d\Omega$  is determined by

$$dN_p = \frac{p^2 \sin\theta dp d\theta d\phi}{(2\pi\hbar/L)^3} = \frac{V p^2 dp d\Omega}{(2\pi\hbar)^3}.$$
 (10.4.2.2)

As for photon E = pc, dp/dE = 1/c, the corresponding density of states is equal to

$$\rho(E) = \frac{dN_p}{dE} = \frac{VE^2 d\Omega}{(2c\pi\hbar)^3} = \frac{V\omega^2 d\Omega}{(2c\pi)^3\hbar}.$$
(10.4.2.3)

Eq. (10.4.1.12) tells us that  $VE_{\circ}^2/(8\pi) = E$  if only one photon with energy *E* is in vacuum space.

The transition rate from  $|k\rangle$  to  $|k'\rangle (E_k > E_{k'})$  with emitting a photon is thus

$$w_{k'k}(t \ge t_{\circ}) \equiv \frac{P_{k'k}(t \ge t_{\circ})}{t_{\circ}} = \frac{e^2}{4\hbar^2 t_{\circ}} \frac{\pi}{3} \frac{E8\pi}{V} \int \rho(E) dE |r_{k'k}|^2 \frac{\sin^2[(E_{k'k} + E)t_{\circ}]/(2\hbar)}{[(E_{k'k} + E)/(2\hbar)]^2}.$$
(10.4.2.4)

Substituting Eq. (10.4.2.3) into Eq. (10.4.2.4) and noting that the spontaneously emitted photon's frequency is exactly equal to the incident photon frequency (in case spontaneous emission, the incident photon comes from zero point electromagnetic oscillation.), we can take out the *E* in  $\rho(E)$  from integral. The interval of integration over energy is the range of dispersion of incident light. Due the the character of the oscillation integrand we can take integration range as  $\pm\infty$ . Noting that the  $\rho(E)$  in Eq. (10.4.2.3) includes  $d\Omega$  and the emitting direction of the spontaneous emitted photon is same as that of the incident photon, we do not need to make integration over solid angle. We have

$$w_{k'k}(t \ge t_{\circ}) = \frac{e^2}{4\hbar^2 t_{\circ}} \frac{\pi}{3} \frac{E8\pi}{V} \frac{VE^2}{(2c\pi\hbar)^3} |r_{k'k}|^2 \int_{-\infty}^{\infty} dE \frac{\sin^2[(E_{k'k} + E)t_{\circ}/(2\hbar)]}{[(E_{k'k} + E)/(2\hbar)]^2} d\Omega$$
  
$$= \frac{1}{12t_{\circ}\pi^2} \frac{e^2\omega}{\hbar^2 c} \left(\frac{|r_{k'k}|\omega}{c}\right)^2 2\hbar t_{\circ} \int_{-\infty}^{\infty} dx \frac{\sin^2 x}{x^2} d\Omega$$
  
$$= \frac{1}{12t_{\circ}\pi^2} \frac{e^2\omega}{\hbar^2 c} \left(\frac{|r_{k'k}|\omega}{c}\right)^2 2\hbar t_{\circ}\pi d\Omega$$
  
$$= \frac{2}{3} \frac{e^2\omega}{\hbar c} \left(\frac{\hbar\omega}{c}\right)^2 \frac{1}{4\pi} d\Omega. \qquad (10.4.2.5)$$

To estimate the order of magnitude of  $w_{k'k}$  ( $t \ge t_{\circ}$ ), we put  $|r_{k'k}| = a$ , where *a* is a quantity of the order of the linear dimensions of the quantum system (atom); we get

$$w_{k'k}(t \ge t_{\circ}) \approx \frac{e^2 \omega}{\hbar c} \left(\frac{a\omega}{c}\right)^2 \approx \frac{\omega}{137} \left(\frac{a\omega}{c}\right)^2 \frac{1}{4\pi} d\Omega.$$
 (10.4.2.6)

For a system with Coulomb interaction  $a \approx e^2/(\hbar\omega)$ , and thus

$$w_{k'k}(t \ge t_{\circ}) \approx \frac{\omega}{137^3} \frac{1}{4\pi} d\Omega.$$
 (10.4.2.7)

It follows from Eq. (10.4.2.7) that for optical radiation ( $\omega \sim 10^{15}$ ) second<sup>(-1)</sup>, the order of magnitude of transition rate is  $\sim 10^9$  second<sup>(-1)</sup>. For  $\gamma$ -radiation ( $\omega \sim 10^{21}$ ) second<sup>(-1)</sup>, the order of magnitude of transition rate is  $\sim 10^{15}$  second<sup>(-1)</sup>.

In this simple case, where the  $w_{k'k}(t \ge t_\circ)$  is independent of time, the relaxation time or, say, lifetime  $\tau \approx 1/w_{k'k}(t \ge t_\circ)$ .

It is interesting to note that the calculation methods in subsections 10.4.1 and 10.4.2 are nearly the same. If the transition probability is proportional to and independent of the number of incident light photons, then we call it stimulating and spontaneous, respectively [87].

#### **10.4.3.** Perturbation in Finite Time

We discuss two cases: constant and variation perturbations in finite time. At first we give correct method, then we introduce the wrong method, existing in some references, and explain where are the mistakes.

(1). Constant perturbations in finite time interval.

Generally speaking, the external perturbation acts only in a finite time interval. Let us discuss a very simple case, i. e., a constant perturbation in finite time  $0 \le t \le T$ . In mathematics,

$$H'(t) = H'[\theta(t) - \theta(t - T)], \qquad (10.4.3.1)$$

where  $\theta(t)$  is called step function, which's definition is

$$\Theta(t) = \begin{cases} 0, & t < 0\\ 1 & t > 0 \end{cases}$$
(10.4.3.2)

According to Eq. (10.2.3), the probability amplitude of transition from state  $|k\rangle$  to  $|k'\rangle$ , caused by H'(t) at *t*, is

$$a_{k'k}^{(1)}(t) = \frac{1}{i\hbar} \int_{-\infty}^{t} e^{i\omega_{k'k}t'} H_{k'k}'(t') dt'.$$
 (10.4.3.3)

After integration by parts, one obtains

$$a_{k'k}^{(1)}(t) = -\frac{H'_{k'k}(t)exp(i\omega_{k'k}t)}{\hbar\omega_{k'k}} + \int_{-\infty}^{t} \frac{exp(i\omega_{k'k}t')}{\hbar\omega_{k'k}} \frac{\partial H'_{k'k}(t')}{\partial t'} dt'.$$
 (10.4.3.4)

When t > T the first term in Eq. (10.4.3.4) is zero.  $a_{k'k}^{(1)}(t)$  is determined by the second term. Substituting the expression of  $a_{k'k}^{(1)}(t)$  into Eq. (10.1.12), one obtains the transition probability from state |k > to state |k' >

$$P_{k'k}(t \ge T) = |a_{k'k}^{(1)}(t \ge T)|^2 = \left| \int_{-\infty}^{t} \frac{\exp(i\omega_{k'k}t')}{\hbar\omega_{k'k}} H'_{k'k}[\theta(t') - \theta(t' - T)]dt' \right|^2$$
  

$$= \left| \frac{H'_{k'k}}{\hbar\omega_{k'k}} \left( 1 - e^{i\omega_{k'k}T} \right) \right|^2$$
  

$$= \frac{|H'_{k'k}|^2}{\hbar^2} \frac{\sin^2(\omega_{k'k}T/2)}{(\omega_{k'k}/2)^2}$$
  

$$\equiv \frac{|H'_{k'k}|^2}{\hbar^2} \times I.$$
(10.4.3.5)



Figure 10.4. The functions  $\sin(x)/x$  (dashed curves) and  $[\sin(x)/x]^2$  (solid curve). The vertical dotted lines denote the region  $|x| \leq \pi$ .

If we neglect the (k')-dependence of  $|H'_{k'k}|$ , then the variation of  $I \propto P_{k'k}(t \ge T)$  with  $\omega_{k'k}$  is shown in Fig. 10.4. It is interesting to note that we have met the similar diagram in Fig. 10.1.

Fig. 10.4 indicates that although under the condition of (k')-independence of  $|H'_{k'k}|$  the main transition process keeps energy conservation, but the transition processes of energy nonconservation has also a non zero transition probability. If we only consider the transition process of energy conservation  $\hbar\omega_{k'} = \hbar\omega_k$ , then

$$P_{k'k}(t \ge T) = \frac{|H'_{k'k}|^2}{\hbar^2} T^2 \frac{\sin^2(\omega_{k'k}T/2)}{(\omega_{k'k}T/2)^2} \quad (\omega_{k'} = \omega_k)$$
  
=  $\frac{|H'_{k'k}|^2}{\hbar^2} T^2 \propto T^2.$  (10.4.3.6)

Eq. (10.4.3.6) indicates that if we do not take the limit  $t \to \infty$ , then the energy conservation process in Eq. (10.4.3.5) gives  $P_{k'k}(t \ge T) \propto T^2$  other than  $P_{k'k}(t \ge T) \propto T$ , and thus, actually, cannot obtain the Fermi golden rule.

We prefer to make legal in mathematics but approximate derivation from Eq. (10.4.3.5) for the transition probability,  $P_{all \leftarrow k} (t \ge T)$ , from initial state  $|k\rangle$  to all possible final states. Similarly to Eq. (10.4.1.6), we introduce an approximate constant average density of states [i. e., the average number of states in a unit energy interval  $\overline{\rho(E)} = constant$  or the average number of states in a unit angle frequency interval  $\overline{\rho(\omega)} = constant$ ], and use energy or angle frequency integrations instead of the summation over discrete states. At the last step,

we take  $\overline{\rho} = 1$ . Assuming that  $|H'_{k'k}|^2$  and  $\overline{\rho(\omega)}$  are independent of (k', k), one obtains

$$P_{all \leftarrow k}(t \ge T) = \sum_{k'} |a_{k'k}^{(1)}(t \ge T)|^2$$
  
=  $\int_{-\infty}^{+\infty} d\omega_{k'} \overline{\rho(\omega_{k'})} |a_{k'k}^{(1)}(t \ge T)|^2$   
=  $\int_{-\infty}^{+\infty} d\omega_{k'} \frac{|H'_{k'k}|^2 \overline{\rho(\omega_{k'})}}{\hbar^2} \frac{\sin^2(\omega_{k'k}T/2)}{(\omega_{k'k}/2)^2}$   
=  $\frac{|H'_{k'k}|^2 \overline{\rho(\omega_{k'})}}{\hbar^2} \int_{-\infty}^{+\infty} d\omega_{k'} \frac{\sin^2(\omega_{k'k}T/2)}{(\omega_{k'k}/2)^2}$   
=  $\frac{2|H'_{k'k}|^2 \overline{\rho(\omega_{k'})}}{\hbar^2} T \int_{-\infty}^{+\infty} dx \frac{\sin^2 x}{x^2}$ 

$$= \frac{2\pi |H'_{k'k}|^2 \overline{\rho(\omega_{k'})}}{\hbar^2} T$$
  
$$= \frac{2\pi |H'_{k'k}|^2 \overline{\rho(E_{k'})}}{\hbar} T, \qquad (10.4.3.7)$$

where  $\overline{\rho(\omega_{k'})}$  and  $\overline{\rho(E_{k'})}$  represent the number of states per unit interval of angular frequency and energy, respectively.

The transition rate from state  $|k\rangle$  to all possible final states is

$$w_{all \leftarrow k}(t \ge T) = \frac{P_{all \leftarrow k}(t \ge T)}{T} = \frac{2\pi |H'_{k'k}|^2 \overline{\rho(E_{k'})}}{\hbar}.$$
 (10.4.3.8)

All textbooks, including this textbook, call the time independence of  $w_{all \leftarrow k} (t \ge T)$  the Fermi golden rule. Note that in our derivations of Fermi golden rule we do not need  $T \rightarrow \infty$ , which leads to energy conservation of transition processes, but we need the (k')-independence of both  $|H'_{k'k}|^2 \rho(\omega)$  and the contributions coming from all transition processes including strong energy nonconservation processes.

Now we introduce the common but wrong method existing in all until now references and textbooks.

The mistake in some references occurs after Eq. (10.4.3.5). The Eq. (10.4.3.5) is

$$P_{k'k}(t \ge T) = \frac{|H'_{k'k}|^2}{\hbar^2} \frac{\sin^2(\omega_{k'k}T/2)}{(\omega_{k'k}/2)^2}.$$
(10.4.3.5)'

Some references use the correct mathematical formula

$$\lim_{\alpha \to \infty} = \frac{\sin^2 \alpha x}{x^2} = \pi \alpha \delta(x), \qquad (10.4.3.9)$$

and think that

$$\lim_{T \to \infty} \frac{\sin^2(\omega_{k'k}T/2)}{(\omega_{k'k}/2)^2} = \pi T \delta(\omega_{k'k}), \qquad (10.4.3.10)$$

set  $T \rightarrow \infty$  in Eq. (10.4.3.5)' and obtain

$$P_{k'k}(t) = \frac{2\pi}{\hbar^2} |H'_{k'k}|^2 \delta(\omega_{k'k}) T.$$
(10.4.3.11)

To avoid the difficulty of appearance of the delta function in Eq. (10.4.3.11), some references, such as Ref. [1], say that although the  $\infty$  of the delta function in Eq. (10.4.3.11) carries difficulty for a perturbation theory, but this difficulty do not have practical trouble by taking the following procedures: in practical problems we often meet integration for the delta function, and thus the delta function does not carry difficulty, and due to that the delta function ensure the energy conservation, in physics, of course, energy in the transition process has to be conservative.

To avoid the difficulty of appearance of the  $T \to \infty$ , and thus  $P_{k'k}(t) \to \infty$ , in Eq. (10.4.3.11), all until now references and textbooks, such as Ref. [1], say that the transition rate

$$w_{k'k}(t) \equiv \frac{P_{k'k}(t)}{T}$$

is time independent, i. e., Fermi golden rule.

This textbook thinks that one cannot *a priory* conclude that the energy has to be conservative for an nonisolated system. (In the quantum transition the system is not an isolated system.) (Remember that the principle of conservation of energy in classical physics states that the energy of an isolated or a conservative system is constant in time, i. e., is conservative [3]. One has to prefer to believe a conclusion, which is legal in mathematics and corresponds to actual case (i. e., all the transition processes are completed in an finite time.), although this conclusion is not to be understood temporarily. One should be not to prefer to believe a conclusion, which is obviously wrong in mathematics, and does not corresponds to actual case, although this conclusion is easy to be understood by the known physical laws or rules.

(B). Perturbation of variation with time in finite time interval.

Assume the external perturbation H'(t) is dependent on time at 0 < t < T, and is zero at other times. The H'(t) can be expressed by Fourier integral:

$$H'(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega H'(\omega) e^{-i\omega t}, \qquad (10.4.3.12)$$

where

$$H'(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt' H'(t') e^{i\omega t'} = \frac{1}{\sqrt{2\pi}} \int_{0}^{T} dt' H'(t') e^{i\omega t'}.$$
 (10.4.3.13)

According to the definition of the  $H'(\omega_{k'k})$  in Eq. (10.4.3.12), its dimension is *enery* × *time*. Similarly to Eq. (10.4.3.5), at  $t \ge T$  the transition probability from state  $|k\rangle$  to state |k'> is

$$P_{k'k}(t \ge T) = |a_{k'k}^{(1)}(t \ge T)|^{2} = \left|\frac{1}{i\hbar}\int_{0}^{T} e^{i\omega_{k'k}t'}H_{k'k}'(t')dt'\right|^{2}$$

$$= \left|\frac{1}{i\hbar}\frac{1}{\sqrt{2\pi}}\int_{0}^{T} dt' e^{i\omega_{k'k}t'}\int_{-\infty}^{\infty} d\omega H_{k'k}'(\omega) e^{-i\omega t}\right|^{2}$$

$$= \left|\frac{1}{i\hbar}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\omega H_{k'k}'(\omega)\int_{0}^{T} dt' e^{i(\omega_{k'k}-\omega)t'}\right|^{2}$$

$$= \left|\frac{1}{i\hbar}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\omega H_{k'k}'(\omega)\frac{exp[i(\omega_{k'k}-\omega)T]-1]}{i(\omega_{k'k}-\omega)}\right|^{2}$$

$$= \left|\frac{1}{i\hbar}\int_{-\infty}^{\infty} d\omega H_{k'k}'(\omega)\frac{exp[i(\omega_{k'k}-\omega)T/2]}{(\omega_{k'k}-\omega)^{0}}\right|^{2}$$

$$\times \frac{\{exp[i(\omega_{k'k}-\omega)T/2]-exp[-i(\omega_{k'k}-\omega)T/2]\}}{i(\omega_{k'k}-\omega)}\Big|^{2}, \quad (10.4.3.14)$$

where

$$H'_{k'k}(\omega) = \langle k' | H'(\omega) | k \rangle, \qquad (10.4.3.15)$$

is a matrix element of operator  $H'(\omega_{k'k})$ . A mathematically correct method has to stop here because we do not know the explicit dependence of  $H'_{k'k}(\omega)$  on  $\omega$ . However, from Eq. (10.4.3.14) we know that the transition process can occur at  $\omega \neq \omega_{k'k}$ .

Next, let us introduce the wrong method in some references. Some references thinks that one can continue the derivations as follows. Seek  $P_{k'k}(t \ge T)$  under the condition of  $T \rightarrow \infty$ . In this case some references use a correct mathematical formula (See Ref. [1]):

$$\lim_{T \to \infty} \frac{\sin Tx}{x} = \pi \delta(x). \tag{10.4.3.16}$$

Substituting Eq. (10.4.3.16) into Eq. (10.4.3.14), some references obtain

$$\lim_{T \to \infty} P_{k'k}(t \ge T) = \frac{2\pi}{\hbar^2} \left| H'_{k'k}(\omega_{k'k}) \right|^2 \bigg|_{\omega_{k'k} = \omega}.$$
 (10.4.3.17)

Eq. (10.4.3.17) clearly indicates that if  $T \to \infty$ , then the transition from state  $|k\rangle$  to state  $|k'\rangle$  can occur only under the condition of the existence of the Fourier component  $\omega_{k'k} = (E_{k'} - E_k)/\hbar$  in Fourier expansion of Eq. (10.4.3.12).

The above conclusions are obviously wrong because:

(i)  $\lim_{T\to\infty} P_{k'k}(t \ge T)$  is independent of t and T. Therefore, the transition rate  $d \lim_{T\to\infty} P_{k'k}(t \ge T)/dt = 0$ , which is wrong in physics obviously.

(ii)  $T \to \infty$  is not reasonable in physics, because the duration time T causing the transition processes cannot be completed in infinitely long time. The duration time should be equal to the relaxation time approximately.

#### 10.4.4. Semiconductor Optical Absorption

Some references's theories of optical absorption in semiconductors are not an exact theory. To clearly make comparisons of theory in this textbook with some references's theories of optical absorption, this subsection introduces briefly the some references's theories.

Some references's D-C transition theories make the  $T \rightarrow \infty$ . When the readers study this subsection, it is not necessary to derive every formula. We just hope readers to know how to correctly calculate the transition probability in D-C transition, to have a bit of impression on the applications of the time dependent perturbation theory, and to know that the energy nonconservation occurs actually in the semiconductor optical absorption.

If light, or, say, photon enters into the semiconductor, the the electron (which's energy is  $E_k = -E_g$ ,  $E_g > 0$  is the energy gap between valence top and conduction bottom) in valence band can absorbs this photon, transits to the conduction band, and energy becomes  $E_{k'}$ . We take that the zero point of  $E_{k'}$  is at the bottom of the conduction band. Therefore, the incident light intensity will be reduced by these absorptions. The absorption coefficient  $\alpha$  can describe this attenuation of the light, and is experimentally observable quantity. The definition of  $\alpha$  is as follows: it indicates the attenuation of the incident light intensity by  $1/e \approx 1/2.7 \approx 0.37$  per unit propagation length. From this definition of  $\alpha$ , one can obtain the following expression: [For detail derivation, refer to Eqs. (4.21), (4.31), (4.39), (4.41), (4.51), and (4.52) in Ref. [128]]

$$\alpha = \frac{2\hbar}{n_{\circ}cA_{\circ}^{2}\varepsilon_{\circ}\omega t}P_{k'k}$$
  
=  $\frac{1}{n_{\circ}cA_{\circ}^{2}\varepsilon_{\circ}\omega t}\frac{1}{\hbar}\int_{0}^{\infty}|H_{k'k}'|^{2}\rho(k')\frac{\sin(E_{k'k}-E)t/2\hbar}{\left((E_{k'k}-E)/2\hbar\right)^{2}}dE_{k'},$  (10.4.4.1)

where *E* is the energy of absorbed photon,  $A_{\circ}$  is the amplitude of the vector potential of electromagnetic field,  $P_{k'k}$  represents the transition probability of an electron from valence band top to conduction band due to optical absorption,  $E_{k'}$  is the energy of an electron in the conduction band,  $E_{k'k} = E_{k'} - E_k \equiv E_{k'} - (-E_g) = \hbar^2 k'^2 / (2\mu^*) + E_g$ ,  $E_g > 0$  is the energy gap between valence band and conduction band,  $n_{\circ}$  is the refractive index, and  $\mu^*$  is called the reduced mass of the electron and hole,  $\rho(k')$  is the (joint) density of states, which is proportional to  $\sqrt{E_{k'}}$ . Let us make an explanation for this. Similarly to Eq. (10.4.2.2), we know that the number of states in volume *V* for free electron with momentum between *p* and p + dp and within a solid angle  $d\Omega$  is determined by

$$dN_p = 2\frac{p^2 \sin\theta dp d\theta d\phi}{(2\pi\hbar/L)^3} = \frac{V p^2 dp d\Omega}{(2\pi\hbar)^3},$$
(10.4.4.2)

where the factor 2 comes from spin of electron. As for electron  $E_{k'} = \hbar^2 k'^2 / 2\mu^*$  and  $p = \hbar k'$ , the corresponding density of states per solid angle and per unit energy interval is equal to

$$\rho(k',\Omega) = \rho(E_{k'},\Omega) = \frac{dN_p}{dE_{k'}} = \frac{V\mu\hbar}{(2\pi\hbar)^3} \sqrt{\frac{2\mu^* E_{k'}}{\hbar^2}}.$$
 (10.4.4.3)

In physics, Eq. (10.4.4.1) is easy to be understood. The large transition probability means more absorption of photon. The more absorption of photon means that the attenuation of

the light intensity in semiconductor is more larger, i. e., larger value of  $\alpha$ . Anyway, we meet with the transition probability in D-C transition. Some references do not make exact numerical integration for the  $P_{k'k}$  in Eq. (10.4.4.1). On the contrary, some references assume  $t \rightarrow \infty$ . Under this limit, the oscillation factor in Eq. (10.4.4.1) becomes a delta function  $\delta(E_{k'} - (-E_g) - E) = \delta(E - E_g - E_{k'})$ . After integration over  $E_{k'}$ , Eq. (10.4.4.1) becomes

$$\alpha \propto \sqrt{E - E_g},\tag{10.4.4.4}$$

where the factor  $\sqrt{E - E_g}$  comes from  $\rho(k')\delta(E - E_g - E_{k'}) \propto \sqrt{E_{k'}}\delta(E - E_g - E_{k'})$  and the integration over  $E_{k'}$ .

The experimental data in Fig. 10.5 shows  $\alpha = 1995$  cm<sup>-1</sup> at  $E = E_g = 1.42$  eV. On the contrary, the preceding theoretical formula of  $\alpha$ , Eq. (10.4.4.2), gives  $\alpha = 0$  at  $E = E_g$ . To extricate theory from a predicament, some references replace the  $\delta(E - E_g - E_k)$  function by the Lorentz function for two cases that there is and is no an interaction between electron and hole. The Lorentz function is characterized by the center located at  $E = E_g$ and by its full-width half-maximum  $\Gamma$ . It is obvious that this replacement of  $\delta(E - E_g - E_k)$  by Lorentz function is very phenomenological, which cannot reveal a bit of origins of the serious departure of some references theory from experimental data. This text book thinks that if we make exact numerical calculations directly for Eq. (10.4.4.1), then the theoretical result should be, at least, better than Eq. (10.4.4.2). For brevity, in the following calculations we only write the  $E_{k'}$ -dependent part in Eq. (10.4.4.1), which is

$$\alpha(E) \propto \int_{0}^{+\infty} \sqrt{E - E_g + E_{k'}} \frac{\sin^2 \frac{E_{k'}t}{2\hbar}}{(E_{k'})^2} dE_{k'} + \int_{0}^{E - E_g} \sqrt{E - E_g - E_{k'}} \frac{\sin^2 E_{k'}t/2\hbar}{(E_{k'})^2} dE_{k'} \equiv I + II.$$
(10.4.4.5)

The solid line in Fig. 10.5 is the theoretical curve given by Eq. (10.4.4.5), which fits the data at  $E \ge E_g$  very well. *II* in Eq. (10.4.4.3) can be called energy reduction part because  $E - E_g \ge E_{k'}$  is necessary. Otherwise, *II* is an imaginary number. *I* in Eq. (10.4.4.5) can be called energy increment part because  $E - E_g < E_{k'}$  is allowed. The ratio of *II*/*I* is given in Fig. 10.6. *I* > *II* means that the energy increment contribution is always larger than that the energy reduction contribution in the absorption of semiconductors.

### 10.4.5. Photoeffect

If the energy  $\hbar\omega$  of photon exceeds the ionization energy of the atom, absorption of photons will be accompanied by the transition of one electron from a bound state to a state of the continuous spectrum (continuum) in vacuum space or conduction band. This is the photoeffect or photoelectric effect. The photoeffect plays an important rule in the absorption of X-rays and  $\gamma$ -quanta and in a number of other physical phenomena.

This subsection will consider the elementary theory of the photoeffect by using the D-C transition theory. Especially, we will remind the readers to note the influences of ultra-fast technology started from 2001 on photoeffect. In that year, attosecond ( $10^{-18}$  second) pulses were generated for the first time. The advent of the attosecond light pulse makes it possible to investigate the much faster electron dynamics, such as real-time observation of



Figure 10.5. The solid line is our theoretical curve of absorption coefficient  $\alpha$  versus photon energy *E* at  $E \ge E_g = 1.42$  eV. The data are for GaAs at 300 K [128]. The unit of  $\alpha$  is cm<sup>-1</sup>. The dotted line comes from the phenomenological Urbach tail.

valence electron, and radiation-matter interaction. Now the attosecond physics has been established. One possible main aspect of the attosecond physics is the attosecond photoeffect. For example, an attosecond pulse photon with energy E shoots a hydrogen atom in ground state, the binding energy of the electron in ground state is  $E_{bin} = -E_k = 13.6$  eV, and the ejected photoelectron energy is  $E_{k'} \ge 0$  if  $E \ge E_{bin} = -E_k$ . However, some references's researches on attosecond photoeffect are still confined in the real-time observation of the motion of ejected photoelectron and the influences of high light intense on the photoeffect. There is still no any research on the possible maximum kinetic energy of ejected photoelectrons. Therefore, it is necessary to study attosecond photoeffect theory, and give some predictions. The aim of this subsection is to study elementary theory for both attosecond and low frequency photoeffect.

Eq. (10.3.1.3)' gives that in case of photon absorption the transition probability of the electron from initial bound state  $|k\rangle$  in an atom to all possible final ejected states  $|k'\rangle$ ,



Figure 10.6. The *I* and *II* represent the energy increment and reduction contributions coming from Eq. (10.4.4.3), respectively. II/I < 1 means that in light absorption of semiconductors the contribution of energy increment part is always more important than the contribution of energy reduction part.

$$P_{all \leftarrow k}(t \ge t_{\circ}):$$

$$P_{all \leftarrow k}(t \ge t_{\circ}) = \int d\Omega \int_{-\infty}^{\infty} d\omega_{k'} \rho(\omega_{k'}) \frac{4|H_{k'k}'|^2}{\hbar^2} \left[ \frac{sin[(\omega_{k'k} - \omega)t_{\circ}/2]]}{(\omega_{k'k} - \omega)} \right]^2$$

$$= \int d\Omega \int_{-\infty}^{\infty} dE_{k'} \rho(E_{k'}) \frac{4|H_{k'k}'|^2}{\hbar^2}$$

$$\times \left[ \frac{sin[(E_{k'k} - E)t_{\circ}/2]}{(E_{k'k} - E)} \right]^2.$$
(10.4.5.1)

In comparison of Eq. (10.4.5.1) with Eq. (10.3.1.3)', there are two changes:

(1) We use the true density of states of the final states  $|k'\rangle$  instead of the imaginary average density of states;

(2) Because the definition of the density of states is within a solid angle  $d\Omega$ , so there is an integration over  $d\Omega$ .

The density of states  $\rho(k')$  in Eq. (10.4.5.1) has been given by Eq. (10.4.4.3). Now let us calculate the matrix element  $H'_{k'k}$ . To simplify, the calculations, we shell neglect in the final state the interaction between the emitted electron and the atom, that is, we write the final state wavefunction of the electron in the form of a plane wave

$$\Psi_{k'}(r) = \frac{1}{\sqrt{V}} e^{ik' \cdot r}, \quad k' = \frac{p}{\hbar} = \frac{\mu v}{\hbar}, \quad (10.4.5.2)$$

normalized in the volume V. This approximation is fully justified, if the energy of the emitted electrons is large compared with the ionization energy I of the atom, that is, if the inequality

$$\frac{1}{2}\mu v^2 >> I = \frac{Z^2 e^4 \mu}{2\hbar^2}, \quad or \quad \xi = \frac{ze^2}{\hbar v} << 1 \tag{10.4.5.2}'$$

is satisfied. The quantity  $\xi^2$  is the ratio of the ionization energy to the kinetic energy of the emitted electron. Since  $\mu v^2/2 = \hbar \omega - I$ , it follows from Eq. (10.4.5.2) that the photon energy must be sufficient large. The photon energy must, on the other hand, be small compared with the rest-mass energy of the electrons, in order that we can solve the problem in the non relativistic approximation.

If the photon energy only just exceeds the ionization energy I of the electron bounded in an atom, then we cannot, in principle, describe the final emitted electron state by plane waves, and we must use the exact electron wavefunctions of the continuous spectrum, because the emitted electron is still in the neighborhood of the atom. Ref. [129] has performed non relativistic calculations using the wavefunctions of the continuous spectrum in a Coulomb field. His calculations show that if one takes the Coulomb interaction between the atom and the emitted electron into account, then the transition probability for the photoeffect decreased by a factor

$$F(\xi) = 2\pi \sqrt{\frac{I}{\hbar\omega}} \frac{exp(-4\xi arccot\xi)}{1 - exp(-2\pi\xi)},$$
(10.4.5.3)

where  $\hbar\omega$  is very close to  $I, \xi \to \infty$ , and  $F(\xi) \to 0.12$ . This estimation indicates that even the emitted electron is just in the neighborhood of the atom, the non plane wave correction is not large.

We choose the electron initial state wavefunction as 1S-state of atom, i. e.,

$$\Psi_i = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}, \quad a = \frac{\hbar^2}{\mu e^2 Z}.$$
(10.4.5.4)

Now let us calculate the matrix element of perturbation Hamiltonian  $H'_{k'k}$ . In photoeffect the atom (system) absorbs photon. Eq. (10.4.2.5) gives

$$H'' = H'e^{i\omega t} = -er \cdot E_{\circ}e^{i\omega t} = -er\cos\theta'' \mathsf{E}e^{i\omega t}, \qquad (10.4.5.5)$$

where  $\theta$  is the angle between electron position vector **r** and electric field  $E_{\circ}$ .

$$H'_{k'k} = < k' |H'|i> = \frac{-e\mathsf{E}}{\sqrt{\pi a^3 V}} \int e^{-ik' r\cos\theta'} r\cos\theta'' e^{-r/a} dr, \qquad (10.4.5.6)$$

where  $\theta'$  is the angle between **r** and **k**'. We use  $\theta$  to denote the angle between **k**' and electric field  $E_{\circ}$ . The integration over **r** in Eq. (10.4.5.6) can be performed by taking **k**' as a polar axis (in this case  $\theta$ " has to be denoted by  $\theta', \theta$ ) or by taking the electric field direction as a polar axis (in this case  $\theta'$  has to be denoted by  $\theta$ ",  $\theta$ ). We take **k**' as the polar axis. In this case

$$\cos\theta'' = \cos\theta'\cos\theta + \sin\theta'\sin\theta\cos(\phi' - \kappa), \qquad (10.4.5.7)$$

where  $\theta', \phi'$  are the polar angles of **r** by taking **k**' as polar axis, and  $\theta, \kappa$  are the polar angles of  $E_{\circ}$  by taking **k**' as polar axis [120].

Now, in Eq. (10.4.5.6), we can take  $r^2 dr d(\cos \theta') d\phi'$  to replace the *dr*. The integration over  $\phi'$  makes the second term in Eq. (10.4.5.7) to vanish. The other calculations for the matrix element is directly. At last, we have

$$H'_{k'k} = < k' |H'|i> = \frac{32\pi i e \mathsf{E}k' a^5 \cos \theta}{\sqrt{\pi a^3 V} (1 + k'^2 a^2)^3}.$$
 (10.4.5.8)

Eq. (10.4.4.3) gives

$$\rho(k',\Omega) = \rho(E_{k'},\Omega) = \frac{V\mu\hbar}{(2\pi\hbar)^3} \sqrt{\frac{2\mu^* E_{k'}}{\hbar^2}}.$$
(10.4.5.9)

Substituting Eqs. (10.4.5.8)  $(H'_{k'k})$  and (10.4.5.9)  $(\rho(k'))$  into Eq. (10.4.5.1), one obtains

$$P_{all \leftarrow k}(t \ge t_{\circ}) \equiv \int P_{all \leftarrow k, d\Omega}(t \ge t_{\circ})$$
  
$$\equiv \frac{256\mu e^{2}E_{\circ}^{2}a^{7}}{\pi\hbar^{3}} \int d\Omega \cos^{2}\theta \int_{-\infty}^{\infty} \frac{d(E_{k'k} - E)}{2\hbar} \frac{k'^{3}}{(1 + k'^{2}a^{2})^{6}}$$
  
$$\times \frac{\sin^{2}[(E_{k'k} - E)t_{\circ}/2\hbar]}{[(E_{k'k} - E)/(2\hbar)]^{2}}, \qquad (10.4.5.10)$$

where  $E_{k'k} - E = E_{k'} - E_k - E = E_{k'} + E_b - E$ .  $-E_b = E_k$  denotes the ground state energy of the atom, and *E* denotes the energy of one photon.

From Eq. (10.4.5.10) we see that transition probability from initial bound state of an electron in an atom to all possible final emitted free states per solid angle is

$$\frac{P_{all \leftarrow k, d\Omega}(t \ge t_{\circ})}{d\Omega} \propto \cos^2 \theta.$$
(10.4.5.11)

The result of Eq. (10.4.5.11) is not strange. We can be expected that the amplitude of transition probability should be proportional to the component of electric field (which causes the electron transition) in this direction. This component is  $-eE\cos\theta$ .

Some references's formula to calculate transition probability of photoeffect are exactly same as our Eqs. (10.4.5.10-11). However, the subsequent calculations are much different. Correspondingly, some references give the conclusion of energy conservation in D-C transition. Let us look at some references's calculation approach. Some references assume  $t_{\circ} \rightarrow \infty$ .

Under these two approximations some references obtain

$$P_{all \leftarrow k}(t \ge t_{\circ}) = \frac{256\mu e^{2}E_{\circ}^{2}a^{7}}{\pi\hbar^{3}(1+k^{\prime2}a_{\circ}^{2})^{6}}\frac{2\pi k^{\prime3}}{3}\int_{-\infty}^{\infty} dE_{k^{\prime}}t_{\circ}\delta(E_{k^{\prime}}+E_{b}-E)$$
  
$$= \frac{256\mu e^{2}E_{\circ}^{2}a^{7}}{\pi\hbar^{3}(1+k^{\prime2}a_{\circ}^{2})^{6}}\frac{2\pi k^{\prime3}}{3}t_{\circ}\Big|_{E_{k^{\prime}}=E-E_{b}},$$
(10.4.5.12)

and the transition rate is

$$W_{all \leftarrow k}(t \ge t_{\circ}) = \frac{P_{all \leftarrow k}(t \ge t_{\circ})}{t_{\circ}} = \frac{256\mu e^{2}E_{\circ}^{2}a^{7}}{\pi\hbar^{3}(1+k'^{2}a_{\circ}^{2})^{6}} \frac{2\pi k'^{3}}{3} \bigg|_{E_{t'}=E-E_{h}},$$
 (10.4.5.13)

where the subscript denotes  $E - E_b = \hbar^2 k'^2 / (2\mu)$ . The prominent character of some references's photoeffect theory is energy conservation.

Without using the time infinite limit, this book makes the following treatments for Eq. (10.4.5.10). From this equation we obtain the transition probability per unit energy of  $E_{kin}$  and per solid angle in the direction perpendicular to the incident direction of photon  $(\cos \theta = \cos 0 = 1)$  is

$$P'_{all \leftarrow k}(t \ge t_{\circ}) = \frac{256\mu e^{2}E_{\circ}^{2}a^{7}}{\pi\hbar^{3}} \frac{1}{(1+2\mu E_{k'}/\hbar^{2}a^{2})^{6}} \left(\frac{2\mu E_{k'}}{\hbar^{2}}\right)^{3/2} \\ \times \frac{\sin^{2}[(E_{k'k} - E)t_{\circ}/2\hbar]}{[(E_{k'k} - E)/(2\hbar)]^{2}} \\ \equiv I \times \frac{\sin^{2}[(E_{k'k} - E)t_{\circ}/(2\hbar)]}{[(E_{k'k} - E)/(2\hbar)]^{2}} \\ \equiv I \times II.$$
(10.4.5.14)

The energy dependence of the factor *I* in Eq. (10.4.5.14) comes from the product of  $|transition matrix element|^2$  and density of states. Eq. (10.4.5.14) shows clearly that factor *I* is dependent on  $E_{k'}$ , which is the kinetic energy of the emitted electron. If a metal (such as copper) is irradiated with light of a given frequency, then electrons can also be ejected from the metal surface. In this case  $E_k = -E_b$  is called work function, and  $E_b = W - E_F$ , where *W* is the depth of the potential well, and  $E_F$  is the Fermi energy.

Let us make comparisons between some references's Eq. (10.4.5.12) and this textbook's Eq. (10.4.5.14). Eq. (10.4.5.14) shows that the kinetic energy  $E_{k'}$  of photoelectron (i. e., the emitted electron) is a complex function of the energy of photons. We can find out the theoretical maximum photoelectron kinetic energies  $E_{kin}$ . According to Eq. (10.4.5.12)  $E_{kin} = E - E_b = E_{photon} - E_b$ . In our numerical calculations we take  $-E_b = -13.6$  eV, which corresponds to the energy of 1S electron of hydrogen atom. (1 eV= $2.418 \times 10^{14}$ Hz) In any cases Eq. (10.4.5.12) always gives an exactly linear relation between  $E_{kin}$  and  $E_{photon}$ , which indicates energy conservation. Fig. 10.7 draws two curves of  $E_{kin}$  versus photon energy  $E_{photon}$  of Eq. (10.4.5.14). If  $t_{\circ}$  is less, then in case of boundary absorption (i. e.,  $E_{photon} = E_b$ ) the energy nonconservation is more obvious. The curve 2 ( $t_{\circ} = 10^{-13}$ second) in Fig. 10.7 is nearly linear and gives  $E_{kin} = 0.02 \approx 0$  eV at  $E_{photon} = E_b = 13.6$  eV  $(E_{photon} = E_b \text{ is called boundary absorption.})$ . The curve 1 ( $t_{\circ} = 10^{-15}$  second.) in the Fig. 10.7  $E_{kin} = 2 \gg 0$  eV at  $E_{photon} = E_b = 13.6$  eV, which means that there is a obvious energy nonconservation in photoeffect. On the contrary, Eq. (10.4.5.12) always give  $E_{kin} = 0$  eV so long as for the boundary absorption, which means that Eq. (10.4.5.12) always gives energy conservation. From Fig. 10.7 we see also that so long as  $t_{\circ} \ge 10^{-13}$  second, the Eq. (10.4.5.12) is good enough.

As is well known, the Millikan's photoeffect experiment in 1916 is generally accepted as the determinant verification for Einstein's photon theory of light and Einstein's photoef-



Figure 10.7. Curves 1 and 2 indicate the relations between maximum photoelectron kinetic energy  $E_{kin}$  and energy of incident photon  $E_{photon}$  due to Eq. (10.4.5.14). In our numerical calculation,  $t_{\circ} = 10^{-15}$  second for the curve 1, and  $t_{\circ} = 10^{-13}$  second for the curve 2.  $E_{bin} =$ 13.6 eV. 1 eV = 2.418×10<sup>14</sup> Hz. Curve 2 indicates the relation between  $E_{kin}$  and  $E_{photon}$ when  $t_{\circ} = 10^{-13}$  second and  $E_{bin} = 13.6$  eV. If  $E_{photon} = E_b = 13.6$  eV, then  $E_{kin} = 2$  eV and  $E_{kin} = 0.02$  eV for curve 1 and curve 2, respectively. However, according to the energy conservation formula Eq. (10.4.5.12), if  $E_{photon} = E_b$ , then always  $E_{kin} = E_{photon} - E_b = 0$ .

fect equation. To compare with the Millikan's experiment [130], we take  $E_b = E_{b,Millikan} =$  1.8156 eV, and draw the Fig. 10.8.

Although the curve 2 ( $t_{\circ} = 10^{-13}$  second) is nearly linear, which fits Millikan'data well. However, the energy, exactly speaking, is still not exactly conservative, because at  $E_{photon} = E_b = 1.8156 \text{ eV} E_{kin} = 0.018 \text{ eV}$  instead of  $E_{kin} = 0$  from Eq. (10.4.5.12). The minimum energy of photon used in Millikan's experiment is 2.2456 eV. The corresponding  $E_{kin} = 0.43 \text{ eV}$ . This value can be obtained theoretically by both Eq. (10.4.5.12) and Eq. (10.4.5.14). However, Millikan did not use the  $E_{photon} = 1.8156 \text{ eV}$ . Therefore, we cannot make comparison between experiment data and theoretical curve. If  $t_{\circ} = 10^{-14}$  second and  $E_{photon} = E_{bin} = 1.8156 \text{ eV}$ , then the curve 1 gives  $E_{kin} = 0.18 \gg 0 \text{ eV}$ , which means that the energy is obviously non conservative. However, Eq. (10.4.5.12) always gives  $E_{kin} = 0$ . The curve 3 in Fig. 10.8 is an imaginary case in which  $t_{\circ} = 10^{-15}$  second.



Figure 10.8. Curve 1 indicates the relation between maximum photoelectron kinetic energy  $E_{kin}$  and energy of incident photon  $E_{photon}$ , when  $t_{\circ} = 10^{-14}$  second and  $E_b = 1.8156$  eV. Curve 2 indicates the relation between  $E_{kin}$  and  $E_{photon}$ , when  $t_{\circ} = 10^{-13}$  second and  $E_b = 1.8156$  eV. If  $E_{photon} = E_b = 1.8156$  eV, then  $E_{kin} = 0.18$  eV and  $E_{kin} = 0.018$  eV for curve 1 and curve 2, respectively. The data are taken from Ref. [130].

In the cases of  $t_{\circ} \ll 10^{-13}$ , the energy nonconservation becomes more stronger. Therefore, it is not convenient to draw diagram. Let us derive a general formula, appropriate for any value of  $t_{\circ}$ , for the maximum kinetic energy of ejected electron in case of boundary absorption. For convenience, we suppose that Eq. (10.4.5.14) is

$$P'_{all \leftarrow k}(t \ge t_{\circ}) \approx E_{kin}^{-1/2} sin^2(\frac{E_{kin}t_{\circ}}{2\hbar}).$$
 (10.4.5.15)

The equation of maximum  $E_{kin}$  of the emitted electron at fixed  $t_o$ ,  $E_{kin}$ , can be obtained from Eq. (10.4.5.15), and has given by Eqs. (10.3.1.9) and (10.3.1.10). It is

$$tan(x) = 4x,$$
 (10.4.5.15)

where  $x = t_{\circ}E_{kin}/(2\hbar) \equiv t_{\circ}\omega/2$ . The solution of Eq. (10.4.5.15) is

$$t_{\circ}\omega_{kin} = 3.10484. \tag{10.4.5.16}$$

Thus, generally speaking, the smaller the  $t_{\circ}$  is, the larger the  $E_{kin}$  is. (As long as for boundary absorption, Eq. (10.4.5.12) gives always  $E_{kin} = 0$ .) If  $t_{\circ} = 10^{-15}$ ,  $10^{-14}$ ,  $10^{-13}$  second, then  $E_{kin} = 2.05$ , 0.205, 0.0205 eV, respectively. These values are nearly equal to the values in Fig. 10.6. In Fig. 10.6  $E_{photon} = E_b = 1.8156$  eV. If we take that  $E_{photon} = E_{bin} = 13.6$  eV, then Eq. (10.4.5.16) gives that for  $t_{\circ} = 10^{-15}$  and  $10^{-13}$  second,  $E_{kin} = 2.05$ , 0.0205 eV, respectively, which approach well the rigorous numerical values in Fig. 10.5. Therefore, Eq. (10.4.5.16) is good enough for applications. For one attosecond  $t_{\circ} = 10^{-18}$  second,  $E_{kin} = 2050 >> 0$  eV, which is much larger than the expected value from Eq. (10.4.5.12). If we note that the Eq. (10.4.5.12) gives  $E_{kin} = 0 << 2050$  eV, then we can say that the energy is strongly non conservative in attosecond photoeffect. To verify this theoretical prediction,  $E_{kin} = 2050$  eV, we need the following experimental conditions: (a). The attosecond light pulse, for which the  $E_{photon} \approx 4135$  eV; (b).  $E_{bin} = E_{photon} = 4135$  eV. Ref. [131] points out that the inner-shell electrons of atoms have widely spaced energy levels from  $10^2$  to  $10^5$  eV. Therefore, it is not difficult to find some inner-shell levels which can give  $E_b \approx 4135$  eV.

The present technique of attosecond light pulse is still very difficult to obtain 1 attosecond pulse. Let us give a now available simple atomic example [131]. Ref. [131] reported that when a helium atom in its ground state absorbs an 100 attosecond light pulse ( $t_o = 10^{-16}$ second) photon with energy of 40.35 eV (= $E_b$ ), a single electron can be emitted, leaving the other electrons in the ground state, through direct attosecond photoeffect. It is a big pity that Ref. [131] did not measure the observed energy  $E_{kin}$  of emitted electron. According to Eq. (10.4.5.12),  $E_{kin} = E_{photon} - E_b = 0$ . However, according to our exact formula, Eq. (10.4.5.16),  $E_{kin} = 20.5$  eV.

The now available experimental photoeffect was done only at picosecond ( $t_{\circ} = 10^{-12}$  second) and subpicosecond ( $t_{\circ} = 10^{-13}$  second), which does not contradict with our Figs. 10.9 and 10.10. Figs. 10.9 and 10.10 show that the obvious energy nonconservation in photoeffect occurs only at  $t_{\circ} < 10^{-13}$  second.

In the famous Millikan's experiment [130], so-called determinant verification for the Einstein equation of photoeffect, there are only five experimental points. All the five points in Fig. 10.8 are at  $E_{photon} > 2.24$  eV, and thus the five points are still quite far from the 2.24 eV. In Millikan's times there were no attosecond and femtosecond pulse techniques. Therefore, Millikan's experiment can neither negative nor confirm our Eq. (10.4.5.14).

Because the strong energy nonconservation in attosecond photoeffect has not yet been verified by experiment, it is very important to analyze its reliability and reasonableness. Let us give this analysis directly, quantitatively, and without any numerical calculation. First, we note that  $t_{\circ} \rightarrow \infty$  is not correct in physics. Therefore, the Eq. (10.4.5.12) is not legitimate, that is, one cannot use the condition  $t_{\circ} \rightarrow \infty$  in photoeffect theory. Second, even if  $t_{\circ} \rightarrow \infty$  is correct, we still need to consider that the factor *I* in Eq. (10.4.5.14) is proportional  $E_{kin}^{3/2} \neq E_{kin}^{0}$ . Thus we have

$$\lim_{t_{o} \to \infty} E_{kin}^{3/2} \times II \neq 2\pi\hbar\delta(E_{kin} - E_{photon} + E_b)t_{o}, \qquad (10.4.5.17)$$

which clearly shows energy nonconservation more or less.

The Einstein equation of photoeffect is

$$E_{kin} = E_{photon} - E_b,$$
 (10.4.5.18)

which is obviously a energy conservation equation. Because this paper has shown that the energy conservation in photoeffect is conditional. If  $t_{\circ} < 10^{-13}$ , then the energy is not conservative obviously, and thus Einstein equation of photoeffect does not hold water exactly.

#### 10.4.6. Scattering

As an application of transition theory, in this subsection we will introduce theory of elastic scattering of an electron by an atomic nucleus, and simultaneously illustrate some concepts of scattering theory. Because our transition theory considers the possibility of energy nonconservation in transition process, our approach will different from some references's approach, and will possibly give new results. As a representative method in some references, in this subsection we will introduce the method in Ref. [6], and in appropriate place we propose more correct method. We examine the scattering of a high velocity electron by a nucleus with the charge number Z. The interaction between electron and nucleus is the pure Coulomb interaction. We treat this interaction as a perturbation:

$$H'(r,R) = \frac{Ze^2}{|r-R|}e^{-|r-R|/d},$$
(10.4.6.1)

where **r** marks the coordinates of the electron, **R** those of the nucleus. The exponential factor in Eq. (10.4.6.1) is introduced because of the screening effect of the electron on the nuclear charge. We need it for mathematical reasons, too, since it helps to avoid divergencies when integrations are performed. The length *d* is a measure for the screening distance. For |r - R| >> d, the interaction disappears, because the charge of the nucleus is then completely shielded by the surrounding electrons.

Before the scattering, the whole system is described by the state  $|\Psi_k\rangle$  and afterwards, by the state  $|\Psi_{k'}\rangle$ . We need to calculate the transition probability for the transition  $|\Psi_k\rangle \rightarrow |\Psi_{k'}\rangle$  in order to learn something about the charge distribution of the nucleus when comparing it with experiments. The electron is in a state of motion with momentum  $p = \hbar k$  and energy  $E_k$  before scattering occurs and is scattered by the Coulomb potential in Eq. (10.4.6.1) into a state with momentum  $p' = \hbar k'$  and  $E_{k'}$ . Since these are continuum states, the transition probability is given by Eq. (10.5.7). The transition probability  $P_{all \leftarrow k}$ of internal conversation of a nucleus from initial state  $|\Psi_k\rangle$  to all possible final states of 400

 $|\Psi_{k'}>$  is

^

$$P_{all \leftarrow k}(t \ge t_{\circ}) = \int d\Omega P_{all \leftarrow k, d\Omega}$$

$$= \int d\Omega \frac{1}{\hbar^{2}} \int_{0}^{+\infty} |H'_{k'k}|^{2} \rho(\omega_{k', d\Omega}) \frac{\sin^{2}(\omega_{k'} - \omega_{k})t_{\circ}/2}{[\omega_{k'} - \omega_{k}/2]^{2}} d\omega_{k'}$$

$$= \int d\Omega \frac{1}{\hbar^{2}} \int_{0}^{+\infty} |H'_{k'k}|^{2} \rho(E_{k', d\Omega})$$

$$\times \frac{\sin^{2}(E_{k'} - E_{k})t_{\circ}/(2\hbar)}{[(E_{k'} - E_{k})/(2\hbar)]^{2}} dE_{k'}, \qquad (10.4.6.2)$$

The total wavefunctions of the electron-nucleus system are product of the wavefunction of the electron and that of the nucleus. We use plane waves as an approximation for the wavefunction of the electron. This approximation is called the Born approximation. But is only valid if the electron-nucleus interaction is small, i. e., the nuclear charge should be not too large and the velocity of the electron has to be great enough. These conditions are summarized by the relation

$$\frac{Z}{137}\frac{c}{v} << 1. \tag{10.4.6.3}$$

Thus the wavefunctions are

$$\Psi_k = e^{ip \cdot r/\hbar} \Phi_i(R), \text{ and } \Psi_{k'} = e^{ip' \cdot r/\hbar} \Phi_f(R), \qquad (10.4.6.4)$$

or, by using Dirac notation,

$$|\Psi_k\rangle = |k\rangle |i\rangle, and |\Psi_{k'}\rangle = |k'\rangle |f\rangle.$$
 (10.4.6.5)

This can also be expressed as

$$\langle r|k\rangle = e^{ip \cdot r/\hbar} = e^{ik \cdot r}, \qquad (10.4.6.6a)$$

$$< r|k'> = e^{ip'\cdot r/\hbar} = e^{ik'\cdot r},$$
 (10.4.6.6b)

$$< R|i> = \Phi_i(R), and < R|f> = \Phi_f(R).$$
 (10.4.6.6c)

The  $\Phi(R)$  are the normalized wavefunctions of the nucleus. We did not normalized the plane waves in Eq. (10.4.6.4).

Let us now evaluate the matrix elements. Since the wavefunction factorizes into an electronic and a nuclear part, the volume element dV also implies integration over both volume  $dV_e$  (electronic space) and  $dV_n$  (nuclear space). The indices e and n stand for electron and nucleus, respectively. Thus

$$<\Psi_{k'}|H'|\Psi_{k}>=Ze^{2}\int\Phi_{f}^{*}(R)\Phi_{i}(R)\int\frac{\exp(-|r-R|/d)}{|r-R|}e^{i(k-k')\cdot r}dV_{e}dV_{n}.$$
 (10.4.6.7)

We first calculate the integration over the electronic coordinates and abbreviate k - k' by the vector s:

$$k - k' = s. \tag{10.4.6.8}$$

Therefore,  $\hbar s = p - p'$  is momentum transfer from the electron to the nucleus during the scattering process. The integration over  $dV_e$  is evidently a function of **R**:

$$J_e(R) = \int \frac{\exp(-|r-R|/d)}{|r-R|} e^{i(k-k')\cdot r} dV_e.$$
 (10.4.6.9)

Since we integrate over the whole space, we can change our system of coordinates and integrate over the whole space again (the integration boundaries do not need be changed). We replace *r* by  $r'=\mathbf{r}\cdot\mathbf{R}$  and introduce spherical coordinates with  $\theta$  being the angle between **s** and r'.

In terms of these coordinates we have

$$dV_e = r^{\prime 2} dr^{\prime} \sin\theta d\theta d\phi, \qquad (10.4.6.10)$$

and, from  $r'=\mathbf{r}+\mathbf{R}$ , we get

$$(k-k') \cdot r = s \cdot r = s \cdot r' + s \cdot R = sr' \cos \theta + s \cdot R.$$
 (10.4.6.11)

Thus the integral becomes

$$J_{e}(R) = \int \frac{e^{-r'/d}}{r'} e^{i(sr'\cos\theta + s\cdot R)} r'^{2} \sin\theta dr' d\theta d\phi$$
  

$$= 2\pi e^{is\cdot R} \int_{0}^{\infty} dr' \int_{0}^{\pi} d\theta r' e^{-r'/d} e^{isr'\cos\theta} \sin\theta$$
  

$$= 2\pi e^{is\cdot R} \int_{0}^{\infty} dr' r' e^{-r'/d} \frac{1}{isr'} (e^{isr'} - e^{-isr'})$$
  

$$= 2\pi e^{is\cdot R} \frac{1}{is} \int_{0}^{\infty} dr' (e^{i(s-1/d)r'} - e^{-i(s-1/d)r'})$$
  

$$= -2\pi e^{is\cdot R} \frac{1}{is} \left(\frac{1}{is-1/d} + \frac{1}{is+1/d}\right)$$
  

$$= e^{is\cdot R} \frac{4\pi}{s^{2} + 1/d^{2}}.$$
(10.4.6.12)

This result can be simplified: the term  $1/d^2$  in the denominator can be neglected if  $s^2d^2 >>$  1. This means that the momentum transfer must be not too small. Hence,

$$J_e(R) \approx e^{is \cdot R} \frac{4\pi}{s^2}.$$
 (10.4.6.13)

Therefore the matrix takes the form

$$<\Psi_{k'}|H'|\Psi_k>=Ze^2rac{4\pi}{s^2}\int\Phi_f^*(R)e^{is\cdot R}\Phi_i(R)dV_n.$$
 (10.4.6.14)

For elastic scattering, the state of the nucleus is not changed. Let the nucleus be in its ground state  $\Phi$ . Thus we have  $\Phi = \Phi_f = \Phi_i$ , and the product  $Z\Phi^*(R)\Phi(R)$  is the density distribution of the protons in the nucleus. Instead of the wavefunctions, we can introduce the

charge density  $\rho_p(R)$  of the atomic nucleus [more accurately:  $\rho_p(R)$  is the charge density without the factor *e*, which we have explicitly taken out]:

$$Z\Phi^*(R)\Phi(R) = \rho_p(R) \quad with \quad \int \rho_p(R)dV_n = Z.$$
 (10.4.6.15)

For further simplification we assume spherical symmetry of the charge distribution:

$$\rho_p(R) = \rho_p(R).$$
(10.4.6.16)

This assumption is only valid for atomic nuclei in the vicinity of the magic numbers. Therefore we obtain for the matrix element

$$<\Psi_{k'}|H'|\Psi_{k}> = \frac{4\pi e^{2}}{s^{2}}\int \rho_{p}(R)e^{is\cdot R}dV_{n}$$
  
$$= \frac{4\pi e^{2}}{s^{2}}F(s). \qquad (10.4.6.17)$$

The quantity F(s) is called a form factor. It is the Fourier-transformed charge distribution and reflects the deviation of the nuclear charge distribution from point structure. Indeed, if the nucleus is assumed to be point-like, i. e.,  $\rho_p(R) = \delta^3(R)$ , we get F = 1.

The form factor can be further evaluated by again introducing spherical coordinates and using the axis defined by **s** as the polar axis. Hence, we get

$$dV_n = R^2 \sin\theta dR d\theta d\phi \quad and \quad s \cdot R = sR \cos\theta, \tag{10.4.6.18}$$

and therefore

$$F(s) = 2\pi \int_0^\infty \int_0^\pi \rho_p(R) e^{is\cos\theta R} R^2 \sin\theta dR d\theta$$
  
=  $2\pi \int_0^\infty \rho_p(R) \frac{1}{isR} (e^{isR} - e^{-isR}) R^2 dR$   
=  $\frac{4\pi}{s} \int_0^\infty \rho_p(R) \sin(sR) R dR.$  (10.4.6.19)

The last integral can be calculated only if the charge distribution  $\rho_p(R)$  is known. Our present result can be summarized as

$$<\Psi_{k'}|H'|\Psi_k>=rac{4\pi e^2}{s^2}F(s).$$
 (10.4.6.20)

The density of states  $\rho(k')$  of the electron in unit volume space has been given by Eq. (10.4.4.3), which is.

$$\rho(k')d\Omega dE_{k'} = \frac{k'^2 dk'}{(2\pi)^3} dE_{k'} d\Omega \equiv \rho(E_{k'}, d\Omega) d\Omega.$$
(10.4.6.21)

$$\rho(E_{k'},\Omega) = \frac{p'^2 dp'}{(2\pi\hbar)^3 dE_{k'}} = \frac{p'^2}{(2\pi\hbar)^3} \frac{1}{dE_{k'}/dp'}.$$
(10.4.6.22)

To calculate the derivative in Eq. (10.4.6.22), we assume that the electron is very fast and therefore proceed from the relativistic energy-momentum relation

$$E_{k'} = \sqrt{p'^2 c^2 + m^2 c^4}, \ (p' = \hbar k'),$$
 (10.4.6.23)

If the kinetic energy of the electron is large enough compared with the rest energy, then the term  $mc^2$  can be neglected and we obtain

$$E_{k'} = p'c. (10.4.6.24)$$

From Eqs. (10.4.6.24) we get

$$\frac{dE_{k'}}{dp'} = c. \tag{10.4.6.25}$$

Substituting Eq. (10.4.6.25) in to Eq. (10.4.6.22) we get the following expression for the density of states:

$$\rho(E_{k'},\Omega) = \frac{p'^2}{(2\pi\hbar)^3} \frac{1}{dE_{k'}/dp'} = \frac{p'^2}{(2\pi\hbar)^3 c}.$$
(10.4.6.26)

Substituting Eqs. (10.4.6.26) and (10.4.6.20) into Eq. (10.4.6.2) yields

$$P_{all \leftarrow k}(t \ge t_{\circ}) \equiv \int d\Omega P_{all \leftarrow k, d\Omega}(t \ge t_{\circ}) \\ = \int d\Omega \frac{1}{\hbar^2} \int_0^{+\infty} \left| \frac{4\pi e^2}{s^2} F(s) \right|^2 \frac{p'^2}{c(2\pi\hbar)^3} \\ \frac{\sin^2(E_{k'} - E_k)t_{\circ}/(2\hbar)}{\left[(E_{k'} - E_k)/(2\hbar)\right]^2} dE_{k'},$$
(10.4.6.27)

where, according to the definition of s,

$$\hbar^2 s^2 = p^2 + p'^2 - 2pp' \cos\Theta.$$
 (10.4.6.28)

Correspondingly, the transition rate is

$$w_{fi} \equiv \frac{P_{all \leftarrow k}(t \ge t_{\circ})}{t_{\circ}}$$
  
=  $\frac{1}{t_{\circ}} \int d\Omega \frac{1}{\hbar^{2}} \int_{0}^{+\infty} \left(\frac{4\pi e^{2}}{s^{2}}\right)^{2} |F(s)|^{2} \frac{p'^{2}}{(2\pi\hbar)^{3}c} \frac{\sin^{2}(E_{k'} - E_{k})t_{\circ}/(2\hbar)}{[(E_{k'} - E_{k})/(2\hbar)]^{2}} dE_{k'}$   
=  $\int d\Omega w_{fi,d\Omega}.$  (10.4.6.29)

The transition probability itself cannot be measured directly, but a quantity can be observed, which is called a cross-section, or, more accurately, a scattering cross-section, and is denoted by  $\sigma$ . Or, more conveniently, we introduce differential cross-section  $d\sigma_{fi,d\Omega}$ , which is defined as the number of particles scattered per unit time and per unit of the incoming particle current into the section of the solid angle ( $\Omega \rightarrow \Omega + d\Omega$ ). Since the initial states  $|i\rangle = |k\rangle$  represent particles, the current of which is  $v_i$ , we obtain

$$d\sigma_{fi,d\Omega} = \frac{w_{fi,d\Omega} d\Omega}{v_i}.$$
 (10.4.6.30)

Since we use the high velocity approximation for the scattering electron,  $v_i \approx c$ . Substituting Eq. (10.4.6.29) into Eq. (10.4.6.30) yields

$$\frac{d\sigma_{fi,d\Omega}}{d\Omega} = \frac{1}{t_o} \frac{1}{\hbar^2 (2\pi\hbar)^3 c^2} \int_0^{+\infty} \frac{(4\pi)^2 e^4 p'^2}{s^4} |F(s)|^2 \frac{\sin^2 \frac{(E_{k'} - E_k)t_o}{2\hbar}}{\left[(E_{k'} - E_k)/(2\hbar)\right]^2} dE_{k'}.$$
 (10.4.6.31)

Eq. (10.4.6.31) is called exact scattering formula.

Although some references do not give the exact formula Eq. (10.4.6.31), but if some references like, then they can give this formula. This means that until now the treatments of both some references and this textbook are the same in essence. (See for example Ref. [6].) However, for treatment of Eq. (10.4.6.31) the significant difference between some references and this textbook manifests. Some references such as Ref. [6] make the following treatments:

(1) Some references make  $t_{\circ} \rightarrow \infty$ , use Eq. (10.4.6.19), and obtain (See, for example, Ref. [6])

$$\frac{d\sigma_{f\leftarrow i,d\Omega}}{d\Omega} = \left(\frac{e^2}{2pc}\right)^2 \frac{1}{\sin^4 \Theta/2} |F(s)|^2.$$
(10.4.6.32)

Eq. (10.4.6.32) is called Rutherford scattering formula.

If the effect of the recoiling nucleus is taken into account, then one can put a recoiling factor, and Eq. (10.4.6.32) becomes

$$\frac{d\sigma_{fi,d\Omega}}{d\Omega} = \left(\frac{e^2}{2pc}\right)^2 \frac{1}{\sin^4 \Theta/2} |F(s)|^2 \frac{1}{1 + (2p/Mc)\sin^2 \Theta/2}.$$
(10.4.6.33)

Eq. (10.4.6.33) is called modified Rutherford scattering formula.

(2) Experiments have given the angular distributions of scattered electrons from many different nuclei, such ad:  ${}^{197}Au$ ,  ${}^{51}V$ , and  ${}^{40}Ca$ . For example, in one observed curve the scattering probability is proportional to the scattered electron number and  $d\sigma_{f \leftarrow i, d\Omega}/d\Omega$  [132].

Some references think that the figure in Ref. [132] tells us that the nucleus is of a spherical distribution of positive charge of essentially constant density, so that the nuclear radius could be modeled by the relationship:  $r = r_0 A^{1/3}$  (this formula is called the Fermi model for nuclear radius), where A=atomic mass number (the number of protons, Z, plus the number of neutrons, N),  $r_0 = 1.2 \times 10^{-15}$  m=1.2 fm.

(3) Actually, the correct function form of  $\rho_p(R)$  is not known. Some references assumed that the function's form of  $\rho_p(R)$  is the following Fermi-distribution:

$$\rho_p(R) = \frac{\rho_o}{1 + \exp[(R - R_H/2)/a]},$$
(10.4.6.34)

where the parameters  $R_H/2$  and *a* are adjusted to obtain the best fit with the experimental curves. By taking  $\rho_0 = 1.65 \times 10^{44}$  nucleons/m<sup>3</sup>, a = 0.55 fermi, and  $R_H = 1.07 \times A^{1/3}$  fermi (*A* is the number of nucleons in a nucleus), for the heavy nuclei many experimental curves can be fitted. Robert Hofstadter, who made systematic measurements of this kind, was awarded the Nobel Prize for this work in 1961. Some of the most accurate charge

distributions of atomic nuclei were measured in the same way by Peter Brix at the electron accelerator in Darmstadt.

We have the following comments for the above points (1)-(3), taking by some references:

(1)' General speaking, the infinite time limit is not good, and thus Eq. (10.4.6.33) should be not exact.

(2)' Actually, the charge distribution of, for example, lead nucleus, which is obtained by using the approximate Eq. (10.4.6.34), is too simple. Ref. [133] gives the charge distributions in many other nuclei, which are obtained by using the approximate Eq. (10.4.6.34).

#### 10.4.7. Internal Conversion

Let us consider quantum transition under the influence of time independent interactions in a time interval. Examples of such transitions are: (1). Internal conversion, that is, the process in which an exited nucleus transfers its energy to the atomic electrons; (2). The Auger effect, that is, the readjustments of the electron shells of atoms with several electrons, accompanied by the ejection of one electron from atom.

In the present section, we shell consider internal conversion. This term reflects the original, incorrect viewpoint according to which the transfer of the excitation energy of the nucleus to the electrons in the atom was considered to be an intranuclear photoeffect, caused by the photons emitted by the nucleus. Afterwards it becomes clear that the excited nucleus can transfer its energy to the electron also when the emission of a single photon is absolutely forbidden, that is, when the transition is between states with zero total angular momentum  $(0 \rightarrow 0$  transitions; see the photoeffect in many textbooks on quantum mechanics such as Ref. [10]. Internal conversion and emission of photons by the nucleus must be considered as two alternative possibilities, which can realized when an atomic nucleus makes a transition from an excited state to the ground state [87]. Many authors have considered the problem of calculating the transition probability for internal conversion; their papers differ from one another in the various approximations made for the wavefunctions of the atomic electrons and for the operator determining the transition. We shell consider here an elementary theory of internal conversion in which we choose the wavefunctions of the ejected electrons in the form of plane waves and use a non-relativistic approximation. Refer to Ref. [87] for this subsection.

We shell thus use for the initial state of the electron

$$\Psi_k(r) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}, \quad a = \frac{\hbar^2}{\mu e^2 Z},$$
(10.4.7.1)

where  $\Psi_k$  can be a wavefunction of hydrogen-like K-electron,  $\mu$  is the mass of electron, Z is the proton's number in a nucleus. For the final state

$$\Psi_{k'}(r) = \frac{1}{\sqrt{V}} e^{ik' \cdot r},$$
(10.4.7.2)

which is a plane wave of the ejected electron. If we denote the wavefunctions of the initial and final states of the nucleus by  $\phi_i(q)$  and  $\phi_f(q)$ , respectively, we have for the wavefunctions of the initial and final states of whole system

$$|ki\rangle = \Psi_k(r)\phi_i(q) \quad and \quad |k'f\rangle = \Psi_{k'}(r)\phi_f(q).$$
 (10.4.7.3)

The transition probability  $P_{all \leftarrow k}$  of internal conversation of a nucleus from initial excited state  $\phi_i(q)$  to final state  $\phi_f(q)$  and one of the atomic K-shell electrons going from initial state  $\Psi_k(r)$  to final ejected state  $\Psi_{k'}(r)$  is

$$P_{all \leftarrow k}(t \ge t_{\circ}) = \int d\Omega P_{all \leftarrow k, d\Omega}$$

$$= \int d\Omega \frac{1}{\hbar^2} \int_0^{+\infty} |H'_{k'k}|^2 \rho(\omega_{k'}) \frac{\sin^2 \frac{(\omega_{k'} - \omega_{\Delta} + \omega_b)t_{\circ}}{2}}{\left[\frac{\omega_{k'} - \omega_{\Delta} + \omega_b}{2}\right]^2} d\omega_{k'}$$

$$= \int d\Omega \frac{1}{\hbar^2} \int_0^{+\infty} |H'_{k'k}|^2 \rho(E_{k'})$$

$$\times \frac{\sin^2 \frac{(E_{k'} - E_{\Delta} + E_b)t_{\circ}}{2\hbar}}{\left[\frac{E_{k'} - E_{\Delta} + E_b}{2\hbar}\right]^2} dE_{k'}, \qquad (10.4.7.4)$$

where  $\omega_{k'}$ ,  $\omega_{\Delta}$ , and  $\omega_b$  are the angular frequency of the ejected electron, the excitation of nucleus, and the atomic K-electron binding, respectively,  $\omega_{k'k} = \omega_{k'} - \omega_k \equiv \omega_{k'} - (\omega_{\Delta} - \omega_b)$ ,  $\rho(\omega_{k'})$  is the density of states per unit angular frequency interval of ejected electron within a solid angle  $d\Omega$ ,  $E_{k'}$ ,  $E_{\Delta}$ , and  $E_b$  are the energies of the ejected electron, excitation of nucleus, and atomic K-electron binding, respectively,  $E_{k'k} = E_{k'} - E_k \equiv E_{k'} - (E_{\Delta} - E_b)$ ,  $\rho(k')$  is the density of states per unit energy interval of ejected electron within a solid angle  $d\Omega$ , and  $t_o$  is the duration time of the perturbation Hamiltonian.

$$\rho(k') = V \frac{\mu \hbar k'}{(2\pi\hbar)^3} d\Omega. \qquad (10.4.7.5)$$

 $H'_{k'k}$  is the matrix element of perturbation Hamiltonian.

$$H'_{k'k} = < k'f|H'|ki> \equiv < k'f|\sum_{j=1}^{Z} \frac{e^2}{|r-q_j|}|ki>, \qquad (10.4.7.6)$$

where H' represents the Coulomb interactions between all Z protons in a nucleus at  $q_j$  and one electron at **r** (take the center of the nucleus as origin), and the summation is over all the protons in the nucleus. Because the perturbation operator H' in Eq. (10.4.7.6) does not contain spin variables, so that we cannot describe nuclear transition corresponding to magnetic multiple radiations.

If  $|r| >> |q_j|$ , we can expand the perturbation operator H' in spherical harmonics,

$$H' = \sum_{j=0}^{Z} \sum_{l=0}^{\infty} \sum_{m} \frac{4\pi e^2}{(2l+1)r} \left(\frac{q_j}{r}\right)^l Y_l^m(\Theta, \Phi) Y_l^{m*}(\Theta_j, \phi_j),$$
(10.4.7.7)

where  $(\Theta, \Phi)$  are the angles defining the direction of **r** and  $(\theta_j, \phi_j)$  are the angles defining the direction of the  $q_j$ 

Using Eqs. (10.4.7.7) and (10.4.7.3), we can write

$$H_{k'k}' = \langle k'f|H'|ki\rangle = \sum_{l,m} \frac{4\pi e^2}{2l+1} \langle f|\sum_j q_j^l Y_l^{m*}(\theta_j \phi_j)|i\rangle \langle k'|\frac{Y_l^m(\Theta\Phi)}{r^{l+1}}|k\rangle, \quad (10.4.7.8)$$

After substituting Eqs. (10.4.7.1-2) into the matrix element containing the integration over the electronic coordinates, we get

$$< k'|Y_l^m(\Theta\Phi)/r^{l+1}|k> = \frac{1}{\sqrt{\pi a^3 V}} \int \frac{Y_l^m(\Theta\Phi)}{r^{l+1}} e^{-r/a} e^{-ik' \cdot r} dr.$$
 (10.4.7.9)

Expanding  $exp(-ik' \cdot r)$  in spherical harmonics,

$$e^{-ik'\cdot r} = 4\pi \sum_{lm} (-i)^l j_l(k'r) Y_l^m(\theta\phi) Y_l^{m*}(\Theta\Phi), \qquad (10.4.7.10)$$

where  $(\theta, \phi)$  are angles defining the direction of the wavevector k', and integrating over angles  $(\Theta, \Phi)$ , we get

$$< k'|Y_l^m(\Theta\Phi)/r^{l+1}|k> = 4\sqrt{\frac{\pi}{a^3V}}(-i)^l Y_l^m(\Theta\phi) \int \frac{1}{r^{l+1}} j(k'r) e^{-r/a} dr.$$
(10.4.7.11)

When evaluating the the integral in Eq. (10.4.7.11), we must bear in mind that in our approximation, k'a >> 1, only small values of *r* are important in the integral because of the fast oscillation of the spherical Bessel function; therefore

$$\int \frac{1}{r^{l+1}} j(k'r) e^{-r/a} dr \approx \frac{k'^{l-2}}{1 \cdot 2 \cdot 3 \cdots (2l-1)}.$$
(10.4.7.12)

Substituting Eq. (10.4.7.12) into Eq. (10.4.7.11), and then Eqs. (10.4.7.8) and (10.4.7.5) into Eq. (10.4.7.4), integrating over the angles defining the direction of the emission of electron, i. e., integrating over the solid angle in Eq. (10.4.7.4) using the orthogonality of the spherical harmonics:

$$\int d\Omega Y_l^{m*}(\theta,\phi) Y_{l'}^{m'}(\theta,\phi) = \delta_{ll'} \delta_{mm'}, \qquad (10.4.7.13)$$

we find the transition probability per ejected electron:

$$P \equiv P_{all \leftarrow k}(t \ge t_{\circ}) = \frac{128\pi e^{4}\mu}{\hbar(a\hbar)^{3}} \sum_{lm} \frac{|\langle f|\sum_{j=1}^{Z}q_{j}^{l}Y_{l}^{m}(\theta_{j}\phi_{j})|^{2}}{((2l+1)!!)^{2}} \int_{0}^{+\infty} dE_{k'}k'^{2l-3}$$

$$\times \frac{\sin^{2}\frac{(E_{k'}-E_{\Delta}+E_{b})t_{\circ}}{2\hbar}}{\left[\frac{E_{k'}-E_{\Delta}+E_{b}}{2\hbar}\right]^{2}}$$

$$\approx \frac{128\pi e^{4}\mu}{\hbar(a\hbar)^{3}} \sum_{lm} \frac{Z^{2}d^{2l}}{((2l+1)!!)^{2}} \int_{0}^{+\infty} dE_{k'}k'^{2l-3} \frac{\sin^{2}\frac{(E_{k'}-E_{\Delta}+E_{b})t_{\circ}}{2\hbar}}{\left[\frac{E_{k'}-E_{\Delta}+E_{b}}{2\hbar}\right]^{2}}$$

$$= \frac{128\pi e^{4}\mu}{\hbar(a\hbar)^{3}} \sum_{lm} \frac{Z^{2}d^{2l}}{((2l+1)!!)^{2}} \left(\frac{2\mu}{\hbar^{2}}\right)^{(2l-3)/2}$$

$$\times \int_{0}^{+\infty} dE_{k'}E_{k'}^{(2l-3)/2} \frac{\sin^{2}\frac{(E_{k'}-E_{\Delta}+E_{b})t_{\circ}}{2\hbar}}{\left[\frac{E_{k'}-E_{\Delta}+E_{b}}{2\hbar}\right]^{2}},$$
(10.4.7.14)

where the matrix element in the first equality of Eq. (10.4.7.14) is approximately taken as

$$\left| < f | \sum_{j=1}^{Z} q_j^l Y_l^m(\theta_j \phi_j) | i > \right|^2 \approx Z^2 d^{2l},$$
 (10.4.7.15)

where *d* is the linear magnitude of the nucleus. The square of the matrix element occurring in Eq. (10.4.7.14) is proportional to the probability of the nuclear transition corresponding to an *El* multiple radiation. We must remind the reader that Eq. (10.4.7.14) was derived under the conditions  $v \ll c$ , and  $Ze^2/(\hbar v) \ll 1$ .

To seek the expression of Eq. (10.4.7.14), Some references calculate the integral in Eq. (10.4.7.14) by taking the following two approximations. First approximation is that the factor in the integrand  $E_{k'}^{(2l-3)/2}$  is taken as a constant independent of integration variable  $E_{k'}$ . Second approximation is to assume that  $t_{\circ}$  approaches to infinity. Then some authors find from Eq. (10.4.7.4) that

$$P_{all \leftarrow k}(t_{\circ} \to \infty) = \lim_{t_{\circ} \to \infty} t_{\circ} \frac{128Z^2 \pi e^4 \mu}{(\hbar a)^3} \sum_{lm} \frac{k^{2l-3} d^{2l}}{(2l+1)!!}.$$
 (10.4.7.16)

Eq. (10.4.7.16) is some author's formula to calculate the internal conversion process. The transition rate is

$$W_{all \leftarrow k}(t_{\circ} \to \infty) \equiv \frac{P_{all \leftarrow k}(t_{\circ} \to \infty)}{t_{\circ}} = \frac{64Z^2 \pi e^4 \mu}{(\hbar a)^3} \sum_{lm} \frac{k'^{2l-3} d^{2l}}{(2l+1)!!}.$$
 (10.4.7.17)

According to the two approximations made by some references the energy in internal conversion is conservative.

Comments for the above some references' treatment of the internal conversion. Generally speaking, the experimental value for time needed by one nucleus to emit one electron through internal conversion is only, for example  $10^{-7}$  second. Therefore, the  $t_{\circ} \rightarrow \infty$  should be bad. The approximation that neglects the energy dependence of  $E_{k'}^{(2l-3)/2}$  in Eq. (10.4.7.14) should be bad as well because the integration up limit is  $\infty$ . From the integrand of Eq. (10.4.7.14), it is possible that the larger the  $E_{k'}$  is, the larger the transition probability is. Therefore, let us try to establish a more exact internal conversion theory by using exact calculations.

The treatment of this textbook for the internal conversion is as follows. For simplicity, we consider parity-favored electric fourth multipole transition E4 (l = 4) in Eq. (10.4.7.14).

The factor  $E_k^{(2l-3)/2} = E_k^{5/2}$  in the integrand of Eq. (10.4.7.14) is strongly  $E_k$ -dependent. For element Bi, Z=83,  $E_b = 95.7 \times 10^3$  eV,  $E_{\Delta} = 5$  MeV, and the lifetime of excited nucleus  $t_o = 10^{-7} \ll \infty$  (second). It is obvious that if we abandon the two approximations taking by some references, then the theoretical results should be better. Therefore, let us continue our calculations.

The exact formula for internal conversion is Eq. (10.4.7.14). To keep that perturbation theory of D-C transition process holds water, we should take, for example, P = 0.05 << 1. In this case the up limit of integral in Eq. (10.4.7.14) should be finite. If we take that the down limit of integral is zero, then the integral should be timed by a factor 2. Numerical calculations give the up limit of integral is  $E_{k,up} = 6.4 \times 10^9$  erg =  $4 \times 10^{15}$  Mev, which is much larger than the excitation energy of nucleus  $E_{\Delta} = 5$  MeV, and even much larger than the Einstain's static mass energy of Bi nucleus  $M_{nucleus}c^2 = 0.3$  erg =  $0.3 \times 0.624 \times 10^6$ MeV.  $E_{k,up} = 2 \times 10^{10} M_{nucleus}c^2$ . If we rewrite Eq. (10.4.7.14) as

$$P \equiv \int_0^{E_{k,up}} P'(E_k) dE_k, \qquad (10.4.7.18)$$

then  $P'(E_k)$  represents the energy density of transition probability. From the expression of  $P'(E_k)$  in Eq. (10.4.7.14), we know that the larger the energy of ejected electron  $E_k$  is, the larger the value of  $P'(E_k)$  is, i. e., the ejected electron with higher energy has higher transition probability. Therefore, the internal conversation process is a strong energy nonconversation process.

It is also interesting to note that if the initial excited state of a nucleus transits to final ground state, and a  $\gamma$  photon is emitted, then the transition probability is proportional to (Refer to any textbook on nuclear physics for derivation)

$$P_{\gamma} \propto \int_{0}^{E_{k,up}} E_{k}^{2l+1} \frac{\sin^{2} \frac{(E_{k} - E_{\Delta})t_{\circ}}{2\hbar}}{\left[\frac{E_{k} - E_{\Delta}}{2\hbar}\right]^{2}} dE_{k}, \qquad (10.4.7.19)$$

where  $E_k$  represents the energy of one photon. Due to that the energy-dependence of factor  $E_k^{2l+1}$  in Eq. (10.4.7.19) is stronger than the factor  $E_k^{(2l-1)/2}$  in Eq. (10.4.7.14), the energy nonconservation in the internal conversion of ejecting  $\gamma$ -rays will be much stronger than that in the internal conversion of electron ejection.

Let us here make some discussions for the above calculations.

(1) Generally speaking, the energy is more or less not conservative in time-dependent and time-independent D-C quantum transition processes.

(2) We can obtain infinite energy from vacuum space in terms of some D-C transitions such as internal conversation of electron ejection. According to our exact calculations for the internal conversation of electron ejection above, the energy will be strongly not conservative.

The internal conversion process can be repeated by three steps:

(2.1) We get the ejected electron in the internal conversion;

(2.2) The ejected electron gives  $4 \times 10^{15}/2$  MeV energy to the environment, and then goes back to the original K-shell;

(2.3) The nucleus absorbs a photon with energy 5 Mev, and transits from the state of lower energy  $\Psi_f$  to the state of higher energy  $\Psi_i$ .

After the above three steps the internal conversion process can occur once again, and we can obtain energy  $E_{one-ejected-electron} = 4 \times 10^{15}/2$  MeV once again by energy loss of 5 MeV only.

If the volume of element Bi is 1 mm<sup>3</sup>, then this volume contains number of Bi atoms

$$N_{Bi} = \frac{9.78}{1000 \times 207 \times 1.6 \times 10^{-24}} = 2.95 \times 10^{19}.$$
 (10.4.7.20)

Assume that the number of the Bi nuclei, for which the internal conversion processes of electron ejection occur in the time interval of the lifetime  $t_{\circ} = 10^{-7}$  second, are only  $N_{ejected-nuclei} = 10^{-2} \times N_{Bi}$ . The energy of oil per gram is  $E_{oil} = 2.5 \times 10^{16}$  eV. The energy, obtained in one second from one mm<sup>3</sup> of Bi atoms, is  $E = E_{one-ejected-electron}N_{ejected-nuclei}/(t_{\circ}E_{oil}) = 4.5 \times 10^{23}$  ton of oil. This is a very high rate of energy generation. For example, everybody in our world can share in the energy about  $10^7$  tons of oil from internal conversation just in one second and in volume  $mm^3$ . Because this energy gain process in the internal conversion can be repeated, we can say that one can obtain infinite energy in terms of internal conversion transition process of electron ejection.

If we can obtain infinite energy from vacuum space, then the vacuum space has to have infinite energy.

(3) Although the high rate of energy generation is so inconceivable and unimaginable, but we have to emphasize that our theoretical result on the energy nonconservation in internal conversion transition process is absolutely reliable, the reason for which is very simple and obvious. Because our basic physical formula to calculate the internal conversion process is exactly the same as that in some references, and the sole difference between our method and the methods in some references is that we make exact numerical calculations without using the two "illegal" approximations, and some references always make the two "illegal". Here we say two "illegal" approximations because: (a). The  $|H_{if}|^2 \rho(E_k) \propto E_k^{5/2}$ in Eq. (10.4.7.14), which is strongly energy-dependent; (b).  $t_o \rightarrow \infty$  is non-physical.

(4) The light absorption in semiconductors are the particular verification for the energy nonconservation in D-C quantum transition process.

(5) According to famous Einstein formula, static mass  $m_{nucleus}$  can be transformed into energy  $m_{nucleus}c^2$ , and at the same time  $m_{nucleus}$  vanishes into the void. However, according to our theory of internal conversation of electron ejection, one excited Bi (or other) nucleus can produce energy  $10^{12} \times m_{Bi-nucleus}c^2 = 1.5 \times 10^{17}m_{free-electron}$ , and at the same time  $m_{Bi-nucleus}$  still exist after transition process.

(6) The reasons that why the energy nonconservation in D-C transition has not yet been reported in a large number are as follows:

(6.1) The until now experiments of the internal conversations are confined to measure the number of the ejected electrons. Therefore, the energy nonconservation cannot be discovered;

(6.2) The until now experiment of the internal conversations are confined to measure low angular quantum number, for which the effect of energy nonconservation is not large;

(6.3) Although some references gave also the curve of transition probability versus energy, which has contained small energy nonconservation, but some references think that the second peak in this curve is too low, and therefore can be neglected in any case. Therefore, the present controversial issue is not that the nonconservation has not yet been reported in a large number, but is that can one neglect the nonconservation just due to its littleness in special case of  $\beta = 0$ ? The obvious answer is: Cannot.

(7) Warning! We have given in this section that the energy, obtained in one second from one mm<sup>3</sup> of Bi atoms contained excited nuclei, is  $E = 4.5 \times 10^{21}$  ton of oil. This is a very high rate of energy generation, and absolute value of energy is also too high. It is well known, in energy aspect, one ton of oil =  $10^{-4}$  ton of TNT. Therefore,  $E = 4.5 \times 10^{17}$  ton of TNT in energy. From this estimation we know that to use many exited Bi nuclei to verify our theoretical prediction has to be prohibited. We give readers an other estimation. The energy of only one ejected electron released in  $t_0 = 10^{-7}$  second by just one exited Bi nucleus is equivalent to 150 Kg of oil. We sincerely hope that the readers consider our estimations.

# 10.5. General Theory of Transition Processes

## 10.5.1. Other Examples of Energy Nonconservation in Transition Process

Example (1).

A charged particle with charge q and mass  $\mu$  is placed in the harmonic oscillator potential of angular frequency  $\omega$ , and is in ground state  $|0\rangle$ . A finite pulse of spatially uniform electric field is applied to it.

$$H'(t) = -qx \mathsf{E}e^{-t^2/\tau^2},\tag{10.5.1.1}$$

where E is electric field intensity,  $\tau$  is the pulse duration. In the approximation of week field,

(1.1) Find the transition probability from the ground state to one of the excited oscillator states  $|n\rangle$  after the pulse;

(1.2) Discuss the condition of producing transition;

(1.3) Discuss that if the energy in transition process is not conservative.

Solution:

(1.1) The transition probability amplitude is

$$a_{n\circ}^{(1)} = \frac{1}{i\hbar} \int_{-\infty}^{\infty} (-q\mathsf{E}) < n|x|0 > e^{-t^2/\tau^2 + i\omega_{n\circ}t} dt, \qquad (10.5.1.2)$$

where  $\omega_{n\circ} = (E_n - E_{\circ})/\hbar = n\omega$ , and  $\langle n|x|0 \rangle = \sqrt{\hbar/(2\mu\omega)}\delta_{n1}$ , which means that the particle can only transit to the first exited state. We have

$$a_{n\circ}^{(1)} = \frac{-q\mathsf{E}}{i\hbar} \sqrt{\frac{\hbar}{2\mu\omega}} \int_{-\infty}^{\infty} dt e^{-t^2/\tau^2 + i\omega t} = iq\mathsf{E}\sqrt{\frac{1}{2\mu\hbar}} \sqrt{\pi}\tau e^{-\omega^2\tau^2/4}.$$
 (10.5.1.3)

Therefore the transition probability from |0> to |1> is

$$P_{10} = |a_{10}^{(1)}|^2 = \frac{q^2 \mathsf{E}^2}{2\mu\hbar\omega} \pi \tau^2 e^{-\omega^2 \tau^2/2}.$$
 (10.5.1.4)

The probability that the particle stays still in the ground state  $|0\rangle$  is  $1 - P_{10}$ .

(1.2) If the time duration  $\tau$  is large enough so that  $\omega \tau >> 1$ , than  $P_{10} \rightarrow 0$ , i. e., the transition does not occur.

(1.3) In the transition process the total momentum transfer by the pulse is

$$P = \int_{-\infty}^{\infty} dt q \mathsf{E} e^{-t^2/\tau^2} = \sqrt{\pi} q \mathsf{E} \tau.$$
 (10.5.1.5)

In one transition the particle gets energy from electric field is

$$\Delta E = \hbar \omega P_{10} = \hbar \omega \frac{q^2 \mathsf{E}^2}{2\mu \hbar \omega} \pi \tau^2 e^{-\omega^2 \tau^2/2} = \frac{P^2}{2\mu} e^{-\omega^2 \tau^2/2}.$$
 (10.5.1.6)

Comparing Eq. (10.5.1.6) with Eq. (10.5.1.5), we find that in the real transition process the energy is not conservative due to the factor  $exp(-\omega^2 \tau^2/2)$  in Eq. (10.5.1.6).

 $\tau \to 0$  means the time duration of the field as a perturbation approaches zero, i. e., the transition does not occur.

 $\tau \rightarrow \infty$  means the time duration of the field as a perturbation is infinite. Eq. (10.5.1.4) tells us that this transition does not occur. The physical basis lies in the fast oscillating character of the motion. The action of the field is compensated during different parts of the period. This is a general rule that slow changing (i. e., adiabatic) tail to excite the system. Instead, the system remains in its original state with the wavefunction adiabatically adjusting to the slow changing perturbation and coming back after the perturbation is switched off.

Example (2).

Free hydrogen atom Hamiltonian  $H_{\circ}$ , Energy level  $E_n$ , energy eigenstate  $\Psi_n$  (for brevity, set *n* denote three quantum numbers *nlm*.). The eigenequation is

$$H_{\circ}\Psi_n = E_n\Psi_n. \tag{10.5.1.7}$$

Take the electric field direction as z axis. Perturbation Hamiltonian is

$$H' = e\mathbf{E}(t) \cdot r = e\mathbf{E}z\delta(t). \tag{10.5.1.8}$$

Find

(2.1) The total transition probability from ground state to all possible excited states;

(2.2) Discuss if the energy is nonconservative.

Solution: (2.1) In electric field

$$i\hbar\frac{\partial}{\partial t}\Psi(r,t) = (H_{\circ} + H')\Psi(r,t). \qquad (10.5.1.9)$$

Initial condition is

$$\Psi(r,0) = \Psi_{100}(r) \equiv \Psi_1(r). \tag{10.5.1.10}$$

Set

$$\Psi(r,t) = \sum_{n} a_n(t) \Psi_n(r) e^{-iE_n t/\hbar}.$$
 (10.5.1.11)

Initial condition rewrites as

$$a_n(0^-) = \delta_{n1}. \tag{10.5.1.12}$$

Substituting Eq. (10.5.1.12) into Eq. (10.5.1.9), taking  $H'\Psi \approx H'\Psi_1$  (H' is a week perturbation), one obtains

$$\sum_{n} i\hbar\Psi_n \frac{da_n}{dt} e^{-iE_n t/\hbar} = H'\Psi_1 = e E z \Psi_1 \delta(t).$$
(10.5.1.13)

Multiplying the left hand side of Eq. (10.5.1.12) by  $\Psi_n^*$ , and integrating over whole space yield

$$i\hbar \frac{da_n}{dt} = e \mathbb{E} z_{n1} \delta(t) e^{iE_n t/\hbar}.$$
(10.5.1.14)

Making integration over *t* from  $-\infty \rightarrow \infty$  yields

$$a_n(t) = \frac{eE}{i\hbar} z_{n1}.$$
 (n \ne 1) (10.5.1.15)

Therefore, after the action of the pulse electric field the transition probability to  $\Psi_n$  state is

$$P_n = |a_n(t)|^2 = \frac{e^2 \mathbf{E}^2}{\hbar^2} |z_{n1}|^2.$$
(10.5.1.16)

According to the selection rule ( $\Delta l = 1, \Delta m = 0$ ), the quantum numbers of final states have to be (nlm) = (n10), i. e., electron can only transits to np states (l = 1, m = 0).

The total transition probability to all possible excited states is

$$\sum_{n}^{\prime} P_{n} = |a_{n}(t)|^{2} = \frac{e^{2} E^{2}}{\hbar^{2}} \sum_{n}^{\prime} |z_{n1}|^{2} = \frac{e^{2} E^{2}}{\hbar^{2}} \left( \sum_{n} |z_{n1}|^{2} - |z_{11}|^{2} \right), \quad (10.5.1.17)$$

where  $z_{11} = \langle \Psi_{100} | z | \Psi_{100} \rangle = 0$  (because z is odd parity operator).

$$\sum_{n} |z_{n1}|^{2} = \sum_{n} \langle \Psi_{100} | z | \Psi_{n} \rangle \langle \Psi_{n} | z | \Psi_{100} \rangle$$
  
=  $\langle \Psi_{100} | z^{2} | \Psi_{n} \rangle = \frac{1}{3} \langle \Psi_{100} | r^{2} | \Psi_{100} \rangle = a_{\circ}^{2},$  (10.5.1.18)

where  $a_{\circ}$  is the Bohr radius. Substituting Eq. (10.5.1.18) into Eq. (10.5.1.17) yields

$$\sum_{n}^{\prime} P_{n} = |a_{n}(t)|^{2} = \frac{e^{2} \mathrm{E}^{2} a_{\circ}^{2}}{\hbar^{2}}.$$
(10.5.1.19)

The probability that the electron stays still in the ground state  $|\Psi_1\rangle$  is  $1 - \sum_{n=1}^{n} P_n$ .

(2.2) In the transition process the total momentum, transferred by the electric field pulse, is  $\int_{-\infty}^{\infty}$ 

$$P = \int_{-\infty}^{\infty} dt (-e\mathsf{E}\delta(t)) = -e\mathsf{E}.$$
 (10.5.1.20)

In the transition process the total energy, transferred by the electric field pulse, is

$$E_{field,total} = \frac{e^2 \mathsf{E}^2}{2\mu}.$$
 (10.5.1.21)

When the electron transits to all possible excited states from ground state under the action of the electric pulse perturbation, the electron gets energy

$$\Delta E = \sum_{n}^{\prime} (-E_{n})P_{n} = \sum_{n} [-E_{n} - (-E_{\circ})]P_{n}$$

$$= \sum_{n} \frac{e^{2}}{2a_{\circ}} \left(\frac{1}{n^{2}} - \frac{1}{1^{2}}\right) \left(\frac{e\mathsf{E}}{\hbar}\right)^{2} |z_{n1}|^{2}$$

$$= \frac{e^{2}}{2a_{\circ}} \left(\frac{e\mathsf{E}}{\hbar}\right)^{2} \sum_{n} \left(\frac{1}{n^{2}} - 1\right) | < \Psi_{n} |z| \Psi_{100} > |^{2}$$

$$= \frac{e^{2}}{2a_{\circ}} \left(\frac{e\mathsf{E}}{\hbar}\right)^{2} \sum_{n} \left(\frac{1}{n^{2}} - 1\right) a_{\circ}^{2}$$

$$= \frac{e^{2}a_{\circ}}{2} \left(\frac{e\mathsf{E}}{\hbar}\right) \left(\frac{\pi^{2}}{6} - 1\right)$$

$$= \frac{e^{2}\mathsf{E}^{2}}{2\mu} \left(\frac{\pi^{2}}{6} - 1\right) \approx 0.5E_{field,total}, \qquad (10.5.1.22)$$

where Bohr radius  $a_{\circ} = \hbar^2/(\mu e^2)$ , and the forth equality comes from Eq. (10.5.1.18).

#### 10.5.2. More General Theory of Transition Processes

**Theorem XXXXI: Energy nonconservation in transition processes.** In quantum transition processes the energy is more or less not conservative except some physical conditions are imposed.

**Proof.** We use two methods to prove this important theorem. First method is not exact. Second method is exact in the sense of first order time-dependence perturbation approximation.

First method. The formula of transition probability given by Eq. (10.2.1.4), which is quoted as follows:

$$P_{k'k}(t) = P_{k'k}^{(1)}(t) = |a_{k'k}^{(1)}(t)|^2 = \frac{1}{\hbar^2} \left| \int_0^t e^{i\omega_{k'k}t} H_{k'k}'(t) dt \right|^2$$
  
=  $\frac{1}{\hbar^2} \left| \int_0^t e^{i(E_{k'} - E_k)t/\hbar} < E_{k'} |H'(t)| E_k > dt \right|^2,$  (10.5.2.1)

where H'(t) is a nonperiodic external perturbation. If the transition process of a system from state  $|k\rangle$  to  $|k'\rangle$  is energy conservation, then the following energy conservation equation has to hold water:

$$\Delta E = E_{external}, \tag{10.5.2.2}$$

where  $E_{external}$  is the energy transfer from the external perturbation into the system, and  $\Delta E$  is the energy obtained in the transition processes from the initial state  $|k\rangle$  of the system to all possible final states of the system.

$$\Delta E = \sum_{k' \neq k} E_{k'} P_{k'k}(t) = \sum_{k'} (E_{k'} - E_k) P_{k'k}(t).$$
(10.5.2.3)

To seek  $E_{external}$ , we can at first find the momentum transfer P (Note that P is no relation with the probability.) by external perturbation

$$P(t_{\circ}) - P(0) = \int_{0}^{t_{\circ}} dt |F|, \qquad (10.5.2.4)$$

where **F** is the force applied on the system by external perturbation, and  $F = -\nabla H'$ .

$$E_{external} = \frac{P^2(t_{\circ})}{2\mu} - \frac{P^2(0)}{2\mu}.$$
 (10.5.2.5)

Eqs. (10.5.2.4-5) are completely independent of Eq. (10.5.2.3). Therefore, transition process does not satisfy generally the energy conservation equation Eq. (10.5.2.2).

Second method. Use Eq. (10.4.3.14). We write the Eq. (10.4.3.14) as the following Eq. (10.5.2.6).

$$P_{k'k}(t \ge T) = |a_{k'k}^{(1)}(t \ge T)|^{2} = \left|\frac{1}{i\hbar}\int_{0}^{T} e^{i\omega_{k'k}t'}H_{k'k}'(t')dt'\right|^{2}$$

$$= \left|\frac{1}{i\hbar}\frac{1}{\sqrt{2\pi}}\int_{0}^{T}dt'e^{i\omega_{k'k}t'}\int_{-\infty}^{\infty}d\omega H_{k'k}'(\omega)e^{-i\omega t}\right|^{2}$$

$$= \left|\frac{1}{i\hbar}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}d\omega H_{k'k}'(\omega)\int_{0}^{T}dt'e^{i(\omega_{k'k}-\omega)t'}\right|^{2}$$

$$= \left|\frac{1}{i\hbar}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}d\omega H_{k'k}'(\omega)\frac{exp[i(\omega_{k'k}-\omega)T]-1]}{i(\omega_{k'k}-\omega)}\right|^{2}$$

$$= \left|\frac{1}{i\hbar}\int_{-\infty}^{\infty}d\omega H_{k'k}'(\omega)\frac{exp[i(\omega_{k'k}-\omega)T/2]}{(\omega_{k'k}-\omega)^{0}}\right|^{2}$$

$$= \frac{4}{\hbar^{2}}\frac{1}{2\pi}\left|\int_{-\infty}^{\infty}d\omega H_{k'k}'(\omega)\frac{sin[(\omega_{k'k}-\omega)T/2]}{\omega_{k'k}-\omega}\right|^{2}, \quad (10.5.2.6)$$

where  $|k'\rangle$  and  $|k\rangle$  represent the quantum states of discrete spectra. For free particles, we use box normalization, and thus Eq. (10.5.2.6) can also be use to free particles. The H'(t)

in Eq. (10.5.2.6), i. e., Eq. (10.4.3.14), generally, has three cases. Correspondingly, Eq. (10.5.2.6) becomes the following results:

$$P_{k'k}(t \ge T) = \begin{cases} \frac{4}{\hbar^2} \frac{1}{2\pi} \left| \int_{-\infty}^{\infty} d\omega H'_{k'k}(\omega) \frac{\sin[(\omega_{k'k} - \omega)T/2]}{\omega_{k'k} - \omega} \right|^2 \\ if H' = H'(x, t); \\ \frac{4}{\hbar^2} \left| V_{k'k}(\omega) \frac{\sin[(\omega_{k'k} \pm \omega)T/2]}{\omega_{k'k} \pm \omega} \right|^2 \\ if H' = V(x) \exp(\pm i\omega t); \\ \frac{4}{\hbar^2} \left| V_{k'k}(\omega) \frac{\sin[(\omega_{k'k})T/2]}{\omega_{k'k}} \right|^2 \\ if H' = V(x) \end{cases}$$
(10.5.2.7)

The three formulas in Eq. (10.5.2.7) show that we can only say that for the transition processes between any assigned two states, the transition of energy conservation is not definitely of the largest probability. We explain this point in detail as follows.

If we ask that what is the transition probability from an assigned initial state  $|k\rangle$  to a possible final states under the perturbation H'(t), for this possible final state the transition of energy nonconservation can have the largest probability. The transition probabilities from an assigned initial state  $|k\rangle$  to any possible final states under the perturbation H'(t) are:

$$\sum_{k' \neq k} P_{k'k}(t \ge T) = \begin{cases} \sum_{k' \neq k} \frac{4}{\hbar^2} \frac{1}{2\pi} \left| \int_{-\infty}^{\infty} d\omega H'_{k'k}(\omega) \frac{\sin[(\omega_{k'k} - \omega)T/2]}{\omega_{k'k} - \omega} \right|^2 \\ if H' = H'(x,t); \\ \sum_{k' \neq k} \frac{4}{\hbar^2} \left| V_{k'k} \frac{\sin[(\omega_{k'k} \pm \omega)T/2]}{\omega_{k'k} \pm \omega} \right|^2 \\ if H' = V(x,t) \exp(\pm i\omega t); \\ \sum_{k' \neq k} \frac{4}{\hbar^2} \left| V_{k'k} \frac{\sin[(\omega_{k'k})T/2]}{\omega_{k'k}} \right|^2 \\ if H' = V(x) \end{cases}$$
(10.5.2.8)

In Eq. (10.5.2.8) the magnitude of  $\sum_{k' \neq k} P_{k'k}(t \ge T)$  is determined by two factors, for example,

$$|V_{k'k}|^2 \left| \frac{\sin[(\omega_{k'k} \pm \omega)T/2]}{\omega_{k'k} \pm \omega} \right|^2 \equiv |V_{k'k}|^2 \times I,$$
(10.5.2.9)

other than just by the factor *I*. In this case, if, for example,  $|V_{k'k}|^2 \propto \omega_{k'}^3$ , then it is obvious that the larger the  $\omega_{k'}$  is, the larger the transition probability from  $|k\rangle$  to this special  $|k'\rangle$  is. QED.

Comment 1: Although in some cases the magnitudes of the energy nonconservation is not large, but we should have an estimation for the magnitude of the energy nonconservation. Especially, in some cases the magnitude of energy nonconservation might be huge. In some processes, such as stimulated emission, the energy conservation is a physical requirement, and thus in these cases we have to impose the energy conversation condition to the transition formula before calculations.

Comment 2: The energy nonconservation in transition processes does not violate the energy conservation proved in chapter 5. The latter says that if H has homogeneity (or
uniformity) of time, then  $\partial H/\partial t = 0$ , and thus dE/dt = 0 from

$$\frac{d\langle H\rangle}{dt} = \frac{dE}{dt} = \left\langle \frac{i}{\hbar} [H, H] + \frac{\partial H}{\partial t} \right\rangle = 0.$$
(10.5.2.10)

The condition to obtain Eq. (10.5.2.10) is that the variation of state with time obeys the time-dependent Schrödinger equation. However, in the case time-dependent transition the system is in external time-dependent perturbation, the time is no longer of homogeneity. On the other hand, the transition between initial and final states is determined by the time-dependent transition probability instead of the time-dependent Schrödinger equation. More simply speaking, in quantum transition process,  $\partial H/\partial t \neq 0$ .

Comment 3: The energy sources of energy nonconservation come from vacuum space because the energy dependence of  $|H'_{k'k}|^2 = |V_{k'k}|^2$  in Eq. (10.5.2.8) or  $|H'_{k'k}\rho(k')|^2$  in Eq. (10.3.2.4) determines the energy nonconservation of transition process. The particular energy dependence of  $|H'_{k'k}|^2\rho(k')$  is determined by the wavefunctions in states  $|k\rangle$  and  $|k'\rangle$ , the form of the perturbation Hamiltonian H', and density of states, which are all dependent on the space structure such as dimensions, and so on. We name  $|H_{k'k}|^2\rho(k')$  vacuum energy support ability.

At the end of this chapter 10, I would like to tell the readers that some references treat the quantum transition problems by using a method, which can be called "cutting up with one time knife". According to this method, all transition processes obey the Fermi golden rule, and, correspondingly, keep the energy conservation.

However, according to the theorem in this subsection, we should consider the energy dependence of  $|H'_{k'k}|^2\rho(k')$  on k'. If the dependence of k' is weak, then we can obtain the time independence of the transition rate, i. e., Fermi golden rule. However, even in the case of approximate time independence of transition rate, the physics between our textbook and some references still has differences. Some references deduce the energy conservation under the hypotheses that duration time of perturbation  $T = (t_0 - 0) \rightarrow \infty$ . On the contrary, this textbook deduces Fermi golden rule without using finite duration time of perturbation.

**Theorem XXXXII: Zero initial transition rate**: The initial transition rate of any nonstable system is certainly zero.

Proof. The survival probability of any nonstable system can be defined as

$$P(t) = |\langle \Psi(0)|\Psi(t)\rangle|^{2}.$$
 (10.5.2.11)

This theorem means

$$\left. \frac{dP(t)}{dt} \right|_{T=0} = 0. \tag{10.5.2.12}$$

The proof for Eq. (10.5.2.12) is as follows: (Refer to Ref. [114].)

$$\frac{d|\Psi(t)>}{dt} = \frac{1}{\hbar}H(t)|Psi(t)>,$$
(10.5.2.13)

and

$$\frac{d < \Psi(t)|}{dt} = -\frac{1}{\hbar} < Psi(t)|.$$
(10.5.2.14)

Therefore,

$$\begin{aligned} \frac{dP(t)}{dt} &= <\Psi(0) \left\{ \frac{d}{dt} |\Psi(t) > \right\} < \Psi(t) |\Psi(0) > +h.c \\ &= \frac{1}{i\hbar} < \Psi(0) |H(t)| \Psi(t) > < \Psi(t) |\Psi(0) > +h.c \\ &\stackrel{t \to 0}{=} 0. \end{aligned}$$
(10.5.2.15)

QED.

Although the above derivations are the same as that in Ref. [114], the physical cause of this theorem is different between this textbook and Ref. [114]. Ref. [114] argues that this theorem is correct just for particle ensemble, and makes many arguments.

On the contrary, this textbook thinks that this theorem is for individual particle. The reasons are as follows:

(i). In this textbook, we think from beginning to end that wavefunction, state, and Schrödinger equation belong to individual particle;

(ii). The theorem can be proved also as follows.

$$\frac{dP(t)}{dt} = \frac{dP_{k' \leftarrow k}(t)}{dt} = \frac{d}{dt} \frac{1}{\hbar^2} \left| \int_0^t dt' < k' |H'(t')| k > \right|_{t=0}^2 = 0$$

#### 10.5.3. Quantum Zeno Effect

**Theorem XXXXIII: Quantum Zeno effect.** The survival probability of a nonstationary initial state increases with increase of observation times *n* in finite time interval  $t = n\delta t$ , where  $\delta t$  represents the time interval between two time observations (i. e., the time interval producing transition) and in continuous transition case, i. e.,  $n \to \infty$  and  $\delta t \to 0$ , the nonstationary state will stop decay or transition, i. e.,

$$P_{ex \to gr,n} \stackrel{n \to \infty}{\overset{\delta t \to 0}{\longrightarrow}} 1.$$

**Proof.**  $n\delta t = infinite$  and  $n \to \infty, \delta t \to 0$  is called continuous observation of transition process. Consider, for example, the spontaneous emission of an  ${}^{9}Be^{+}$  ion [134]. The transition probability from excited state to ground state and emitting a photon with frequency  $\omega$  during time interval  $\delta T$  is

$$P_{ex \to gr}(\delta t) \equiv A \int_0^\infty d\omega |H'_{gr,ex}|^2 \rho(\omega) \frac{\sin^2(\omega_{gr,ex} + \omega)\delta t/2}{(\omega_{gr,ex} + \omega)^2} \stackrel{\text{sum}}{\equiv} B(\delta t)^2, \ B > 0.$$
(10.5.3.1)

chant

If the duration time  $\delta t$  is short, then we obtain the last equality of Eq. (10.5.3.1).

If we make observations to know if the ion is still in the excited state in finite time interval  $n\delta t$ , and make *n* time observations, then the survival probability that the ion keeps in excited state is [60]

$$\lim_{n \to \infty} \left\{ P_n(t) = \left[ 1 - B\left(\frac{t}{n}\right)^2 \right]^n \to e^{-Bt^2/n} = e^{-Bt(\delta t)^2/2} \right\} \stackrel{\delta t \to 0}{=} 1, \quad (10.5.3.2)$$

which means that the continuous observations will stop the transition or the decay. This phenomenon is called quantum Zeno effect [103, 114]. The observed data are if n = 64, then  $P_{n=64} = C$ , and if n = 1, then  $P_{n=1} = 0.09C$ . Therefore, experiment confirmed Zeno effect.

Quantum Zeno effect needs  $P_{ex \to gr} \equiv Bt^{\alpha}$  ( $\alpha > 1$ ), which indicates that the Fermi golden rule is not correct, and further indicates indirectly that the energy in transition process is not conservative.

Quantum Zeno effect is a present interesting subject. Readers can refer to Refs. [103, 114]. The quantum Zeno effect was proposed as a paradox by Refs. [135]. All until now references and textbooks like to connect the so-called measurement with Zeno effect. However, according to our statement and proof of Zeno effect, it is not necessary to connect measurements with Zeno effect.

### 10.6. Exercises and Solutions

(1) This exercise is for subsection 10.3.1.

Eq. (10.3.1.3) can be found in some references, such as Refs. [1, 103]. We would like to say that our understanding for the Eq. (10.3.1.3) is different from some references in both physical and mathematical aspects. For reader to make clear distinction between right and wrong, to be skilful at transition theory, and to have significant contributions in both energy sources and quantum mechanics, as an exercise we require readers to know theory of transition probability and transition rate, given by some references, and make comments for these theories in both physics and mathematics.

Some references, such as Refs. [1], use the mathematical formula

$$\lim_{t \to \infty} \frac{\sin^2 xt}{x^2} = \lim_{t \to \infty} \pi t \,\delta(x),\tag{1}$$

or, such as Refs. [103], use mathematical formula equivalent to Eq. (1), and obtain from Eq. (10.3.1.3)

$$P_{k'k}(t \to \infty) = \lim_{t \to \infty} \frac{|H'_{k'k}|^2}{\hbar^2} \frac{\sin^2[(\omega_{k'k} - \omega)t/2]}{[(\omega_{k'k} - \omega)/2]^2}$$
  
$$= \lim_{t \to \infty} \frac{2\pi |H'_{k'k}|^2 t}{\hbar^2} \delta(\omega_{k'k} - \omega)$$
  
$$= \lim_{t \to \infty} \frac{2\pi |H'_{k'k}|^2 t}{\hbar} \delta(E_{k'} - E_k - \hbar\omega).$$
(2)

Some references obtain the corresponding transition rate from initial state  $|k\rangle$  to state  $|k'\rangle$  is

$$w_{k'k}(t \to \infty) = \lim_{t \to \infty} \frac{d}{dt} P_{k'k}(t \to \infty) = \frac{2\pi |H'_{k'k}|^2}{\hbar^2} \delta(\omega_{k'k} - \omega)$$
$$= \frac{2\pi |H'_{k'k}|^2}{\hbar} \delta(E_{k'} - E_k - \hbar\omega).$$
(3)

The delta function in the some references's Eq. (3) represents the energy conservation in the quantum transition process. That the  $w_{k'k}$  does not depend on time is the so-called Fermi golden rule.

As is well known, the  $\delta(x)$  function in Eqs. (2-3) is a distribution function of x, i. e., x is a continuous variable distributed in the range  $-\infty < x < +\infty$ , and the dimension of  $\delta(x)$  is [1/x]. Therefore,  $\omega_{k'}$  can continuously vary. Ref. [1] suggests a method to take out the  $\delta$  function from Eqs. (2) and (3). Ref. [1] introduces density of states  $\rho(k')$ , puts  $\rho(k')$  into Eqs. (1-2), and makes integration, and obtains:

$$P_{k'k}(t \to \infty) = \lim_{t \to \infty} \frac{2\pi |H'_{k'k}|^2 t}{\hbar} \rho, \quad w_{k'k}(t \to \infty) = \frac{2\pi |H'_{k'k}|^2}{\hbar} \rho. \tag{2-3}$$

Here we finish the introductions on the derivations for the transition probability and transition rate by some references.

Solution:

We make some comments for the above derions in Eqs. (2-3), or, in other words, makes some comments for some references's transition theory:

(1.1) The limit  $t \to \infty$  in the second equality of Eq. (2) violates the validity of perturbation theory because of the unlimited growth of the transition probability;

(1.2) The limit  $t \to \infty$  in Eq. (2) is not physical, because any physical transition process has a finite lifetime. For example, for many transition processes in atoms the observed lifetime is  $10^{-10} - 10^{-7} << \infty$  second;

(1.3) Some references, such as Refs. [103], think that if the physics of the condition of long time limit is in that the duration time *t* of periodic perturbation is considerably greater than typical period  $2\pi/(\omega_{k'} - \omega_k)$ .

Let us give readers a numerical example to explain that  $t >> 2\pi/(\omega_{k'} - \omega_k)$  does not satisfy the condition of long time approximation. It is clear from Eq. (13.1.4.1.9) that the exact mathematical condition of the long time approximation is  $(\omega_{k'k} - \omega)t >> 1$  other than  $\omega_{k'k}t >> 1$ . Take  $\hbar\omega_{k'} - \hbar\omega_k = 5 - 4 = 1 eV$ . According to some references the condition of long time approximation is  $t >> 2\pi/(\omega_{k'} - \omega_k) = 2\pi\hbar/(E_{k'} - E_k) = 2\pi\hbar/(1.602 \times 10^{-12}) = 4.118 \times 10^{15}$  second. Because some references think that from the condition  $\omega_{k'k}t >> 1$  one can obtain  $\hbar\omega_{k'} - \hbar\omega_k - \hbar\omega = 0$ . To make numerical comparison, let us take  $\hbar\omega_{k'} - \hbar\omega_k - \hbar\omega = 0.001 \ eV$ . From the exact mathematical condition of the long time approximation, one can obtain that  $t >> 2\pi\hbar/(\hbar\omega_{k'} - \hbar\omega_k - \hbar\omega) = 2\pi\hbar/(0.001 \ eV) = 2\pi\hbar/(0.001 \times 1.602 \times 10^{-12}) = 1000 \times 4.118 \times 10^{15}$  second. It is clear that  $t >> 4.118 \times 10^{15}$  second cannot ensure  $t >> 1000 \times 4.118 \times 10^{15}$  second;

(1.4) Some references, such as Refs. [103], think that the conclusions of quantum transition theory represent behavior of quantum ensemble.

On the contrary, our transition theory thinks that any conclusion, including that from quantum transition theory, in quantum mechanics represents the individual behavior of the studied system;

(1.5) Some references, such as Refs. [103], think that the conclusions of quantum transition theory do not change, if  $|H'_{k'k}|^2$  is a smooth function of k' and k.

On the contrary, we think that if  $|H'_{k'k}|^2$  is a smooth function of  $E_{k'} - E_k$ , then the problems in some references's transition theory are even more serious. Let us cite an exemple to illustrate why. Let us consider the energy dependence of  $|H'_{k'k}|^2 = |H''|^2 (E_{k'} - E_k)^{1-\beta}$ , and calculate  $P_{all \leftarrow k}$ , which represents transition probability from initial state  $|k\rangle$  to all possible final states of the system. To avoid the mathematical divergence, in the following calculations we take  $\beta = a \rightarrow 0$ .

$$\begin{split} P_{all \leftarrow k}(t \rightarrow \infty) &\equiv \lim_{t \rightarrow \infty} \sum_{k' \neq k} P_{k'k}(t) \\ &\approx \lim_{t \rightarrow \infty} \int_{-\infty}^{+\infty} d\omega_{k'} \overline{\rho(\omega_{k'})} P_{k'k}(t) \\ &= \lim_{t \rightarrow \infty} \int_{-\infty}^{+\infty} d\omega_{k'} \overline{\rho(\omega_{k'})} \frac{4|H'_{k'k}|^2}{\hbar^2} \left[ \frac{\sin[(\omega_{k'} - \omega_k - \omega)t/2]}{(\omega_{k'k} - \omega)} \right]^2 \\ &= \lim_{t \rightarrow \infty} \frac{4|H''|^2}{\hbar^2} \overline{\rho(\omega_{k'})} \int_{-\infty}^{+\infty} d\omega_{k'} (\omega_{k'} - \omega_k)^{1-\beta} \\ &\left[ \frac{\sin[(\omega_{k'} - \omega_k - \omega)t/2]}{(\omega_{k'k} - \omega)} \right]^2 \\ &= \lim_{t \rightarrow \infty} \frac{4|H''|^2}{\hbar^2} \overline{\rho(\omega_{k'})} \\ &\int_{-\infty}^{+\infty} d\omega_{k'} \frac{t}{2} \left[ (\omega_{k'} - \omega_k - \omega)^{1-\beta} + \omega^{1-\beta} \right] \frac{t}{2} \\ &\left[ \frac{\sin[(\omega_{k'} - \omega_k - \omega)t/2]}{(\omega_{k'k} - \omega)t/2} \right]^2 \\ &= \lim_{t \rightarrow \infty} \frac{4|H''|^2}{\hbar^2} \overline{\rho(\omega_{k'})} \int_{-\infty}^{+\infty} d\omega_{k'} \frac{t}{2} \left\{ t^{\beta} \frac{\sin^2[(\omega_{k'} - \omega_k - \omega)t/2]}{[(\omega_{k'} - \omega_k + \omega)t/2]^{1+\beta}} \\ &+ \frac{\omega^{1-\beta}t}{2} \frac{\sin^2[(\omega_{k'} - \omega_k - \omega)t/2]}{[(\omega_{k'} - \omega_k + \omega)t/2]^2} \right\} \\ &= \lim_{t \rightarrow \infty} \frac{4|H''|^2}{\hbar^2} \overline{\rho(\omega_{k'})} \left[ t^{\beta} \int_{-\infty}^{+\infty} dx \frac{\sin^2 x}{x^{1+\beta}} + \frac{\omega^{1-\beta}t}{2} \int_{-\infty}^{+\infty} dx \frac{\sin^2 x}{x^2} \right] \\ &= \lim_{t \rightarrow \infty} \frac{4|H''|^2}{\hbar^2} \overline{\rho(\omega_{k'})} \left[ \frac{-2t^{\beta}\Gamma(-\beta)\cos(\beta\pi)/2}{2^{1-\beta}} + \frac{\omega^{1-\beta}t\pi}{2} \right] \end{split}$$

$$= \lim_{t \to \infty} \frac{4|H''|^2}{\hbar^2} \overline{\rho(\omega_{k'})} \left[ \frac{-2t^{\beta} \Gamma(-\beta)}{2} + \frac{\omega^{1-\beta} t\pi}{2} \right]$$
  
$$= I + II \quad (\beta = a \to 0). \tag{4}$$

The second term is recognized by some references as a term corresponding to energy conservation transition. Even though we agree with some references's this opinion, the first term belongs definitely to energy nonconservation transition. Due to that the  $\beta$  can be very small and  $\Gamma(-0) = -\infty$ , the probability of energy nonconservation transition can, in principle, much larger than that of the energy conservation transition;

(1.6). The oscillation factor in Eqs. (2) and (10.3.1.3),  $sin^2[(\omega_{k'k} - \omega)t/2]/[(\omega_{k'k} - \omega)/2]^2$ , gives that the first peak is at  $\omega_{k'k} - \omega = 0$ , the height of the first peak is very height, and the first zero point is at  $(\omega_{k'k} - \omega)t/2 = \pm \pi$  (For example, see our Fig. 10.1 or Fig. 2.1 in Ref. [103]). From these features of the oscillation factor, some references confirm that:

(1.6.1) The quantum transition process is energy-conservative;

(1.6.2) The width  $2 \times (\omega_{k'k} - \omega)t/2 = \pi$  between two zero points  $((\omega_{k'k} - \omega)t/2 = -\pi$  and  $(\omega_{k'k} - \omega)t/2 = \pi)$  comes from Heisenberg uncertainty relation, and thus does not need to be considered;

(1.6.3) (The height of the first peak):(The height of the second peak) $\approx 22$ . Thus, some references think that although the oscillation factor does not equal zero at  $|\omega_{k'k} - \omega| > 0$ , but due to theirs smallness one can neglect all the contributions from  $|\omega_{k'k} - \omega| > 0$ .

Let us make some comments for the some references's opinions in points (1.6.1-3). Eq. (10.3.1.8) contains two terms, *I* and *II*. Correspondingly, the oscillation factor in the seventh equality of Eq. (4) contains the following two terms as well, named as *I'* and *II'*. Noting that  $\beta = a \rightarrow 0$ , and the second term can be neglected, we have

$$I' + II' = \frac{[(\omega_{k'} - \omega_k - \omega)^{1-\beta}]t}{2} \frac{sin^2[(\omega_{k'} - \omega_k - \omega)t/2]}{[(\omega_{k'k} - \omega)t/2]^2} + \frac{\omega t}{2} \frac{sin^2[(\omega_{k'} - \omega_k - \omega)t/2]}{[(\omega_{k'k} - \omega)t/2]^2} \approx \frac{[(\omega_{k'} - \omega_k - \omega)^{1-\beta}]t}{2} \frac{sin^2[(\omega_{k'} - \omega_k - \omega)t/2]}{[(\omega_{k'k} - \omega)t/2]^2} = \frac{sin^2[(\omega_{k'} - \omega_k - \omega)t/2]^{1+\beta}}{[(\omega_{k'} - \omega_k - \omega)t/2]^{1+\beta}}.$$
(5)

The oscillation factor in Eq. (5) gives that the first peak is at  $(\omega_{k'k} - \omega)t/2 = \pi/2$ , the height of the first peak is very high, and the zero points, nearest to the first peak of the oscillation factor, are at  $(\omega_{k'k} - \omega)t/2 = 0$  and  $(\omega_{k'k} - \omega)t/2 = \pi$ , which are much different from Fig. 10.1 and Fig. 2.1 of Ref. [103]. From these features of the oscillation factor, the author of this book confirms with a tit-for-tat that:

(1.6.1)' The quantum transition process is energy-nonconservative;

(1.6.2)' (The height of the first peak):(The height of the second peak):(The height of the third peak)= 1 : 1/3 : 1/5. We think that due to that the second and third peaks do not too low, one cannot neglect the contributions from second and third peaks;

(1.6.3)' The width of the first peak does not connect with Heisenberg uncertainty relation. Our reason is simple. The second and third peaks do not too low. Therefore, anybody cannot think that just the peak width of the first peak connects with Heisenberg uncertainty relation.

(1.7) The quantum transition process of the system's initial state  $|k\rangle$  to any other final state  $|k'\rangle$  belongs to a still more microscopic process. In chapter 4 we have pointed out that in a still more microscopic process, the energy is generally not conservative;

(1.8) In the simple case that  $H'_{k'k}$  does not depend on k', the inverse of transition rate is called lifetime of initial state  $|k\rangle$ . This lifetime can be measured by experiment. We have to stress that this observed lifetime connects with all possible final states instead of connection with just the single energy conservation transition.

(1.9) Although Ref. [1] suggests a method to take out the  $\delta$  function from Eqs. (2-3) by introducing a physical quantity, density of state, and, formally, Eqs. (2-3)' are same as our Eqs. (2) and (10.3.1.3)'. However, we have to point out that:

(1.9.1) Our Eqs. (10.3.1.6) and (10.3.1.3)' do not need  $t \to \infty$ , and Eqs. (2-3) need;

(1.9.2) In mathematics, the procedure to obtain Eqs. (10.3.1.4) and (10.3.1.3)' are legitimate, but that of Eqs. (10.3.1.6-7) is not legitimate;

(1.9.3) In physics, our Eqs. (10.3.1.6) and (10.3.1.3)' say that that the transition process with large probability is energy conservation just occurs under the condition of k'-independence of  $|H'_{k'k}|\rho(k')$ . On the contrary, Eqs. (2-3) think that their delta function can ensure the k'-independence of  $|H'_{k'k}|\rho(k')$ , and in treating any particular problems some references always use Fermi golden rule, and affirm energy conservation in transition processes.

(1.10) The condition of long time approximation in some references is  $(\omega_{k'k} - \omega)t >> 1$ . This condition is self-contradictory in mathematics. This condition leads to energy conservation, i. e.,  $\omega_{k'k} - \omega = 0$ . Then, from  $(\omega_{k'k} - \omega)t >> 1$  we conclude that  $t \to \infty$ . However, in practical experiments on transition processes experimentalists cannot wait with infinite long time. If t = 1 second, then some references's condition  $(\omega_{k'k} - \omega)t >> 1$  is equivalent to condition  $\omega_{k'k} = \omega_{k'} - \omega)k >> \omega$ , which shows serious energy non conservation.

(1.11) Some authors have recognized that the limit  $t \to \infty$  in the second equality of Eq. (2) violates the validity of perturbation theory because of the unlimited growth of the transition probability [103]. However, these authors also provide explanation to still legitimately use the  $t \to \infty$ . They said: "However, the transition process is finished after a few period of the transition frequency so that use the  $t \to \infty$  rather safely."

On the contrary, our viewpoint and logic are: "Just due to that the transition process is finished after a few period of the transition frequency,  $t \to \infty$  is not legitimate. Any mathematician knows that limit procedure cannot be taken randomly. Otherwise, one can derive even an absolutely ridiculous conclusion."

(2) This exercise is for section 10.3.1.

List, in mathematics, some cases in which the oscillation factor appears.

Solution:

$$I = \int_0^{k_o} dt e^{ikx} = \frac{1}{ix} e^{ik_o x/2} \left( e^{ik_o x/2} - e^{-ik_o x/2} \right)$$
$$I^2 = \frac{\sin^2 k_o x/2}{(k_o x/2)^2}.$$

That is, Fourier transform of a constant in some interval is of this oscillation certainly.

(3) This exercise is for section 10.4.3.

In point (B) of subsection 10.4.3 we studied the variation perturbation in finite time interval. All the until now references and text books, such as Ref. [1], studied this problem as well. However, they made the following derivations, and gave the following different expression, Eq. (13.1.5.11)', for the transition probability from  $|k > to |k' > at t \ge T$ :

$$P_{k'k}(t \ge T) = |a_{k'k}^{(1)}(t \ge T)|^{2} = \left|\frac{1}{i\hbar}\int_{0}^{T} e^{i\omega_{k'k}t'}H_{k'k}'(t')dt'\right|^{2}$$

$$= \left|\frac{1}{i\hbar}\int_{-\infty}^{\infty} e^{i\omega_{k'k}t'}H_{k'k}'(t')dt'\right|^{2}$$

$$= \left|\frac{1}{i\hbar}\int_{-\infty}^{\infty} dt' e^{i\omega_{k'k}t'}\int_{-\infty}^{\infty} d\omega H_{k'k}'(\omega)e^{-i\omega t}\right|^{2}$$

$$= \left|\frac{1}{i\hbar}\int_{-\infty}^{\infty} d\omega H_{k'k}'(\omega)2\pi\delta(\omega_{k'k}-\omega)\right|^{2} = \left|\frac{2\pi}{i\hbar}H_{k'k}'(\omega_{k'k})\right|^{2}$$

$$= \frac{4\pi^{2}}{\hbar^{2}}|H_{k'k}'(\omega_{k'k})|^{2}.$$
(10.4.3.14)'

Eq. (10.4.3.14)' is different from our Eq. (10.4.3.14). Please point out the mistake in the derivations of Eq. (10.4.3.14)'.

(4) This exercise is for section 10.4.3. Similarly to Eq. (10.4.3.7), seek  $P_{all \leftarrow k}(t \ge T)$ .

Solution:

We hope that readers can confirm that  $H'_{k'k}(\omega)$  has to be dependent, at least, on  $\omega$ . Otherwise, the integration over  $\omega_{k'}$  will be divergent.

(5) Exercise for subsection 10.3.2.

Discuss the physical meaning of the term neglected in Eq. (10.3.2.3). Estimate the scale of the neglected term.

(6) Exercise for the theorem XXXIX in subsection 10.3.2.

Some references give the same result as the case  $\beta = 0$  of theorem XXXIX, and the same curve as Fig. 10.1. Some references's interpretation and treatment for their obtained transition formula and Fig. 10.1 is as follows. Some references only take the value of  $P_{k'k}$  at  $f = (E_{k'} - E_k - E)/h = 0$  as the transition probability in any cases. Some references think that the k'-dependence of  $|H'_{k'k}|^2 \rho k'$  always can be neglected. Some references's

reasons for this are:

(a)  $f = (E_{k'} - E_k - E)/h \neq 0$  violates the energy conservative law;

(b) The width of the first peak at  $E_{k'} - E_k - E = 0$  comes from Heisenberg uncertainty relation, and therefore does not need to be considered;

(c) The heights of second peak and so on are too small, and thus can be neglected.

Please make comments.

Solution:

This book thinks that some references's viewpoints are wrong because:

(a) Every body should do not negative rashly his (hers) direct calculation results according to apriorism. Therefore, we have to study deeply this small energy nonconservation shown in Fig. 10.1. If some processes violate the energy conservation law, then we should ask a question that is the energy conservation law really true in any cases?

(b) From derivation we see that the width of the first peak in Fig. 10.1 does not have even a wee bit of connection with Heisenberg uncertainty relation. This point can be understood by Fig. 10.2.

(c) It might be that in some D-C transitions the transition at f >> 0 becomes important, and thus the transition of energy nonconservation becomes important. We should do not give a simple negation only due to its littleness. Actually, this paper demonstrates in subsequent subsections that the transition at  $\omega_{k'} - \omega_k - \omega >> 0$  becomes important in  $\beta > 0$  cases.

(7) This exercise is an exercise for subsections 10.4.4 and 10.3.1.

We have indicated in subsection 10.4.4 that both experimental data and our theory show that the energy in the optical absorption of semiconductor is not conservative. The origin of the energy non conservation comes from the factor  $\sqrt{E_{k'}}$  in the density of states. In subsection 10.4.4 the density of states is three dimensional. Discuss the energy nonconservation in case of one and two dimensions.

Solution:

Do not need to write the whole expression of  $\alpha$ . First, write the energy-dependence of density of states in one and two dimensional systems; Second, put this energy-dependence in the integrand, and make integration over energy; Third, make comparisons of the magnitudes of energy non conservation in one, two, and three dimensions. We hope readers to know from these comparisons that energy non conservation of D-C transition is related to the vacuum energy support ability.

(8) Exercise for subsection 10.4.5.

Obtain the time dependence of transition rate for photoeffect, and negative Fermi golden rule.

#### Solution:

It is easy to show that for photoeffect the transition rate is nearly proportional to  $t_{\circ}^{-1/2}$ .

(9) Exercise for subsection 10.4.5.

By numerical analysis, explain the characters of theoretical curve 1 and 2 of Fig. 10.10 under boundary absorption.

Solution:

In the case of photoeffect of atom, if  $t_o << 10^{-13}$ , the energy nonconservation becomes more stronger. Therefore, it is not convenient to draw diagram. Let us derive a general formula, appropriate for any value of  $t_o$ , for the maximum kinetic energy of ejected electron in case of boundary absorption ( $\omega = \omega_b$ ). For convenience, we neglect the complex energy denominator in Eq. (13.1.6.5.14). Then, we have

$$P'_{all \leftarrow k}(t \ge t_{\circ}) \approx E_{kin}^{-1/2} sin^2(\frac{E_{kin}t_{\circ}}{2\hbar}).$$
(1)

The equation of maximum  $E_{kin}$  of emitted electron at fixed  $t_{\circ}$ ,  $E_{kin}$ , can be obtained from Eq. (1), and has been given by Eqs. (13.1.4.1.9) and (13.1.4.1.10). It is

$$tan(x) = 4x,\tag{2}$$

where  $x = t_{\circ} E_{kin} / (2\hbar) \equiv t_{\circ} \omega / 2$ . The solution of Eq. (2) is

$$t_{\circ}\omega_{kin} = 3.11484.$$
 (3)

Thus, generally speaking, the smaller the  $t_{\circ}$  is, the larger the  $E_{kin}$  is. (As long as for boundary absorption, Eq. (3) gives always  $E_{kin} = 0.$ ) If  $t_{\circ} = 10^{-14}$ ,  $10^{-13}$  second, then  $E_{kin} = 0.205$ , 0.0205 eV, respectively. These values are nearly equal to the values in Fig. 10.10. In Fig. 10.10  $E_{photon} = E = E_b = 1.8156$  eV.

(10) Exercise for subsection 10.4.5.

If the following experimental conditions:

(a) The attosecond light pulse, for which the  $E_{photon} = E \approx 4135 \text{ eV}$ ;

(b)  $E_{bin} = E_b = E_{photon} = E = 4135$  eV. (Ref. [131] points out that the inner-shell electrons of atoms have widely spaced energy levels from  $10^2$  to  $10^5$  eV. Therefore, it is not difficult to find some inner-shell levels which can give  $E_b \approx 4135$  eV.) can be fulfilled, then under the boundary absorption of atom photoeffect seek the magnitude of energy nonconservation.

Solution:

From Eq. (3) of the last exercise (2), if  $t_{\circ} = 10^{-18}$  second, then the kinetic energy of emitted electron  $E_{kin} = \hbar \omega_{kin} = 2050 \text{ eV}$ , which is much larger than the expected value 0 eV from energy conservation theory. We can say that the energy is strongly nonconservative in attosecond photoeffect.

(11) Exercise for subsection 10.4.5.

The 2010 available ultrafast technology is 100 attosecond [131]. Ref. [131] reported when a helium atom in its ground state with energy -40.35 eV absorbs an 100 attosecond light pulse ( $t_{\circ} = 10^{-16}$  second, photon energy = 40.35 eV= $E_b$ ), a single electron can be emitted, leaving the other electrons in the ground state, through direct attosecond photoeffect. It is a big pity that Ref. [131] did not measure the observed kinetic energy  $E_{kin}$ of emitted electron. Would you please give the theoretical expected value.

Solution: According to Eq. (3),  $E_{kin} = E_{photon} - E_b = 20.5$  eV.

(12) Exercise for subsection 10.4.5.

What are the reasons that the famous Millikan's experiment [130], so-called determinant verification for the Einstein equation of photoeffect, looks like to support the photoeffect theory of energy conservation?

Solution:

In Millikan's experimental data there are only five experimental points. All the five points are at  $E_{photon} > 2.24$  eV. In Millikan's times there were no attosecond and femtosecond pulse techniques. For boundary absorption in Millikan's experiment the photon energy has to be  $E_{photon} = E_b = 1.85$  eV. Therefore, Millikan's experiment can neither negative nor confirm our energy nonconservation photoeffect theory.

The now available experimental photoeffect was done only at picosecond ( $t_{\circ} = 10^{-12}$  second) and subpicosecond ( $t_{\circ} = 10^{-13}$  second), which does not contradict with our Figs. 10.7 and 10.8. Figs. 10.7 and 10.18 show that the obvious energy nonconservation in photoeffect occurs only at  $t_{\circ} < 10^{-13}$  second.

(13) Exercise for subsection 10.4.5.

The Einstein equation of photoeffect is

$$E_{kin} = E_{photon} - E_b$$

which is obviously a energy conservation equation, and is verified by Millikan's photoeffect experiment. Would you please argue that Einstein equation of photoeffect does not hold water exactly.

(14) Exercise for subsection 10.4.5.

Design an experiment to verify the obvious energy nonconservation under boundary absorbtion condition of photoeffect.

Solution:

Refer to the discussion on the attosecond technology in photoeffect at subsection 13.1.6.5 (after Eq. (10.4.5.16)).

(15) Exercise for subsection 10.4.5.

Point out the significance of the above experiment.

#### Solution:

According to Einstein photoeffect equation, which is an energy conservation equation and is thought as a correct equation until now, under the bound absorbtion the emitted electron energy is equal to zero. Therefore, if your experimental data is that the emitted electron energy is equal to 2050 eV, then this is definitely an interesting experimental result because this is a direct energy nonconservation observation.

(16) Exercise for section 10.4.6.

The following quotation on the elastic scattering problem comes from Ref. [133]. The author does not agree with this method. But for reader to be familiar with our energy nonconservation transition theory, this exercise will at first quote, then ask the readers to point out which equation is wrong and why?

Ref. [133] wrote after our Eq. (10.4.6.22) that:

To calculate the derivative, the energy condition of the collision have to be examined. We assume that the electron is very fast and therefore proceed from the relativistic energymomentum relation

$$\sqrt{p^2 c^2 + m^2 c^4} + Mc^2 = \sqrt{p'^2 c^2 + m^2 c^4} + \sqrt{\hbar^2 s^2 c^2 + M^2 c^4} = E,$$
(1)

where the first and second terms represent the system (one electron and one nucleus) initial and final state energy. That the two energies are equal to each other means energy conservation in scattering process. If the kinetic energy of the electron is large enough compared with the rest energy, then the term  $mc^2$  can be neglected and we obtain

$$\frac{E}{c} = p + Mc^2 = p' + \sqrt{\hbar^2 s^2 + M^2 c^2}.$$
(2)

According to the definition of  $\mathbf{s}$ , we have

$$\hbar^2 s^2 = p^2 + p'^2 - 2pp' \cos \Theta.$$
 (3)

Because the great mass M of nucleus, the energy transfer can be considered small compared with  $Mc^2$ , and therefore  $p \approx p'$  and  $(p'-p)^2 \approx 0$ , so that  $p'^2 + p^2 = 2p'p$ . Thus we get

$$\hbar^2 s^2 = 2pp'(1 - \cos\Theta) = 4pp'\sin^2\frac{\Theta}{2}.$$
(4)

From Eq. (4) we find for E/c that

$$(p - p' + Mc^{2})^{2} = \hbar^{2}s^{2} + M^{2}c^{4}$$
  
=  $4pp'\sin^{2}\frac{\Theta}{2} + M^{2}c^{2}.$  (5)

On the other hand, we have

$$(p - p' + Mc^2)^2 = (p - p')^2 + 2(p - p')Mc + M^2c^2 \approx 2(p - p')Mc + M^2c^2,$$
(6)

because  $p - p' \approx 0$  and thus the square  $(p' - p)^2$  is vanishingly small. From Eqs. (5) and (6) we have

$$(p-p')Mc \approx 2pp'\sin^2\frac{\Theta}{2},$$
 (7)

and with this, finally,

$$p' = \frac{p}{1 + (2p/Mc)\sin^2\Theta/2}.$$
 (8)

Now the expression  $dE_{k'}/dp'$  has to be calculated. For this purpose we start with

$$E_{k'} = p'c + \sqrt{\hbar^2 s^2 c^2 + M^2 c^4},$$
(9)

from which we get

$$\frac{dE_{k'}}{dp'} = c + \frac{\hbar^2 c^2 (ds^2 dp')}{2\sqrt{\hbar^2 s^2 c^2 + M^2 c^4}} \\
\approx \frac{\hbar^2 c^2}{2M c^2} \frac{ds^2}{dp'},$$
(10)

and if we make use of Eqs. (4) and (8), then we obtain

$$\frac{dE_{k'}}{dp'} \approx c\left(1 + \frac{2p}{Mc}\sin^2\frac{\Theta}{2}\right) = c\frac{p}{p'}.$$
(11)

Finally, we get the following expression for the density of states in Eq. (10.4.6.22):

$$\rho(E_{k',d\Omega}) = \frac{p'^2}{(2\pi\hbar)^3} \frac{1}{dE_{k'}/dp'} = \frac{p'^3}{(2\pi\hbar)^3 cp}.$$
(12)

Substituting Eqs. (12) and (10.46.20) into Eq. (10.4.6.2) yields

$$P_{all \leftarrow k}(t \ge t_{\circ}) = \int d\Omega \frac{1}{\hbar^2} \int_0^{+\infty} |\frac{4\pi e^2}{s^2} F(s)|^2 \frac{p'^3}{(2\pi\hbar)^3 cp} \frac{\sin^2 \frac{(E_{k'} - E_k)t_{\circ}}{2\hbar}}{\left[\frac{E_{k'} - E_k}{2\hbar}\right]^2} dE_{k'}.$$
 (13)

Correspondingly, the transition rate is

$$w_{fi} = w_{all \leftarrow k} (t \ge t_{\circ}) = P_{all \leftarrow k} (t \ge t_{\circ})$$

$$= \int d\Omega \frac{1}{\hbar^2} \int_0^{+\infty} |\frac{4\pi e^2}{s^2} F(s)|^2 \frac{p'^3}{(2\pi\hbar)^3 cp} \frac{\sin^2 \frac{(E_{k'} - E_k)t_{\circ}}{2\hbar}}{\left[\frac{E_{k'} - E_k}{2\hbar}\right]^2} dE_{k'}$$

$$\equiv \int d\Omega w_{fi,d\Omega}.$$
(14)

The transition probability itself cannot be measured directly, but a quantity can be observed, which is called a cross-section, or, more accurately, a scattering cross-section, and is denoted by  $\sigma$ . Or, more conveniently, we introduce differential cross-section  $d\sigma_{f\leftarrow i,d\Omega}$ , which is defined as the number of particles scattered per unit time and per unit of the incoming

particle current into the section of the solid angle  $(\Omega \rightarrow \Omega + d\Omega)$ . Since the initial states  $|i\rangle = |k\rangle$  represent particles, the current of which is  $v_i$ , we obtain

$$d\sigma_{f \leftarrow i, d\Omega} = \frac{w_{f \leftarrow i, d\Omega} d\Omega}{v_i}.$$
(15)

Since we use the high velocity approximation for the scattering electron,  $v_i \approx c$ . Substituting Eq. (14) into Eq. (15) yields

$$\frac{d\sigma_{f \leftarrow i, d\Omega}}{c} = \frac{1}{\hbar^2 (2\pi\hbar)^3 c^2 p} \int_0^{+\infty} \frac{(4\pi)^2 e^4 p'^3}{s^4} |F(s)|^2 \\
\times \frac{\sin^2 \frac{(E_{k'} - E_k)t_\circ}{2\hbar}}{\left[\frac{E_{k'} - E_k}{2\hbar}\right]^2} dE_{k'} \\
= \left(\frac{e^2}{2pc} \frac{p'}{p} \frac{1}{\sin^4 \Theta/2}\right)^2 |F(s)|^2.$$
(16)

The last equality in Eq. (16) comes from assumptions of p'-independence of  $p'^3/s^4|F(s)|^2$ and  $t_o \to \infty$ .

Solution:

According our transition theory the energy before and after scattering does not be conservative, therefore Eq. (1) is wrong. Eqs. (2-8) and (11) are wrong because the energy before and after scattering does not be conservative. Eq. (10) is wrong because after scattering p' can be infinite, it is might be that  $\hbar^2 s^2 >> Mc^2$ . Although in comparison of Eq. (10) with our Eq.(10.4.6.26)

$$\rho(E_{k',d\Omega}) = \frac{p'^2}{(2\pi\hbar)^3} \frac{1}{dE_{k'}/dp'} = \frac{p'^2}{(2\pi\hbar)^3 c},$$
(10.4.6.26)

formally, the difference is little, but, in essence, the difference is big, the reason of which is that p' can be equal to  $\infty$ . Of course, Eqs. (13-16) are wrong.

(17) Exercise for section 10.4.6.

Assume that the nuclear charge density distribution is given by the so-called Fermi distribution

$$\rho_p(R) = \frac{\rho_o}{1 + \exp[(R - R_H/2)/a]}.$$
(10.4.6.34)

The values of parameters in Eq. (10.4.6.34) are as follows. p is determined by the experimental value, i. e., the incident electron energy is 200 MeV.  $t_{\circ}$  represents the duration time of scattering. Although we cannot exactly determine it, but we can approximately estimate it. Due to that the Coulomb interaction is proportional to |r - R|, which is the distance between initial position of incident electron and the target position, we take |r - R| = 1 cm. Thus  $t_{\circ} \approx 2/c = 0.7 \times 10^{-10}$  second. Take  $M = M_{Au} = 197 \times 1.67 \times 10^{-27}$  Kg. A = 197.  $R_H \approx (1.0 - 1.2)A^{1/3}$  fermi.  $\rho_{\circ} = 1.65 \times 10^{44}$  nucleons/m<sup>3</sup>. Substituting all these values and Eq. (10.4.6.34) into Eq. (10.4.6.31), you can obtain a theoretical

curve of  $d\sigma_{fi,d\Omega}/d\Omega \propto$  the scattering probability versus scattering angle  $\Theta$ . Based on the comparison of your theoretical curve and the experimental data in Ref. [132], please make conclusion.

#### Solution:

If your theoretical curve fits the data, then the conclusion is that the nuclear charge density distribution is given by the so-called Fermi distribution correctly.

If your theoretical curve departures from the data seriously, then the conclusion is that the nuclear charge density distribution does not obey the so-called Fermi distribution, and scientists have to find true nuclear charge density distribution. If your theoretical curve departures from the data seriously, then would you please write a paper to negative the so called Fermi distribution model of nucleus, accepted by some references.

(18) Exercise for subsection 10.4.6.

According to the shell model of nucleus, inside the nucleus there should be some places where there are no charges. The shell model was awarded the Nobel Prize. Do you have ability to propose a nucleus charge density distribution model instead of the so called Fermi distribution model, and to put your model distribution function into Eq. (10.4.6.31) to explain the experimental data given by Ref. [133]?

Solution:

To approach the shell model of nucleus, the distribution model can have many possibility. Even you have not yet had enough reasons to negative the Fermi distribution model, but if you have enough reasons to doubt the Fermi distribution model, then it also has significance for science.

#### (19) Exercise for subsection 10.4.6.

Using the Eq. (10.4.6.31), calculate the transition probability in direction of  $\Theta = \pi/2$ .  $\Theta = \pi/2$  represents the angle between electron incident direction **p** and scattered electron direction **p**'.

Solution:

The transition probability is proportional to

$$\int_0^\infty dp' \frac{p'^2}{(p^2 + p'^2)^3} \int_0^\infty dR \rho_p(R) \sin(\sqrt{p^2 + p'^2} R/\hbar) R \frac{\sin^2[(p' - p)ct_\circ/\hbar]}{[(p' - p)c/\hbar]^2}$$

To continue the calculation, we need to make some assumptions about the charge density distribution in nucleus.

(20) This exercise is for subsection 10.4.6, and might be a paper if you have enough time to finish it.

Please study that which formula is better for the  $\alpha$  scattering: Rutherford's and modified Rutherford's formulas Eq. (10.4.6.2-3) or this textbook's exact formula Eq. (10.4.6.31)? The related experimental data are in the Table 1.1 of Ref. [133]. Table 1.1 of Ref. [133] gives the experimental values of scattering angle  $\theta$  and the scattered  $\alpha$  particle

number  $N(\theta)$ , which is proportional to differential scattering cross section, and also gives the calculated values of  $N(\theta) \sin^4(\theta/2)$ .

(A) Do you think that Rutherford's formula has been verified by the experimental data?(B) Can the modified Rutherford's formula explain the experimental data good enough?(C) Use the exact formula to explain the data.

Solution:

(A) According to Rutherford's formula,  $N(\theta) \sin^4(\theta/2)$  has to be a constant. However, the data are:, for example,  $N(15^\circ) \sin^4(15^\circ/2) = 38.4$ ,  $N(30^\circ) \sin^4(30^\circ/2) = 35.0$ ,  $N(105^\circ) \sin^4(105^\circ/2) = 27.5$ ,... Therefore, Rutherford'd formula is not good.

(B) Use the modified Rutherford's formula to calculate  $N(\theta) \propto$  differential scattering cross section and make comparisons with the experimental data in the Table 1.1.

(C) Use the exact scattering formula to calculate  $N(\theta) \propto$  differential scattering cross section and make comparisons with the experimental data in the Table 1.1.

(D) Use the exact scattering formula with recoil effect to calculate  $N(\theta) \propto$  differential scattering cross section and make comparisons with the experimental data in the Table 1.1.

(21) The newest textbook Ref. [10] proves the same formula as our

$$\lim_{T \to \infty} P_{k'k}(t \ge T) = \frac{2\pi}{\hbar^2} \left| H'_{k'k}(\omega_{k'k}) \right|^2$$
(10.4.3.17)

for the D-D transition. Do you think that is the result of Ref. [10] correct?

#### Solution:

No. It is still wrong although Ref. [10] is the newest textbook. We still insist that

$$P_{k'k}(t \ge T) = \frac{4}{\hbar^2} \frac{1}{2\pi} \left| \int_{-\infty}^{\infty} d\omega H'_{k'k}(\omega) \frac{\sin[(\omega_{k'k} - \omega)T]}{\omega_{k'k} - \omega} \right|^2,$$
(10.4.3.14)

is correct.

Our reason, besides the reason mentioned in that subsection, is as follows. Assume that  $H'_{k'k}(\omega) \approx constant$ . Eq. (10.4.3.14) becomes

$$P_{k'k}(t \ge T) = \frac{4}{\hbar^2} \frac{1}{2\pi} |H'_{k'k}|^2 \left| \int_{-\infty}^{\infty} d\omega \frac{\sin[(\omega_{k'k} - \omega)T]}{\omega_{k'k} - \omega} \right|^2$$
  
$$= \frac{4}{\hbar^2} \frac{1}{2\pi} |H'_{k'k}|^2 \times \left| \int_{-\infty}^{\infty} dx \frac{\sin x}{x} \right|^2$$
  
$$= \frac{4}{\hbar^2} \frac{1}{2\pi} |H'_{k'k}|^2 \times \pi^2 = \frac{2\pi}{\hbar^2} |H'_{k'k}|^2.$$
(10.4.3.14)'

Although our Eq. (10.4.3.14)' looks like the formula in Ref. [10] apparently, but there is significant difference, i. e., the formula in Ref. [10] is based in the non-physical limit  $T \rightarrow \infty$ , on the contrary, our formula is based on that: (i). The *T* can be long or short; (ii). The energy is not conservative in transition process. We prefer to believe a physical new effect (which does not contract with any known experimental facts), and do not prefer to

believe an obviously wrong assumption  $T \rightarrow \infty$ .

(22) The transition from continuous state into discrete states can occur in many actual processes, e.g, the capture of electron by ions, the absorption of an electron a valence band into an acceptor state in a doped semiconductor, the neutron capture by nuclei, and in plasma or early evolution of universe [10]. There are many papers to calculate the radiative capture cross section for electron-proton recombination into arbitrary hydrogen shells [10]. However, until 2012, the calculations results of the electron capture cross section for ions from radiative recombination were much too small to explain the experimental values. To set theoretical result to fit better the experimental values people proposed many model on the scattering process and so on. Ref. [115] found from experiment that if the electron energy is high, then the theoretical result is better, and if the electron energy is low, then the theoretical result is worse.

(A) Do you have other method other than present scattering model to make a new theoretical calculations? Is it might be that your calculations have important significance?

(B) Can you qualitatively explain the experimental values in Ref. [115]?

#### Solution:

(A) There is an obvious weak point for the treating the quantum transition in some references, i. e., all they neglect the possible energy nonconservation processes. We can try to make an exact numerical calculations for the transition probability. Qualitatively speaking, our theoretical calculations will definitely can give larger cross section, because we consider both the contribution from the energy conservation process (which is considered solely by some references) and all contributions from energy nonconservation processes (which have not been considered by some references). Of course, if we really can quantitatively explain the experimental values, then the significance is: (i). Many models should be wrong; (ii). We can conclude that the energy nonconservation in transition processes is verified by this  $C \rightarrow D$  transition.

(B) At first, we should remember that theories in some references for  $C \rightarrow D$  transition do not consider the contribution of energy nonconservation. The theorem in this chapter denotes that for high energy electron the contribution of energy conservation in  $C \rightarrow D$  transition is important, and thus the theories in some references are easy to fit the experimental values [10]. However, the theorem in this chapter denotes that for the low energy electron the contribution of energy nonconservation in  $C \rightarrow D$  transition process is important, thus the theoretical results in some references will be bad definitely.

(23) Let us systematically discuss Fermi golden rule in case of D-C transition, make detail comparisons between the methods of some references and this textbook.

#### Solution:

We calculate the differential transition probability in first order approximation

$$dP_{k \to k'} = dE' \rho(E') | < k' |U_I(t, t_\circ)|k > |^2$$
  
=  $dE' \rho(E') |S_{k'k}(t, t_\circ)|^2$   
=  $dE' \rho(E') \frac{1}{\hbar^2} \frac{| < k' |H'|k > |^2}{[(\omega_{k'k} - \omega)/2]^2} sin^2 [(\omega_{k'k} - \omega)(t - t_\circ)/2].$  (23.1)

Under first order approximation, the differential transition rate into a final state energy interval  $E' \rightarrow E' + dE'$  is

$$dw_{k \to k'} = \frac{\partial}{\partial t} dP_{k \to k'}(t, t_{\circ})$$
  
= 
$$dE' \rho(E') \frac{1}{\hbar^2} \frac{|\langle k'|H'|k \rangle|^2}{[(\omega_{k'k} - \omega)/2]^2} \frac{\partial}{\partial t} sin^2 [(\omega_{k'k} - \omega)(t - t_{\circ})/2].$$
(23.2)

Integration over the final state energy E' then yields an expression for the transition rate of initial state |k>

$$\begin{split} w_{k \to a l l \ k's} &= \int_{0}^{\infty} dw_{k \to k'} \\ &= \int_{0}^{\infty} dE' \rho(E') \frac{1}{\hbar^{2}} \frac{|\langle k'|H'|k \rangle|^{2}}{[(\omega_{k'k} - \omega)/2]^{2}} \\ &\times \frac{1}{t - t_{\circ}} sin^{2} [(\omega_{k'k} - \omega)(t - t_{\circ})/2] \\ &\approx \frac{1}{\hbar^{2}} |\langle k'|H'|k \rangle|^{2} \rho(E') \frac{1}{t - t_{\circ}} \\ &\times \int_{0}^{\infty} dE' \frac{sin^{2} [(\omega_{k'k} - \omega)(t - t_{\circ})\hbar/2\hbar]}{[(\omega_{k'k} - \omega)\hbar/2\hbar]^{2}} \\ &= \frac{1}{\hbar^{2}} |\langle k'|H'|k \rangle|^{2} \rho(E') \frac{\partial}{\partial t} 2\hbar(t - t_{\circ}) \\ &\times \int_{-(E_{k} - \hbar\omega)(t - t_{\circ})/2\hbar}^{\infty} dx \frac{sin^{2}x}{x^{2}} \\ &\approx \frac{1}{\hbar^{2}} |\langle k'|H'|k \rangle|^{2} \rho(E') \frac{1}{t - t_{\circ}} 2\hbar(t - t_{\circ}) \\ &\times \int_{-\infty}^{\infty} dx \frac{sin^{2}x}{x^{2}} \\ &= \frac{1}{\hbar^{2}} |\langle k'|H'|k \rangle|^{2} \rho(E') \frac{1}{t - t_{\circ}} 2\hbar(t - t_{\circ}) \pi \\ &= \frac{2\pi}{\hbar} |\langle k'|H'|k \rangle|^{2} \rho(E'). \end{split}$$

The fourth equality is an approximate expression, because we assume the E'(k')independence of  $|\langle k'|H'|k\rangle|^2\rho(E')$ . The sixth equality is also an approximate expression,
because we take the lower limit of the integration is  $-\infty$ . Under the three conditions of these

two approximations and allowing the strong energy nonconservation in transition, we derive the Fermi golden rule (= time independence of the transition rate of initial state  $|k\rangle$ ). From our derivation, we can see that Fermi golden is not an exactly rule. On the contrary, it is an quite approximate rule. This rule requires the independence of energy of final state of  $|\langle k'|H'|k\rangle|^2\rho(E')$ . In fact, generally, this condition cannot be satisfied. For example, always  $\rho(E') \propto \sqrt{E'}$ .

Next, we introduce the method of some references to obtain the time-independence of  $w_{k\rightarrow all\ k's}$ . Would the readers please to make comparisons with our Eq. (23.3), and points out the mistakes in the derivations.

Some references (such as [10]) make the following derivations (Suppose  $H'(t) = H' \exp(-i\omega t)$ ):

$$dP_{k\to k'} = dE'\rho(E') \left| -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt_1 e^{i\omega_{k'k}t_1} < k'|H'(t_1)|k > \right|^2$$
  

$$= dE'\rho(E') \frac{1}{\hbar^2} | < k'|H'|k > |^2(2\pi)^2 [\delta(\omega_{k'k} - \omega)]^2$$
  

$$= dE'\rho(E') \frac{1}{\hbar^2} | < k'|H'|k > |^2(2\pi)^2 \delta(\omega_{k'k} - \omega)$$
  

$$\times \lim_{(\omega_{k'k} - \omega) \to 0} \lim_{T \to \infty} \frac{1}{2\pi} \int_{T/2}^{T/2} dt e^{i(\omega_{k'k} - \omega)t}$$
  

$$= dE'\rho(E') \frac{1}{\hbar^2} | < k'|H'|k > |^2(2\pi)^2 \delta(\omega_{k'k} - \omega)$$
  

$$\times \lim_{T \to \infty} \frac{T}{2\pi}.$$
(23.4)

Therefore,

$$w_{k \to all \ k's} = \int_{0}^{\infty} dw_{k \to k'} = \lim_{T \to \infty} \int_{0}^{\infty} \frac{1}{T} dP_{k \to k'}$$
  
=  $\int_{0}^{\infty} dE' \rho(E') \frac{1}{\hbar^{2}} | < k' |H'| k > |^{2} (2\pi)^{2} \delta[(\omega_{k'k} - \omega)\hbar]\hbar$   
 $\times \lim_{T \to \infty} \frac{1}{T} \frac{T}{2\pi} = \frac{2\pi}{\hbar} \rho(E') | < k' |H'| k > |^{2} \Big|_{E' = E_{k} + \hbar\omega}$  (23.5)

Eq. (23.5) is exactly same as the Eq. (13.29) in Ref. [10], and is used by some references. Let us discuss Eqs. (23.3) and (23.5).

(i) It is obviously that the duration time *T* of time-dependence perturbation has to have a magnitude order of relaxation time of the transition process. Generally, the relaxation time is from  $10^{-7}$  to  $10^{-15}$  second. Therefore, the limit  $T \to \infty$  is not reasonable in physics. Generally, the condition that  $\rho(E')| < k'|H'|k > |^2$  does not be satisfied.

Therefore, when one uses the Fermi golden rule, one has to use the rule based on the proof of this textbook, i. e., we should know that the Fermi golden rule is not exact, and thus one should: (a). consider the conditions in any particular cases, and make an estimations for the error; (b). abandon the often energy conservation of transition process.

(ii) As is well known, when some references treat the problems in solid state, particle physics, nuclear physics, and so on, some references use the Fermi golden rule, and make

further analyses based on the Fermi golden rule. By using this "cutting up with just one knife", from 1930 up to 2013, some references make conclusions, the number of which will be more than  $10^3$ . This textbook believe that in the  $10^3$  conclusions there are, at least, more than 500, which are of serious mistakes. If a person makes derivations once again, then one the person might have new discoveries.

(24) Would reader please read and understand in both physics and mathematics the paper in "F. S. Liu, Energy and Power Engineering, 2010, 2, 137-142", and then design some interesting experiments to verify the possible strong energy nonconservation in quantum transition processes. In my coming textbook "Advanced quantum mechanics upon theorems" I will give some of them.

(25) At beginning of this chapter, we write: "(5). We would like to point out that the mathematical treatment for transition processes and scattering processes in the until now all references and textbooks exists one very seriously purely mathematical mistake on the limit *time*  $\rightarrow \infty$ ."

Would you please point out the serious consequences in physics due to this mistake.

(26) Born and Fock proposed adiabatic (approximate) theory in 1928 [136] for quantum transition. All until now references and textbooks prefer to use adiabatic theory to treat quantum transition processes [120, 114, 57, 7]. However, after first strongly criticizing this adiabatic theory by Ref. [137], and then supporting Ref. [137] by Ref. [138], now many references want to modify the adiabatic theory, and the adiabatic theory in quantum transition of open system becomes a modern open hot problem. The physical idea of adiabatic theory in all until now references and textbooks is simple. The idea is to find a better conditions to set the limit  $t \to \infty$  reasonable. If one takes  $t \to \infty$ , and obtains energy conservation result and keeping Fermi golden rule, then one thinks that his method is nearly with confidence.

This textbook does not agree the above idea, and suggest to stop using the adiabatic theory since 1928 to now. Our reasons are also very simple, and are listed as follows:

(i) The limit  $t \rightarrow \infty$  in transition processes is not physical, i. e., violates all experimental facts;

(ii) The limit  $t \to \infty$  is wrong completely in mathematics. We have to remember that the actual quantum transition is a short time problem. The treatment for a physical problem is not a game. One cannot play a mathematical infinite limit game, one cannot also take mathematical infinite limit as an approximation arbitrarily.

(iii) No anybody and no any theory have proved that an open system has to obey energy conservation and Fermi golden rule. Actually, this chapter exactly proves that the quantum transition in an open system does not maintain energy conservation.

Do you think that the critiques of this textbook for the adiabatic theory are excessive?

Solution: No. They are balanced criticism. (27) As you know, transition process requires to find a matrix element, which is independent of pictures. Until now this textbook uses Schrödinger picture to study quantum transition. Please use the interaction picture in chapter 5 to give quantum Zeno effect a more general proof.

Solution: From Eqs. (5.7.4.18) and (5.7.4.3), we obtain

$$P_{exci \to groun}(\delta t) = |\langle \Psi_I(t=0)|\Psi_I(\delta t)\rangle|^2 \stackrel{shout}{=} 1 - B'(\delta t)^{\alpha}.$$

Using the same method as that in subsection 10.5.3, we obtain if  $\alpha > 1$ , then there is quantum Zeno effect. However, if  $\alpha = 1$ , then the transition or decay process do not be suppressed.

(28) Using interaction picture in chapter 5 derives the first approximation theory of quantum transition. (Refer to Refs. [120, 114].)

(29)

(i) Would readers, including students and beginners, please argue that quantum mechanics upon theorems will cause fourth science and technology revolution in our world; [The first, second, and third are steam engine (1765, Watt), electric motor(1821, Faraday) $\rightarrow$ applications of electricity(1880, Edison), and computer(1946)  $\rightarrow$  internet(1960) $\rightarrow$ information, respectively.]

(ii) Would readers please appraise classical mechanics, quantum mechanics upon postulates, special and general theory of relativity;

(iii) Would readers please estimate influences of quantum mechanics upon theorems to social science, especially, philosophy.

(iv) Do you agree that the quantum theory from Planck quantum (1900) to basic quantum field theory (1929) cannot be a cause of third world science revolution? Why?

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