Unit 1

Application of Schrodinger wave equation

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Motion of Free particle

The simplest form of time independent schrodinger equation is the case of **Particle moving freely**

- Free particle is either at rest or moving with constant momentum p.

Total Energy = $p^2/2m$

To predict the behavior of particle quantum mechanically we have to solve Schrodinger time independent equation:

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\Psi = 0$$

$$\frac{d^2\Psi}{dx^2}+\frac{2m}{\hbar^2}(E-V)\Psi=0$$

With V=o

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

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

$$\frac{d^2\Psi}{dx^2}+k^2\Psi=0$$

$$\Psi=e^{ikx} \text{ or } \Psi=e^{-ikx}$$

$$\frac{2mE}{\hbar^2}=\frac{8m\pi^2p^2}{h^2\ 2m}=\frac{4\pi^2p^2}{h^2}=\frac{4\pi^2h^2}{\lambda^2h^2}=k^2$$

$$\frac{d}{dx}=D$$

$$D^2\Psi+k^2\Psi=0$$

$$(D^2+k^2)\Psi=0$$

$$D^2+k^2=0$$

$$D^2=-k^2$$

$$D=\pm\sqrt{-k^2}$$

$$D=k\sqrt{-1}$$

$$D=\pm ik$$

$$D\Psi=\pm ik\Psi$$

$$\frac{d\Psi}{dx}=\pm ik\Psi$$

$$\Psi=e^{\pm ikx}$$

$$\Psi=Ae^{ikx}+B\,e^{-ikx}$$

$$\Psi(x,t)=\Psi(x)\,\varphi(t)$$

$$= Ae^{ikx}\, e^{-i\omega t}$$

$$E = \frac{h^2k^2}{8\pi^2 m}$$

Since particle is moving freely there is no restriction on k and all values of energy are allowed

$E \propto k^2$

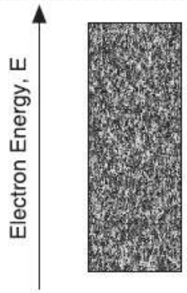


Fig. 20.15

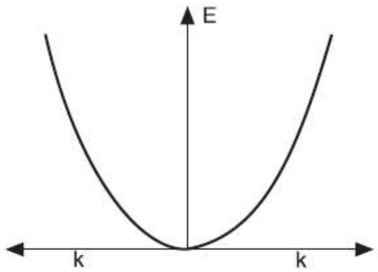


Fig. 20.16

The k-vector describes the wave properties of the particle. It may be seen from equ. (20.70) that $E \propto k^2$. The plot of E as a function of k gives a parabola, as illustrated in Fig.

INFINITE POTENTIAL WELL

- A **potential well is a potential energy function** ***V(x)*** that has a minimum
- In classical mechanics a particle trapped in a potential well can vibrate back and forth with periodic motion but cannot leave the well.
- In quantum mechanics, such a trapped state is called a

bound state.

one-dimensional Infinite potential box.

- Let us consider a particle confined to the region $0 < x < L$.
- *It can move freely within the region $0 < x < L$*

Region I

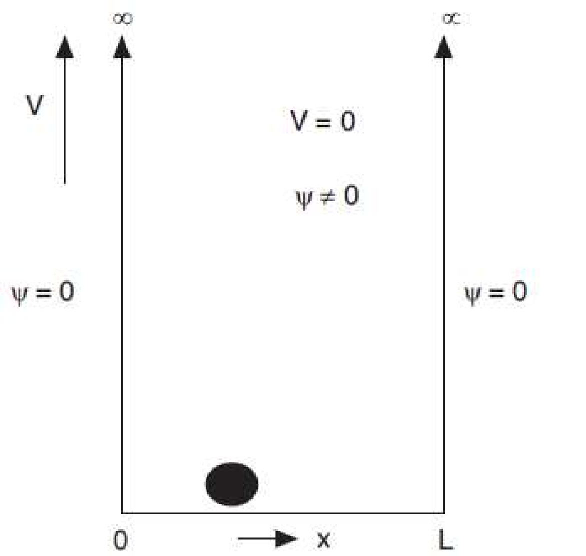
$X \leq 0$, $V = \infty$, $\Psi = 0$

Region II

$0 < x < L$, $V = 0$

Region III

$X \geq L$, $V = \infty$, $\Psi = 0$



Potential has a feature that it binds the particle within $x=0$ to $x=L$, with any finite energy $E \geq 0$

- Let us consider one- dimensional motion along X-axis of a particle between two points x=o and x=L
- Particle is free to move between o and L.
- It cannot cross left of x=o and to the right of x=L, the situation is represented by potential function V

Region I

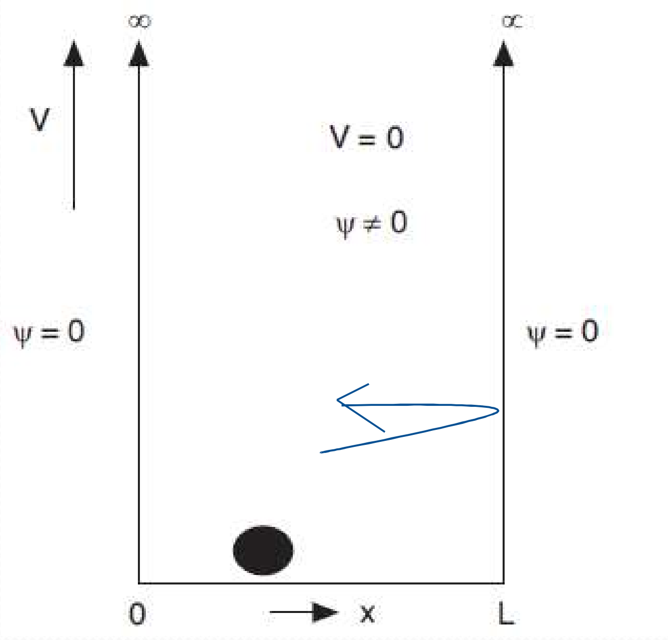
$X \leq 0 \quad , \quad V = \infty \quad , \quad \Psi = 0$

Region II

$0 < x < L \quad , V = 0$

Region III

$X \geq L , \qquad V = \infty \, , \ \Psi = 0$



In the region within potential well

Schrodinger time independent equation-

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\,\Psi = 0$$

In the region $0 < x < L$,

$V=0$

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

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

$$\frac{d^2\Psi}{dx^2} + k^2\Psi = 0$$

This is second order linear homogeneous differential equation

Solution of above equation

$$\Psi = Ae^{ikx} + B\,e^{-ikx} \qquad (1)$$

We can evaluate the constants A and B with the help of boundary conditions

At $x=0$, $\Psi=0$

$x=L$, $\Psi=0$

$$\Psi_{x=0} = A + B = 0$$

$$B=-A\text{--------}(2)$$

Substitute in equation (1)

$$\Psi = A\,(e^{ikx} - e^{-ikx})$$

$$\Psi = 2iA\,\sin kx\text{----}(3)$$

$\Psi=0$ *at* $x=L$

$$\Psi_L = 2iA\sin kL = 0$$

The factor 2iA cannot be zero hence sinkL is zero

$\sin kL=0$

$kL=n\pi$

As $k=2\pi/\lambda$

$$\cos\theta = \frac{e^{j\theta} + e^{-j\theta}}{2}$$

$$\sin\theta = \frac{e^{j\theta} - e^{-j\theta}}{2j}$$

$\lambda=2L/n$ or $k=n\pi/L$

$$\Psi_n = 2iA\,\sin\{(n\pi x)/L\}$$

$$\Psi_n = C\sin\frac{n\pi x}{L}$$

Quantization of energy

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

$$\frac{n^2\pi^2}{L^2} = \frac{2mE}{\hbar^2}$$

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

n= 1,2,3-----

Only certain values of energy are allowed

$$E = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

- As n is integer, there is thus infinite sequence of discrete energy levels which corresponds to positive integer n
- Quantum state with lowest n=1 is called ground state
- Levels corresponding to n=2,3,4----- are called exited states
- Energy for n=1 is

$$E = \frac{\pi^2 \hbar^2}{2mL^2}$$

Zero point energy or ground state energy

- Classically zero point energy can be zero but quantum mechanically ground state energy cannot have zero energy

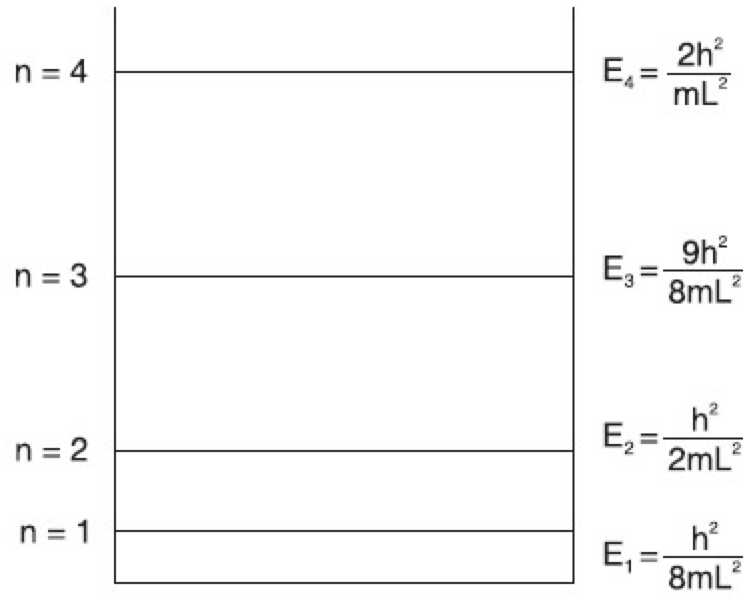
- Higher energy levels are

$$E_2 = \frac{4\pi^2\hbar^2}{2mL^2}$$

E2=4E1

Similarly

E3=9E1



Wave Function

$$\Psi_n = C \sin \frac{n\pi x}{L}$$

Normalize this wave function

C=???????

$$\int_0^L \psi_n \psi_n^* dx = 1$$

$$\therefore \qquad C^2 \int_0^L \sin^2 \frac{n\pi\, x}{\mathrm{L}} dx = 1$$

$$\frac{C^2}{2} \int_0^L \left[1 - \cos\frac{2n\pi\, x}{L}\right] dx = 1$$

$$\frac{C^2}{2} \left[x - \frac{\sin \dfrac{2n\,\pi\, x}{L}}{\dfrac{2n\pi}{L}} \right]_0^L = 1$$

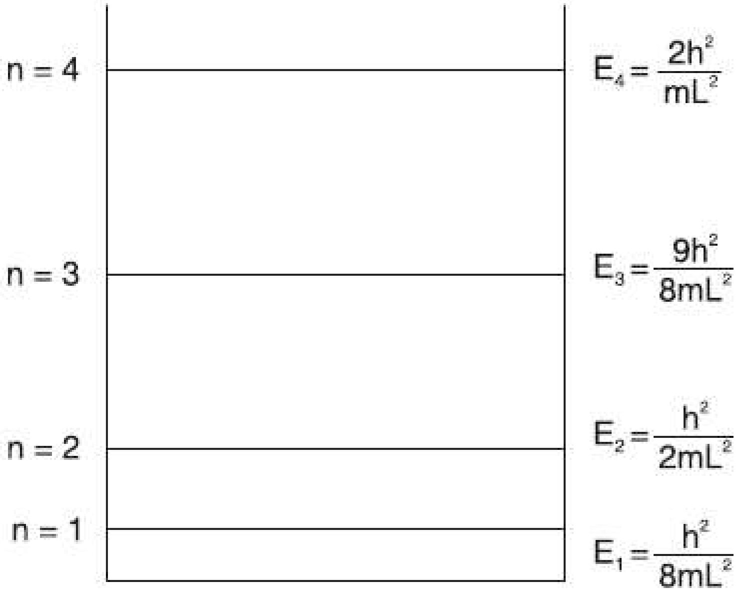


Fig. 20.24

$$\therefore \qquad C^2 \frac{L}{2} = 1$$

i.e.,
$$C^2 = \frac{2}{L}$$

or
$$C = \sqrt{2/L} \tag{20.97}$$

Using the value of C into eq.(20.96), we obtain the wave function as

$$\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \tag{20.98}$$

Plot of Wave function and probability density for different energy levels

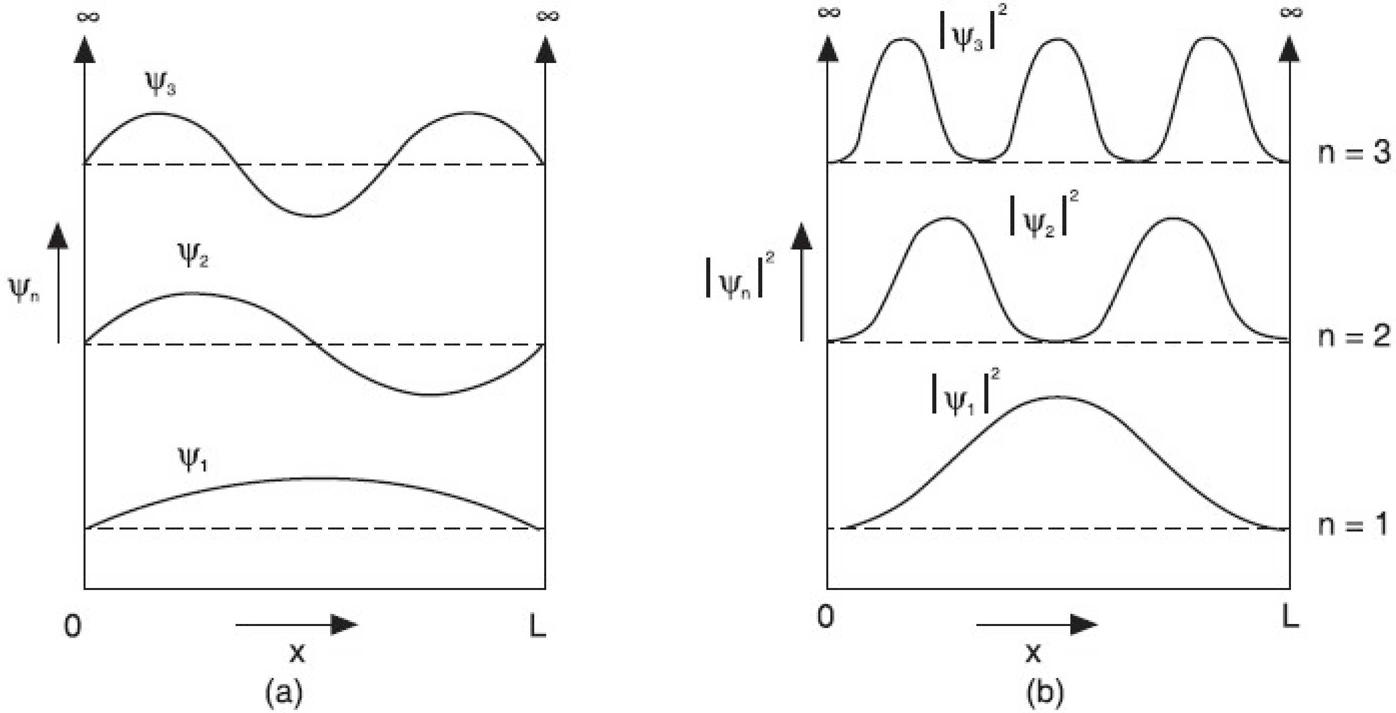


Fig. 20.25

Problems

Q-1 Find the energy of an electron confined to move in a one dimensional potential box of 1 A (given $m=9.11 \times 10^{-31}$ kg ,$\hbar=9.11 \times 10^{-34}$ Js)

Q-2 The wavefunction for a particle in infinite potential well is given by

$$\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

Where $0 \le x \le L$, find $\langle x \rangle$ and $\langle p \rangle$.

Q-3 A small object of mass 1.00 μg is confined to move between two rigid walls seperated by distance of 1.00 mm. (a) Calculate the minimum speed of the object. (b) if the speed is 3×10^6 m/s, find the corresponding value of n.

Q-4 A proton is confined to move in a one-dimensional box of width 0.200 nm. (a) Find the lowest possible energy of proton. (b) What is the lowest possible energy of electron of an electron confined to the same box?

Q-5 A ruby laser emits light of wavelength 693.4 nm. If this light is due to transition from n=2 to n=1 state of an electron in a one-dimensional box, find the width of the box.

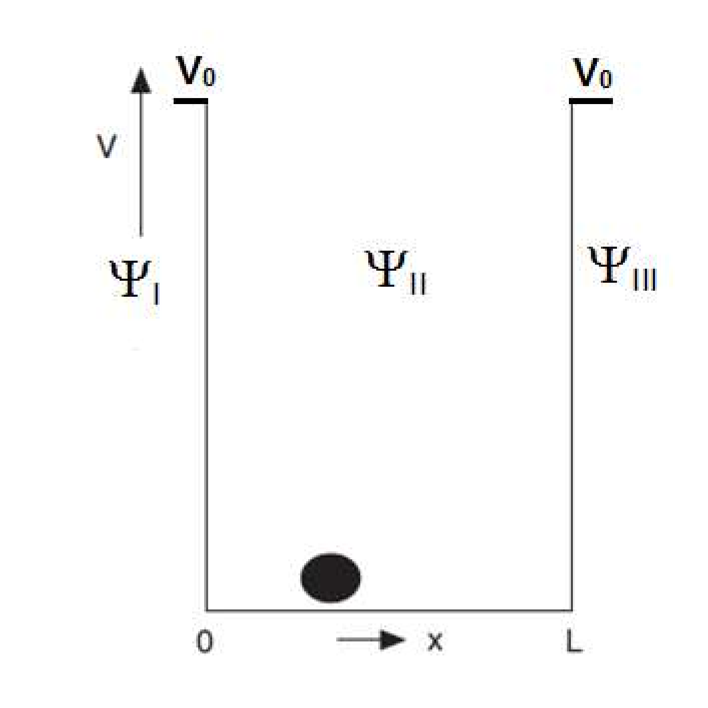
Q-6 An electron is trapped in an infinitely deep potential well 3.0 A in length. If the electron is in the ground state, what is the probability of finding it within the 1.0 A of the left hand wall.

Q-7 An electron is confined to move between two rigid walls seperated by 1nm. Find the de Broglie wavelength representing first two allowed energy states of the electron and the corresponding energies.

Q-8 Calculate the energy required for an electron to jump from ground state to second exited state in a potential well of width L.

One Dimensional Finite potential well

This type of potential is also known as square well potential



Region I

$X \leq o \quad , \quad V = Vo \ , \ \Psi_I$

Region II

$o < x < L \ , V = o, \ \Psi_{II}$

Region III

$X \geq L, \quad V = Vo \ , \ \Psi_{III}$

Case I

E > Vo

E< Vo

$E < Vo$ $$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\Psi = 0$$

Region I

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V_0)\Psi = 0$$

$$\frac{\partial^2\Psi}{\partial x^2} - \frac{2m}{\hbar^2}(V_0 - E)\Psi = 0$$

Substitute $\frac{2m}{\hbar^2}(V_0 - E) = k'$

$$\frac{\partial^2\Psi}{\partial x^2} - k'\Psi = 0$$

$$\Psi_I(x) = Ce^{k'x} + De^{-k'x}$$

As $x \to -\infty$ $e^{-kx} \to \infty$

$$\Psi_I(x) = Ce^{k'x}$$

Region III

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V_0)\Psi = 0$$

$$\frac{\partial^2\Psi}{\partial x^2} - \frac{2m}{\hbar^2}(V_0 - E)\Psi = 0$$

$$\frac{2m}{\hbar^2}(V_0 - E) = k'$$

$$\frac{\partial^2\Psi}{\partial x^2} - k'\Psi = 0$$

$$\Psi_{III}(x) = Fe^{k'x} + Ge^{-k'x}$$

As $x \to \infty$ $e^{kx} \to \infty$

$$\Psi_{III}(x) = Ge^{-k'x}$$

Region II

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

$$\frac{d^2\Psi}{dx^2} + k^2\Psi = 0$$

$$\Psi = Ae^{ikx} + B\,e^{-ikx}$$

$$\Psi_{II}(x) = \ Asinkx$$

so, ψ_{III}

• Now, by Continuity conditions of wavefunction we have at $\boxed{x = L}$,

$$\psi_{II}\Big|_{x=L} = \psi_{III}\Big|_{x=L} \Rightarrow A\sin kL = G e^{-k'L}$$

(by ⑥ & ⑦)

Also,

$$\frac{\partial \psi_{II}}{\partial x}\Big|_{x=L} = \frac{\partial \psi_{III}}{\partial x}\Big|_{x=L} \Rightarrow Ak\cos kL = -k' G e^{-k'L}$$

(by ⑥ & ⑦)

Dividing above eqns

$$\frac{\tan kL}{k} = \frac{1}{-k'}$$

$$\tan kL = \frac{-k}{k'} = -\frac{E^{1/2}}{(V_0 - E)^{1/2}}$$

• If $V_0 >> E$ i.e. $V_0 \to \infty$ then,

$$\tan kL \to \frac{1}{\infty} \to 0 \Rightarrow kL = 0, \pi, 2\pi \ldots$$

i.e. $kL = n\pi$

that will be infinite well case

• But if $V_0 << E$ OR $V_0 \sim E$ then,

$$\tan kL \to \frac{1}{0} \to \infty \Rightarrow kL = \frac{\pi}{2}, \frac{3\pi}{2} \ldots \text{etc}$$

i.e. $kL = \frac{(2p+1)}{2}\pi$ where $p = 0, 1, 2 \ldots$ etc.

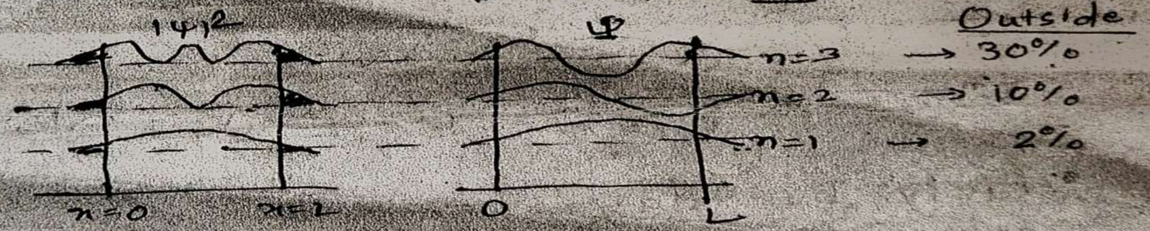
As $E = \frac{\hbar^2 k^2}{2m}$

$$= \frac{\hbar^2\left(\frac{(2p+1)}{2}\frac{\pi}{L}\right)^2}{2m}$$

$$\boxed{E_p = \frac{h^2}{8mL^2}\left(\frac{2p+1}{2}\right)^2} \quad p = 0, 1, 2 \ldots \text{etc.}$$

These are energy eigenvalues.

- The net wavefunction for this problem will be $\psi = \psi_I + \psi_{II} + \psi_{III}$



Properties —

i> More deep is the well, it can accomodate more quantum states.

ii> As quantum no. increases, probability to determine outside increases significantly

iii> Energies of finite well are lower than infinite well.