

## UNIT 1

# FUNDAMENTALS OF QUANTUM PHYSICS BEHIND COMPUTING

### 1.0 INTRODUCTION

Quantum theory is the theoretical basis of modern physics that explains the behavior of matter and energy on the scale of atoms and subatomic particles / waves where classical physics does not always apply due to wave-particle duality and the uncertainty principle.

In 1900, physicist Max Planck presented his quantum theory to the German Physical Society. Planck had sought to discover the reason that radiation from a glowing body change in color from red, to orange, and, finally, to blue as its temperature rises.

#### **The Development of Quantum Theory**

- In 1900, Planck made the assumption that energy was made of individual units, or quanta.
- In 1905, Albert Einstein theorized that not just the energy, but the radiation itself was *quantized* in the same manner.
- In 1924, Louis de Broglie proposed the wave nature of electrons and suggested that all matter has wave properties. This concept is known as the de Broglie hypothesis, an example of wave-particle duality, and forms a central part of the theory of quantum mechanics.

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- In 1927, Werner Heisenberg proposed uncertainty principle. It states that the more precisely the position of some particle is determined, the less precisely its momentum can be known, and vice versa. The formal inequality relating the standard deviation of position  $\sigma_x$  and the standard deviation of momentum  $\sigma_p$  was derived by Earle Hesse Kennard<sup>[3]</sup> later that year and by Hermann Weyl in 1928

$$\sigma_x \sigma_y \geq \frac{h}{4\pi}$$

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

### **1.1 ELECTROMAGNETIC WAVES**

Electric and magnetic fields in an electromagnetic wave are perpendicular to each other, *and* to the direction of propagation. The existence of electromagnetic waves, the only familiar electromagnetic waves was the visible light waves. The existence of ultraviolet and infrared waves was barely established. By the end of the nineteenth century, X-rays and gamma rays had also been discovered. We now know that, electromagnetic waves include visible light waves, X-rays, gamma rays, radio waves, and microwaves, ultraviolet and infrared waves. The classification of electromagnetic waves according to frequency is the electromagnetic spectrum. There is no sharp division between one kind of wave and the next. The classification is based roughly on how the waves are produced and/or detected.

The electric and magnetic fields  $E_x$  and  $B_y$  are perpendicular to each other, and to the direction  $z$  of propagation. We can write  $E_x$  and  $B_y$  as follows:

$$E_x = E_0 \sin(kz - \omega t)$$

$$B_y = B_0 \sin(kz - \omega t)$$

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Here  $k$  is related to the wave length  $\lambda$  of the wave by the usual equation

$$k = \frac{2\pi}{\lambda}$$

### **Radio waves**

Radio waves are produced by the accelerated motion of charges in conducting wires. They are used in radio and television communication systems. They are generally in the frequency range from 500 kHz to about 1000 MHz. The AM (amplitude modulated) band is from 530 kHz to 1710 kHz. Higher frequencies upto 54 MHz are used for *short wave* bands. TV waves range from 54 MHz to 890 MHz. The FM (frequency modulated) radio band extends from 88 MHz to 108 MHz. Cellular phones use radio waves to transmit voice communication in the ultrahigh frequency (UHF) band.

### **Microwaves**

Microwaves (short-wavelength radio waves), with frequencies in the gigahertz (GHz) range, are produced by special vacuum tubes (called klystrons, magnetrons and Gunn diodes). Due to their short wavelengths, they are suitable for the radar systems used in aircraft navigation. Radar also provides the basis for the speed guns used to time fast balls, tennis serves, and automobiles. Microwave ovens are an interesting domestic application of these waves. In such ovens, the frequency of the microwaves is selected to match the resonant frequency of water molecules so that energy from the waves is transferred efficiently to the kinetic energy of the molecules. This raises the temperature of any food containing water.

### **Infrared waves**

Infrared waves are produced by hot bodies and molecules. This band lies adjacent to the low-frequency or long-wave length end of the visible spectrum.

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Infrared waves are sometimes referred to as *heat waves*. This is because water molecules present in most materials readily absorb infrared waves (many other molecules, for example, CO<sub>2</sub>, NH<sub>3</sub>, also absorb infrared waves).

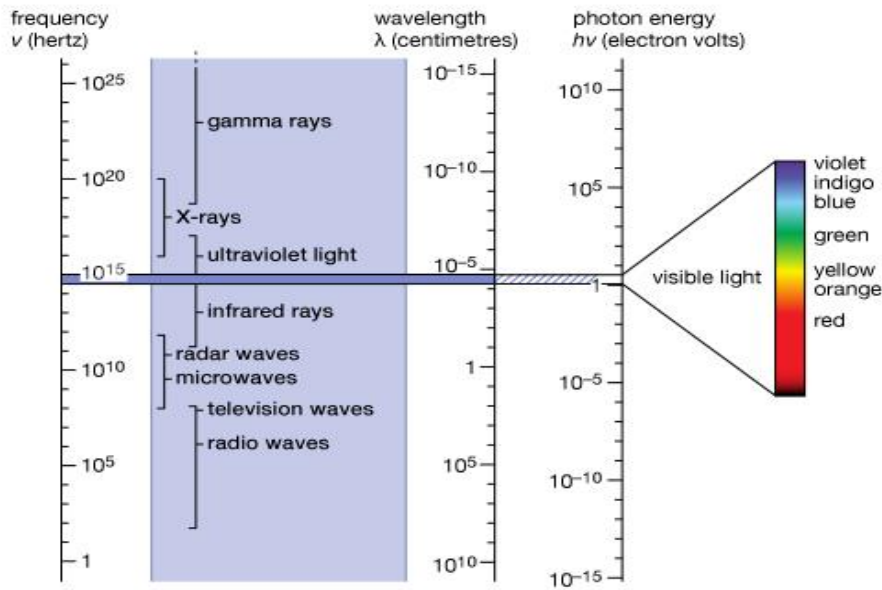
### **Visible rays**

It is the most familiar form of electromagnetic waves. It is the part of the spectrum that is detected by the human eye. It runs from about  $4 \times 10^{14}$  Hz to about  $7 \times 10^{14}$  Hz or a wavelength range of about 700 – 400 nm. Visible light emitted or reflected from objects around us provides us information about the world. Our eyes are sensitive to this range of wavelengths.

### **Ultraviolet rays**

It covers wavelengths ranging from about  $4 \times 10^{-7}$  m (400 nm) down to  $6 \times 10^{-10}$  m (0.6 nm). Ultraviolet (UV) radiation is produced by special lamps and very hot bodies. The sun is an important source of ultraviolet light. But fortunately, most of it is absorbed in the ozone layer in the atmosphere at an altitude of about 40 – 50 km. UV light in large quantities has harmful effects on humans. Exposure to UV radiation induces the production of more melanin, causing tanning of the skin. UV radiation is absorbed by ordinary glass. Hence, one cannot get tanned or sunburn through glass windows.

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**Fig.1.1 Electromagnetic Spectrum**

### X-rays

Beyond the UV region of the electromagnetic spectrum lies the X-ray region. We are familiar with X-rays because of its medical applications. It covers wavelengths from about  $10^{-8}$  m (10 nm) down to  $10^{-13}$  m ( $10^{-4}$  nm). One common way to generate X-rays is to bombard a metal target by high energy electrons. X-rays are used as a diagnostic tool in medicine and as a treatment for certain forms of cancer. Because X-rays damage or destroy living tissues and organisms, care must be taken to avoid unnecessary or over exposure.

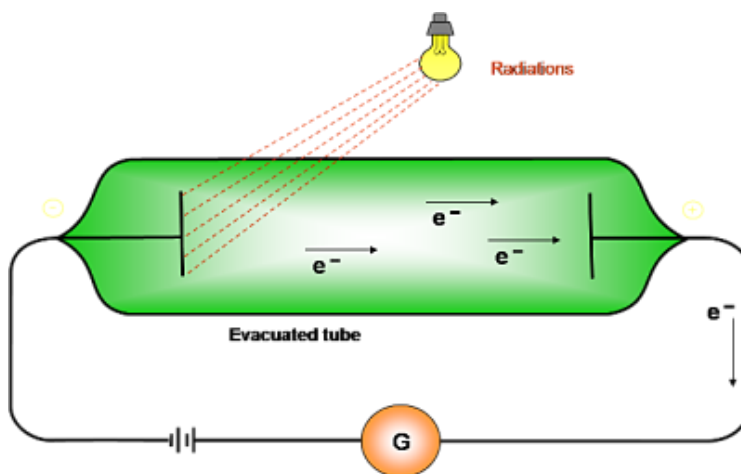
### Gamma rays

They lie in the upper frequency range of the electromagnetic spectrum and have wavelengths of from about  $10^{-10}$ m to less than  $10^{-14}$ m. This high frequency

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radiation is produced in nuclear reactions and also emitted by radioactive nuclei. They are used in medicine to destroy cancer cells.

### **1.2 PHOTOELECTRIC EFFECT**



**Fig.1.2**

J.J. Thomson, observed that when a light of certain frequency strikes the surface of a metal, electrons are ejected. This phenomenon is known as photoelectric effect and the ejected electrons are called photoelectrons.

A few metals, which are having low ionization energy like Cesium, show this effect under the action of visible light but many more show it under the action of more energetic ultraviolet light.

An evacuated tube contains two electrodes connected to a source of variable voltage, with the metal plate whose surface is irradiated as the anode. Some of the photoelectrons that emerge from this surface have enough energy to reach the cathode despite its negative polarity, and they constitute the measured current. The slower photoelectrons are repelled before they get to the cathode. When the voltage is

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increased to a certain value  $V_0$ , of the order of several volts, no more photoelectrons arrive, as indicated by the current dropping to zero.

This extinction voltage (or also referred as stopping potential) corresponds to the maximum photoelectron kinetic energy.

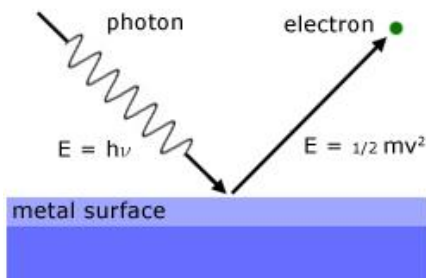
$$\text{i.e., } eV_0 = \frac{1}{2} mv^2$$

### **The experimental findings are summarized as below:**

- Electrons come out as soon as the light (of sufficient energy) strikes the metal surface.
- The light of any frequency will not be able to cause ejection of electrons from a metal surface. There is a minimum frequency, called the threshold (or critical) frequency, which can just cause the ejection. This frequency varies with the nature of the metal. The higher the frequency of the light, the more energy the photoelectrons have. Blue light results in faster electrons than red light.
- Photoelectric current is increased with increase in intensity of light of same frequency, if emission is permitted i.e., a bright light yields more photoelectrons than a dim one of the same frequency, but the electron energies remain the same.

Light must have stream of energy particles or quanta of energy ( $h\nu$ ). Suppose, the threshold frequency of light required to eject electrons from a metal is  $\nu_0$ , when a photon of light of this frequency strikes a metal it imparts its entire energy ( $h\nu_0$ ) to the electron.

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**Fig.1.3**

**“This energy enables the electron to break away from the atom by overcoming the attractive influence of the nucleus”.** Thus each photon can eject one electron. If the frequency of light is less than  $\nu_0$  there is no ejection of electron. If the frequency of light is higher than  $\nu_0$  (let it be  $\nu$ ), the photon of this light having higher energy ( $h\nu$ ), will impart some energy to the electron that is needed to remove it from the atom. The excess energy would give a certain velocity (i.e, kinetic energy) to the electron.

$$h\nu = h\nu_0 + \text{K.E}$$

$$h\nu = h\nu_0 + \frac{1}{2}mv^2$$

$$\frac{1}{2}mv^2 = h\nu - h\nu_0$$

**Where,  $\nu$  = frequency of the incident light**

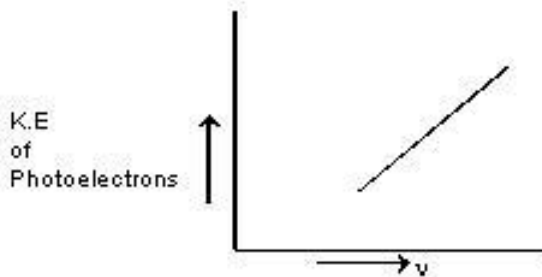
**$\nu_0$  = threshold frequency**

$h\nu_0$  is the threshold energy (or) the work function denoted by  $\Phi = h\nu_0$  (minimum energy of the photon to liberate electron). It is constant for particular metal and is also equal to the ionization potential of gaseous atoms.



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The kinetic energy of the photoelectrons increases linearly with the frequency of incident light. Thus, if the energy of the ejected electrons is plotted as a function of frequency, it results in a straight line whose slope is equal to Planck's constant 'h' and whose intercept is  $h\nu_0$ .



**Fig.1.4**

### **1.3 COMPTON SCATTERING**

Photoelectric effect provides evidence that energy is quantized. In order to establish the particle nature of radiation, it is necessary that photons must carry momentum. In 1922, Arthur Compton studied the scattering of x-rays of known frequency from graphite and looked at the recoil electrons and the scattered x-rays. According to wave theory, when an electromagnetic wave of frequency is incident on an atom, it would cause electrons to oscillate. The electrons would absorb energy from the wave and re-radiate electromagnetic wave of a frequency  $\nu_s > \nu_o$ . The frequency of scattered radiation would depend on the amount of energy absorbed from the wave, i.e. on the intensity of incident radiation and the duration of the exposure of electrons to the radiation and not on the frequency of the incident radiation. Compton found that the wavelength of the scattered radiation does not depend on the intensity of incident radiation but it depends on the angle of scattering and the wavelength of the incident beam. The wavelength of the radiation scattered at an angle  $\theta$  is given by

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$$\lambda_x = \lambda_0 + \frac{h}{m_0 c} (1 - \cos \theta)$$

Where  $m_0$  is the rest mass of the electron. The constant  $\frac{h}{m_0 c}$  is known as the Compton wavelength of the electron and it has a value 0.0024nm.

The spectrum of radiation at an angle  $\theta$  consists of two peaks, one at  $\lambda_0$  and the other at  $\lambda_x$ . The Compton effect can be explained by assuming that the incoming radiation is a beam of particles with

The energy

$$E = h\nu_0$$

The momentum

$$p = \frac{h}{m_0 c}$$

For energy momentum relation

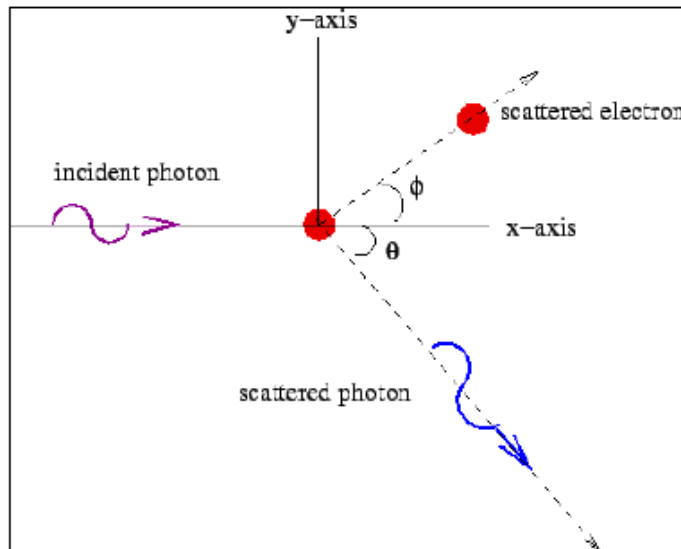
$$E^2 = p^2 c^2 + m c^2$$

### **1.4 PHOTON**

A photon is the smallest discrete amount or quantum of electromagnetic radiation. It is the basic unit of all light.

Photons are always in motion and, in a vacuum, travel at a constant speed to all observers of  $2.998 \times 10^8$ m/s. This is commonly referred to as the speed of light, denoted by the letter  $c$ .

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**Fig.1.5**

As per Einstein's light quantum theory, photons have energy equal to their oscillation frequency times Planck's constant. Einstein proved that light is a flow of photons, the energy of these photons is the height of their oscillation frequency, and the intensity of the light corresponds to the number of photons. Essentially, he explained how a stream of photons can act both as a wave and particle.

### **Photon properties**

The basic properties of photons are:

- Zero mass and rest energy and exist as moving particles.
- Elementary particles despite lacking rest mass.
- No electric charge.
- Stable.

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- Carry energy and momentum which are dependent on the frequency.
- Have interactions with other particles such as electrons, such as the Compton effect.
- They can be destroyed or created by many natural processes, for instance when radiation is absorbed or emitted.
- When in empty space, they travel at the speed of light.

### **1.5 WAVE-PARTICLE DUALITY OF RADIATION AND MATTER**

The dual nature of matter and the dual nature of radiation were revolutionary concepts of physics. In case of light some phenomenon like diffraction and interference can be explained on the basis of its wave character. However, the certain other phenomenon such as black body radiation and photoelectric effect can be explained only on the basis of its particle nature. Thus, light is said to have a dual character. Such studies on light were made by Einstein in 1905. Louis de Broglie, in 1924 extended the idea of photons to material particles such as electron and he proposed that matter also has a dual character-as wave and as particle.

S. No.	Radiation	Material
1	Radiation spreads in the form of waves.	Material shoots in straight line.
2	It has no mass.	Material has mass.
3	Radiation can only be experienced.	Material is Visible, it has volume etc.
4	Radiation has energy known as radiation energy.	It has energy known as mechanical energy.
5	Main representative of radiation is	Main representative of material is

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	light.	electron.
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### **1.5.1 Derivation of de-Broglie Equation**

The wavelength of the wave associated with any material particle was calculated by analogy with photon.

In case of photon, if it is assumed to have wave character, its energy is given by

$$E = h\nu \quad \dots(i)$$

(According to the Planck's quantum theory)

Where  $\nu$  frequency of the wave and 'h' is Planck's constant

If the photon is supposed to have particle character, its energy is given by

$$E = mc^2 \quad \dots\dots (ii)$$

(according to Einstein's equation)

where 'm' is the mass of photon, 'c' is the velocity of light.

By equating (i) and (ii)

$$h\nu = mc^2$$

$$\text{But } \nu = c/\lambda$$

$$h c/\lambda = mc^2$$

$$(\text{or}) \lambda = h /mc$$

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The above equation is applicable to material particle if the mass and velocity of photon is replaced by the mass and velocity of material particle. Thus for any material particle like electron.

$$\lambda = h/mv \quad \text{or} \quad \lambda = h/p$$

where  $mv = p$  is the momentum of the particle.

### **1.5.2 De-Broglie wave**

De-Broglie first proposed that the light has both wave like and particle like properties. Electrons can also have wave like properties. The De Broglie equation is given by,

$$\lambda = \frac{h}{mv}$$

Here,  $\lambda$  is the de-Broglie wavelength,  $h$  is the Planck's constant, and  $p$  is the momentum.

For heavy particles which are having momentum, and can create a relation with the plank's constant, those particles are associated the de Broglie wavelength.

This relationship between the wavelength and momentum holds good for all types of matter, i.e. all matters exhibit the particle and wave nature properties.

De Broglie states that any particle should exhibit wave like nature and also particle like nature. The particle velocity should be always equal the group velocity of the corresponding wave.

The wave like nature of light is having two supportive experimental proofs as suggested in the De Broglie hypothesis. The experimental proofs are

- The discrete atomic energy levels of the atom in the electronic structure.

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- And the diffraction pattern of electrons from the crystal planes in solid materials. The atomic energy levels, the electron waves can be analyzed as a constructive interference pattern by using the Bohr model.
- Again, the wave nature of the electrons can be explained, by the particle in box analysis in quantum mechanics. In this case, to explain the behavior of the electron wave, we can use a box in which the electron is confined, and is having the dimensions in the order of the size of an atom.

### **1.6 Physical interpretation of a wave function**

A wave function of quantum mechanical system is some thing associated with its wave nature. To arrive at results consistent with real time observations, we have imposed several requirements on the wave function of a quantum mechanical system. Wave function is a quantity which describe the particle. **Wave function must be single valued and continuous everywhere and it should approach to zero as  $r$  is tending to infinity.**

It is a mathematical function that describes some of the properties of the wave. the shape of the wave is described by the sine function, and the amplitude describes strength (intensity) of the wave. The wave function can be interpreted as  $\psi(r,t)$ .

$$\psi = A \sin \theta$$

The probability of finding a particle at a position  $x_1 < x < x_2$  and time  $t$

$$\int_{x_1}^{x_2} |\Psi(x)|^2 dx$$

OR

$$\int_{x_1}^{x_2} \psi^* \psi dx$$

The probability per unit length of finding the particle at the position  $r$  at time  $t$ .  $\psi^*(r,t)$  is complex conjugate of  $\psi(r,t)$

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### **Requirements for An Acceptable Wavefunction**

1. The wave function  $\psi$  **must be continuous**. All its **partial derivatives must also be continuous** (partial derivatives are  $\left(\frac{\partial\psi}{\partial x}, \frac{\partial\psi}{\partial y} \text{ etc.}\right)$  This makes the wave function “smooth”.
2. The wave function  $\psi$  must be **quadratically integrable**. This means that the integral  $\int \psi^* \psi d\tau$  must exist.
3. Since  $\int \psi^* \psi d\tau$  is the probability density, **it must be single valued**.
4. The wave functions must form an **orthonormal set**. This means that

- the wave functions must be **normalized**.

$$\int_{-\infty}^{\infty} \psi_i^* \psi_i d\tau = 1$$

- the wave functions must be **orthogonal**.

$$\int_{-\infty}^{\infty} \psi_j^* \psi_i d\tau = 0$$

$$\int_{-\infty}^{\infty} \psi_j^* \psi_j d\tau = \delta_{ij} \text{ where } \delta_{ij} = 1 \text{ when } i = j; \delta_{ij} = 0 \text{ when } i \neq j$$

$\delta_{ij}$  is called Kronecker delta

5. The wave function must be **finite everywhere**.
6. The wave function must satisfy the **boundary conditions** of the quantum mechanical system it represents.

### **1.7 HEISENBERG UNCERTAINTY PRINCIPLE**

**Uncertainty principle**, also called **Heisenberg uncertainty principle** or **indeterminacy principle**, statement, articulated (1927) by the German physicist Werner Heisenberg, that the position and the velocity of an object cannot both be measured exactly, at the same time, even in theory. The very concepts of exact position and exact velocity together, in fact, have no meaning in nature.



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The uncertainty principle is alternatively expressed in terms of a particle's momentum and position. The momentum of a particle is equal to the product of its mass times its velocity. Thus, the product of the uncertainties in the momentum and the position of a particle equals  $h/(4\pi)$  or more, where  $h$  is Planck's constant, or about  $6.6 \times 10^{-34}$  joule-second). It is impossible to know the precise position and momentum. This relationship also applies to energy and time, in that one cannot measure the precise energy of a system in a finite amount of time. Uncertainties in the products of "conjugate pairs" (momentum/position) and (energy/time) were defined by Heisenberg as having a minimum value corresponding to Planck's constant divided by  $4\pi$ . More clearly:

$$\Delta p * \Delta x \geq \frac{h}{4\pi}$$

$$\Delta t * \Delta E \geq \frac{h}{4\pi}$$

Where  $\Delta$  refers to the uncertainty in that variable.

Qualitatively this principle states that "the order of magnitude of the product of the uncertainties in the knowledge of two variables must be at least Planck's constant  $h$ ". Considering the position and momentum is the pair of physical variables, we have

$$\Delta p \Delta x \approx h \quad \dots (1)$$

where  $\Delta p$  is the uncertainty in determining the momentum and

$\Delta x$  is the uncertainty in determining the position of the particle.

Similarly, we have

$$\Delta E \Delta t \approx h \quad \dots (2)$$

$$\Delta J \Delta \theta \approx h \quad \dots (3)$$

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where  $\Delta E$  and  $\Delta t$  are uncertainties in determining the energy and time while  $\Delta J$  and  $\Delta \theta$  uncertainties in determining the angular momentum and angle.

### **Applications of Uncertainty Principle**

#### **Eigenvalues and Eigen functions:**

If there is a class of functions which, when operated by an operator  $\alpha$ , are merely multiplied by some constant  $\lambda$ , i.e., if

$$\alpha f(x) = \lambda f(x)$$

then the functions  $f(x)$  are called eigenfunctions of the operator  $\alpha$  and the various possible values  $\lambda$  are called eigenvalues of the operator.

For example, let us consider the function  $\sin 4x$ . If it is operated by an operator  $\frac{-d^2}{dx^2}$ , the result is

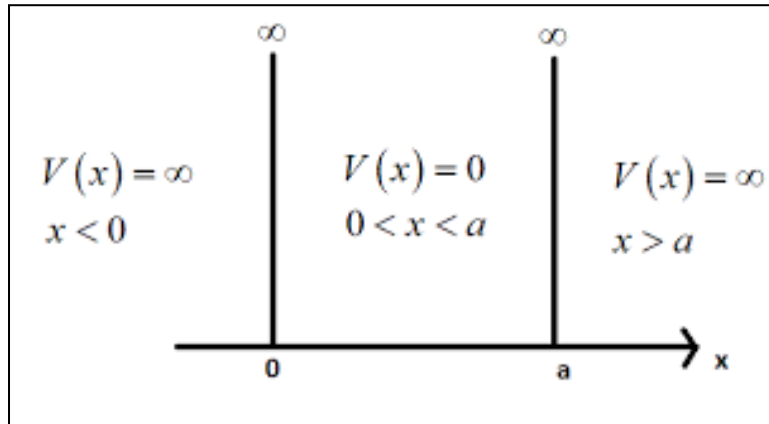
$$\frac{-d^2}{dx^2}(\sin 4x) = 16 \sin 4x$$

Thus  $\sin 4x$  is eigen function and 16 is the eigenvalue of the operator  $\frac{-d^2}{dx^2}$ . In quantum mechanics, the allowed eigenfunctions are continuous, finite and single valued.

#### **Calculation of energy of particle in 1D box:**

Consider a particle of mass 'm' moving along the x-axis between the two rigid walls of the well with  $x = 0$  and  $x = a$ .

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**Fig.1.8 Particle in a box**

When the force acting on the particle between the walls is zero, its potential energy is constant in this region and it is duly taken to be zero. As the walls are assumed to be rigid, the force acting on the particle abruptly increases from zero to finite value at the boundaries and hence the potential energy of the particle becomes infinitely large at  $x = 0$  and  $x = a$ .

Thus, potential function  $V(x)$  is expressed as

$$V(x) = 0 \text{ for } 0 < x < a$$

$$V(x) = \infty \text{ for } 0 \geq x \geq a$$

This potential function is known as square well potential.

The particle cannot move out of the box. Also, it cannot exist on the walls of the box. So its wave function  $\Psi$  is 0 for  $x \leq 0$  and  $x \geq a$  and for zero potential the Schrodinger equation can be written as:

$$\frac{d^2 \psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0 \quad \dots (1)$$

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$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \dots (2)$$

where  $k^2 = \frac{2mE}{\hbar^2}$

The general solution of equation (2) is

$$\Psi(x) = A \sin kx + B \cos kx \quad \dots (3)$$

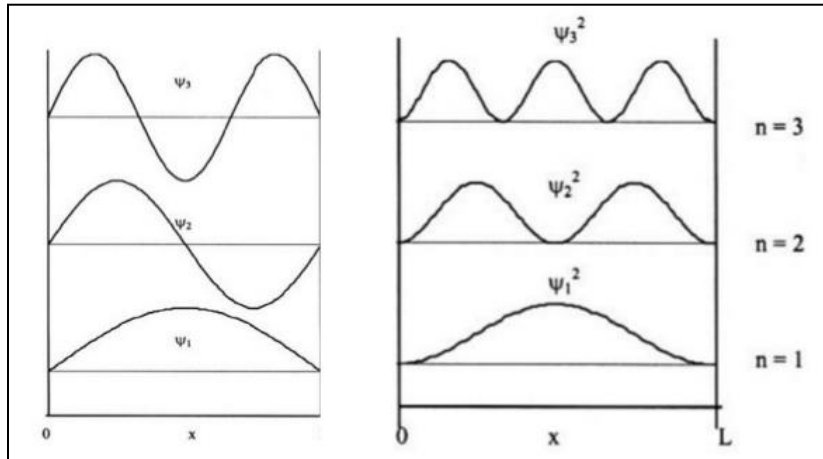
Applying the boundary conditions  $\Psi(x) = 0$  at  $x = a$  and  $x = 0$ , one gets  $k = \frac{n\pi}{a}$  where  $n = 1, 2, 3, \dots$  and  $B = 0$ .

Thus the wave function associated with the electron is:

$$\Psi_n = A \sin \left[ \frac{n\pi x}{a} \right] \quad \dots (4)$$

$$E_n = \frac{k^2 \hbar^2}{2m} = \frac{n^2 \hbar^2}{8ma^2} \quad \dots (5)$$

This equation gives the energy of the particle in the  $n^{\text{th}}$  energy state.



**Fig.1.9 Energy levels and wave functions**

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The particle in the box cannot possess any arbitrary amount of energy. Rather, it can have discrete energy values specified by the equation (5). In other words, its energy is quantized. Each value of  $E_n$  is called as Eigen value and the corresponding  $\Psi_n$  is called Eigen function.

### **Eigenvalues and Eigen functions:**

If there is a class of functions which, when operated by an operator  $\alpha$ , are merely multiplied by some constant  $\lambda$ , i.e., if

$$\alpha f(x) = \lambda f(x)$$

then the functions  $f(x)$  are called eigenfunctions of the operator  $\alpha$  and the various possible values  $\lambda$  are called eigenvalues of the operator.

For example, let us consider the function  $\sin 4x$ . If it is operated by an operator  $\frac{-d^2}{dx^2}$ , the result is

$$\frac{-d^2}{dx^2}(\sin 4x) = 16 \sin 4x$$

Thus  $\sin 4x$  is eigen function and 16 is the eigenvalue of the operator  $\frac{-d^2}{dx^2}$ . In quantum mechanics, the allowed eigenfunctions are continuous, finite and single valued.

## **1.9 SCHRÖDINGER WAVE EQUATION**

Schrodinger wave equation describes the wave nature of a particle in mathematical form. It is the basis equation of wave mechanics originally proposed by Austrian Scientist Erwin Schrödinger.

Schroedinger connected the expression of De-Broglie wavelength with the classical wave equation for a moving particle and obtained a new wave equation.

### **Forms of Schroedinger wave equation**

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There are two forms of Schrodinger wave equation. They are

- i) Time independent wave equation
- ii) Time dependent wave equation

### **1.9.1 Schrodinger's time independent wave equation (Stationary states)**

According to De-Broglie's hypothesis, a particle of mass  $m$  moving with velocity  $v$  is always associated with a wave whose wavelength is given by  $\lambda = \frac{h}{mv}$ . If the particle has wave properties, then it is expected that there should be some sort of wave equation to describe the behaviour of the particle.

The classical differential equation of wave system is

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2} \quad \dots (1)$$

where  $\Psi$  is wave displacement for De-Broglie's waves at time  $t$ ;

$x, y, z$  are coordinates of the particle ; and  $v$  is wave velocity

Equation (1) may be rewritten as

$$\nabla^2 \Psi = \frac{1}{v^2} \frac{\partial^2 \Psi}{\partial t^2} \quad \dots (2)$$

where  $\nabla^2 \Psi = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$  is Laplacian operator.

The solution of equation (2) gives the periodic displacement in terms of time  $t$ ,

$$\text{i.e. } \Psi(x, y, z, t) = \Psi_0(x, y, z)e^{-i\omega t} \quad \dots (3)$$

where  $\Psi_0$  is amplitude at the point considered . It is a function of position and not of time ( $t$ ).

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Differentiating equation (3) twice with respect to t, we get

$$\begin{aligned}\frac{\partial \Psi}{\partial t} &= -i \omega \Psi_0 e^{-i\omega t} \\ \text{and } \frac{\partial^2 \Psi}{\partial t^2} &= (-i\omega)(-i\omega)\Psi_0 e^{i\omega t} = i^2 \omega^2 \Psi_0 e^{-i\omega t} \quad \dots (4) \\ &= -\omega^2 \Psi \quad [i^2 = -1]\end{aligned}$$

Substituting this in equation (2), we get

$$\nabla^2 \Psi = -\frac{\omega^2}{v^2} \Psi \quad \dots (5)$$

$$\text{or} \quad \nabla^2 \Psi + \frac{4\pi^2}{\lambda^2} \Psi = 0 \quad \dots (6)$$

$$\nabla^2 \Psi + \frac{4\pi^2 m^2 v^2}{h^2} \Psi = 0 \quad \dots (7)$$

If E is total energy of the particle, V is potential energy and  $\frac{1}{2}mv^2$  is kinetic energy, then

$$E = \text{P.E.} + \text{K.E.}$$

$$\text{i.e., } E = V + \frac{1}{2}mv^2 \quad \text{or } E - V = \frac{1}{2}mv^2$$

$$mv^2 = 2(E - V)$$

Multiply m on both sides

$$\text{or } m^2 v^2 = 2m(E - V) \quad \dots (8)$$

Substituting equation (8) in equation (7), we get

$$\nabla^2 \Psi + \frac{8\pi^2 m}{h^2} (E - V) \Psi = 0 \quad \dots (9)$$

## ***Basic Quantum Physics***

This  $\Psi$  is independent of time. This is the steady state (stationary state) form of Schrodinger equation. The equation is known as **Schrodinger's time independent wave equation.**

If we consider one-dimensional motion, i.e., particle moving along x-direction only, then Schrodinger's equation (9) reduces to

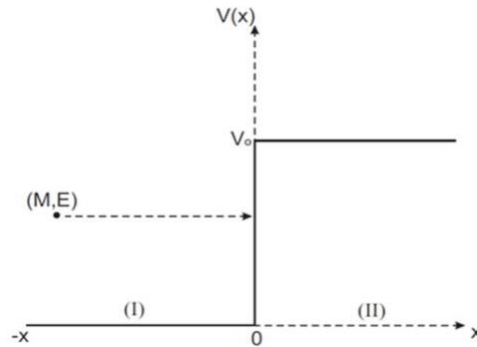
$$\frac{d^2\Psi(x)}{dx^2} + \frac{8\pi^2m}{h^2}(E - V)\Psi(x) = 0 \quad \dots (10)$$

Taking  $\hbar = \frac{h}{2\pi}$  (where  $\hbar$  is a reduced Planck's constant) in equation (9), Schrodinger's wave equation may be rewritten as

$$\nabla^2\Psi + \frac{2m}{\hbar^2}(E - V)\Psi = 0 \quad \dots (11)$$

### **1.10 PHYSICAL APPLICATIONS OF SCHRODINGER'S EQUATION TO SQUARE WELL POTENTIAL IN ONE DIMENSION: TRANSMISSION AND REFLECTION COEFFICIENT AT A BARRIER:**

A potential barrier corresponds to the force field acting on a particle being zero everywhere except in a limited region. A single potential barrier is shown in Fig.1.



**Fig.1.6**



## ***Basic Quantum Physics***

For  $x < 0$ , the potential  $V(x) = 0$

For  $x > 0$ , the potential  $V(x) = V_0$

So we may define the potential function of a potential step as Fig.1.6.

$V(x) = 0$  for  $x < 0$

$V_0$  for  $x > 0$

$V_0$  is considered as the height of the potential barrier. Now consider the case of electrons carrying energy  $E$  moving from left to right (i.e.) along the positive  $X$ -directing. The energy of the electron may be greater than  $V_0$  or less than  $V_0$ . According to quantum mechanics, the electrons behave like a wave and while moving from left to right, it faces a sudden shift in potential at  $x = 0$ . This is analogous to the propagation of light wave when it strikes a glass plate and faces a change in refractive index. The ray is partly reflected and partly transmitted. In a similar way, the electrons will be partly reflected and partly transmitted at  $x = 0$  i.e., at the discontinuity.

The Schrodinger wave equation is applied to region I and II at the condition  $E > V_0$ .

In region I, the Schrodinger wave equation is given by

$$\frac{d^2\psi_1}{dx^2} + \frac{2mE}{\hbar^2}\psi_1 = 0$$

it may be written as

$$\text{or} \quad \frac{d^2\psi_1}{dx^2} + k_1^2\psi_1 = 0 \quad \text{where} \quad \frac{2mE}{\hbar^2} = k_1^2 \quad \dots (1)$$

In region II, the Schrodinger wave equation is given by

## ***Basic Quantum Physics***

$$\frac{d^2\Psi_2}{dx^2} + \frac{2mE}{\hbar^2}(E - V_0)\Psi_2 = 0$$

or 
$$\frac{d^2\Psi_2}{dx^2} k_2^2 \Psi_2 = 0 \quad \text{where} \quad \frac{2m(E-V)}{\hbar^2} = k_2^2 \quad \dots (2)$$

The general solutions of equations (1) and (2) takes the form

$$\Psi_1 = A e^{ik_1x} + B e^{-ik_1x} \quad (x < 0) \quad \dots (3)$$

and 
$$\Psi_2 = C e^{ik_2x} + D e^{-ik_2x} \quad (x > 0) \quad \dots (4)$$

Where A, B, C and D are constants which may be found boundary conditions.

In equation (3), the first term corresponds to a wave propagating along +ve X-direction while the second term corresponds to wave travelling along negative X-direction in the region I. While the first will represent incident wave, the second will represent reflected wave. Since in the first region both incident and reflected rays will be present, so equation (3) represents the solution of Schrodinger's equation in region I.

In equation (4), the first term corresponds to a wave travelling along positive X-direction i.e., transmitted wave and second term corresponds to the wave travelling in negative X-direction i.e., reflected wave in region II. Since there is no discontinuity in region II, so there will not be a reflected wave i.e., D = 0, and so we have the solution of wave equation as

$$\Psi_2 = C e^{ikx} \quad \dots (5)$$

So equations (3) and (5) will represent the solutions of Schrodinger wave equation in I and II region respectively.

From probability interpretation of wave function,  $\psi$  must be finite i.e., it must be continuous. So we will have the following boundary conditions.

### ***Basic Quantum Physics***

$$(\Psi_1)_{x=0} = (\Psi_2)_{x=0}$$

$$\text{And} \quad \left(\frac{d\Psi_1}{dx}\right)_{x=0} = \left(\frac{d\Psi_2}{dx}\right)_{x=0} \quad \dots (6)$$

Applying these boundary conditions, to equations (3) and (5), we get

$$A + B = 0 \quad \dots (7)$$

$$\text{and} \quad k_1 A - k_1 B = k_2 C \quad \dots (8)$$

Putting the value of C in equation (8), we have

$$k_1 A - k_1 B = k_2 (A + B)$$

$$(k_1 - k_2)A = (k_1 + k_2)B$$

$$\text{Which gives} \quad B = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)A \quad \dots (9)$$

Putting the value of B from equation (9) in equation (7), we get

$$A + \frac{(k_1 - k_2)}{(k_1 + k_2)}A = C$$

$$\text{Which gives} \quad C = \left(\frac{2k_1}{k_1 + k_2}\right)A \quad \dots (10)$$

In this case B and C represent the amplitudes of reflected and transmitted beam respectively in terms of amplitude of incident wave.

Now  $\psi\psi^*$  represents the probability density. Let  $v$  be the velocity of a stream of particles then  $\psi\psi^*v$  represents the current density i.e., number of particles crossing unit area placed perpendicular to the direction of motion. If  $N_i$  be the incident flux, then we have by definition

$$N_i = |A \Psi_i \Psi_i^*|^2 v = |A|^2 v = |A|^2 \frac{k_1 \hbar}{m} \dots (11)$$

## ***Basic Quantum Physics***

Similarly the reflected flux  $N_r$  is given by the relation

$$N_r = |B|^2 v = \left| \left( \frac{k_1 - k_2}{k_1 + k_2} \right) \right|^2 |A|^2 \frac{k_2 \hbar}{m} \quad \dots (12)$$

Now 
$$N_t = \frac{4k_1}{(k_1 + k_2)^2} \frac{k_1 k_2 \hbar}{m} |A|^2 = \frac{4k_1 k_2}{(k_1 + k_2)^2} N_i \quad \dots (13)$$

We have from equation (11), (12) and (13)

$$N_t + N_r = N_i$$

So quantum mechanically, there is some probability of reflection and some probability of transmission. The reflection coefficient  $R$  and transmission coefficient  $T$  are defined as under

$$\begin{aligned} \text{Reflection coefficient } R &= \frac{\text{Magnitude of reflected flux}}{\text{Magnitude of incident flux}} = \frac{N_r}{N_i} \\ &= \left( \frac{k_1 - k_2}{k_1 + k_2} \right)^2 \end{aligned}$$

$$\begin{aligned} \text{Transmission coefficient } T &= \frac{\text{Magnitude of transmitted flux}}{\text{Magnitude of incident flux}} = \frac{N_t}{N_i} \\ &= \frac{4k_1 k_2}{(k_1 + k_2)^2} \end{aligned}$$

So we have 
$$T + R = \frac{4k_1 k_2}{(k_1 + k_2)^2} + \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} = 1$$

## **Application of quantum mechanics in computational physics:**

Computational physics is the study of scientific problem using computational methods i.e. the study and implementation of numerical analysis to solve problems in physics for which a quantitative theory already exists. It combines computer science, physics, and applied mathematics to develop scientific solutions to complex problems.

### **Computational Methods in Quantum Mechanics**

There are several computational methods available to analyze quantum systems. Among them two commonly used methods are known as the matching method and the Monte Carlo method. Using them the correct wave function, energy Eigen values of different quantum systems like – infinite square well, linear harmonic oscillator, Lenard Jones potential can be evaluated. The basis of all calculations in a quantum system will typically be based on the time independent Schrödinger equation, so let's first analyze this equation to see how it can be used computationally.

Time independent Schrodinger equation in three -dimensional form is -

$$1) \quad -\frac{\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = E\psi$$

We can approximate the double partial derivative of the wave function as:

$$\frac{\partial^2 \psi_n}{\partial x^2} = \frac{1}{\Delta x} \left( \frac{\partial \psi_{n+1}}{\partial x} - \frac{\partial \psi_n}{\partial x} \right) = \frac{1}{\Delta x} \left( \frac{\psi_{n+1} - \psi_n}{\Delta x} - \frac{\psi_n - \psi_{n-1}}{\Delta x} \right) = \frac{\psi_{n+1} + \psi_{n-1} - 2\psi_n}{(\Delta x)^2}$$

Thus ,

$$2) \quad \frac{\partial^2 \psi_n}{\partial x^2} = \frac{\psi_{n+1} + \psi_{n-1} - 2\psi_n}{(\Delta x)^2}$$

Now that we have an equation for the double partial derivative, we put this in the Schrödinger equation and rearrange the terms in the following way-

## Basic Quantum Physics

$$3) \quad \psi_{n+1} = 2\psi_n - \psi_{n-1} - \frac{2m}{\hbar}(\Delta x)^2 (E - V_n)\psi_n$$

Using this equation, the numerical method to find eigen energy can thus be started-

### 1. Matching Method

Now that we can calculate a wave function we must find the Eigen energies associated with a system in order to determine the Eigen state. There are multiple ways to do this; one such is the matching method which is particularly useful for asymmetric potential systems. The goal of the matching function is to generate a smooth and continuous wave function by combining two wave functions which are generated from the left and right corners of the potential array using some initial inputs. The inputs of a matching method function are- an initial energy guess, the potential array, the spatial step size, and an indexing point which we will use to check the slope of each wave function. In order to calculate each wave function, there are unique initial conditions for even and odd parity solutions:

For even parity, set  $\frac{\partial \psi_0}{\partial x} = 0$ , ( $\psi_{-1} = \psi_0 = 1$ )

For odd parity, set  $\frac{\partial \psi_0}{\partial x} > 0$ , ( $\psi_{-1} = -\Delta x$ ,  $\psi_0 = \Delta x$ )

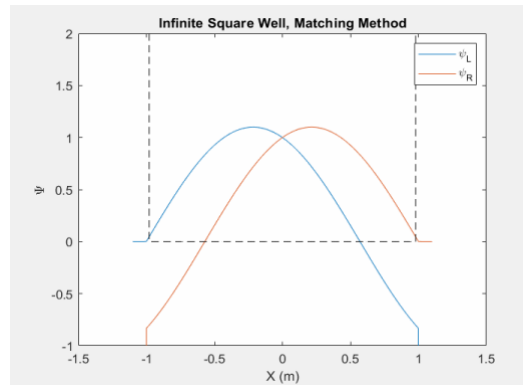


Figure (1) – Matching method inside an infinite square well.

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The steps are given below -

Step 1:

Using equation 3 and the initial conditions, calculate the first wavefunction using the initial energy guess. Then, repeat this process by first flipping the potential array and generating a second wavefunction with the same initial conditions. The flip this second wavefunction so that we have effectively generated one array from left to right and a second array from right to left. After this normalize each wavefunction at the indexed point so that they intersect.

Step 2:

Calculate the slope of each wavefunction at the index. We then call a secondary matching function which keeps track of the orientation of the slopes. If each slope's relative orientation remains the same, then our 'change in energy' value, which we will add afterwards, remains the same. If each slope's relative orientation changes, then our 'change in energy' value is halved and negated. In either case, we then add a 'change in energy' value to the original energy guess, recalculate the left and right wavefunctions and repeat the process.

Step 3:

This function allows us to find eigenstates and the eigen energies of a system. Once we reach a certain limit, the 'change in energy' value will be so small that we can stop the program and merge the two functions at the index point.

**The second method is –**

### **Monte Carlo Method**

Another useful computational method is the Monte Carlo method. Rather than guessing at the energy as in the matching method, in this method we will be guessing at the wavefunction and iterating on this guess. The idea of a Monte Carlo method is that we randomly change a system and only keep the changes that bring us closer to a solution we would expect. In the case of quantum mechanics, this will be used to randomly change the wavefunction and only keep the changes that lower the energy of the system.

In order to implement this approach, we must first understand how to calculate energy using equation 4 below:

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$$4) \quad E = \frac{\int \psi^* H \psi dx}{\int \psi^* \psi dx}$$

Where H is the Hamiltonian operator.

With further processing

$$E = \frac{\int \psi^* H \psi dx}{\int \psi^* \psi dx} = \frac{\sum_{n \geq 1} \frac{\Delta x}{2} (\psi_n E \psi_n + \psi_{n+1} E \psi_{n+1})}{\sum_{n \geq 1} \frac{\Delta x}{2} (\psi_n^2 + \psi_{n+1}^2)}$$

But now we have energy on both sides of the equation. In order to resolve this, we need to substitute in the time independent Schrödinger equation (Eq. 1) which gives us

$$8) \quad E = \frac{\sum_{n \geq 1} \frac{\Delta x}{2} (\psi_n (-\frac{\hbar^2}{2m} \frac{\psi_{n+1} + \psi_{n-1} - 2\psi_n}{(\Delta x)^2} + V \psi_n) + \psi_{n+1} (-\frac{\hbar^2}{2m} \frac{\psi_{n+2} + \psi_n - 2\psi_{n+1}}{(\Delta x)^2} + V \psi_{n+1}))}{\sum_{n \geq 1} \frac{\Delta x}{2} (\psi_n^2 + \psi_{n+1}^2)}$$

This is the final solution which will allow us to calculate the energy in any system given a wave function and potential array.

### Step 1:

We create a function that takes in an arbitrary guess of the wave function and calculate the energy of this guess.

### Step 2:

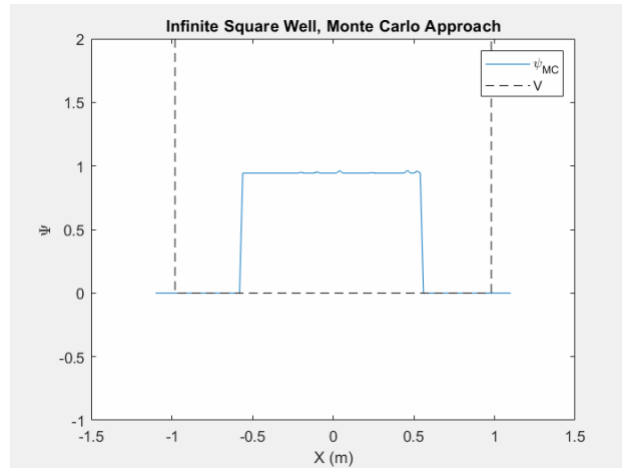
Then we randomly pick a point of the wave function and change it by a random amount. Then we recalculate the energy of the system and if the energy has decreased, we can keep that random change, otherwise discard the change and revert to the previous wave function.

### Step 3:

We repeat this process over and over again until we reach a point in which the energy does not change after a certain number of attempts. At this point we can assume we reached the ground state of our potential system.



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Typically when using the Monte Carlo method on a new potential system, it is actually quite difficult in order to tell when we have reached the ground state unless we actually watch the iterations as they happen. As the wave function starts to change less and less we can assume that we are nearing the ground state. This is still a very slow process and it can take vastly different times to reach the ground state depending on your initial wave function guess and the step size of your random changes. While the Monte Carlo method is significantly slower than the matching method, it is still incredibly useful in finding the ground state energy of an arbitrary system. We typically need little to no intuition as to what the ground state looks like when we make our initial wave function guess.

## Quantum mechanics aspects of solar energy conversion

### a. Interaction photon-solids

#### The energy-moment space in semiconductors

The electron energy-momentum (**E-k**) relationship is well known to be fundamental for obtaining the physical properties of solids. It governs many optical and electronic related phenomena in solids, in particular photoelectric related processes. This relationship is very sensitive to the periodicity of the crystal potential in which the electron propagates. The (**E- k**) relationship is obtained in the one-electron

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approximation by solving the Schrodinger equation for electron in effective periodic crystal field. The crystal periodic field renormalizes the electron momentum and defines a new complex energy-momentum ( $\mathbf{E}-\mathbf{k}$ ) relationship, given in *Brillouin zone that essentially differs from the simple parabolic energy- momentum relationship shown in Figure 1(a) for free electron with  $m_e$  the electron mass in the free space*. Figure 1(b) and (c) show the very well-known energy-momentum for Si and GaAs, respectively, to remind the complexity of the energy band structure of solids. The ( $\mathbf{E}-\mathbf{k}$ ) relationship is a multifold function of momentum, since the same momentum refers to different electron energies. The ( $\mathbf{E}-\mathbf{k}$ ) is chiefly parabolic near the crystal lattice symmetry points (  $L, X, \dots$  ) only, but the concavity variation is characteristic, in a first order approximation, of crystal symmetry in these points and the band energy variation in the vicinity of the considered point. This variation commensurate with the *electron effective mass*. Because *Pauli Exclusion Principle* limits the occupation of the same energy-momentum-spin electronic state to one electron, some energy bands are completely filled with electrons while others are either empty or partially filled in the vicinity of the symmetry points as shown in Figure 1(b) and (c). Like free electrons, in the vicinity of the symmetry points, the *energy and* to be conserved even though the interaction with other particles, in the solid, can be very strong and can occur in stages. All interactions are bound by the complex ( $\mathbf{E}-\mathbf{k}$ ) relation. Changes in electron energy-momentum ( $\mathbf{E}-\mathbf{k}$ ) relationship in solids are essentially *quantum mechanical effects*, and can be found by solving the Schrödinger Equation.

### **1.1.1 Absorption and emission, direct and indirect electron transitions**

Engineering semiconductors that fully absorb the entire energy of incident photons over the entire solar spectrum constitute an ambitious goal. This can be at best approached by nanotechnology and used for by third generation PV cells. To better utilize the photoelectric effect, solid state *fundamental processes* must be addressed individually at various time, space, and energy scales. These basically include *photon absorption and emission* and subsequent *electron-hole generation, recombination, separation, and collection*. Additionally, other processes such as the

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involvement of phonon cascades, surface plasmons and polarons,... must be taken into account for nanoscale investigations, Single or cascade of such processes move electrons from one energy level to another, which brakes the equilibrium of the electronic system and leads to a cascade of other processes that ultimately bring the system back to its thermodynamic equilibrium.

The blue arrows and red curly-arrows in Figure 1(b) and (c) illustrate photon absorption resulting in the electron transfer from the valence band into the conduction band. The reverse process is the electron transfer from the conduction band into the valence band, which results in photon emission (illustrated by green arrows and red curly-arrows in Figure 1(b) and (c)).

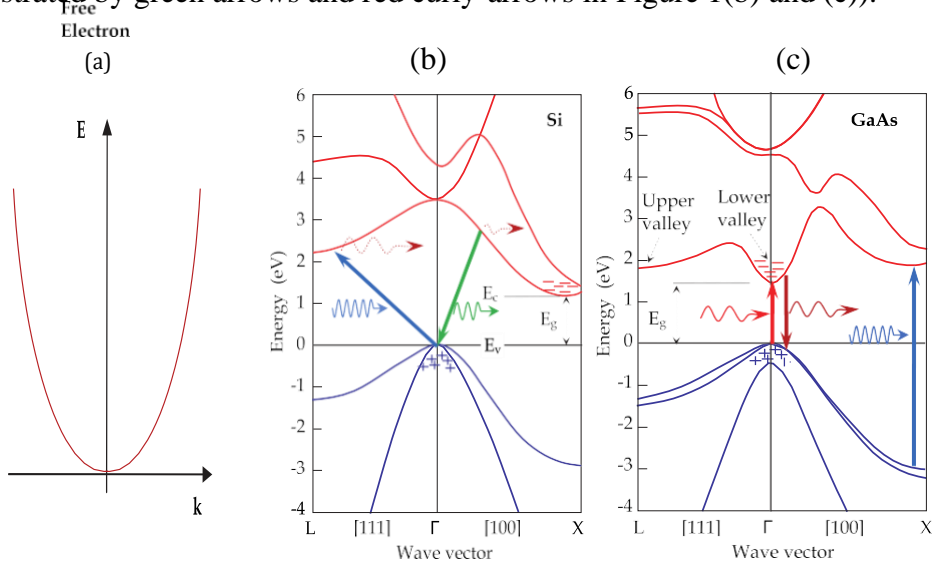


Fig. 1. Electron energy-momentum ( $E-k$ ) relationship and electron transitions in: a) the freespace; b) the indirect bandgap silicon; c) the direct bandgap GaAs.

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Since photon momentum is very small compared to that of electron, the momentum conservation allows only electron transitions between energy levels with practically no electron momentum variation (thus the same wave vector) in the Brillouin zone. The vertical blue and green arrows display such *direct electron transitions* in Figure 1(c) for a direct bandgap semiconductor, here GaAs. When there is not an empty state that enables photon induced electron transition with momentum conservation, phonon assistance is required to ensure momentum conservation. *Indirect electron transitions* must involve both phonon and photon, as illustrated in Figure 1(b), where dotted curly-arrows represent phonons.

### Problems

1. Calculate the minimum energy of an electron can possess in an infinitely deep potential well of width 4nm.

Given:

$$a = 4\text{nm}; n = 1 \text{ (for minimum energy)}$$

**Solution:**

$$E = \frac{n^2 h^2}{8ma^2}$$

$$E = \frac{1^2 (6.625 \times 10^{-34})^2}{8 \times 9.11 \times 10^{-31} (4 \times 10^{-9})^2}$$

$$E = 3.7639 \times 10^{-21} \text{ J or } E = 0.0235 \text{ eV}$$

2. An electron is trapped in a one-dimensional box of length 0.1nm. Calculate the energy required to excite the electron from its ground state to the sixth excited state.

### ***Basic Quantum Physics***

Given:

$a = 0.1 \text{ nm}$ ;  $n = 1$  (for ground energy)

**Solution:**

$$E = \frac{n^2 h^2}{8ma^2}$$

$$E = \frac{1^2 (6.625 \times 10^{-34})^2}{8 \times 9.11 \times 10^{-31} (0.1 \times 10^{-9})^2}$$

$$E = 6.0223 \times 10^{-18} \text{ J}$$

For sixth state,  $n = 6$

$$E = \frac{6^2 (6.625 \times 10^{-34})^2}{8 \times 9.11 \times 10^{-31} (0.1 \times 10^{-9})^2}$$

$$E = 2.1680 \times 10^{-16} \text{ J}$$

The energy required to excite the electron from its ground state to the sixth excited state is  $E = E_6 - E_1$

$$E = 2.1680 \times 10^{-16} - 6.0223 \times 10^{-18}$$

$$E = 2.1078 \times 10^{-16} \text{ J}$$

$$E = 1317 \text{ eV}$$

3. If the uncertainty in position of an electron is  $4 \times 10^{-10} \text{ m}$ , calculate the uncertainty in its momentum.

**Solution:**

$$\Delta p_x \Delta x \approx h$$

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$$\begin{aligned}\Delta p_x &\approx \frac{h}{\Delta x} \approx \frac{6.6 \times 10^{-34}}{4 \times 10^{-10}} \\ &= 1.65 \times 10^{-24} \text{ kg} \frac{\text{m}}{\text{sec}}\end{aligned}$$

## ***Basic Quantum Physics***

### **QUESTIONS**

#### **Part A:**

1. Define electromagnetic wave
2. Define the following
  - a) Radio waves
  - b) Microwaves
  - c) infrared waves
  - d) Visible rays
  - e) Ultraviolet rays
  - f) X- Rays
  - g) Gamma rays
3. Explain Photo electric effect.
4. Define Compton scattering
5. Define photon and write any four properties of photon.
6. Write postulates of Bohr Atom model.
7. Define electron diffraction.
8. Write dual nature of the particle.
9. Define De-Broglie wavelength.
10. Define wave function with the basic equation.
11. What is Heisenberg Uncertainty principle?
12. Write the importance of Heisenberg Uncertainty principle.
13. State Schroedinger's time dependent wave equation.
14. State Schroedinger's time independent wave equation.
15. Write down Schroedinger's time dependent and independent wave equations for matter waves.

### ***Basic Quantum Physics***

16. What is operator?
17. What do you mean by eigen values and eigen functions of the operators?
18. What is transmission and reflection coefficient?
19. What is quantum mechanical tunnelling?
20. Write the principle behind the STM.

### **Part B:**

1. Explain Photo electric effect with its experimental evidences.
2. Explain in detail about Franck-Hertz experiment to give Quantum mechanical evidences for Bohr Atom Model.
3. State Compton Scattering and write relationship between relativistic energy and momentum of the particle.
4. What is uncertainty principle? Explain how it is the out come of the wave description of a particle.
5. Derive Schroedinger's time dependent wave equations for matter waves.
6. Derive stationary state wave equations for matter waves.
7. State Schroedinger's time independent wave equation for a one-dimensional case. Use it to prove that a particle enclosed in a one-dimensional box has quantised energy values.
8. Obtain expression for Eigen function of particle in one dimensional potential well of infinite height.
9. A particle of some mass number and total energy  $E$  moves from a region of zero potential to a region of constant potential  $V_0$ . Derive an expression for reflection and transmission coefficients when  $E < V_0$ .
10. Explain in detail potential barrier and quantum mechanical tunnelling.
11. Discuss in detail the applications of quantum tunneling.