

A Mini Project Report on

Physics [PH 101]



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Prologue^[1]

Before the theory of relativity and quantum mechanics, classical physics describes many aspects of nature on an ordinary scale. But when the quantum mechanics came, it helped us to explain the aspects of nature at small (atomic and subatomic) scales, where classical mechanics is insufficient. In that time classical physics was failed to explain several microscopic phenomena, such as black-body radiation, the photoelectric effect, atomic stability. It was a big obstacle in the way of seeking new ideas outside its purview.

So, in 1900, when Max Planck introduced the concept of the quantum of energy then the first real breakthrough came. He gave a perfect explanation of blackbody radiation, prompted new thinking, and all the solutions to the most outstanding problems of the time.

Historically, in this quantum mechanics, there were two independent formulations. The first one is called matrix mechanics which was developed by Heisenberg (1925) to describe atomic structure starting from the observed spectral lines. The second formulation is called wave mechanics, which was given by Schrödinger (1926) explains the energy spectrum and the wave function of the system under consideration.

Quantum mechanics is the founding basis of all modern physics such as solid-state, molecular, atomic, nuclear, and particle physics, optics, thermodynamics, statistical mechanics, and so on. Also, it is considered to be the foundation of chemistry and biology.

Wavefunction^[2]

In quantum mechanics, wave function is a variable quantity that mathematically describes the wave characteristics of a particle. It describes the quantum state of an isolated quantum system. In easy words it is defined to be a function describing the probability of a particle's quantum state as a function of position, momentum, time, and/or spin.

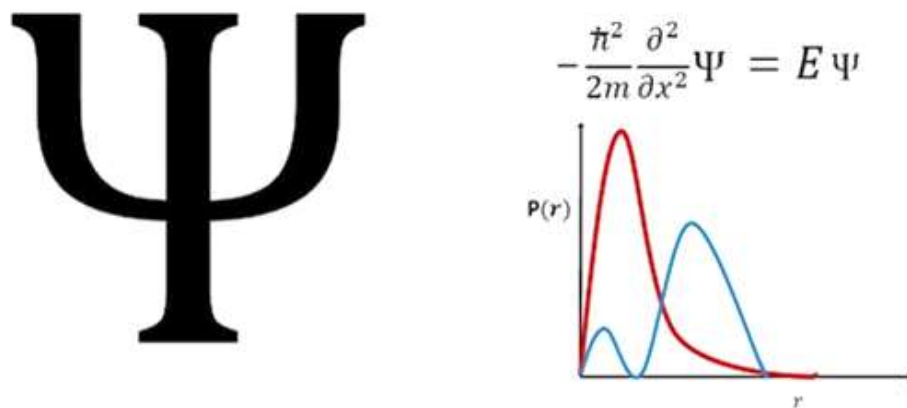


Figure: Wavefunction

A wave function may be used to describe the probability of finding an electron within a matter wave. To do this, the wave function, which may include an imaginary number, is squared to yield a real number solution. Then, the probability of an electron being within a certain area can be assessed. The wave function is a complex-valued probability amplitude, and the probabilities for the possible results of measurements made on the system can be derived from it. . The most common symbols for a wave function are the Greek letters ψ and Ψ (lower-case and capital psi, respectively). The value of the wave function of a particle at a given point of space and time is related to the likelihood of the particle's being there at the time. By analogy with waves such as those of sound, a wave function, , may be thought of as an expression for the amplitude of the particle wave (or de Broglie wave), although for such waves amplitude has no physical significance. The square of the wave function, Ψ^2 , however, does have physical significance: the probability of finding the particle described by a specific wave function Ψ at a given point and time is proportional to the value of Ψ^2 .

- **Properties of Wavefunction^[3]**

Some of the major properties of wavefunction are:

1. All the measurable information about the particle is available.
2. ψ should be continuous and single-valued.
3. Probability distribution in three dimensions is established using the wave function.
4. The probability of finding a particle, if it exists, is 1.
5. Using the Schrodinger equation, energy calculations become easy to solve.

- **Constraints on Wavefunction^[4]**

In order to represent a physically observable system, the wavefunction must satisfy certain constraints:

1. It must be a solution of the Schrodinger Equation.
2. It must be normalisable. This implies that the wavefunction approaches zero as x approaches infinity.
3. It must be a continuous function of x .
4. The slope of the function in x must be continuous, specially, $\frac{\partial \psi(y)}{\partial x}$ must be continuous.

These constraints are applied to the boundary conditions on the solutions and in the process help determine the energy eigenvalues.

- **Postulates of Quantum Mechanics^[5]**

The properties of a quantum mechanical system are determined by a wavefunction $\psi(r,t)$ that depends upon the spatial coordinates of the system and time, r and t . For a single particle system, r is the set of coordinates of that particle, i.e., $r = (x_1, y_1, z_1)$. For more than one particle, r is used to represent the complete set of coordinates $r = (x_1, y_1, z_1, x_2, y_2, z_2, \dots, x_n, y_n, z_n)$. Since the state of a system is defined by its properties, ψ specifies or identifies the state and sometimes is called the state function rather than the wavefunction.

The postulates of quantum mechanics are:

1. With the help of time-dependent Schrodinger equation, the time evolution of wave function is given.
2. For a particle in a conservative field of force system, using wave function, it becomes easy to understand the system.
3. Linear set of independent functions is formed from the set of eigen functions of operator Q .
4. Operator Q associated with a physically measurable property q is Hermitian.
5. By performing the expectation value integral with respect to the wave function associated with the system, the expectation value of the property q can be determined.
6. For every physical observable q , there is an operator Q operating on wave function associated with a definite value of that observable such that it yields wave function of that many times.

- **Interpretation of Wavefunction^[6]**

During the studying of the wavefunction, three main questions arose. Understanding these question helped the physicists to illustrate the nature of the wavefunction.

The questions were:

1. For a travelling particle described by $\psi(x,t) = A \sin(kx - \omega t)$, what is 'waving'?
2. How is the wavefunction used to make predictions?
3. If the matter wave is given by the wavefunction $\psi(x, t)$, where exactly is the particle?

Wavefunction is a mathematical function that can, among other things, be used to determine where the particle is likely to be when a position measurement is performed. When the observer is not looking (or the particle is not being otherwise detected), the particle is everywhere (i.e., $x = [-\infty, +\infty]$), and when the observer is looking (or the particle is being detected), the particle 'jumps into' a particular position state ($x, x + dx$) with a probability given by,

$$P(x, x + dx) = |\psi(x, t)|^2 dx$$

via a process called state reduction or wavefunction collapse. This principle is called Copenhagen interpretation of the wavefunction.

To illustrate this interpretation, consider the simple case of a particle that can occupy a small container either at x_1 or x_2 . In classical physics, we assume the particle is located either at x_1 or x_2 when the observer is not looking. However, in quantum mechanics, the particle may exist in a state of indefinite position—that is, it may be located at x_1 and x_2 when the observer is not looking. The assumption that a particle can only have one value of position (when the observer is not looking) is abandoned. Similar comments can be made of other measurable quantities, such as momentum and energy.

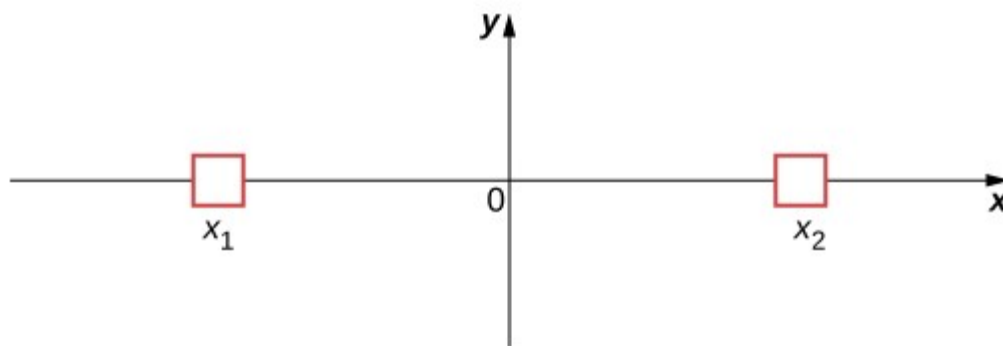


Figure: A two-state system of position of a particle.

The bizarre consequences of the Copenhagen interpretation of the quantum mechanics are illustrated by a creative thought experiment first articulated by Erwin Schrodinger. A cat is placed in a steel box along with a Geiger counter, a vial of poison, a hammer, and a radioactive substance. When the radioactive

substance decays, the Geiger detects it and triggers the hammer to release the poison, which subsequently kills the cat. The radioactive decay is a random [probabilistic] process, and there is no way to predict when it will happen. Physicists say the atom exists in a state known as a superposition—both decayed and not decayed at the same time. Until the box is



Figure: Schrodinger's Cat experiment

opened, an observer doesn't know whether the cat is alive or dead—because the cat's fate is intrinsically tied to whether or not the atom has decayed and the cat would [according to the Copenhagen interpretation] be “living and dead; in equal parts” until it is observed. This experiment is widely known as “Schrodinger's Cat”. Schrödinger took the absurd implications of this thought experiment (a cat simultaneously dead and alive) as an argument against the Copenhagen interpretation. However, this interpretation remains the most commonly taught view of quantum mechanics.

Schrodinger Wave Equation^[7]

In the year 1926, Erwin Schrodinger reasoned that if electrons behave as waves, then it should be possible to describe them using a wave equation. Schrodinger wave equation describes the behaviour of a particle in a field of force or the change of a physical quantity over time. Schrodinger wave equation is a mathematical expression describing the energy and position of the electron in space and time, taking into account the matter wave nature of the electron inside an atom.

The Schrodinger equation plays the role of Newton's laws and conservation of energy in classical mechanics, i.e., it predicts the future behaviour of a dynamic system. It is a wave equation in terms of the wavefunction which predicts analytically and precisely and probability of events or outcome. The detailed outcome is not strictly determined, but given a large number of events, the Schrodinger equation will predict the distribution of results.

Schrodinger basically gave wave equations with two considerations:

1. Time Dependent Wave Equation

$$\hat{H}|\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle$$

2. Time Independent Wave Equation

$$E\psi(x) = \left[\frac{-\hbar^2}{2m} \nabla^2 + V(x) \right] \psi(x)$$

• Derivation of the Time Dependent Schrodinger Wave Equation^[8]

The wave function of a particle of fixed energy E could most naturally be written as a linear combination of wave functions of the form,

$$\Psi(x, t) = Ae^{i(kx - \omega t)} \quad - (i)$$

representing a wave travelling in the positive x direction, and a corresponding wave travelling in the opposite direction, so giving rise to a standing wave, this being necessary in order to satisfy the boundary conditions.

the appropriate wave function for a free particle of momentum $p = \hbar k$ and energy $E = \hbar \omega$,

$$\frac{\partial^2 \psi(t)}{\partial x^2} = -k^2 \psi(t) \quad - (ii)$$

which can be written as, using $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(t)}{\partial x^2} = \frac{p^2}{2m} \psi(t) \quad - (iii)$$

Similarly,

$$\frac{\partial \psi(t)}{\partial t} = -i\omega \psi(t) \quad - (iv)$$

which can be written as, using $E = \hbar \omega$,

$$i\hbar \frac{\partial \psi(t)}{\partial t} = \hbar \omega \psi(t) = E \psi(t) \quad - (v)$$

generalising this to the situation in which there is both a kinetic energy and a potential energy present, then $E = \frac{p^2}{2m} + V(x)$ so that,

$$E \psi(t) = \frac{p^2}{2m} \psi(t) + V(x) \psi(t) \quad - (vi)$$

Assuming, the results in equations (iii) and (iv) apply in this case, we get the famous time dependent Schrodinger wave equation.

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(t)}{\partial x^2} + V(x) \psi(t) = i\hbar \frac{\partial \psi(t)}{\partial t} \quad - (vii)$$

Here, $\psi(t)$ is the wave function of a particle moving in the presence of a potential $V(x)$.

\hbar is reduced Plank Constant

m is electron mass

The obtained Schrodinger wave equation in (vii) can finally be written as,

$$\hat{H}\psi(t) = ih \frac{\partial \psi(t)}{\partial t} \quad - \text{(viii)}$$

Here, \hat{H} is Hamiltonian Operator (Energy operator) and $\hat{H} = -\frac{h^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$

• Derivation of the Time Independent Schrodinger Wave Equation^[9]

The time-independent Schrodinger equation can be expressed in highly compressed mathematical shorthand as,

$$\hat{H}\psi = E\psi \quad - \text{(i)}$$

The solution to extract the time dependence of the Schrodinger wave equation is,

$$\psi(x, t) = \psi(x) e^{-\frac{iEt}{\hbar}} \quad - \text{(ii)}$$

Substituting this solution into the Schrodinger wave equation, and making use of the partial derivations, we get,

$$-\frac{h^2}{2m} \frac{d^2 \psi(x)}{dx^2} e^{-\frac{iEt}{\hbar}} + V(x) \psi(x) e^{-\frac{iEt}{\hbar}} = ih \frac{-iE}{\hbar e^{-\frac{iEt}{\hbar}}} = E \psi(x) e^{-\frac{iEt}{\hbar}} \quad - \text{(iii)}$$

Cancelling the factor exponential $-i \frac{Et}{\hbar}$ from both sides, we get,

$$-\frac{h^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x) \quad - \text{(iv)}$$

This can also be written as,

$$E \psi(x) = \left[\frac{-h^2}{2m} \nabla^2 + V(x) \right] \psi(x) \quad - \text{(v)}$$

Here, E is energy eigen value

$$\nabla^2 \text{ is Laplacian operator and } \nabla^2 \psi(x) = \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right)$$

This obtained equation in (iv) is the time independent Schrodinger wave equation.

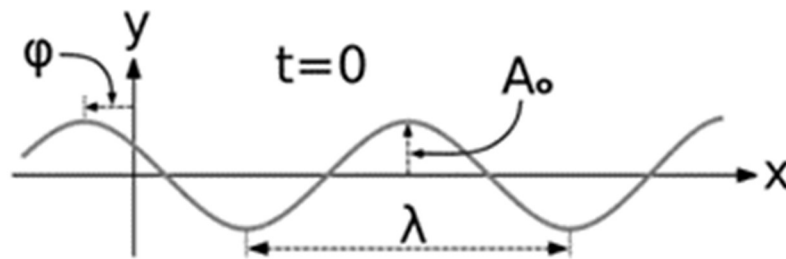
- **Schrodinger Wave Equation Considerations^[10]**

Schrodinger wave equation is a mathematical expression describing the energy and position of the electron in space and time, taking into account the matter wave nature of the electron inside an atom. It is based on three considerations:

1. Classical Plane Wave Equation
2. Broglie's Hypothesis of Matter-Wave
3. Conservation of Energy

- **Classical Plane Wave Equation^[11]**

A wave is a disturbance of a physical quantity undergoing simple harmonic motion or oscillations about its place. The disturbing gets passed on to its neighbours on a sinusoidal form.



The equation for the wave is a second-order partial differential equation of a scalar variable in terms of one or more space variable and time variable. The one-dimensional wave equation is,

$$\nabla^2 \psi = \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) \quad - (i)$$

The amplitude (y) for example of a plane progressive sinusoidal wave is given by,

$$y = A \cos \left(\frac{2\pi}{\lambda} \times \frac{-2\pi t}{T} + \phi \right) \quad - (ii)$$

where, A is the maximum amplitude
 T is the Time period
 φ is the phase difference of the wave
 t is the time in seconds

For a standing wave, there is no phase difference, so that,

$$y = A \cos\left(\frac{2\pi}{\lambda} \times \frac{-2\pi t}{T}\right) = A \cos\left(\frac{2\pi x}{\lambda} - 2\pi vt\right) \quad - \text{ (iii)}$$

In general, the same equation can be written in the form of,

$$y = e^{i\left(\frac{2\pi}{\lambda} - 2\pi vt\right)} = e^{-i\left(2\pi vt - \frac{2\pi x}{\lambda}\right)} \quad - \text{ (iv)}$$

• Broglie's Hypothesis of Matter Wave^[12]

Planck's quantum theory states that, the energy of waves is quantized such that

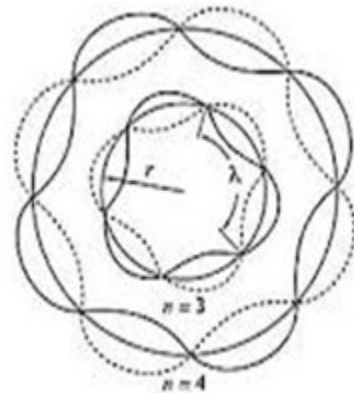
$$E = h\nu = 2\pi h\nu, \quad - \text{ (i)}$$

where,
$$h = \frac{h}{2\pi}$$
$$\nu = \frac{E}{2\pi h}$$

Smallest particles exhibit dual nature of particle and wave. De Broglie related the momentum of the particle and wavelength of the corresponding wave as follows,

$$\lambda = \frac{h}{mv} \quad - \text{ (ii)}$$

where, h is Planck's constant
 m is the mass of the particle
 v is the velocity of the particle



De-Broglie relation can be written as

$$-\lambda \frac{2\pi h}{mv} = \frac{2\pi h}{p} \quad - \text{ (ii)}$$

where, p is the momentum

Electron as a particle-wave moving in one single plane with total energy E has

$$\text{Amplitude} = \text{Wave function} = \psi = e^{-i\left(2\pi vt - \frac{2\pi x}{\lambda}\right)} \quad - \text{ (iii)}$$

Substituting for the wavelength and energy in this equation,

$$\text{Amplitude} = \text{Wave function} = \psi = e^{-i\left(\frac{2\pi Et}{2\pi h} - \frac{2\pi px}{2\pi h}\right)} = e^{-\frac{i}{h}(Et - px)} \quad - \text{(iv)}$$

Partial differentiating w.r.t. x, we get,

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{p^2}{h^2} \psi \quad - \text{(v)}$$

or,

$$E\psi = -\frac{h}{i} \frac{\partial \psi}{\partial t} = i\hbar \frac{\partial \psi}{\partial t} \quad - \text{(vi)}$$

• Conservation of Energy^[13]

Total energy is the sum of kinetic and potential energy of the particle,

$$E = K.E. + P.E. = \frac{mv^2}{2} + U = \frac{p^2}{2m} + U \quad - \text{(i)}$$

Substituting the above obtained equation in wave function equation, we get,

$$E\psi = \frac{p^2}{2m} \psi + U\psi \quad - \text{(ii)}$$

Substituting for $E\psi$ and $p^2\psi$, we get the wave function for one-dimensional wave or the Time-dependent Schrodinger wave equation,

$$E\psi = i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U\psi \quad - \text{(iii)}$$

Time dependent Schrodinger equation for three-dimensional progressive wave is,

$$E\psi = -\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + U\psi \quad - \text{(iv)}$$

On rearranging,

$$\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + \frac{2m}{\hbar^2} (E - U)\psi = 0 \quad - \text{(v)}$$

This equation can also be written as,

$$\nabla^2 \psi + \frac{2m}{\hbar^2} (E - U)\psi = 0 \quad - \text{(vi)}$$

- **Applications of Schrodinger Wave Equation^[14]**

Schrodinger equation is a second order differential equation. It can be used to solve problems for a particle given its mass, its energy and the potential it is in. The solution is a wave function which gives the information about the particle's behavior in time and space. Schrodinger wave equation is also helpful in finding the possible energies that the particle can have in that quantum system.

Some of the applications of Schrodinger Wave Equation can be figured out with the following points.

1. Particle in One Dimensional Deep Potential Well

Let us consider a particle of mass 'm' in a deep well restricted to move in a one dimension (say x). Let us assume that the particle is free inside the well except during collision with walls from which it rebounds elastically.

The potential function is expressed as,

$$\begin{aligned} V &= 0 & , \text{ for } 0 \leq x \leq L \\ V &= \infty & , \text{ for } x < 0; x > L \end{aligned}$$

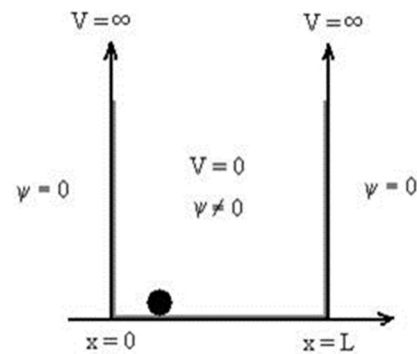


Figure: Particle in Deep Potential Well

The probability of finding the particle outside the well is zero (i.e., $\psi = 0$). Inside the well, the Schrödinger wave equation is written as

$$\nabla^2 \psi + \frac{2m}{\hbar^2} W \psi = 0 \quad - (i)$$

Substituting $\frac{2mE}{\hbar^2} = k^2$ and writing the Schrodinger Wave Equation for one-dimension,

We get,

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \quad - (ii)$$

The general equation of above equation may be expressed as

$$\psi = A \sin(kx + \phi) \quad - (iii)$$

where, A and ϕ are constants to be determined by boundary condition

Condition I: We have $\psi = 0$ at $x = 0$, therefore from above equation,

$$0 = A \sin \phi \quad - (iv)$$

As, $A \neq 0$, then $\sin \phi = 0$ or, $\phi = 0$

Condition II: Further $\psi = 0$ at $x = L$, and $\phi = 0$, therefore from the same above equation,

$$0 = A \sin L \quad - (v)$$

As, $A \neq 0$, then $\sin kL = 0$ or, $kL = n\pi$

Therefore, $k = \frac{n\pi}{L}, n = 1, 2, 3, 4, \dots \quad - (vi)$

Substituting the value of k in $\frac{2mE}{\hbar^2} = k^2$, we get,

$$\left(\frac{n\pi}{L}\right)^2 = \frac{2mE}{\hbar^2} \quad - (viii)$$

This gives, $E = E_n$ (say)

Then, $E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}, n = 1, 2, 3, 4, \dots$

Here, E_n is the energy eigen value of the particle in the well.

Clearly, the energy values of the particle in the well are discrete and not continuous.

Using equations (v) and (vi), the equation (viii) becomes,

$$\psi = \psi_n(\text{say}) = A \sin \frac{n\pi x}{L} \quad - (ix)$$

The probability density, $|\psi|^2 = \psi\psi$,

So,

$$|\psi|^2 = A^2 \sin^2 \frac{n\pi x}{L} \quad - (x)$$

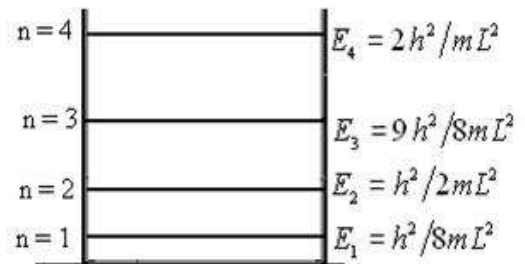


Figure: The energy values for an electron in a potential box

The probability density is zero at $x = 0$ and $x = L$ since the particle is always within the well,

So,

$$\int_0^L |\psi|^2 dx = 1$$

Therefore,

Substituting this value of A in equation (ix), we get,

$$\int_0^L A^2 \sin^2 \frac{n\pi x}{L} dx = 1$$

$$A^2 \int_0^L \sin^2 \frac{n\pi x}{L} dx = 1$$

$$A^2 \frac{L}{2} = 1$$

$$A = \sqrt{\frac{2}{L}}$$

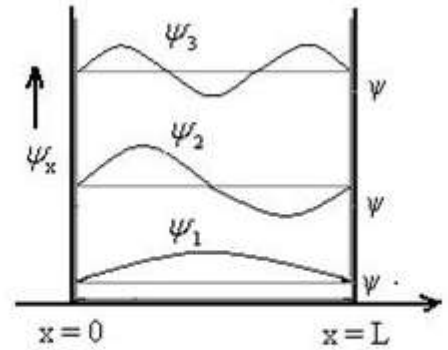


Figure: The allowed wave functions for an electron trapped in a one dimensional potential box

The above equation is normalized wave function (Eigen function) belonging to energy value E_n .

$$\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \quad n=1,2,3,4,\dots \quad - (xi)$$

2. A Free Particle

A particle is said to be free when no external force is acting on during its motion in the given region of space, and its potential energy V is constant.

Let us consider an electron is freely moving in space in positive x -direction and not acted by any force, there potential will be zero. The Schrodinger wave equation reduces to

$$\nabla^2 \psi + \frac{2m}{\hbar^2} E \psi = 0$$

Substituting, we get,

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

As the electron is moving in one direction (say x axis), then the above equation can be written as,

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0$$



Figure: The Energy Continuum of Free Electron

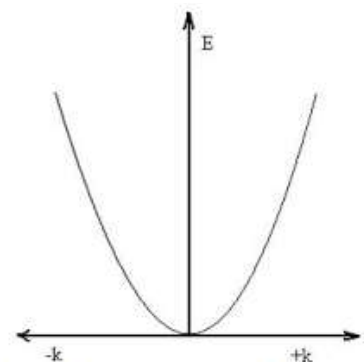


Figure: The Parabolic Relationship between E and k for free Electron

The generalized solution of the above equation is of the form $\psi = \psi_0 e^{-i\omega t}$

The electron is not bounded and hence there are no restrictions on k . This implies that all the values of energy are allowed. The allowed energy values form a continuum and are given by,

$$E = \frac{h^2 k^2}{2m}$$

The wave vector k describes the wave properties of the electron. It is seen from the relation that $E \propto k^2$. Thus the plot of E as a function of k gives a parabola.

The momentum is well defined and in this case given by,

$$p_x \psi = \frac{h}{i} \frac{\partial \psi}{\partial x}$$

Therefore, according to uncertainty principle it is difficult to assign a position to the electron.

- **Physical Significance of Schrodinger Wave Function^[15]**

Bohr concept of an atom is simple. But it cannot explain the presence of multiple orbitals and the fine spectrum arising out of them. It is applicable only to the one-electron system.

Schrodinger wave function has multiple unique solutions representing characteristic radius, energy, amplitude. Probability density of the electron calculated from the wave function shows multiple orbitals with unique energy and distribution in space.

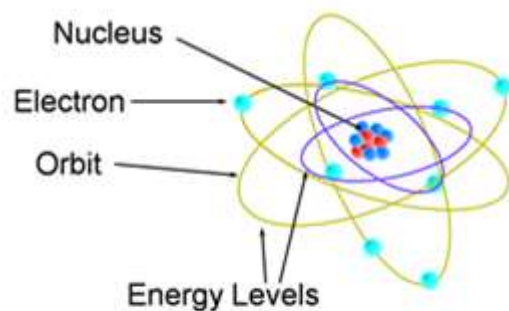


Figure: Bohr's Model

Schrodinger equation could explain the presence of multiple orbitals and the fine spectrum arising out of all atoms, not necessarily hydrogen-like atoms.

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