College of Science
Department of Physics
Fourth Class
Lecture 17

Quantum Mechanics

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Lecture 17: Potential well & Harmonic oscillator

Preparation

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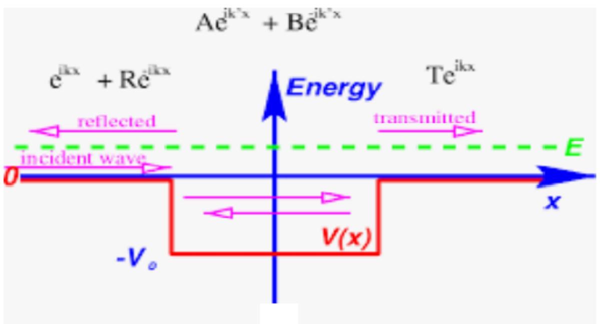
Unit 8

Potential well & Harmonic oscillator

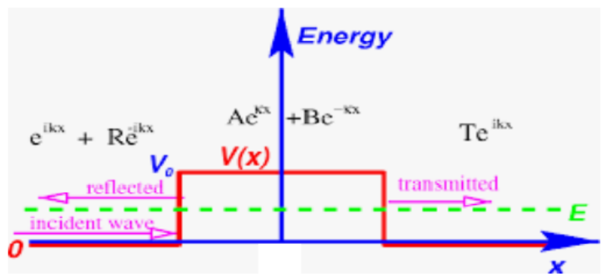
8.1 The square well potential:

We consider a one dimensional problem where the potential function is attractive rather than repulsive i.e. the potential function is defined as:

$$V(x) = \left.\begin{matrix} 0 & for \quad x < 0 \\ -V_0 & for \quad 0 < x < a \\ 0 & x > a \end{matrix}\right\} - - - 1$$



The Potential Well with *



The Potential Barrier
quantummechanics.ucsd.edu

The potential well have a depth V_o between x=0 and x= a.

If a particle having energy E approaches this well from left, according to classical physics none of the particles will turn back, but according to wave theory the particle, will be reflected from the sharp edges at x = 0 and x = a. Consequently, there will be reflected and transmitted beams along with incident one. To solve the problem let us write the schröedinger eq. for each region

for **region I** is

$$\frac{\partial^2 \Psi_1}{\partial x^2} + \frac{2m}{\hbar^2} E\Psi_1 = 0 - - - - 2$$

for **region II** is

$$\frac{\partial^2 \Psi_2}{\partial x^2} + \frac{2m}{\hbar^2} (E + V_o)\Psi_2 = 0 - - - - - - 3$$

for **region III** is

$$\frac{\partial^2 \Psi_3}{\partial x^2} + \frac{2m}{\hbar^2} E\Psi_3 = 0 - - - - - - -4$$

The general solutions of eq. 2,3 &4 may be written as

$$\Psi_1 = A_1 e^{\frac{iP_1 x}{\hbar}} + B_1 e^{-\frac{iP_1 x}{\hbar}} - - - - - - 5$$

$$\Psi_2 = A_2 e^{\frac{iP_2 x}{\hbar}} + B_2 e^{-\frac{iP_2 x}{\hbar}} - - - - - - -6$$

$$\Psi_3 = A_3 e^{\frac{iP_1 x}{\hbar}} + B_3 e^{-\frac{iP_1 x}{\hbar}} - - - - - - -7$$

P_1 and P_2 , the momenta of particles in the corresponding regions, are given by

$$P_1 = \sqrt{2mE} \quad , \quad P_2 = \sqrt{2m(E + V_o)} - - - - - - 8$$

As there is no wave move along the -ve x- axis in region III B = 0 and

$$\Psi_3 = A_3 e^{\frac{iP_1 x}{\hbar}} - - - - - - 9$$

For evaluating A_1, B_1, A_2, B_2, & A_3 we have to apply the conditions at the two boundaries x = 0 and x = a .

Condition one: continuity of Ψ at boundaries, i.e.

$$\left.\begin{array}{l} \Psi_1 = \Psi_2 \ \ at\ x = 0 - - - - - - -(i) \\ \Psi_2 = \Psi_3\ at\ x = a - - - - - - - - (ii) \end{array}\right\} - - - 10$$

Condition two: continuity $\frac{\partial \Psi}{\partial x}$ at the boundaries

$$\left.\begin{array}{l} \frac{\partial \Psi_1}{\partial x} = \frac{\partial \Psi_2}{\partial x} \ \ at\ x = 0 - - - (i) \\ \frac{\partial \Psi_2}{\partial x} = \frac{\partial \Psi_3}{\partial x} \ \ at\ x = a - - - (ii) \end{array}\right\} - - - 11$$

Differentiating eqs.5,6,9 we get

$$\frac{\partial \Psi_1}{\partial x} = \frac{iP_1}{\hbar}\left[A_1 e^{\frac{iP_1 x}{\hbar}} - B_1 e^{-\frac{iP_1 x}{\hbar}}\right] - - - -12$$

$$\frac{\partial \Psi_2}{\partial x} = \frac{iP_2}{\hbar}\left[A_2 e^{\frac{iP_2 x}{\hbar}} - B_2 e^{-\frac{iP_2 x}{\hbar}}\right] - - - -13$$

$$\frac{\partial \Psi_3}{\partial x} = \frac{iP_1}{ħ}\left[A_3\, e^{\frac{iP_1 x}{ħ}}\right] ----14$$

Apply the boundary condition in eq. 5,6 & 9 we get

$$A_1 + B_1 = A_2 + B_2 \quad \text{at } x=0 \text{ --------------15}$$

$$A_2\, e^{\frac{iP_2 a}{ħ}} + B_2 e^{-\frac{iP_2 a}{ħ}} = A_3\, e^{\frac{iP_1 a}{ħ}} \quad at\ x = a \text{ -------------16}$$

Applying the boundary condition in eqs. 12,13 & 14 we get

$$A_1 - B_1 = \frac{P_2}{P_1}(A_2 - B_2) ------17$$

$$A_2\, e^{\frac{iP_2 a}{ħ}} - B_2 e^{-\frac{iP_2 a}{ħ}} = \frac{P_1}{P_2} A_3\, e^{\frac{iP_1 a}{ħ}} ----18$$

Solving eq.15,17 for A_1 and B_1 we get

$$A_1 = \frac{A_2}{2}\left(1 + \frac{P_2}{P_1}\right) + \frac{B_2}{2}\left(1 - \frac{P_2}{P_1}\right) ----19$$

$$B_1 = \frac{A_2}{2}\left(1 - \frac{P_2}{P_1}\right) + \frac{B_2}{2}\left(1 + \frac{P_2}{P_1}\right) ----20$$

Solving eq.16 , 18 for A_2 and B_2 we get

$$A_2 = \frac{A_3}{2}\left(1 + \frac{P_1}{P_2}\right) e^{\frac{i(P_1 - P_2)a}{ħ}} ----21$$

$$B_2 = \frac{A_3}{2}\left(1 - \frac{P_1}{P_2}\right) e^{\frac{i(P_1 + P_2)a}{ħ}} ----22$$

Substituting values of A_2 and B_2 in eqs.19, 20 we get

$$A_1 = \frac{A_3}{4} e^{\frac{iP_1 a}{ħ}}\left[\left(1 + \frac{P_2}{P_1}\right)\left(1 + \frac{P_1}{P_2}\right) e^{-\frac{iP_2 a}{ħ}} + \left(1 - \frac{P_2}{P_1}\right)\left(1 - \frac{P_1}{P_2}\right) e^{\frac{iP_2 a}{ħ}}\right] --23$$

$$B_1 = \frac{A_3}{4} e^{\frac{iP_1 a}{ħ}}\left[\left(1 - \frac{P_2}{P_1}\right)\left(1 + \frac{P_1}{P_2}\right) e^{-\frac{iP_2 a}{ħ}} + \left(1 + \frac{P_2}{P_1}\right)\left(1 - \frac{P_1}{P_2}\right) e^{\frac{iP_2 a}{ħ}}\right] — 24$$

Equation 23 may be written as

$$\frac{A_3}{A_1} = \frac{4e^{\frac{-iP_1 a}{\hbar}}}{\left[\left(1+\frac{P_2}{P_1}\right)\left(1+\frac{P_1}{P_2}\right)e^{-\frac{iP_2 a}{\hbar}} + \left(1-\frac{P_2}{P_1}\right)\left(1-\frac{P_1}{P_2}\right)e^{\frac{iP_2 a}{\hbar}}\right]}$$

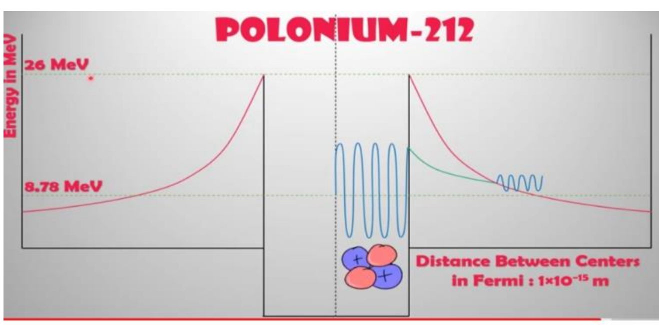
$$\frac{A_3}{A_1} = \frac{4e^{\frac{-iP_1 a}{\hbar}}}{\left(\frac{P_1}{P_2}+\frac{P_2}{P_1}\right)\left(e^{-\frac{iP_2 a}{\hbar}} - e^{\frac{iP_2 a}{\hbar}}\right) + 2\left(e^{-\frac{iP_2 a}{\hbar}} + e^{\frac{iP_2 a}{\hbar}}\right)}$$

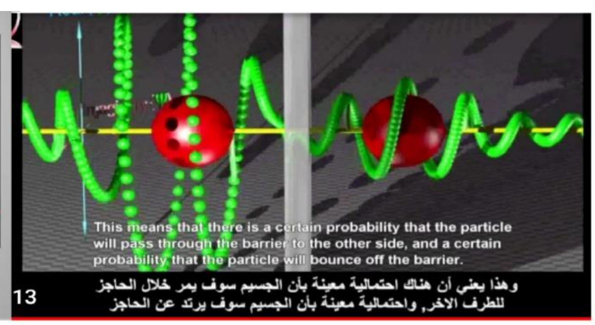
$$\frac{A_3}{A_1} = \frac{e^{\frac{-iP_1 a}{\hbar}}}{-\frac{i}{2}\left(\frac{P_1}{P_2}+\frac{P_2}{P_1}\right)\sin\left(\frac{P_2 a}{\hbar}\right) + \cos\left(\frac{P_2 a}{\hbar}\right)} ----25$$

Transmission coefficient (T)= $\frac{magnitude\ of\ transmitted\ current}{magnitude\ of\ incident\ current} = \frac{(A_3 A_3^*)}{(A_1 A_1^*)}$

$$\boxed{T = \frac{1}{1+\frac{1}{4}\left(\frac{P_1}{P_2}-\frac{P_2}{P_1}\right)^2 \sin^2\left(\frac{P_2 a}{\hbar}\right)}} ----26$$

Clearly T is less than unity. It indicates that some reflection has taken place(T+R=1). This reflection is due to wave nature of matter and is analogous to the reflection of sound waves from the open end of an orqan pipe.





If $P_1 = P_2$, $T = 1$. this is the case when there is no potential well at all. But there is the case in which T= 1, when $P_1 \neq P_2$ but $\sin^2\left(\frac{P_2 a}{\hbar}\right) = 0$, i.e.when $\frac{\boldsymbol{P_2 a}}{\hbar} = \boldsymbol{n\pi}$ ***or*** $\boldsymbol{P_2} = \frac{\boldsymbol{n\pi\hbar}}{\boldsymbol{a}}$

The result may be understood as follows: the wave which reflects from the surface x = a , arrives back at that from x = 0 with a phase shift of nπ, then it interferes constructively with next wave coming in end the transmitted wave is reinforced. Thus, for certain wavelength T is unity.

8.2 One dimensional linear harmonic oscillator.

For a one –dimensional harmonic oscillator (i.e. a particle undergoing simple harmonic oscillations in one dimension), the restoring force is proportional to the displacement "x" from the equilibrium position i.e.

$$F = -kx$$

Where k is +ve constant. According to Newton's 2nd law ,

$m\frac{d^2x}{dt^2} = -kx$ where m is the mass of oscillating particle

$\frac{d^2x}{dt^2} + \frac{k}{m}x = 0 - - - - 27$

The general solution of this eq. written as

$$x = A\, sin(Bt + C) - - - - 28$$

Where A, B and C are constant to be determined. As the motion is periodic, we must have $B = 2\pi\vartheta$

Where ϑ is the frequency of oscillations of the particle under condition. Substituting value of B in eq.28, we get

$x = A\sin(2\pi\vartheta t + c) - - - - - 29$

So that $\frac{d^2x}{dt^2} = -4\pi^2\vartheta^2 x$ sub. value of x and $\frac{d^2x}{dt^2}$ in eq. 27 we get

k = $4\pi^2\vartheta^2 m$ $- - - - 30$

The pot. Energy for the H.O. is

$$F = -\frac{dV}{dx} \quad \rightarrow V = -\int F dx = -\int -kx\, dx = \int kx\, dx$$

$$V = \frac{1}{2}kx^2 + V_o$$

V_o const. of integration. Assuming potential energy to be zero at X=0 , we have $V_o = 0$, so the pot. Energy of H.O.

$$\boxed{V = \frac{1}{2}kx^2 = 2\pi^2\vartheta^2 mx^2}$$

Sub. In schröedinger eq.

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

The wave eq. for H.O.

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}kx^2\right)\Psi = 0 - - - -31$$

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{2m}{\hbar^2}\ \sqrt{k}\left(\frac{E}{\sqrt{k}} - \frac{1}{2}\sqrt{k}x^2\right)\Psi = 0$$

$$\frac{1}{\sqrt{\frac{mk}{\hbar^2}}}\frac{\partial^2\Psi}{\partial x^2} + \left[2\sqrt{\frac{m}{\hbar^2 k}}E - \sqrt{\frac{mk}{\hbar^2}}x^2\right]\Psi = 0 - - - -32$$

Let us put $\sqrt{\frac{mk}{\hbar^2}} = \alpha^2$, $2\sqrt{\frac{m}{\hbar^2 k}}E = \lambda - - - -33$

In eq. 32, then we have $\boxed{\frac{1}{\alpha^2}\frac{\partial^2\Psi}{\partial x^2} + (\lambda - \alpha^2x^2)\Psi = 0} - - - 34$

Let us introduce a new variable (q) related to x, such that $q = \alpha\ x \quad \rightarrow \frac{\partial q}{\partial x} = \alpha$

Where $\frac{\partial\Psi}{\partial x} = \frac{\partial\Psi}{\partial q}.\frac{\partial q}{\partial x} = \alpha\frac{\partial\Psi}{\partial q}$ --------35

And $\frac{\partial^2\Psi}{\partial x^2} = \alpha^2\frac{\partial^2\Psi}{\partial q^2}$ sub. These in eq.34, we get

$$\boxed{\frac{\partial^2\Psi}{\partial q^2} + (\lambda - q^2)\Psi = 0} - - - 36$$