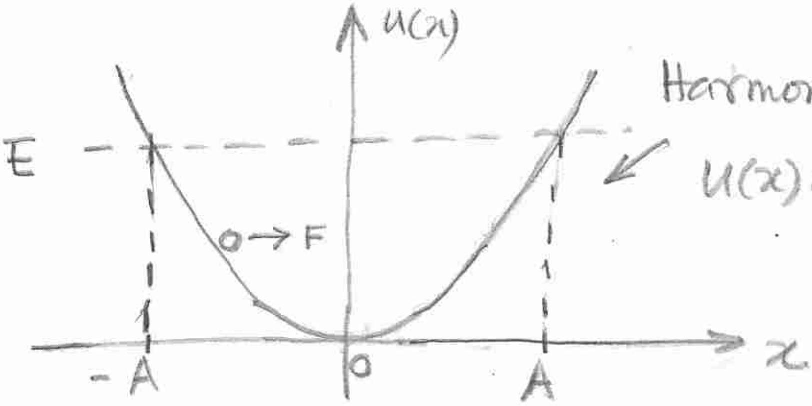
PC2232: (Lecture 8) Harmonic Oscillation & Tunneling

29/03/2013

Classical Harmonic Oscillator:



$u(x) = \frac{1}{2} k_p x^2$

E = Energy of particle, A = Amplitude of oscillation.

Force on particle: $F = -\frac{du(x)}{dx} = -\frac{d}{dx}\left(\frac{1}{2}k_p x^2\right) = -k_p x$

By Newton's 2nd law: $F = m\frac{d^2x}{dt^2}$, m = mass of particle.

So, $m\frac{d^2x}{dt^2} = -k_p x \Rightarrow \frac{d^2x}{dt^2} + \frac{k_p}{m}x = 0$ --- (1)

The general solution of (1) is:

$x(t) = A\cos(\omega_0 t + \theta)$ where $\omega_0 = \sqrt{\frac{k_p}{m}} \Rightarrow k_p = \omega_0^2 m$ --- (2)

natural frequency of oscillation

At any point of time, the total energy E of the particle is the sum of its kinetic and potential energies: $E = E_K + E_p = \frac{p^2}{2m} + \frac{1}{2}k_p x^2$ --- (3)

where p = momentum.

$\frac{p^2}{2m} = \frac{m^2v^2}{2m} = \frac{1}{2}mv^2$ = kinetic energy E_K

$u(x) = \frac{1}{2}k_p x^2$ = potential energy E_p

Using (2), we have

$$v = \frac{dx(t)}{dt} = \frac{d}{dt}\left[A\cos(\omega_0 t + \theta)\right] = -A\omega_0 \sin(\omega_0 t + \theta)$$

So,
$$\left.\begin{aligned} E_K &= \frac{m\omega_0^2}{2} A^2 \sin^2(\omega_0 t + \theta) \\ &= \frac{K_p A^2}{2} \sin^2(\omega_0 t + \theta) \end{aligned}\right\} \quad \cdots (4) \text{ using (2)}$$

&
$$E_p = \frac{1}{2} K_p x^2 = \frac{1}{2} K_p \left[A\cos(\omega_0 t + \theta)\right]^2$$
$$\left.\begin{aligned} &= \frac{K_p A^2}{2} \cos^2(\omega_0 t + \theta) \\ &= \frac{m\omega_0^2}{2} A^2 \cos^2(\omega_0 t + \theta) \end{aligned}\right\} \quad \cdots (5) \text{ using (2)}$$

So, total energy: $E = \frac{K_p A^2}{2}\left[\sin^2(\omega_0 t + \theta) + \cos^2(\omega_0 t + \theta)\right]$

using (3), (4), (5)
$$\Rightarrow E = \frac{K_p A^2}{2} = \frac{m\omega_0^2}{2} A^2 \quad \cdots (6)$$

Quantum Harmonic Oscillator:

We use the same harmonic potential well $U(x) = \frac{1}{2} K_p x^2 = \frac{1}{2} m\omega_0^2 x^2$ as in the previous section.

Then the time independent Schrödinger equation is:

$$E\tilde{\psi}(x) = -\frac{\hbar^2}{2m}\frac{\partial^2 \tilde{\psi}(x)}{\partial x^2} + \frac{1}{2} m\omega_0^2 x^2 \tilde{\psi}(x) \quad \cdots (7)$$

The general solution of (7) is:

$$\left.\begin{aligned} &\tilde{\psi}_n(x) = A_n H_n(\beta x)\, e^{-\frac{\beta^2 x^2}{2}} \\ &\text{where } \beta = \sqrt{\frac{m\omega_0}{\hbar}}, \quad n = 0, 1, 2, 3 \cdots \end{aligned}\right\} \quad \cdots (8)$$

In (8): $A_n = \left(\frac{\beta}{2^n n! \sqrt{\pi}}\right)^{1/2}$ --- (9)

and $H_n(x)$ represent Hermite polynomials:

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}\left[e^{-x^2}\right] \text{--- (10)}$$

The energy corresponding to the above is:

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega_0 \qquad \text{--- (11)}$$

using (8), (9), (10) & (11)

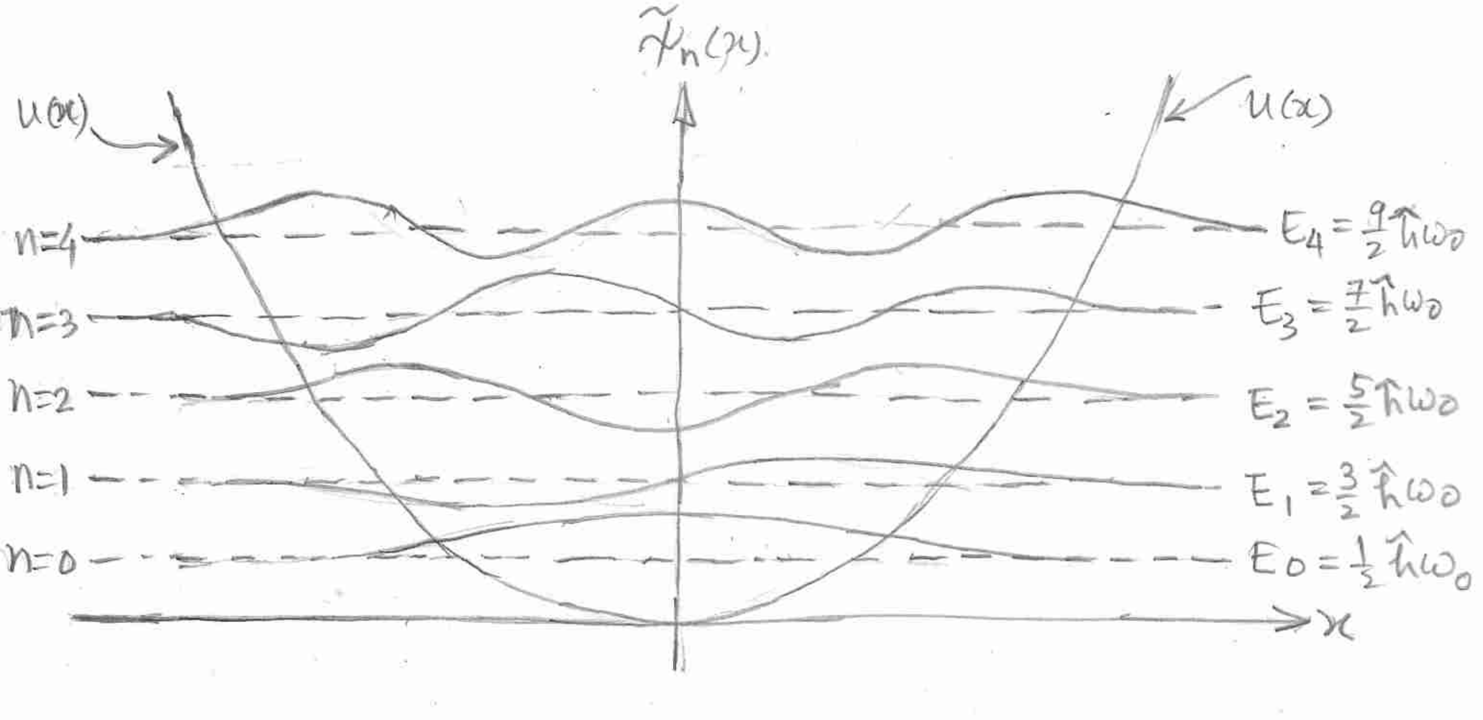
$$\tilde{\psi}_0(x) = \left(\frac{\beta}{\sqrt{\pi}}\right)^{1/2} e^{-\frac{\beta^2 x^2}{2}} \quad ; E_0 = \frac{\hbar\omega_0}{2}$$

$$\tilde{\psi}_1(x) = \left(\frac{\beta}{2\sqrt{\pi}}\right)^{1/2} (2\beta x) e^{-\frac{\beta^2 x^2}{2}} \quad ; E_1 = \frac{3\hbar\omega_0}{2}$$

$$\tilde{\psi}_2(x) = \left(\frac{\beta}{8\sqrt{\pi}}\right)^{1/2} (4\beta^2x^2 - 2) e^{-\frac{\beta^2 x^2}{2}} \quad ; E_2 = \frac{5\hbar\omega_0}{2}$$

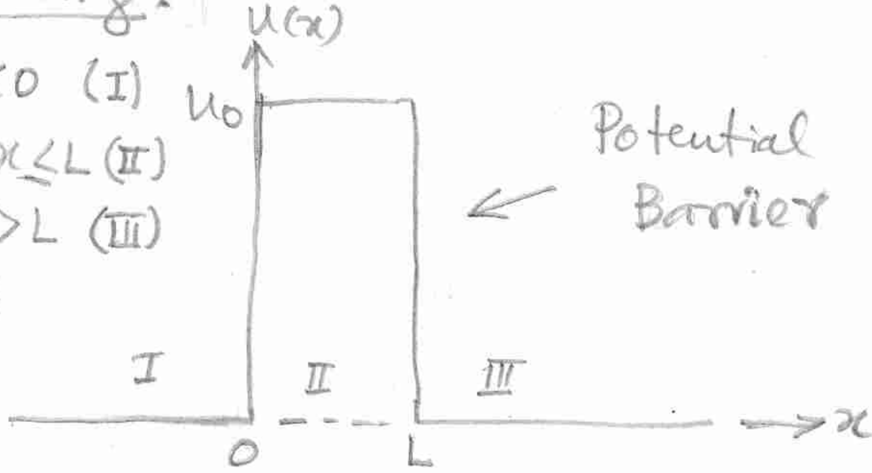
$$\tilde{\psi}_3(x) = \left(\frac{\beta}{48\sqrt{\pi}}\right)^{1/2} (8\beta^3x^3 - 12\beta x) e^{-\frac{\beta^2 x^2}{2}} \quad ; E_3 = \frac{7\hbar\omega_0}{2}$$

$$\vdots$$



Quantum Tunneling:

$$U(x) = \begin{cases} 0 & \text{for } x < 0 \quad (\mathrm{I}) \\ U_0 & \text{for } 0 \le x \le L \quad (\mathrm{II}) \\ 0 & \text{for } x > L \quad (\mathrm{III}) \end{cases} \qquad \text{--- (1)}$$



Assume the following time independent solutions:

$$\tilde{\psi}(x) \begin{cases} = \underset{\text{(incident)}}{Ae^{jkx}} + \underset{\text{(reflected)}}{Be^{-jkx}} & : \text{Region I} \\ = \underset{\text{(evanescent)}}{Fe^{\alpha x} + Ge^{-\alpha x}} & : \text{Region II} \\ = \underset{\text{(tunneled)}}{Ce^{jkx}} + \underset{\text{(reflection after tunneling, if any)}}{De^{-jkx}} & : \text{Region III} \end{cases} \qquad \text{--- (2)}$$

Knowing E, we can find k & α as before:

$$E = \frac{\hbar^2 k^2}{2m} = U_0 - \frac{\hbar^2 \alpha^2}{2m} \qquad \text{--- (3)}$$

(a) Matching boundary conditions at $x = 0$:

$$\tilde{\psi}_{\mathrm{I}}(0) = \tilde{\psi}_{\mathrm{II}}(0) \Rightarrow A + B = F + G \Rightarrow B - G = -A + F \quad \text{--- (4)}$$

$$\psi'_{\mathrm{I}}(0) = \psi'_{\mathrm{II}}(0) \Rightarrow jkA - jkB = \alpha F - \alpha G \Rightarrow jkB - \alpha G = jkA - \alpha F \quad \text{--- (5)}$$

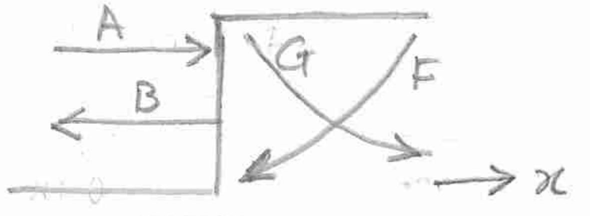
Expressing (4) & (5) in matrix form:

$$\begin{pmatrix} 1 & -1 \\ jk & -\alpha \end{pmatrix} \begin{pmatrix} B \\ G \end{pmatrix} = \begin{pmatrix} -1 & 1 \\ jk & \alpha \end{pmatrix} \begin{pmatrix} A \\ F \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} B \\ G \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ jk & -\alpha \end{pmatrix}^{-1} \begin{pmatrix} -1 & 1 \\ jk & -\alpha \end{pmatrix} \begin{pmatrix} A \\ F \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} B \\ G \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ F \end{pmatrix}$$

scattering matrix at interface $x=0$



$x=0$

Where $$\begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} \frac{jk+\alpha}{jk-\alpha} & \frac{-2\alpha}{jk-\alpha} \\ \frac{2jk}{jk-\alpha} & \frac{-jk-\alpha}{jk-\alpha} \end{pmatrix} \quad \text{---(6)}$$

(b) Matching boundary conditions at $x=L$,

$$\tilde{\psi}_{II}(L) = \psi_{III}(L) \Rightarrow Fe^{\alpha L} + Be^{-\alpha L} = Ce^{jkL} - De^{-jkL}$$

$$\Rightarrow Fe^{\alpha L} - Ce^{jkL} = -Ge^{-\alpha L} + De^{-jkL} \quad \text{---(7)}$$

$$\tilde{\psi}_{II}'(L) = \tilde{\psi}_{III}'(L) \Rightarrow \alpha Fe^{\alpha L} - \alpha Ge^{-\alpha L} = jkCe^{jkL} - jkDe^{-jkL}$$

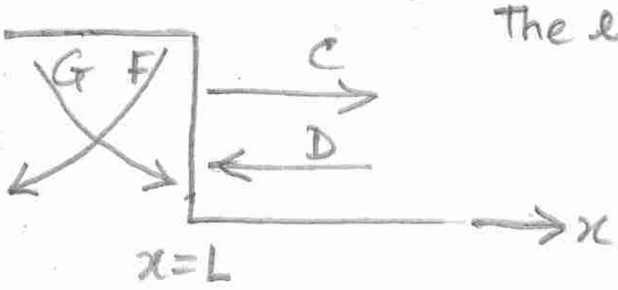
$$\Rightarrow \alpha Fe^{\alpha L} - jkCe^{jkL} = \alpha Ge^{-\alpha L} - jkDe^{-jkL} \quad \text{---(8)}$$

Using (7) & (8):

$$\begin{pmatrix} Fe^{\alpha L} \\ Ce^{jkL} \end{pmatrix} = \begin{pmatrix} S_{22} & S_{21} \\ S_{12} & S_{11} \end{pmatrix} \begin{pmatrix} Ge^{-\alpha L} \\ De^{-jkL} \end{pmatrix} \quad \text{---(9)}$$

scattering matrix at interface $x=L$

The elements are given by (6).



$x=L$

From (6) & (9) we can write:

$$\text{Transmission Coefficient } T = \frac{Ce^{jkL}}{A} = \frac{S_{12}S_{21}e^{-\alpha L}}{1-S_{22}^2 e^{-2\alpha L}} \quad \text{--- (10)}$$

$$\text{Reflection Coefficient } R = \frac{B}{A} = S_{11} + \frac{S_{12}S_{22}S_{21}e^{-2\alpha L}}{1-S_{22}^2 e^{-2\alpha L}} \quad \text{--- (11)}$$

From (10) & (11), probability of tunneling:

$$P_T = |T|^2 = \left|\frac{Ce^{jkL}}{A}\right|^2 = \frac{|C|^2}{|A|^2} = \frac{|S_{12}S_{21}|^2 e^{-2\alpha L}}{|1-S_{22}^2 e^{2\alpha L}|^2} \quad \text{--- (12)}$$

If L is large so that the evanescent wave decays severely, $S_{22}^2 e^{-2\alpha L} << 1$, then from (12)

$$P_T \simeq |S_{12}S_{21}|^2 e^{-2\alpha L} = \frac{16\alpha^2 k^2}{(k^2+\alpha^2)^2} e^{-2\alpha L} = 16\frac{E}{U_0}\left(1-\frac{E}{U_0}\right)e^{-2\alpha L} \quad \text{--- (13)}$$

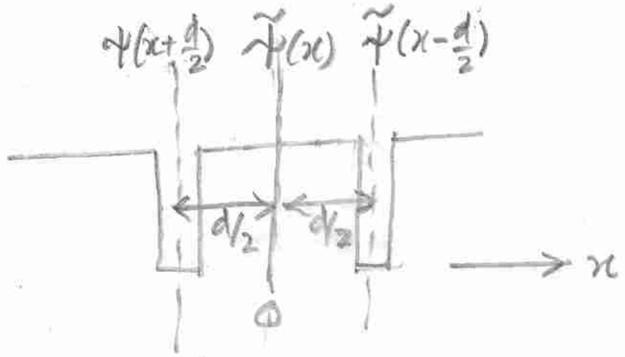
using (6)   using (3)

Large barrier height

Now if $E << U_0$, from (13) $P_T \to 0$.

Tunneling of Bound States:

Consider two identical potential wells a small distance 'd' apart



Let wave function of the well at $x=0$ be $\tilde{\varphi}(x)$

Then the wavefunction at the well on the right will be $\tilde{\psi}(x - d/2)$ and the same at the well on the left will be $\tilde{\psi}(x + d/2)$. There will be back and forth tunneling between the two wells. It can be shown that the overall time dependent wavefunction for the wells is given by:

$$\psi(x,t) \propto \left[\tilde{\psi}(x+\tfrac{d}{2})\cos(\Delta\omega t) + j\tilde{\psi}(x-\tfrac{d}{2})\sin(\Delta\omega t)\right]e^{-j\omega t} \quad \text{---(14)}$$

where $\Delta\omega$ is frequency of back & forth tunneling that reduces with increasing distance d between the wells

Since $\cos(\Delta\omega t) = \dfrac{e^{j\Delta\omega t} + e^{-j\Delta\omega t}}{2}$

and $\sin(\Delta\omega t) = \dfrac{e^{j\Delta\omega t} - e^{-j\Delta\omega t}}{2j}$

We can re-write (14) as:

$$\left.\begin{aligned} \tilde{\psi}(x,t) &\propto \left[\tilde{\psi}_+(x)e^{-j(\omega-\Delta\omega)t} + \tilde{\psi}_-(x)e^{-j(\omega+\Delta\omega)t}\right] \\ \text{where } \tilde{\psi}_+(x) &= \tfrac{1}{2}\left[\tilde{\psi}(x+\tfrac{d}{2}) + \tilde{\psi}(x-\tfrac{d}{2})\right] \\ \text{and } \psi_-(x) &= \tfrac{1}{2}\left[\tilde{\psi}(x+\tfrac{d}{2}) - \tilde{\psi}(x-\tfrac{d}{2})\right] \end{aligned}\right\} \text{---(15)}$$

We see that:

Two frequencies are involved in $\tilde{\psi}(x,t)$: $(\omega - \Delta\omega)$ and $(\omega + \Delta\omega)$ and this corresponds to two energies $\hbar(\omega - \Delta\omega)$ and $\hbar(\omega + \Delta\omega)$. This, in turn, means a single energy state $\hbar\omega$ in the identical wells will be split into two: one higher and one lower due to back and forth tunneling between them because of the proximity 'd'.