

# SSPD\_CHAPTER1\_PART 8\_ELECTRON IN A POTENTIAL WELL\_FORMULATION OF SCHRODINGER EQUATION.\*

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## Abstract

SSPD\_Chapter 1\_Part 8 deals with Electron in a Potential Well. To solve this problem we first write the Hamiltonian and formulate the Schrodinger Equation.

## SSPD\_Chapter 1\_Part 8\_ELECTRON IN 1-D POTENTIAL WELL\_Formulation of Schrodinger Equation.

One Dimensional Potential Well can be of three types:

- (i) 1-D Potential Well of infinite height;
- (ii) 1-D Potential Well of finite height;
- (iii) 1-D Potential Well of finite height and finite thickness;

Before analyzing electron in a potential well we will give the physical significance of matter wave.

Like electromagnetic waves, matter wave is a progressive or traveling harmonic wave.

For mathematical simplicity we will deal with waves having plane wavefront. These are called Plane Waves.

There can be traveling waves of spherical wavefront or cylindrical wavefront and these are known as spherical waves or cylindrical waves respectively.

In fact a spherical wave or cylindrical wave becomes a plane wave after they have traveled for a very long distance. As long as radius of curvature is finite we have cylindrical or spherical curvature and curvature is defined as  $1/r$  where  $r$  is the radius of curvature. As soon as radius of curvature is infinite as it would be if the wave has traveled for a very long distance, the curvature becomes zero and the wave assumes a plane wavefront and it is called Plane Wave.

In Fig.(1.21) a Plane Transverse Electro-Magnetic Wave is shown.

$$\mathbf{E}(\mathbf{z},\mathbf{t}) = \mathbf{E} \mathbf{x0} \text{ Exp}[\mathbf{j}(\mathbf{k} \mathbf{z} \cdot \mathbf{z} - \omega \cdot \mathbf{t})]$$

$$\mathbf{H}(\mathbf{z},\mathbf{t}) = \mathbf{H} \mathbf{y0} \text{ Exp} [\mathbf{j}(\mathbf{k} \mathbf{z} \cdot \mathbf{z} - \omega \cdot \mathbf{t})] \quad \mathbf{1.41}$$

Where  $k_z = 2\pi/\lambda_z =$  wave propagation vector or wave number;

And  $\omega = 2\pi\nu =$  circular frequency;

A wave front is defined as front on which all points have same phase. If this front is plane we say we have a plane wave. If the front is cylindrical, we have cylindrical waves and if the wave front is spherical we have spherical waves.

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The wave front moves with a velocity  $v$ . This wave front velocity is the velocity of wave propagation.

i.e.  $k_z \cdot z - \omega \cdot t = \text{constant} = K$

Taking the time derivative we obtain:

$$k_z \cdot \partial z / \partial t - \omega = 0$$

rearranging the terms we get:  $v = \omega / k_z$

$v = \omega / k_z = \lambda \cdot \nu = \text{velocity of the progressive wave front.}$

A phase term of the form  $(k_z \cdot z - \omega \cdot t)$  gives a forward traveling wave

whereas a phase term of the form  $(k_z \cdot z + \omega \cdot t)$  gives a backward traveling wave.

In absolute vacuum Electromagnetic Wave travels with velocity of light  $c = 3 \times 10^8 \text{ m/sec.}$

In absolute vacuum,  $\omega / k_z = \lambda \cdot \nu = c = 3 \times 10^8 \text{ m/sec}$  (velocity of light, in absolute vacuum, is supposed to be an invariant quantity i.e. invariant with respect to the frame of reference [Lorentz Invariance or Gauge Invariance – Appendix XXIX]). This fact was established by Albert Abraham Michelson (1852-1931) and Edward Williams Morley (1838-1923) in their celebrated experiment known as Michelson-Morley experiment [Appendix XXXIII]. This is called Special Theory of Relativity which was propounded by Einstein in 1905). The Eq. (1.41) is the solution of the wave equation given in Appendix (XXXIV).



**Figure 1.21. A progressive Electro-Magnetic Wave.**

**Figure 1**

Fig(1.21) A Progressive Plane Electro-Magnetic Wave.

An electromagnetic wave is a transverse wave because the oscillation is transverse to the direction of propagation. Electric field is oscillating in X direction and Magnetic Field is oscillating in Y direction whereas Z axis is the direction of propagation. Here X and Y axes are transverse to Z-axis. Maxwell equations constrain Electric field and Magnetic Field to be perpendicular to each other and also to the direction of propagation.

In contrast sound wave is a longitudinal wave because the medium particles oscillate in the same direction as the direction of propagation.

In an identical manner Schrodinger [Appendix XXXV] proposed the progressive matter wave:

In 1926 Schrodinger stated the Hamiltonian Equation:

$$H \cdot \psi = E \cdot \psi$$

where  $H$  is the Hamiltonian [Appendix XXXVI | Energy Operator =  $p^2/(2m) + V(r)$ ];  
and  $E$  is the total energy;

Using this Schrodinger Equation, solutions are obtained for an electron in a Hydrogen atom and the four quantum numbers are predicted namely Principal Quantum Number ( $n$ ), Azimuthal Quantum Number ( $l$ ), Magnetic Quantum Number ( $m$ ) and Spin Quantum Number ( $s$ ). These quantum numbers correctly explain the experimental results.

Still there was no direct proof for the existence of matter wave.

The mathematical form of the solution of Schrodinger Equation is :

$$\psi(\mathbf{z}, \mathbf{t}) = \psi_0 \cdot \text{Exp}[\mathbf{j}(\mathbf{k} \cdot \mathbf{z} - \omega \cdot \mathbf{t})] \quad \mathbf{1.42}$$

Where  $k_z = 2\pi/\lambda_z =$  wave propagation vector or wave number;

And  $\omega = 2\pi\nu =$  circular frequency;

And  $\psi =$  probability amplitude;

And  $\psi \cdot \psi^* = |\psi|^2 =$  probability density = probability of finding the particle per unit volume;

$|\psi|^2 dV =$  probability of finding the particle in an elemental volume.

If  $|\psi|^2 dV$  is integrated over the total volume where the particle is likely to be found then the integral will come out to be unity. This means the particle is certainly present in the given volume over which the integration has been carried out.

If the integral is zero then it means it is impossible to find the particle in the given volume.

If integral is between 0 and 1 say 0.5 that means if hundred observations are made within the given volume then in fifty observations the particle is likely to be detected.

If integral is 0.25 then it implies that out of 100 observations 25 times the particle will be observed.

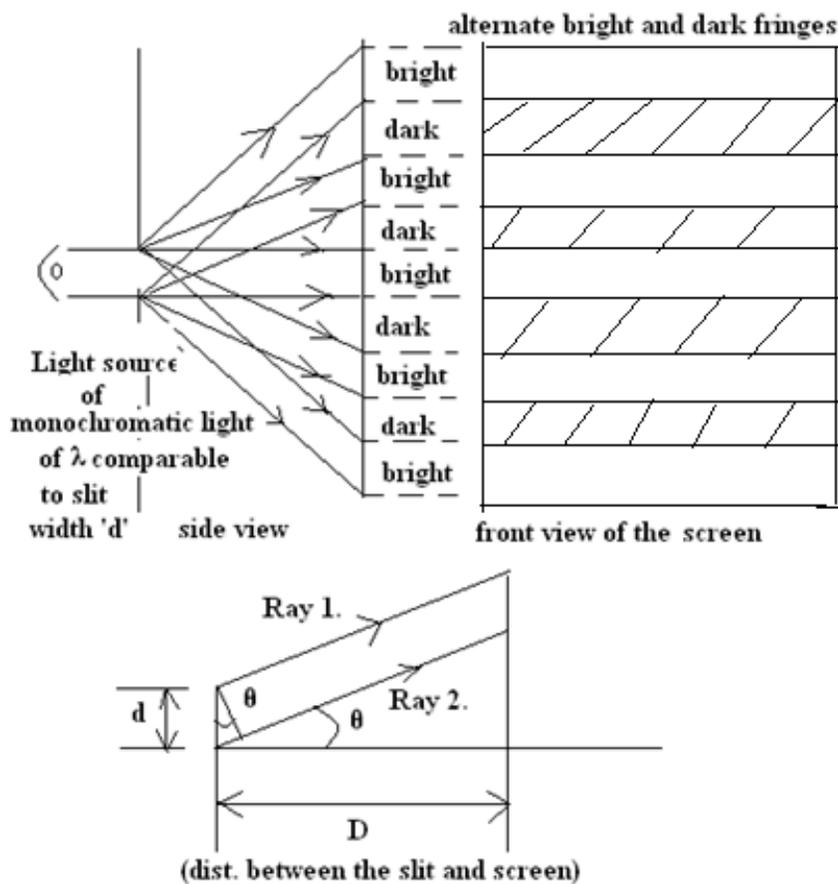
Therefore closed  $\int_V [|\psi|^2 dV] =$  probability of finding the particle in volume  $V$ ;

Therefore  $\int_V [|\psi|^2 dV] = 1$  implies certainty of finding the particle in  $V$  **1.43**

And  $\int_V [|\psi|^2 dV] < 1$  implies less than 100% probability of finding the particle in volume  $V$  **1.44**

In spite of this correctness there were no direct experimental proofs for the matter wave though a THOUGHT EXPERIMENT had been proposed in early 70's.

In 1985 this thought experiment was practically performed as shown in Figure(1.22).



**Bright Fringe** is obtained when there is **constructive interference** between Ray 1 and Ray 2. Condition for **constructive interference** is that **path difference** between Ray 1 and Ray 2 should be  $n \lambda$ .

**Figure 1.22. Single Slit Diffraction Experiment.**

Figure 2

Fig(1.22) Single slit light diffraction experiment.

Path length of ray 1 is =  $D/\cos$

Path length of ray 2 is =  $D/\cos + d.\sin$

Therefore the path difference =  $d.\sin$

When  $d.\sin = n\lambda$  then we have a bright fringe and

When  $d.\sin = (n + \frac{1}{2})\lambda$  then we obtain a dark fringe. Thus Single Slit Diffraction pattern of light consists

of alternate bright and dark fringes.

If instead of light we use a very weak source of electrons then instead of bright and dark fringes we obtain the high and low probability of finding the electrons on different parts of the screen.

For this experiment the electron source should be weak enough to pass singly or one by one through the single slit. As a detector the positively charged anode plate should be used and the whole diffraction set up should be installed in an evacuated chamber as shown in Fig(1.23). The strength of current picked up from different parts of the screen is directly proportional to the probability of incidence of the incident electrons. In place of bright fringe we will obtain a large current and in place of dark fringe we will obtain a small current.

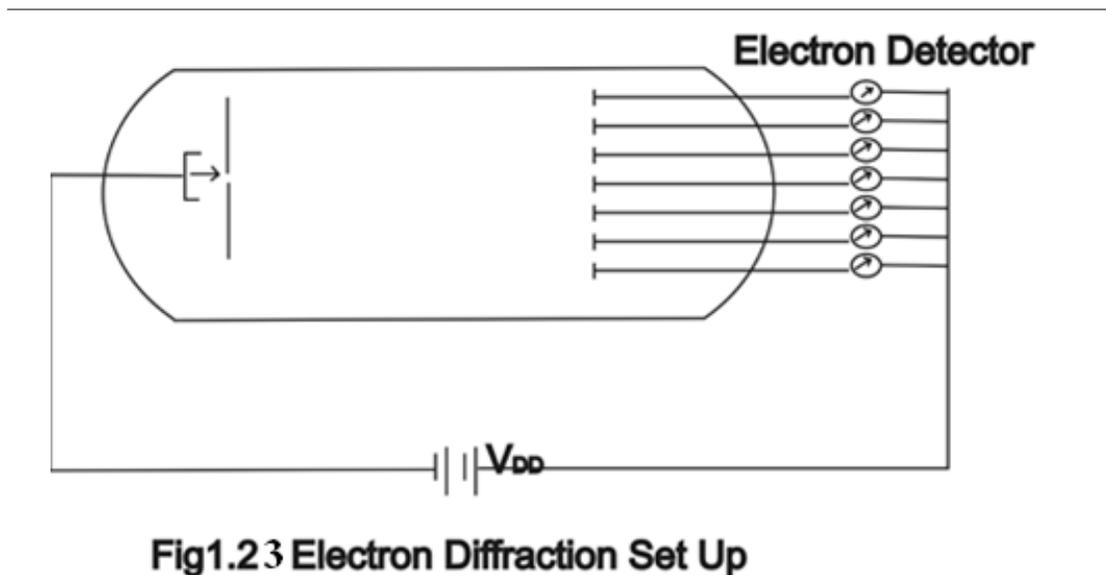


Figure 3

Fig(1.23) Electron Diffraction Set Up.

After giving a physical interpretation of the matter wave we will come to the statement of Schrodinger Equation.

Position ( $z$ ) and momentum in  $z$  direction ( $p_z$ ) are defined as canonical conjugate variables.

Similarly time ( $t$ ) and energy ( $E$ ) are also defined as canonical conjugate variables.

Momentum  $p_z$  is defined as operator  $i\hbar\partial/\partial z$  and

Energy  $E$  is defined as  $-i\hbar\partial/\partial t$ .

Schrodinger used

Hamiltonian Operator  $H = \text{Kinetic Energy Operator} + \text{Potential Energy Operator}$ .

Therefore  $\mathbf{H} = \mathbf{p}^2/(2m) + \mathbf{V}(z)$  1.45

When Operator  $H$  operates upon a matter wave then it yields the Eigen value of the energy of the matter wave.

Therefore  $\mathbf{H}\psi = \mathbf{E}\psi$  1.46

Therefore  $[\mathbf{p}^2/(2m) + \mathbf{V}(z)] \psi = \mathbf{E}\psi$

Substituting  $p$  operator we get:

$[-(\hbar^2/2m) \partial^2/\partial x^2 + \mathbf{V}(z)]\psi = \mathbf{E}\psi$

Therefore  $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial z^2} = [E - V(x)] \psi$

**Or  $\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial z^2} + [E - V(z)] \psi = 0$  1.47**

This is a second order linear differential equation known as the Schrodinger Equation and this has a standard procedure for its solution.