Lectures in Applied 8 (Wave Mechanics) For 3rd-Level Faculty of Education Second Term

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Contents

1 Introduction **5**

1.1 Wave-particle duality 7

1.1.1 Compton effect and particle-like quanta 7

1.1.2 Diffraction by two slits wave-like quanta 11

1.2 Schrödinger Equation 13

1.2.1 Sinusoidal waves 14

1.2.2 Linear superpositions of sinusoidal waves 16

1.2.3 Dispersive and non-dispersive waves 20

1.3 Probability 26

1.3.1 Discrete random variables 26

1.3.2 Continuous random variables . . . 29

1.4 The Heisenberg Uncertainty Principle . . . 33

1.5 Diffraction by two slits 36

2 Motion of free particles in space **47**

2.1 Confined particle in a box 47

2.2 Examples 54
2.2.1 Example .1 54
2.3 Excercises 59

3 Linear harmonic oscillator 61
3.1 Classical harmonic oscillator 62
3.2 Quantum harmonic oscillator 64
3.3 Eigenvalues and eigenfunctions 68
3.3.1 Some Hermit polynomials properties 73
3.3.2 Calculating the normalization constant Q_n 76
3.3.3 The number operator 77

Chapter 1

Introduction

Classical physics is dominated by two fundamental concepts. The first is the concept of a particle, a discrete entity with definite position and momentum which moves in accordance with Newton's laws of motion. The second is the concept of an electromagnetic wave, an extended physical entity with a presence at every point in space that is provided by electric and magnetic fields which change in accordance with Maxwell's laws of electromag-

netism. The classical world picture is neat and tidy: the laws of particle motion account for the material world around us and the laws of electromagnetic fields account for the light waves which illuminate this world.

This classical picture began to crumble in 1900 when Max Planck published a theory of black-body radiation; i.e. a theory of thermal radiation in equilibrium with a perfectly absorbing body. Planck provided an explanation of the observed properties of black-body radiation by assuming that atoms emit and absorb discrete quanta of radiation with energy $\epsilon = h\nu$, where ν is the frequency of the radiation and h is a fundamental constant of nature with value

$$h = 6.626 \times 10^{-34} Js$$

This constant is now called Planck's constant. In the future parts of the course we will see that Planck's constant has a strange role of linking wave-like and particle-like properties. In so doing it reveals that physics cannot be based on two distinct, unrelated concepts, the concept of a particle and the concept of a wave. These classical concepts, it seems, are at best approximate descriptions of reality.

1.1 Wave-particle duality

1.1.1 Compton effect and particle-like quanta

Photons are particle-like quanta of electromagnetic radiation. They travel at the speed of light c with momentum

p and energy ϵ given by

$$p = \frac{h}{\lambda}; \epsilon = \frac{hc}{\lambda}$$

where λ is the wavelength of the electromagnetic radiation. In comparison with macroscopic standards, the momentum and energy of a photon are tiny. For example, the momentum and energy of a visible photon with wavelength $\lambda = 663nm$ are

$$p = 10^{-27}Js, \epsilon = 3 \times 10^{-19}j \tag{1.1}$$

We note that an electronvolt, $1eV = 1.602 \times 10^{-19}J$, is a useful unit for the energy of a photon: visible photons have energies of the order of an eV and X-ray photons have energies of the order of $10keV$.

Actually, the evidence for the existence of photons emerged

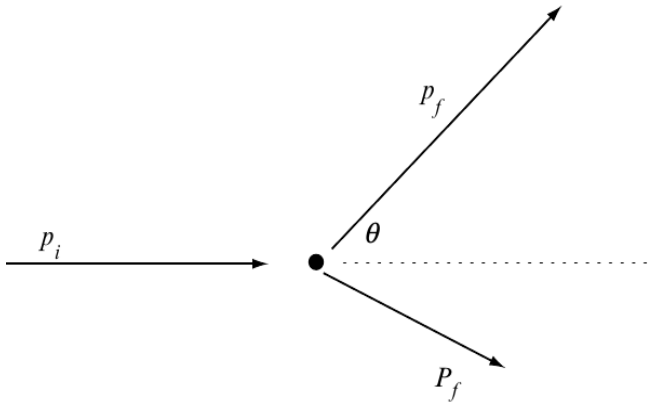

Figure 1.1: A photon-electron collision in which a photon is scattered by a stationary electron through an angle θ. Because the electron recoils with momentum P_f , the magnitude of the photon momentum decreases from p_i to p_f and the photon wavelength increases.

when A. H. Compton showed that the wavelength of an X-ray increases when it is scattered by an atomic electron. This effect, which is now called the Compton effect, can be understood by assuming that the scattering process is a photon-electron collision in which energy and momentum are conserved. As illustrated in Fig. (1.1), the incident photon transfers momentum to a stationary

electron so that the scattered photon has a lower momentum and hence a longer wave-length. In fact, when the photon is scattered through an angle θ by a stationary electron of mass m_e , the increase in wavelength is given by

$$\Delta\lambda = \frac{h}{m_e c}(1 - \cos\theta) \tag{1.2}$$

We note that the magnitude of this increase in wavelength is set by

$$\frac{h}{m_e c} = 2.43 \times 10^{12} m,$$

a fundamental length called the Compton wavelength of the electron. Moreover, the concept of a photon provides a natural explanation of the Compton effect and of other particle-like electromagnetic phenomena such as the photo-electric effect.

1.1.2 Diffraction by two slits wave-like quanta

When electromagnetic radiation passes through the two slits it forms a pattern of interference fringes on a screen (an interference experiment which was first used by Thomas Young in 1801 to measure the wavelength of light), see Fig.(1.2). These fringes arise because wave-like disturb-

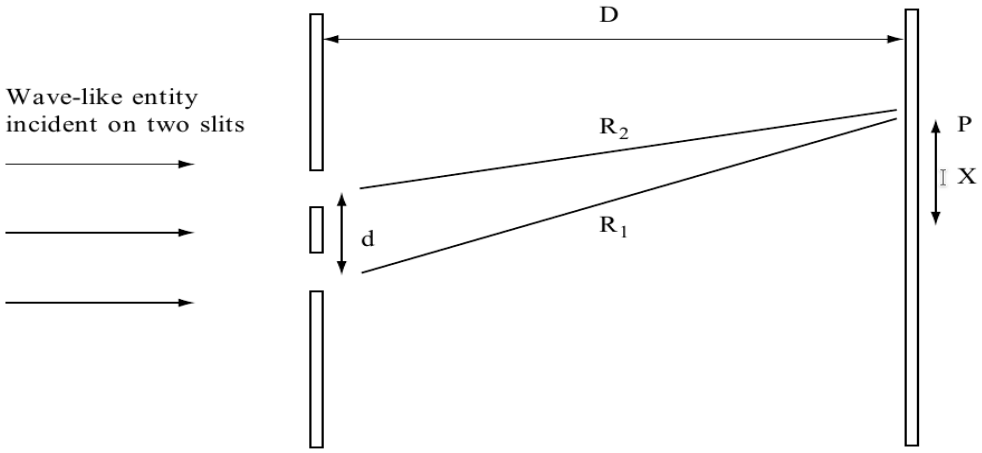

Figure 1.2: A schematic illustration of a two-slit interference experiment consisting of two slits with separation d and an observation screen at distance D. Equally spaced bright and dark fringes are observed when wave-like disturbances from the two slits interfere constructively and destructively on the screen. Constructive interference occurs at the point P, at a distance x from the centre of the screen, when the path difference $R_1 - R_2$ is an integer number of wavelengths. This path difference is equal to xd/D if $d << D$.

ances from each slit interfere constructively or destructively when they arrive at the screen. But a close examination of the interference pattern reveals that it is the result of innumerable photons which arrive at different points on the screen, as illustrated in Fig.(1.3). In fact, when the intensity of the light is very low, the interference pattern builds up slowly as photons arrive, one by one, at random points on the screen after seemingly passing through both slits in a wave-like way. These photons are not behaving like classical particles with well-defined trajectories. Instead, when presented with two possible trajectories, one for each slit, they seem to pass along both trajectories, arrive at a random point on the screen and build up an interference pattern.

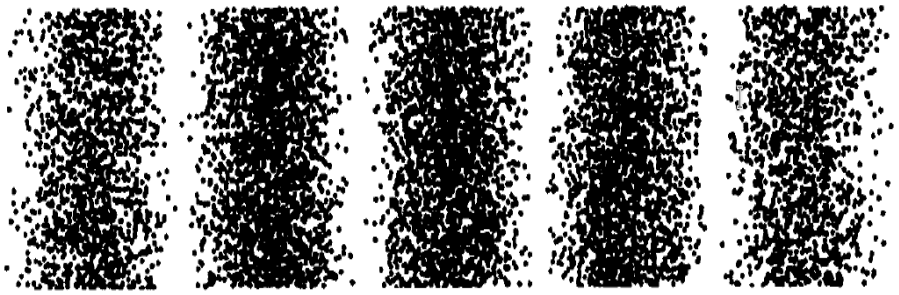

Figure 1.3: A computer generated simulation of the build-up of a two-slit interference pattern. Each dot records the detection of a quantum particle on a screen positioned behind two slits.

1.2 Schrödinger Equation

The role of the Schrödinger equation in quantum mechanics is analogous to that of Newton's Laws in classical mechanics. Both describe motion. Newton's Second Law is a differential equation which describes how a classical particle moves, whereas the Schrödinger equation is a partial differential equation which describes how the wave function representing a quantum particle ebbs and

flows. In addition, both were postulated and then tested by experiment.

1.2.1 Sinusoidal waves

The most elegant wave is a sinusoidal travelling wave with definite wavelength λ and period τ, or equivalently definite wave number, $k = 2\pi/\lambda$, and angular frequency, $\omega = 2\pi/\tau$. Such a wave may be represented by the mathematical function

$$\psi(x,t) = A\cos(kx - \omega t)$$

where A is a constant. At each point x, the function $\psi(x,t)$ oscillates with amplitude A and period $2\pi/\omega$. At each time t, the function $\psi(x,t)$ undulates with amplitude A and wavelength $2\pi/k$. Moreover, these undula-

tions move like a Mexican wave, in the direction of increasing x with velocity ω/k for example, the maximum of $\psi(x,t)$ corresponding to $kx - \omega t = 0$ occurs at the position $x = \omega t/k$, and the minimum corresponding to $kx - \omega t = \pi$ occurs at the position $x = \lambda/2 + \omega t/k$ in both cases the position moves with velocity ω/k.

The function $\sin(kx - \omega t)$, like $\cos(kx - \omega t)$, also represents a sinusoidal travelling wave with wave number k and angular frequency ω. Because

$$\sin(kx - \omega t) = \cos(kx - \omega t - \pi/2)$$

The most general sinusoidal travelling wave with wave number k and angular frequency ω is the linear superpo-

sition

$$\psi(x,t) = A\cos(kx - \omega t) + B\sin(kx - \omega t)$$

where A and B are arbitrary constants.

1.2.2 Linear superpositions of sinusoidal waves

Two sinusoidal waves moving in opposite directions may be combined to form standing waves. For example, the linear superposition

$$A\cos(kx - \omega t) + A\cos(kx + \omega t)$$

gives rise to the wave $2A\cos kx\cos\omega t$. This wave oscillates with period $2\pi/\omega$ and undulates with wavelength $2\pi/k$, but these oscillations and undulations do not propagate; it is a non-Mexican wave which merely stands and waves.

Alternatively, many sinusoidal waves may be combined to form a wave packet. For example, the mathematical form of a wave packet formed by a linear superposition of sinusoidal waves with constant amplitude A and wave numbers in the range $k - \Delta k$ to $k + \Delta k$ is

$$\psi(x,t) = \int_{k-\Delta k}^{k+\Delta k} A\cos(k'x - \omega' t)dk' \qquad (1.3)$$

If k is positive, this wave packet travels in the positive x direction, and in the negative x direction if k is negative. The initial shape of the wave packet, i.e. the shape at $t = 0$, may be obtained by evaluating the integral

$$\psi(x,0) = \int_{k-\Delta k}^{k+\Delta k} A\cos k'x dk'$$

This gives

$$\psi(x,0) = S(x)\cos kx; \quad S(x) = 2A\Delta k\frac{\sin \Delta kx}{\Delta kx}$$

If $\Delta k << k$, we have a rapidly varying sinusoidal,

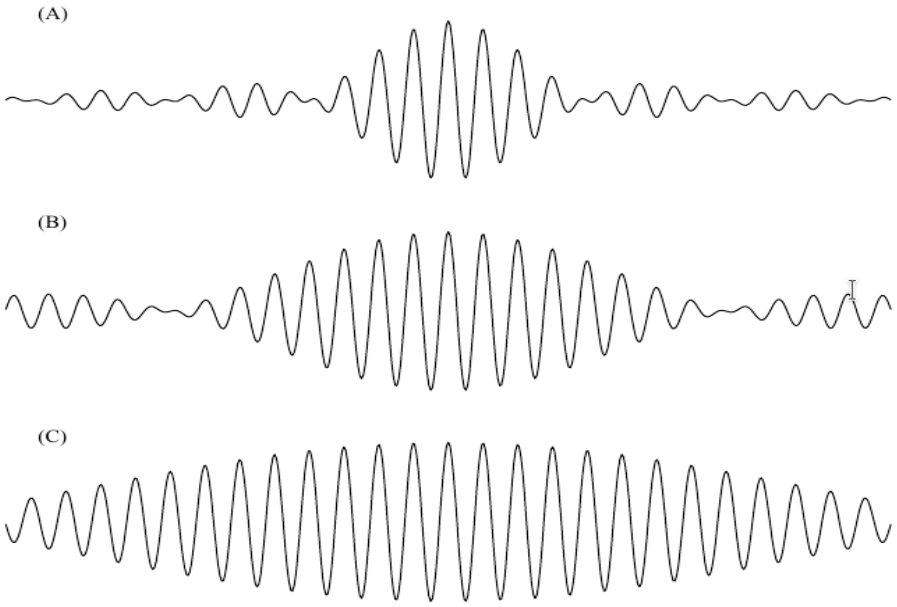

Figure 1.4: The initial shapes of the wave packets given by a linear superposition of sinusoidal waves with constant amplitude A and wave numbers in the range $k - \Delta k$ to $k + \Delta k$. The three diagrams show how the length of a wave packet increases as the range of wave numbers Δk decreases. The value of $A\Delta k$ is constant, but Δk equals $k/8$ in diagram (A), *Deltak* equals $k/16$ in diagram (B) and Δk equals $k/32$ in diagram (C). In general, the length of a wave packet is inversely proportional to Δk and becomes infinite in extent as $\Delta k \to 0$

$\cos kx$, with an amplitude modulated by a slowly varying function $S(x)$ which has a maximum at $x = 0$ and zeros when x is an integer multiple of $\pi/\Delta k$. The net result is

a wave packet with an effective length of about $2\pi/\Delta k$. Three such wave packets, with different values for Δk, are illustrated in Fig.(1.4). We note that the wave packets increase in length as the range of wave numbers decreases and that they would become "monochromatic" waves of infinite extent as $\Delta k \to 0$. Similar behaviour is exhibited by other types of wave packets.

The velocity of propagation of a wave packet, and the possible change of shape as it propagates, depend crucially on the relation between the angular frequency and wave number. This relation, the function $\omega(k)$, is called the dispersion relation because it determines whether the waves are dispersive or non-dispersive.

1.2.3 Dispersive and non-dispersive waves

The most familiar example of a non-dispersive wave is an electromagnetic wave in the vacuum. A non-dispersive wave has a dispersion relation of the form $\omega = ck$, where c is a constant so that the velocity of a sinusoidal wave, $\omega/k = c$ is independent of the wave number k. A wave packet formed from a linear superposition of such sinusoidal waves travels without change of shape because each sinusoidal component has the same velocity.

Non-dispersive waves are governed by a partial differential equation called the classical wave equation. For waves travelling in three dimensions, it has the form

$$\nabla^2\psi - \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} = 0$$

where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

and for waves travelling in one dimension, the x direction say, it has the form

$$\frac{\partial^2 \psi}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2} = 0 \tag{1.4}$$

The classical wave equation has an infinite number of solutions corresponding to an infinite variety of wave forms. For example, the sinusoidal waves,

$$A\cos(kx - \omega t), \quad A\sin(kx - \omega t), \quad Ae^{i(kx-\omega t)}$$

are solutions provided $\omega^2 = c^2k^2$, as may be shown by direct substitution into Eq. (1.4); solutions with $k = +\omega/c$ describe waves travelling in the positive x direction and solutions with $k = -\omega/c$ describe waves travelling in the

negative x direction. Because each term in the classical wave equation is linear in ψ, a linear superposition of sinusoidal waves is also a solution. For example, a superposition like Eq. (1.3) is a solution which describes a wave packet which propagates without change of shape. However, the majority of waves encountered in classical and in quantum physics are dispersive waves. A dispersive wave is governed by a partial differential equation which is more complicated than the classical wave equation, Eq. (1.4). The dispersion relation is more complicated than $\omega = ck$ so that the velocity of propagation of a sinusoidal wave, ω/k, depends upon the wave number k. Hence a packet of dispersive waves will, in general, change shape as it propagates. However, if the packet

is composed of waves with a narrow range of wave numbers, it has a well-defined velocity of propagation. This velocity is called the group velocity and it is given by

$$v_{group} = \frac{d\omega}{dk} \tag{1.5}$$

whereas the velocity of a simple sinusoidal wave, ω/k, is called the phase velocity.

To understand Eq. (1.5), we note that the group velocity describes the motion of a localized disturbance due to constructive interference of many sinusoidal waves. Let us focus on the point of constructive interference of two sinusoidal waves with wave numbers k_1 and k_2 and angular frequencies ω_1 and ω_2 which is formed when the

waves are in phase; i.e. when

$$k_1 x - \omega_1 t = k_2 x - \omega_2 t$$

By rearranging this equation, we find that the position of this point of constructive interference is given by

$$x = \left(\frac{\omega_1 - \omega_2}{k_1 - k_2} \right) t$$

Thus our point of constructive interference is located at $x = 0$ when $t = 0$ and it moves with a velocity given by $\left(\frac{\omega_1 - \omega_2}{k_1 - k_2} \right)$, or by Eq. (1.5) if $|k_1 - k_2|$ is small. Of course, with two sinusoidal waves, there are an infinite number of points of constructive interference, but many sinusoidal waves can form a localized region of constructive interference which moves with a velocity given by Eq. (1.5).

To illustrate how a group velocity can be derived from

Eq. (1.5), we consider the example of water waves of long wavelength which obey the dispersion relation

$$\omega = \sqrt{gk}$$

where g is the acceleration due to gravity. The velocity of a sinusoidal water wave, the so-called phase velocity, is

$$v_{phase} = \frac{\omega}{k} = \sqrt{\frac{g}{k}}$$

and the velocity of a packet of water waves with a narrow range of wave numbers near k is

$$v_{group} = \frac{d\omega}{dk} = \frac{1}{2}\sqrt{\frac{g}{k}}$$

Thus, for water waves, the group velocity is exactly one-half of the phase velocity. In other words, the sinusoidal waves forming the packet, travel at twice the speed of the

region of maximum disturbance formed by the interference of these waves. However, the shape of the disturbance will change as it propagates; in general it will tend to spread out.

1.3 Probability

Due to the importance of Probility in quantum measurement, let's briefly consider how discrete and continuous random variables are governed by probability distributions.

1.3.1 Discrete random variables

Let us consider a process or experiment with possible outcomes described by a discrete random variable which can take on the values $x_0, x_1, x_2, \ldots$, with probabilities

$p_0, p_1, p_2, \ldots$. The set of probabilities p_n is called a probability distribution. Because the total probability of all the possible outcomes is equal to one, the probability distribution p_n must satisfy the normalization condition

$$\sum_{alln} p_n = 1$$

The probability distribution p_n can be used to evaluate the expectation value for the random variable x_n. This is the average value of the many possible outcomes that may occur when the process or experiment takes place an infinite number of times. It is given by

$$\langle x \rangle = \sum_{alln} x_n p_n$$

The likely spread in the outcomes about this expectation value is given by the standard deviation or uncertainty

in x. We shall denote this by Δx. The square of the standard deviation is called the variance and the variance is given by

$$(\Delta x)^2 = \sum_{all n} (x_n - \langle x \rangle)^2 p_n \tag{1.6}$$

In this expression $(x_n - \langle x \rangle)$ is the deviation of x_n from the expected value; this deviation may be positive or negative and its average value is zero. However, the variance is the average of the square of this deviation; it is zero when there is only one possible outcome and it is a positive number when there is more than one possible outcome.

Rewrite Eq. (1.6) in the following way, using

$$(x_n - \langle x \rangle)^2 = x_n^2 - 2x\langle x \rangle + \langle x \rangle^2$$

and bearing in mind that $\langle x \rangle$ is a number that does not depend on n, we find

$$(\Delta x)^2 = \sum_{alln} x_n^2 p_n - 2\langle x \rangle \sum_{alln} x_n p_n + \langle x \rangle^2 \sum_{alln} p_n$$

or in the form

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

1.3.2 Continuous random variables

Consider a process or experiment in which the outcomes are described by a continuous variable x. The probability of an outcome between x and $x + dx$ can be denoted by $\rho(x)dx$. The function $\rho(x)$ is called a probability density. It satisfies the normalization condition

$$\int_{allx} \rho(x)dx = 1$$

The expectation value of x is given by the integral

$$\langle x \rangle = \int_{allx} x\rho(x)dx$$

Similarly, the expectation value of x^2 is given by

$$\langle x^2 \rangle = \int_{allx} x^2\rho(x)dx$$

From previous details, we can conclude that, the square

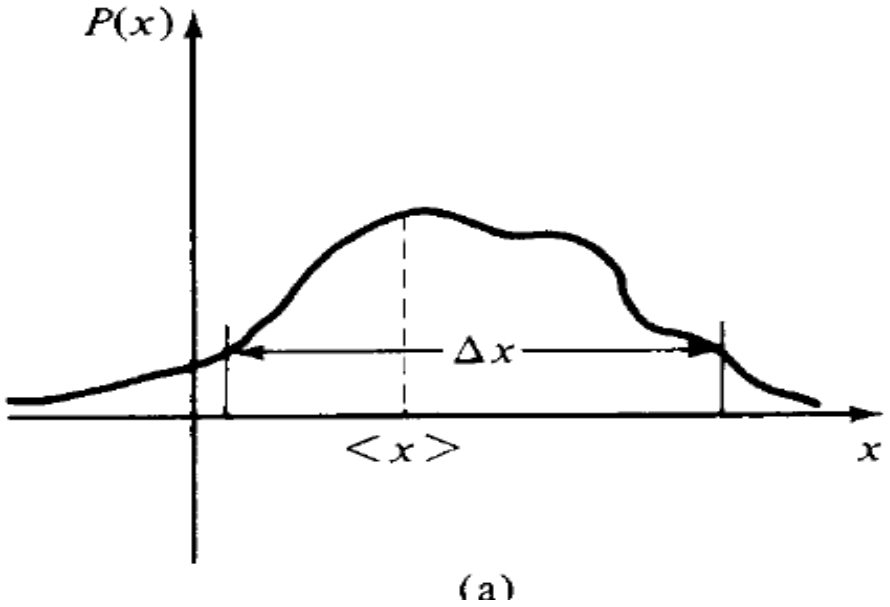

Figure 1.5: (a) Large uncertainty in x; $(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2$

magnitude, $|\psi|^2$, of the wave function $\psi(x, y, z, t)$ can

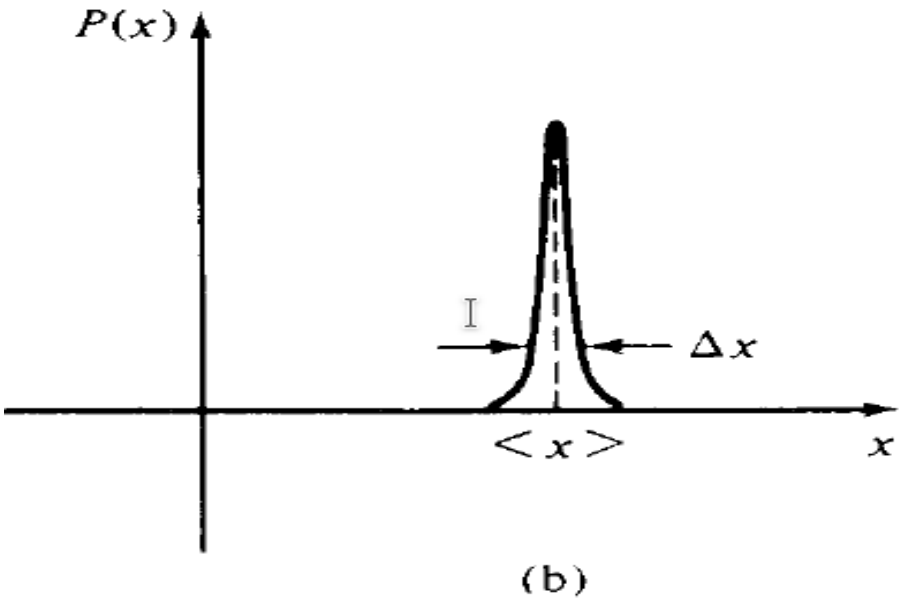

Figure 1.6: (a) Small uncertainty in x; $(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2$

be shown in Fig.(1.7) as grey tones (darker where the magnitude is larger). Now, the physical meaning of the wave function is known as Borns statistical interpretation: darker regions are regions where the particle is more likely to be found if the location is narrowed down. More

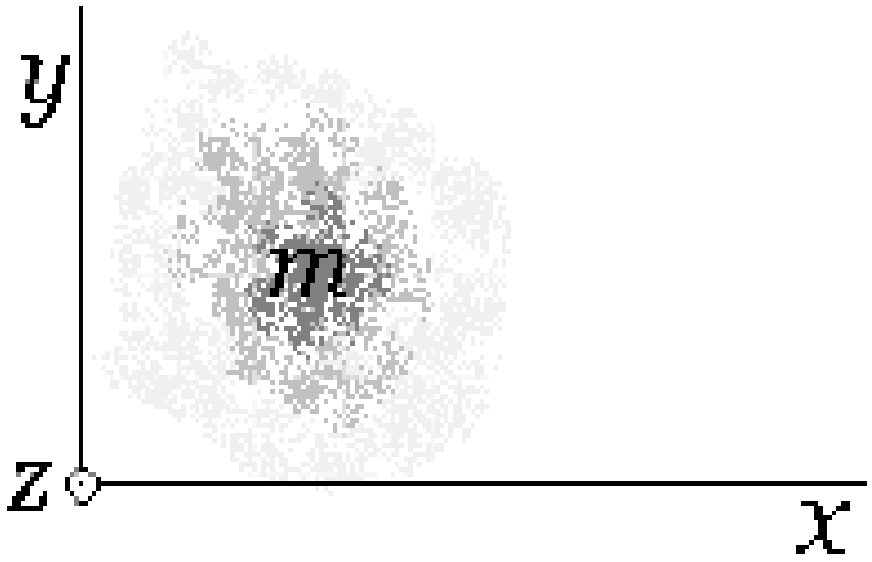

Figure 1.7: A visualization of an arbitrary wave function.

precisely, if $\vec{r} = (x, y, z)$ is a given location, then

$$|\psi(\vec{r}, t)|^2 d^3\vec{r}$$

is the probability of finding the particle within a small volume, of size $d^3\vec{r} = dxdydz$, around that given location, if such a measurement is attempted. **And if such a position measurement is actually done, it affects**

the wave function: after the measurement, the new wave function will be restricted to the volume to which the position was narrowed down. But it will spread out again in time if allowed to do so afterwards.

However, the particle must be somewhere. In quantum mechanics, that is expressed by the fact that the total probability to find the particle, integrated over all possible locations, must be 100% (certainty):

$$\int_{allr} |\psi(\vec{r},t)|^2 d^3\vec{r} = 1$$

1.4 The Heisenberg Uncertainty Principle

The Heisenberg uncertainty principle is a way of expressing the qualitative properties of quantum mechanics in

an easy to visualize way.

Fig. (1.8) is a combination plot of the position x of a particle and the corresponding linear momentum $p_x = mu$, (with m the mass and u the velocity in the x-direction). Fig.(1.9) shows what happens if we squeeze down on the

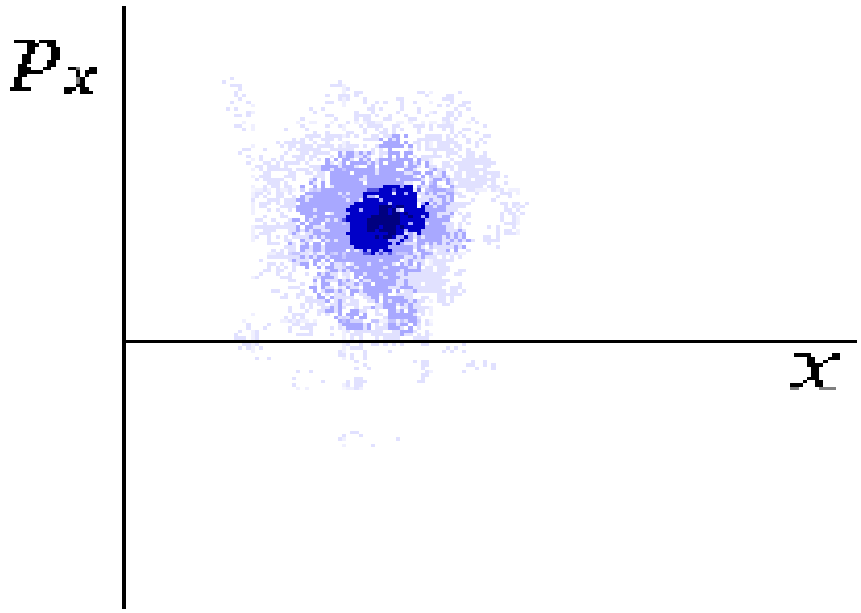

Figure 1.8: Combined plot of position and momentum components.

particle to try to restrict it to one position x: it stretches out in the momentum direction: Heisenberg showed that

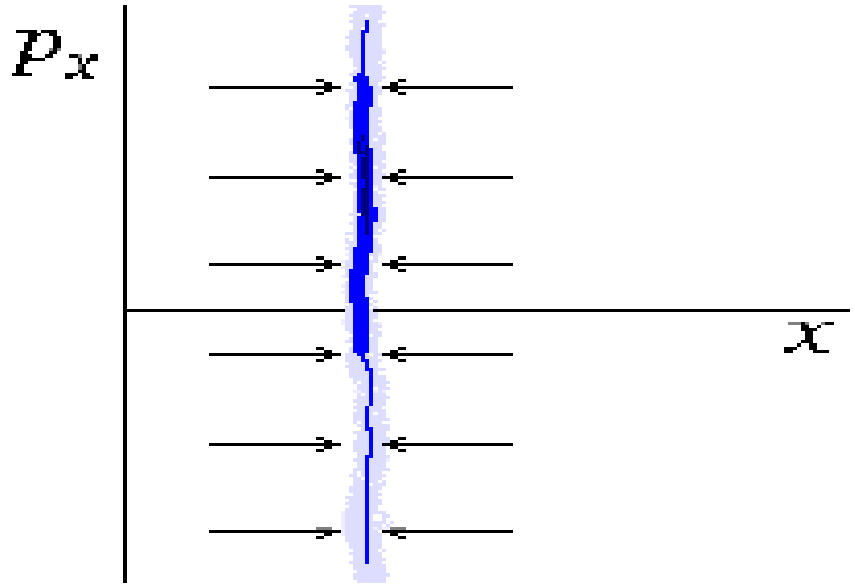

Figure 1.9: Combined plot of position and momentum components.

according to quantum mechanics, **the area of the blue blob cannot be contracted to a point. When we try to narrow down the position of a particle, we get into trouble with momentum. Conversely, if we try to pin down a precise momentum, we lose all hold on the position.**

or in other words: **If a precise measurement of the**

position is made, the new wave packet describing the particle must be very short, a superposition of sinusoidal waves with a very wide range of wavelengths. Similarly, if a precise measurement of the momentum is made, the new wave packet is very long with a sharply defined wavelength.

1.5 Diffraction by two slits

With our interpretation of $|\psi(r)|^2$ as proportional to the probability of find the particle at position r, we are now in a position to calculate a simple electron diffraction problem, that of an electron wave being diffracted by a pair of slits. We need some algebra and wave mechanics to set

up this problem. This behavior is not only one we can use relatively directly to see and verify the wave nature of electrons; it is also a conceptually important "thought experiment" in understanding some of the most bizarre aspects of quantum mechanics. We consider two open

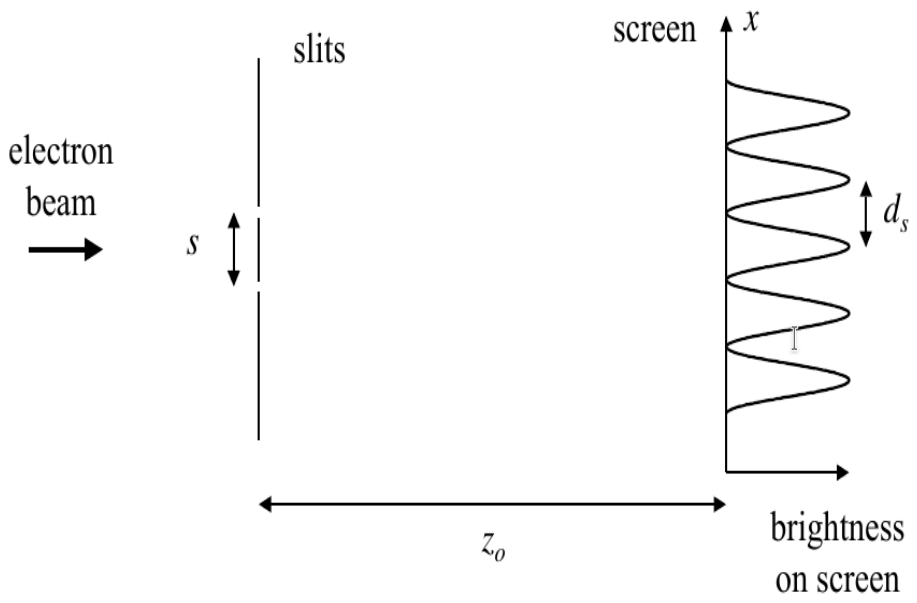

Figure 1.10: A top view of diffraction from two slits, showing the form of the brightness of the interference pattern on a phosphorescent screen.

slits, separated by a distance s, in an otherwise opaque

screen, see Fig.(1.10). We are shining a monochromatic electron beam of wavevector k at the screen, in the direction normal to the screen. For simplicity, we presume the slits to be very narrow compared to both the wavelength $\lambda = 2\pi/k$ and the separation s. We also presume the screen is far away from the slits for simplicity, i.e., $z_0 >> s$, where z_0 is the position of the screen relative to the slits.

For simplicity of analysis, we will regard the slits as essentially point sources of expanding waves, in the spirit of Huygens principle. We write could write these waves in the form $\exp(ikr)$, where r is the radius from the source point. We have therefore one source (slit) at $x = s/2$, and another at $x = -s/2$. The net wave should be the

sum of the waves from these two sources. Remembering that in the $x - z$ plane the equation of a circle of radius r centered about a point $x = a$ and $z = 0$ is $r^2 = (x - a)^2 + z^2$, the net wave at the screen is

$$\psi_s(x) \propto \exp\left[ik\sqrt{(x - s/2)^2 + z_0^2}\right] + \exp\left[ik\sqrt{(x + s/2)^2 + z_0^2}\right]$$

where the first term corresponds to a wave expanding from the upper slit, and the second corresponds similarly with the wave from the lower slit. Note that we are adding the wave amplitudes here. If we presume we are only interested in the pattern on the screen for relatively small angles, i.e., $x << z_0$, then

$$\sqrt{(x - s/2)^2 + z_0^2} = z_0\sqrt{1 + (x - s/2)^2/z_0^2}$$

$$\cong z_0 + (x - s/2)^2/2z_0$$

$$\cong z_0 + x^2/2z_0 + s^2/8z_0 - sx/2z_0$$

and similarly for the other exponent (though with opposite sign for the term in s). Hence, using $2\cos(\theta) = \exp(i\theta) + \exp(-i\theta)$, we obtain

$$\psi_s(x) \propto \exp(i\phi)\cos(ksx/2z_0) = \exp(i\phi)\cos(\pi sx/\lambda z_0)$$

where ϕ is a real number; $\phi = k(z_0 + x^2/2z_0 + s^2/8z_0)$, so $\exp(i\phi)$ is simply a phase factor. Hence, on the screen,

$$|\psi_s(x)|^2 \propto \cos^2(\pi sx/\lambda z_0) = \frac{1}{2}\Big[1 + \cos(2\pi sx/\lambda z_0)\Big]$$

So, if we shine a beam of monoenergetic electrons at the slits, and put some phosphorescent screen (like our cathode ray tube screen) some distance behind the slits, we should expect to see a (co)sinusoidal interference pattern, or fringes, on the screen, with the fringes separated by

a distance $d_s = \lambda z_0/s$. This simple fringe pattern is somewhat idealized; with a more sophisticated diffraction model, and with finite width for the slits, the intensity of the fringes falls off for larger x, but the basic interference fringes we predict here will be observed near the axis as long as the slit separation is much larger than the slit width.

The existence of these interference effects for the quantum mechanical amplitudes has some bizarre consequences that we simply cannot understand classically. For example, suppose that we block one of the slits so the electrons can only go through one slit. Then we would not see the interference fringes. Near the axis we would see a broad featureless band that is readily understood from

wave diffraction from a single slit. Such a broad band is already difficult to explain based on a classical model of a particle; in a classical model, with the electron particles all traveling from left to right in straight lines, we would expect to see a relatively sharp spot on the screen. If we were determined to explain this broad band classically we might come up with some explanation, involving electrons bouncing off the edges of the slit, that would at least be qualitatively plausible (if ultimately incorrect). If we now uncover the second slit, however, we see something that cannot be explained by a classical particle picture parts of the screen that were formerly bright now become dark (the minima of the (co)sinusoidal interference pattern described above). How can we explain that opening

a second source of particles actually reduces the number of particles arriving at some point in the screen?

We might try to argue that the particles from the second slit were somehow bouncing off the ones from the first slit, and hence avoiding some particular part of the screen because of these collisions. If we repeat the experiment with extremely low electron currents so that there are never two electrons in the apparatus at a given time, and take a time-exposure picture of the phosphorescent screen, we will, however, see exactly the same interference pattern emerge, and we cannot now invoke some explanation that involves particles colliding with one another. Hence we are forced even qualitatively to describe the behavior of the electrons in terms of some process in-

volving interference of amplitudes, and we also find that the wave description postulated above does explain the behavior quantitatively.

Though a two-slit diffraction experiment of exactly the form described here might be quite difficult to perform in practice with electrons, diffraction phenomena such as this can be seen quite readily with electrons. Such diffraction is routinely used as a diagnostic and measurement tool. Electrons can be accelerated by electric fields and, if necessary, focused using magnetic and electric techniques. The wavelength associated with such accelerated electrons can be very small (e.g., an Ångstrom (1Å), which is 0.1 nm). Diffractive effects are particularly strong when the wavelength is comparable to the size of

an object (e.g., comparable to the slit spacing, s, above). Electrons can diffract quite strongly off crystal surfaces, for example, where the spacings between the atoms are on the order of ngstroms or fractions of a nanometer.

One diagnostic technique, reflection high-energy electron diffraction (RHEED), for example, monitors the form of a crystal surface during the growth of crystalline layers; an electron beam incident at a shallow angle relative to the surface (i.e., nearly parallel with the crystal surface) is reflected and diffracted onto a phosphorescent screen to give a diffraction pattern characteristic of the precise form of the surface. Electron diffraction is also intrinsic to the operation of some kinds of electron microscope. In general, the fact that the electron wavelength can be

so small means that electron microscopes can be used to view very small objects; it is practically difficult to image objects much smaller than a wavelength with any optical or wave-based technique because of diffractive effects, but the small wavelength possible in electron beams means that small objects or features can be seen.

Chapter 2

Motion of free particles in space

2.1 Confined particle in a box

As we see before that, for the wave function $\psi(x) = A\exp(ikx)$, it integration $\int_{\infty}^{\infty} |\psi(x)|^2 dx$ will goes to infinity, i.e, $\int_{\infty}^{\infty} |\psi(x)|^2 dx \rightarrow \infty$, in this case it is tradationally to study the state in a finite region (particle confinment) such as a cubic region, see Fig.(2.1) of side l with initial condition of periodicity of the wave function (or the wave function equal to zero at these sides). The

periodicity condition means that the wave fucntion has the same values on every two opposite sides or mathematically as

$$\psi(x,y,z) = \psi(x+l,y,z) = \psi(x,y+l,z) = \psi(x,y,z+l)$$

Applying the normalization condition, we have

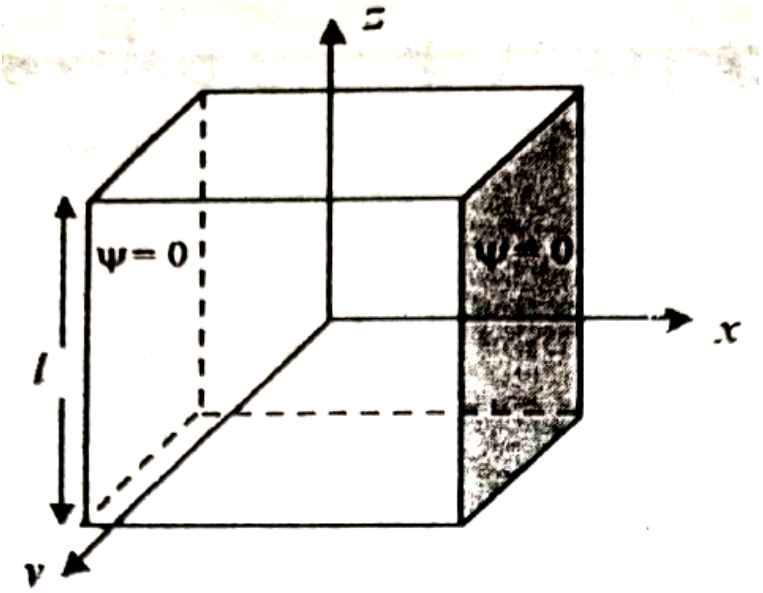

Figure 2.1: Quantization cube.

$$\int_{-l/2}^{l/2} \psi^*(x)\psi(x)dx = \int_{-l/2}^{l/2} |\psi(x)|^2 dx$$

$$|A|^2 \int_{-l/2}^{l/2} dx = |A|^2 l = 1$$

which mena that $A = \frac{1}{\sqrt{l}}$, and the normalixed wave function becomes

$$\psi(x) = \frac{1}{\sqrt{l}} \exp(ikx)$$

Applying the periodicity condition on the last function we obtain

$$\psi(x) = \psi(x + l)$$

or

$$\exp[ikx] = \exp[ik(x + l)] \rightarrow \exp(ikl) = 1$$

this implies that

$$kl = 2n\pi \rightarrow k_n = \frac{2n\pi}{l}$$

where n are positive and negative integrs. In this case, the change in k, ie, Δk is the difference between any two

consecutive values, or $\Delta k = 2\pi/l$. Note, the periodicity condition, that is equivalent to the condition of particle confinment, implies that the wave vector $\vec{k}$ was taking a series of separate values determined from the last equation.

In case of 3D, the wave function ψ takes the form

$$\psi(r) = \frac{1}{l^{3/2}} \exp[ikr] = \frac{1}{\sqrt{V}} \exp[ikr]$$

where V is the cube volume. Now, it convienet to index the wave function with label related to the wave number k, i.e,

$$\psi_k(x) = \frac{1}{\sqrt{V}} \exp[ik_n x]$$

or in terms of n

$$\psi_n(x) = \frac{1}{\sqrt{V}} \exp[2in\pi x/l]$$

Now all these normalized wave functions corresponding to the possible values of the wave vector $\vec{k}$ constitute among each other a set of orthogonal functions (or in short orthonormal set), i.e,

$$\int_V \psi_k^*(r)\psi_{k'}(r)d\tau = \delta_{kk'}$$

or

$$\int_V \psi_n^*(r)\psi_{n'}(r)d\tau = \delta_{nn'}$$

the last two equations known as the orthonormalization condition, where

$$d\tau = dxdydz, \qquad \delta_{kk'} = \delta_{k_1k_1'}\delta_{k_2k_2'}\delta_{k_3k_3'}$$

and $\delta_{kk'}$ is the kroniker-delta function

$$\delta_{kk'} = \begin{cases} 1, & k = k' \\ 0, & k \neq k' \end{cases}$$

or in terms of the quantum number n as

$$\delta_{nn'} = \begin{cases} 1, & n = n' \\ 0, & n \neq n' \end{cases}$$

The case that $k \neq k'$ $(n \neq n')$ means the probability of finding the particle in a two distinct states, that means we cann't find a particle of distinct values of the number $k(n)$ that be found in single state.

Let's now prove the last relation begining from the integration

$$\int \psi_k^*(x)\psi_{k'}(x)dx = \frac{1}{l}\int_{-l/2}^{l/2} \exp[-ikx]\exp[ik'x]$$
$$= \frac{1}{l}\int_{-l/2}^{l/2} \exp[i(k'-k)x]$$

in the case where $k = k'$ $(n = n')$, we have $(k' - k = 0,$ that implies

$$\int \psi_k^*(x)\psi_k(x)dx = \int |\psi_k(x)|^2 dx = 1$$

but in the case where $k \neq k'(n \neq n')$, we have

$$\int \psi_k^*(x)\psi_{k'}(x)dx = \frac{1}{l}\frac{2i\sin[\frac{l}{2}(k'-k)]}{i(k'-k)}$$

$$= \frac{\sin[\frac{l}{2}(k'-k)]}{\frac{l}{2}(k'-k)}$$

the last equation represents the general case of the previous integration where if we substitute about $k = k_n = \frac{2n\pi}{l}$, $k' = k_{n'} = \frac{2n'\pi}{l}$, we find that

$$\int \psi_k^*(x)\psi_{k'}(x)dx = \frac{\sin[\pi(n'-n)]}{\pi(n'-n)} = 0$$

that is the case where $n \neq n'$, but when $n = n'$, putting such a quantity in the form $\frac{\sin x}{x}$, with $x = \frac{l}{2}(k'-k) = \pi(n'-n)$, in this case

$$\lim_{x\to 0}\frac{\sin x}{x} = 1$$

2.2 Examples

2.2.1 Example .1

Calculate $\psi(x,0)$ for the Gaussian wave packet $\phi(k) = A\exp[-a^2(k-k_0)^2/4]$, where A is the normalization constant. Calculate the normalization constant and the probability of finding the particle in the region $-a/2 \leq x \leq a/2$, find also the function $\phi(k)$ for the quadratic wave packet

$$\psi_0(x) = \begin{cases} A\exp(ik_0x), & |a| \leq a \\ 0, & |a| > a \end{cases}$$

Also, find the the normalization constant

Solution

To find the normalization constant, we do

$$1 = \int_{-\infty}^{\infty} |\phi(k)|^2 dk = \int_{-\infty}^{\infty} \exp\Big[-\frac{a^2}{2}(k-k_0)^2\Big]dk$$

put $z = k - k_0$, and with aid of the rule

$$\int_{-\infty}^{\infty} \exp\Big[-\frac{a^2 z^2}{2}\Big] dz = \sqrt{2\pi}/a$$

we find

$$A = \sqrt{a/\sqrt{2\pi}} = [a^2/2\pi]^{1/4}$$

in this case, the normalized wave packet becomes

$$\phi(k) = \left(\frac{a^2}{2\pi}\right)^{1/4} \exp\Big[-\frac{a^2}{4}(k-k_0)^2\Big]$$

and the function $\psi(x,0)$ becomes

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) \exp(ikx) dk$$

$$= \frac{1}{\sqrt{2\pi}} \left(\frac{a^2}{2\pi}\right)^{1/4} \int_{-\infty}^{\infty} \exp\Big[-\frac{a^2}{4}(k-k_0)^2 + ikx\Big] dk$$

to evaluate the integration, we should rearrange the power part as

$$-\frac{a^2}{4}(k-k_0)^2 + ikx = -\Big[\frac{a}{2}(k-k_0) - \frac{ix}{a}\Big]^2 - \frac{x^2}{a^2} + ik_0 x$$

Now, put $y = \frac{a}{2}(k - k_0) - \frac{ix}{a}$, hence $dk = 2dy/a$, and the wave function takes the form

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}}\left(\frac{a^2}{2\pi}\right)^{1/4}\int_{-\infty}^{\infty}\exp\Big(-\frac{x^2}{a^2}\Big)\exp(ik_0x)$$

$$\times\exp(-y^2)\Big(\frac{2}{a}dy\Big)$$

$$= \frac{1}{\sqrt{\pi}}\left(\frac{2}{\pi a^2}\right)^{1/4}\exp\Big(-\frac{x^2}{a^2}\Big)\exp(ik_0x)\int_{-\infty}^{\infty}\exp(-y^2)dy$$

but

$$\int_{-\infty}^{\infty}\exp(-y^2)dy = \sqrt{\pi}$$

hence, the wave function becomes

$$\psi(x,0) = \left(\frac{2}{\pi a^2}\right)^{1/4}\exp\Big(-\frac{x^2}{a^2}\Big)\exp(ik_0x)$$

where $\exp(ikx_0)$ represents the phase function for the wave function $\psi(x,0)$. Here we realize that $\psi(x,0)$ represents an oscillating wave of the modified wave number

k_0 by a Gaussian function centered around the origin. Also, note that $\psi(x,0)$ like $\phi(k)$ a normalized function, that means the forier transform for the Gaussian wave packet is also Gaussian wave packet.

The probability of finding the particle in the region $-a/2 \leq x \leq a/2$ is given by

$$P = \int_{-a/2}^{a/2} |\psi(x,0)|^2 dx = \left(\frac{2}{\pi a^2}\right)^{1/2} \int_{-a/2}^{a/2} \exp\left(-\frac{2x^2}{a^2}\right) dx$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-1}^{+1} \exp\left(-\frac{z^2}{2}\right) dz$$

where we put $z = 2x/a$. To normalize the function

$$\psi_0(x) = \begin{cases} A\exp(ik_0x), & |a| \leq a \\ 0, & |a| > a \end{cases}$$

as previous we do

$$1 = \int_{-\infty}^{\infty} |\psi_0(x)|^2 dx$$

$$= |A|^2 \int_{-a}^{a} \exp[-ik_0 x] \exp[ik_0 x] dx = 2a|A|^2$$

Or $A = \frac{1}{\sqrt{2a}}$, and the Fourier transform of the function $\psi_0(x)$ becomes

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi_0(x) \exp(-ikx) dx$$

$$= \frac{1}{2\sqrt{\pi a}} \int_{-a}^{a} \exp(-ik_0 x) \exp(-ikx) dx$$

$$= \frac{1}{\sqrt{\pi a}} \frac{\sin(k - k_0)a}{k - k_o}$$

2.3 Excercises

1. Find the Fourier transform for the function

$$\phi(k) = \begin{cases} A(a - |k|), & |k| \leq a \\ 0, & |k| > a \end{cases}$$

where a is a positive parameter and A is the normalization constant that should be found also.

2. Consider the functions

$$\psi_1 = A_1 \exp(-y^2), \quad \psi_2 = A_2 \exp(-y^2/2),$$

$$\psi_3 = A_3[\exp(-y^2) + y \exp(-y^2/2)],$$

where A_1, A_2, A_3 are normalization constants.

i. find the normalization constants A_1, A_2, A_3

ii. calculate the probability of finding each case in the intervals $-1 < y < 1, 0 < y < 1$

3. Finf Fourier transform for the following functions and also calculate the normalization constant if found

$$\psi(x) = \begin{cases} 1 - |x|, & |x| < 1 \\ 0, & |x| \geq 1 \end{cases}$$

$$\psi(x) = \frac{A}{1+x^2}, \quad \phi(k) = A\exp(-a|k| - ibk)$$

$$\phi(p) = \begin{cases} 0, & p < -p_0 \\ A, & -p_0 < p < p_o \\ 0, & p_0 < p \end{cases}$$

Chapter 3

Linear harmonic oscillator

In this chapter, we will discuss the wave function for a moving particle in an harmonic oscillating potential. The harmonic oscillating potential is considered as an important example as a lot of physical phenomena like internal molecules' vibrations and atomic motion inside solid objects can be described using harmonic oscillating potential.

3.1 Classical harmonic oscillator

It is well know in classical mechanics that the stored energy that proportional to distance from equilibrium point, i, e, $F = -Cx$, implies a simple harmonic motion. Such a force can be derived from the potential

$$V = \frac{Cx^2}{2}$$

using the relation between the force and potential

$$\frac{dV}{dx} = -F$$

in this case, the 1D equation of motion for the classical harmonic oscillator in the form

$$E = \frac{Mv^2}{2} + \frac{Cx^2}{2}$$

the solution of such an equation can be wrote in the form

$$x = A\sin(\omega t)$$

to determine the constants we do the following

$$E = \frac{MA^2}{2}\omega^2\cos^2(\omega t) + \frac{CA^2}{2}\sin^2(\omega t)$$

or

$$\frac{2E}{CA^2} = \frac{M\omega^2}{C}\cos^2(\omega t) + \sin^2(\omega t)$$

this equality satisfied when

$$\omega^2 = \frac{C}{M}, \quad A^2 = \frac{2E}{C}$$

in this case, the solution will be

$$x = \sqrt{\frac{2E}{C}}\sin\left(\sqrt{\frac{C}{M}}t\right)$$

wihch means that the calssical harmonic oscillator can has any amplitude, hence total energy, but with one fre-

quency

$$\omega = \sqrt{\frac{C}{M}},$$

3.2 Quantum harmonic oscillator

Now let's examine how quantum mechanics works. The

begin with 1D Schrödinger equation for such an oscillator

$$-\frac{\hbar^2}{2M}\frac{d^2u}{dx^2} + \frac{\omega^2 M x^2}{2}u = Eu$$

Now, let's simplify such equation by putting it in the form

$$-\frac{\hbar}{M\omega}\frac{d^2u}{dx^2} + \frac{\omega^2 M x^2}{\hbar}u = \frac{2Eu}{\hbar\omega} = \lambda u$$

with $\lambda = \frac{2E}{\hbar\omega}$. Also, the last equation may be simpler if we use the substitution $x = y\sqrt{\hbar/M\omega}$, then we have

$$-\frac{d^2u}{dy^2} + y^2 u = \lambda u$$

or

$$\frac{d^2u}{dy^2} + (\lambda - y^2)u = 0 \tag{3.1}$$

To solve the last equation, we should make some approximations where for very big values of x we have $\lambda u << y^2 u$, then we obtain

$$\frac{d^2u_\infty}{dy^2} = y^2 u_\infty$$

where we cancel the term λu, in this case, the solution will be for very big values of x thay we can obtain as follows: multiplying the last equation by the quantity $2\frac{du_\infty}{dy}$, we get

$$\frac{d}{dy}\Big(\frac{du_\infty}{dy}\Big)^2 - y^2\frac{du_\infty^2}{dy} = 0$$

or

$$\frac{d}{dy}\Big[\Big(\frac{du_\infty}{dy}\Big)^2 - y^2u_\infty^2\Big] = -2yu_\infty^2$$

if we make the term $-2yu_\infty^2$ small enough, we could cancel it and have

$$\frac{d}{dy}\Big[\Big(\frac{du_\infty}{dy}\Big)^2 - y^2u_\infty^2\Big] = 0$$

implementing the integration, we obtain

$$\frac{du_\infty}{dy} = \sqrt{G + y^2u_\infty^2}$$

where G is the constant of integration. From previous, u_∞^2 and $\frac{du_\infty}{dy}$ go to zero as y goes to $infty$, the we obtain that $G = 0$, and finally have

$$\frac{du_\infty}{dy} = \pm yu_\infty$$

or

$$\frac{du_\infty}{u_\infty} = \pm ydy$$

with solution

$$u_\infty = A\exp(-y^2/2) + B\exp(y^2/2)$$

We shall cancel the term $\exp(y^2/2)$ as it diverges as $y \to \infty$, then we have

$$u_\infty = A\exp(-y^2/2)$$

up to this stage, we implemented all needed approximations for suitable slution for equation of motion of the oscillator, but the remaining step is the constant of integration A, that may be a function of y due to such approximations, then we write

$$u(y) = f(y)\exp(-y^2/2)$$

To determine $f(y)$, substituting in Eq.(3.1) as

$$\frac{d^2u}{dy} = \exp(-y^2/2)[-f(y) - 2yf'(y) + f''(y) + y^2f(y)]$$

we have

$$\exp(-y^2/2)[-f(y) - 2yf'(y) + f''(y) + y^2 f(y)]$$

$$+(\lambda - y^2)f(y)\exp(-y^2/2) = 0$$

or

$$f''(y) - 2yf'(y) + (\lambda - 1)f(y) = 0$$

if we put $\lambda - 1 = 2n$ or $\lambda = 2n+1, n = 0, 1, 2, \ldots$, the solution of the last equation will be the Hermit polynomial, i. e, $f(y) = H_n(y)$, hence

$$u_n(y) = H_n(y)\exp(-y^2/2)$$

3.3 Eigenvalues and eigenfunctions

Using the quantity $\lambda = \frac{2E}{\hbar\omega}$ as

$$\frac{2E}{\hbar\omega} = 2n + 1$$

this implies

$$E = E_n = \frac{1}{2}\hbar\omega(2n+1) = \hbar\omega(n+\frac{1}{2})$$

which represents the allowed energy values that can the oscillator take in a quantum form which correspond to the energy eigen vlaues with the unnormalized eigen functions

$$u_n(y) = Q_n H_n(y)\exp(-y^2/2)$$

substituting with $y = \sqrt{M\omega/\hbar}x$, we have

$$u_n(x) = Q_n H_n(\sqrt{M\omega/\hbar}\, x)\exp[-M\omega x^2/2\hbar]$$

with Q_n is the normalization constant. Here we recapulate some important remarks on the eigenvalues of the harmonic oscillator:

1. Quantum oscillator energy levels are separated by

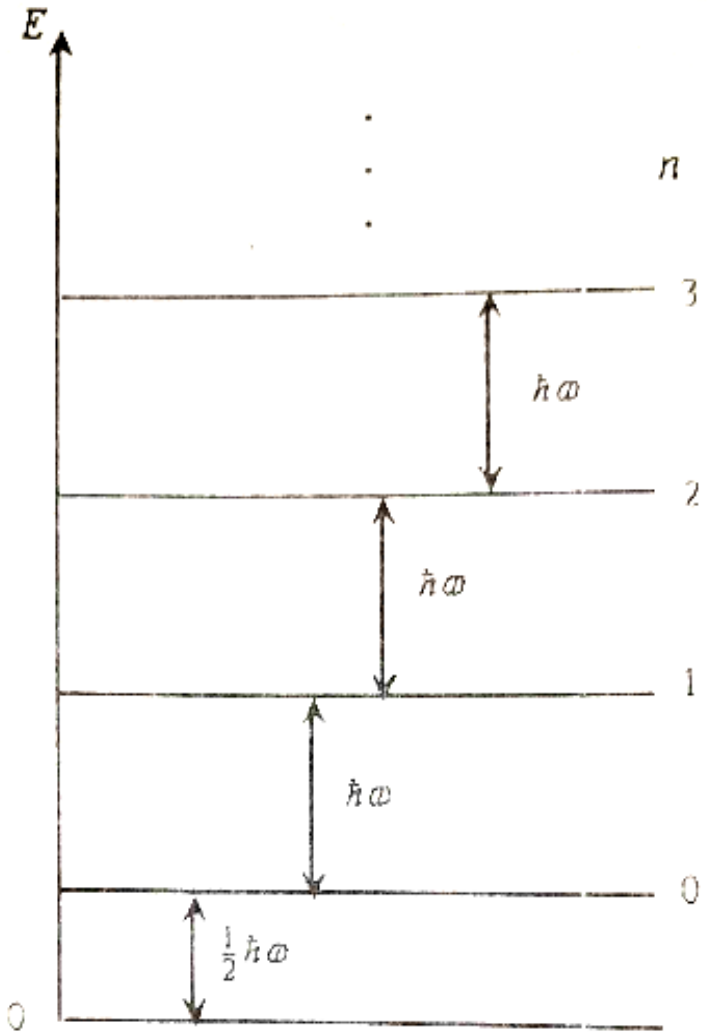

Figure 3.1: Quantization cube.

equal values, that is extinguish laboratory specrta for some materials molecules and nucli. In this context, we find that quantum harmonic oscillator represents a adquate and good model for describing such specrta.

2. For every eigenvalue, there exist only one eigenfunction, that represents a common advantigue for 1D bound potential that remain bound for bound values of x.

3. For every $n = 0$, that is called ground state, the oscillator energy is $E_0 = \frac{1}{2}\hbar\omega$ that represents the zero energy of the oscillator.

4. As Hermit polynomials correspond to the eigenval-

ues of the quantum number n are function of order n, it follows that the oscillator eigenfunctions have n nodes. Note, the number of nodes is directly proportional to energy value, namely, the higher number of nodes the greater the value of energy, that could be understood easily as the momentum is proportional to the arc curvature or the wave function curvature (d^2u/dx^2), that means the greater the curvature of the arc, the greater the momentum(i. e, the greater wave function curvature back and forth to reach zero, the greater the energy).

5. Figures (3.2, 3.3) show a comparison between probability density of the particle at different distances from the origin in case of classical and quantum sit-

uations, respectively. We see easily the coincidence between them developes gradually as the quantum number increases. Finally, we conclude that, the quantum systems, in general, their behaviours converges the classical behaviour as we move towards the greater values of the quantum number n.

3.3.1 Some Hermit polynomials properties

$$H_0(y) = 1$$

$$H_1(y) = 2y$$

$$H_2(y) = -2 + 4y^2$$

$$H_3(y) = -12y + 8y^3$$

$$H_4(y) = 12 - 48y^2 + 16y^4$$

$$H_5(y) = 120y - 160y^3 + 32y^5$$

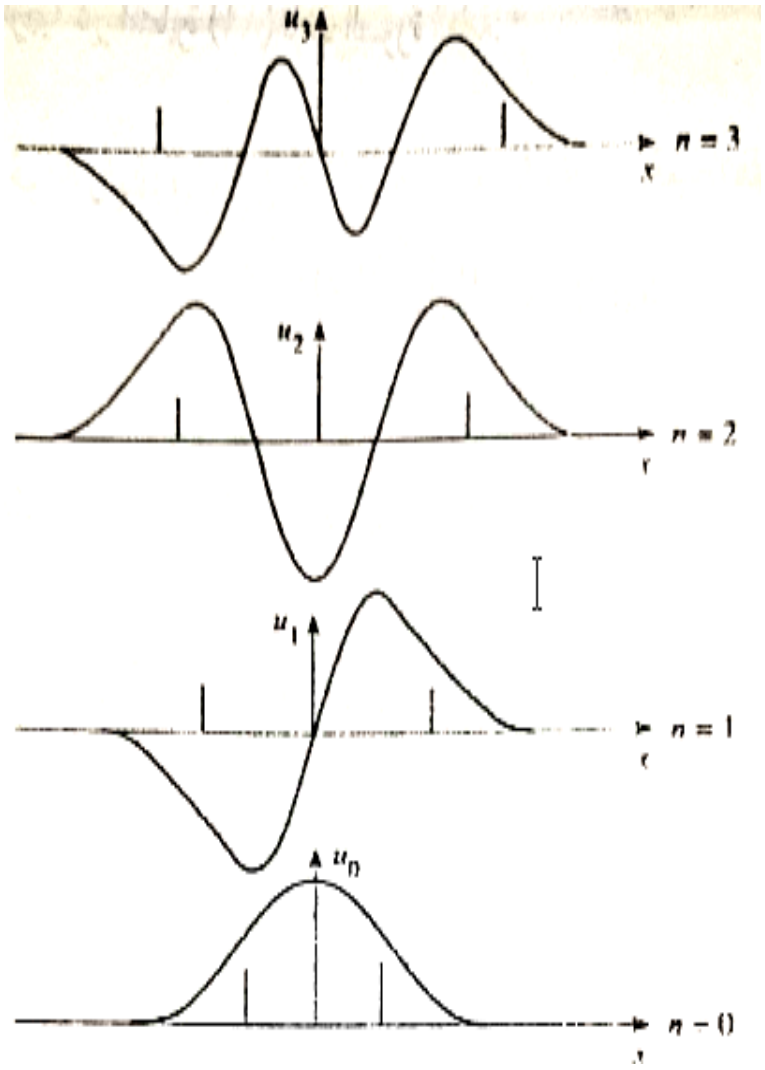

Figure 3.2: Quantum wave function.

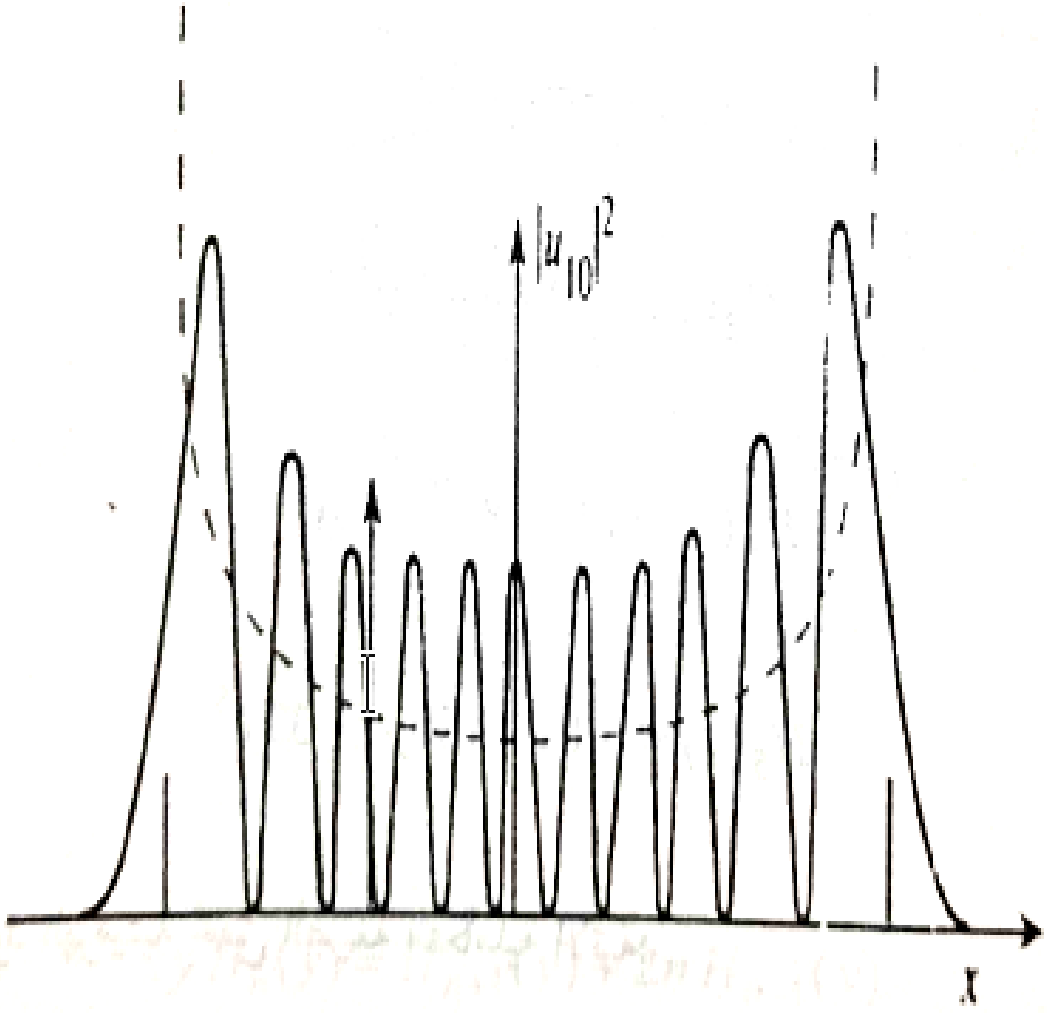

Figure 3.3: Classical wave function

Also, Hermit polynomials satisfy the integration form

$$\int_{\infty}^{\infty} dy H_n(y) H_m(y) \exp[-y^2] = \sqrt{\pi} 2^n n! \delta_{nm}$$

3.3.2 Calculating the normalization constant Q_n

Exploiting the last property of Hermit polynomials, we can easily calculate the normalization constant Q_n as follows:

$$\int_{\infty}^{\infty} dx u_n^2(x) = Q_n^2 \sqrt{\hbar/M\omega} \sqrt{\pi} 2^n n! = 1$$

or

$$Q_n = \frac{(M\omega/\pi\hbar)^{1/4}}{\sqrt{2^n n!}}$$

hence, the normalized wave functions take the form

$$u_n(x) = \frac{(M\omega/\pi\hbar)^{1/4}}{\sqrt{2^n n!}} H_n(\sqrt{M\omega/\hbar}\, x) \exp[-M\omega x^2/2\hbar] \tag{3.2}$$

From the last form of the wave functions we can easily conclude that orthogonality of the wave functions for different values of the quantum number n comes from Hermit polynomials orthogonality.

3.3.3 The number operator

The following three recurrence relations of Hermit polynomials are important in calculating the expectation (average) value for the quantum harmonic oscillator via the aid of the eigenfunctions $u_n(x)$. These three recurrence relations area

$$\frac{dH_n(y)}{dy} = 2nH_{n-1}(y) \tag{3.3}$$

$$2yH_n(y) = H_{n+1}(y) + 2nH_{n-1}(y) \tag{3.4}$$

$$yH_n(y) = nH_{n-1}(y) + \frac{1}{2}H_{n+1}(y) \tag{3.5}$$

Now, from Eq.(3.2), by putting $\mu = \sqrt{M\omega/\hbar}\, x$, and

$$\gamma = (M\omega/\pi\hbar)^{1/4} \exp[-\mu^2/2]$$

we have

$$u_n(\mu) = \frac{\gamma}{\sqrt{2^n n!}} H_n(\mu)$$

now,

$$\begin{aligned} u_{n-1}(\mu) &= \frac{\gamma}{\sqrt{2^{n-1}(n-1)!}} H_{n-1}(\mu) \\ &= \sqrt{2n} \frac{\gamma}{\sqrt{2^n n!}} H_{n-1}(\mu) \end{aligned}$$

and

$$\begin{aligned} u_{n+1}(\mu) &= \frac{\gamma}{\sqrt{2^{n+1}(n+1)!}} H_{n+1}(\mu) \\ &= \frac{1}{\sqrt{2(n+1)}} \frac{\gamma}{\sqrt{2^n n!}} H_{n+1}(\mu) \end{aligned}$$

or

$$\gamma\ H_n = \sqrt{2^n n!}\ u_n \tag{3.6}$$

now,

$$\gamma\ H_{n-1} = \frac{1}{\sqrt{2n}}\sqrt{2^n n!}\ u_{n-1} \tag{3.7}$$

and

$$\gamma\ H_{n+1} = \sqrt{2(n+1)}\sqrt{2^n n!}\ u_{n+1} \tag{3.8}$$

Inserting Eqs. (3.3-3.5) into Eqs. (3.6-3.8) with replacing the variable y by the variable μ, we obtain

$$\mu\ u_n = \frac{n}{\sqrt{2n}}\ u_{n-1} + \frac{1}{2}\sqrt{2(n+1)}\ u_{n+1} \tag{3.9}$$

$$\mu\ u_n = \sqrt{n/2}\ u_{n-1} + \sqrt{\frac{n+1}{2}}\ u_{n+1} \tag{3.10}$$

Also, from Eq.(3.2), putting $R = \frac{(M\omega/\pi\hbar)^{1/4}}{\sqrt{2^n n!}}$, we have

$$u_n(\mu) = R\ H_n(\mu)\exp[-\mu^2/2]$$

by differentiating the last equation with respect to μ, we obtain

$$u_n' = R\ \exp[-\mu^2/2][H_n' - \mu H_n]$$

orb br using Eq.(3.3)

$$u'_n = R\ \exp[-\mu^2/2][2nH_{n-1} - \mu H_n]$$

and by using Eq.(3.5), we obtain

$$u'_n = R\ \exp[-\mu^2/2][2nH_{n-1} - nH_{n-1} - \frac{1}{2}H_{n+1}]$$

$$= R\ \exp[-\mu^2/2][nH_{n-1} - \frac{1}{2}H_{n+1}]$$

$$= \frac{\gamma n}{\sqrt{2^n n!}}H_{n-1} - \frac{\gamma}{2\sqrt{2^n n!}}H_{n+1}$$

Using Eqs. (3.7,3.8), we have

$$u'_n = \sqrt{n/2}\ u_{n-1} - \sqrt{\frac{n+1}{2}}\ u_{n+1} \qquad (3.11)$$

From the last Eq.(3.11) and Eq.(3.10), we obtain

$$\frac{1}{\sqrt{2}}\Big(\mu + \frac{\partial}{\partial\mu}\Big)\ u_n = \sqrt{n}\ u_{n-1}$$

$$\frac{1}{\sqrt{2}}\Big(\mu - \frac{\partial}{\partial\mu}\Big)\ u_n = \sqrt{n+1}\ u_{n+1}$$

Bu using the operator $\hat{p}_\mu = -i\frac{\partial}{\partial\mu}$ that is related to the momentum operator $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$ by the relation $\hat{p}_x = \sqrt{\hbar M\omega}\ \hat{p}_\mu$, the last relations take the forms

$$\hat{a}\ u_n = \sqrt{n}\ u_{n-1} \tag{3.12}$$

$$\hat{a}^\dagger\ u_n = \sqrt{n+1}\ u_{n+1} \tag{3.13}$$

with the operators $\hat{a}$ and $\hat{a}^\dagger$ are given by

$$\hat{a} = \frac{1}{\sqrt{2}}\Big(\mu + \frac{\partial}{\partial\mu}\Big) = \frac{1}{\sqrt{2}}\Big(\mu + ip_\mu\Big)$$
$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\Big(\mu - \frac{\partial}{\partial\mu}\Big) = \frac{1}{\sqrt{2}}\Big(\mu - ip_\mu\Big)$$

From Eq.(3.13), with by operating n times with the operator $\hat{a}^\dagger$ on the wave function u_0, we obtain

$$u_n = \frac{1}{\sqrt{n!}}\Big(\hat{a}^\dagger\Big)^n\ \ u_0$$

Note that, the ground state wave function could be obtained from the condition $\hat{a}^\dagger\ u_0 = 0$, i.e, by solving the

equation

$$\left(\mu + \frac{\partial}{\partial \mu}\right) u_0 = 0$$

that has a solution given by

$$u_0 = R_0 \exp[-\mu^2/2]$$

with R_0 is the normalization constant and given by

$$R_0 = \left(\frac{M\omega}{\pi\hbar}\right)^{1/4}$$

also, using Eq.(3.12, 3.13), by the recurrence operating with the operators $\hat{a}$ and $\hat{a}^\dagger$, we obtain

$$\hat{a}\hat{a}^\dagger \; u_n = (n+1) \; u_n \tag{3.14}$$

and

$$\hat{a}^\dagger \hat{a} \; u_n = n \; u_n \tag{3.15}$$

substituting the last two equations and using the unti-commutator $[\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}$, we obtain

$$(\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a})\ u_n = [(n+1) - n]\ u_n$$

or

$$[\hat{a}, \hat{a}^\dagger]\ u_n = u_n$$

that yields

$$[\hat{a}, \hat{a}^\dagger] = 1$$

also, adding the two equations we obtain

$$(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a})\ u_n = [(n+1) + n]\ u_n$$

or

$$\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} = 2n + 1$$

but we have from previous that

$$\hat{a} = \frac{1}{\sqrt{2}}\Big(\mu + ip_\mu\Big)$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\Big(\mu - ip_\mu\Big)$$

or

$$\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} = \mu^2 + p_\mu^2 = 2n + 1$$

in this case, the Hamiltonian (Hamilton function operator) is given by

$$\hat{H} = \frac{\hat{p}_x^2}{2M} + \frac{M\omega^2}{2}\hat{x}^2 = \frac{\hbar\omega}{2}(\mu^2 + p_\mu^2)$$

or

$$\hat{H} = \frac{\hbar\omega}{2}(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a})$$

It is abovious From Eqs. (3.14, 3.15) that the eigenvalues of the operators $\hat{a}^\dagger\hat{a}$ and $\hat{a}\hat{a}^\dagger$ equal, respectively, n and $n+1$, hence, we can calculate the eigenvalues of Hamilton operator for the harmonic oscillator as

$$\hat{H} = E_n = \frac{\hbar\omega}{2}(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}) = \frac{\hbar\omega}{2}(2n+1) = \hbar\omega(n + \frac{1}{2})$$