Phy 330 Spring 2020

Lec #8: 1 Dim Bound States

$\sim \quad (\,)$

$$-\frac{\hbar^2}{2m}\phi_E''(x) + V\phi_E(x) = E\phi_E(x)$$

Boundary conditions -

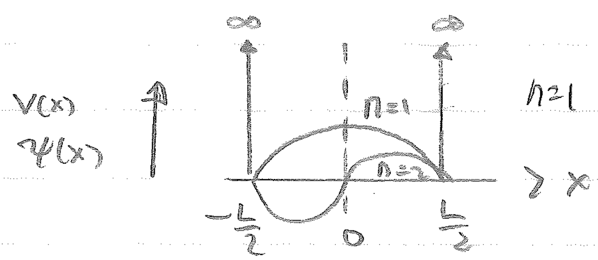
① normalizable $\quad \Phi_E(x)\Big|_{-\infty}^{+\infty} = 0$

② $\Phi_E(x)$ continuous
propability density $|\Phi_E|^2$ continuous

③ $\frac{d\Phi}{dx}$ continuous everywhere V ~~continuous~~ finite

momentum finite

Particle in box $\quad -\frac{L}{2} < x < \frac{L}{2}$



n=1 Ground state, least curvature
zero nodes

n=2 First excited state
one node

Symmetric $(x \to -x)$ potential implies
P.D.F. symmetric implies $\phi_E(x)$ even or odd.
Ground state is always symmetric

$$\phi_E'' = -\frac{2mE}{\hbar^2}\phi_E \equiv -k^2\phi_E$$

oscillatory solutions - even, cosine odd sine boundary condition: $\phi_E(x)\Big|_{-L/2}^{L/2} = 0$

requirement ③ doesn't apply as $V\Big|_{-L/2}^{L/2} = \infty$
force $\frac{dV}{dx}\Big|_{-L/2}^{L/2} = \pm\infty$

$$\phi_n^S = \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right) \Bigg\{ \phi_n^A = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

n odd integer $\qquad$ n even integer

$$E_n = n^2\left(\frac{\hbar^2\pi^2}{2mL^2}\right) \quad n \text{ integer}, \quad k_n = \frac{n\pi}{L}$$

$$(E_{n+1} - E_n)/E_n = [(n+1)^2 - n^2]/n^2 = \frac{2n+1}{n^2}$$

lowest energy ground state has $p_1 = \hbar k = \frac{\hbar\pi}{L}$

$$\Delta p\,\Delta x \leq \frac{\hbar}{2}$$

Orthogonality:
Generally, energy eigenfunctions are orthogonal (linear vector space of functions)

$$\int \phi_n^* \phi_m \, dx = \delta_{nm} \equiv \begin{cases} 1 & n = m \\ 0 & n \neq m \end{cases}$$

Completeness: Generally, energy eigenfunction complete;

Any solution can be written as linear superposition:

$$\phi(x) = \sum_{\substack{n=1 \\ n \text{ odd}}}^{\infty} A_N \phi_N^S + \sum_{\substack{N=2 \\ N \text{ even}}}^{\infty} B_N \phi_N^A$$

<u>Example</u>

$$\phi_{2x} = \frac{1}{\sqrt{3}}\,\phi_1^S + i\sqrt{\frac{2}{3}}\,\phi_2^A$$

not an energy eigenstate.

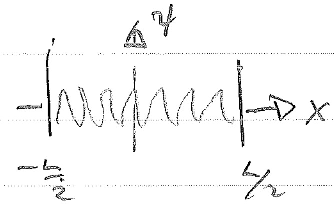
$\boxed{\text{Collapse postulate}}$:

Measurement gives eigenvalue with probability $|\text{amplitude}|^2$ & leaves Q.M. system in eigenstate

So in our example,

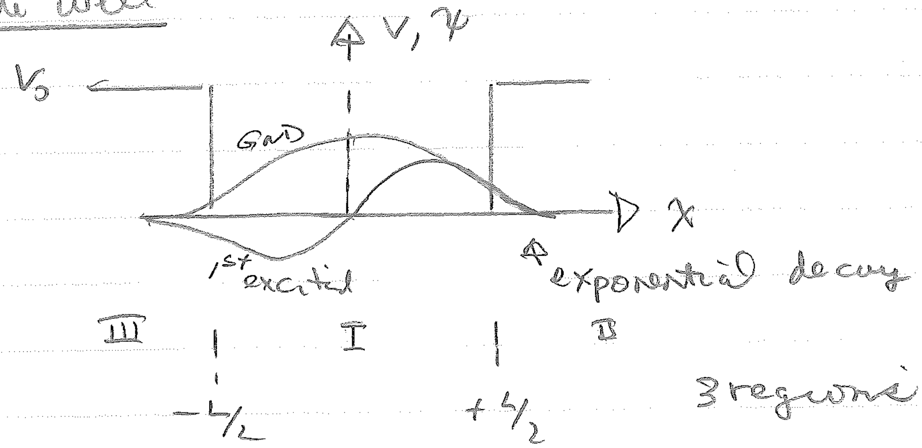
$$P(E_1) = \left|\frac{1}{\sqrt{3}}\right|^2 = \frac{1}{3} \qquad P(E_2) = \left|i\sqrt{\frac{2}{3}}\right|^2 = \frac{2}{3}$$

<u>Classical limit</u> $n \to \infty$



$|\phi_n|^2 \to \frac{1}{L}$ classically, equally likely to be anywhere in box

Finite well



Wave function normalizable implies exponential decay in region II, III.

$$k^2 \equiv \frac{2mE}{\hbar^2} \qquad q^2 \equiv 2m(V_0 - E)/\hbar^2$$

region I $\qquad \phi_E'' = -k^2 \phi_E$

region II, III $\qquad \phi_E'' = +q^2 \phi_E$

region I, $\quad \phi_E \propto \cos kx,\ \sin kx \qquad$ choose even, odd because of V parity symmetry $V(x) = V(-x)$

region II, III $\quad \phi_E \propto e^{\pm qx}$

Symmetry of potential implies even, odd solution

Even:

$$\phi^{I}(x) = A \cos kx$$
$$\phi^{II}(x) = B\ e^{-qx}$$
$$\phi^{III}(x) = B\ e^{+qx}$$

boundary conditions -

$$A \cos\left(\frac{kL}{2}\right) = B e^{-q L/2} \qquad \phi \text{ continuity}$$

$$-k \sin\left(\frac{kL}{2}\right) = -q B e^{-q L/2} \qquad \phi' \text{ continuity}$$

transcendental equation:

$$k \tan\left(\frac{kL}{2}\right) = q$$

and $\quad k^2 + q^2 = \frac{2mV_0}{\hbar^2}$

introduce dimensionless variables:

$$\xi = \frac{kL}{2} \quad \eta = \frac{qL}{2} \quad ; \quad a^2 = \frac{2mV_0}{\hbar^2}\left(\frac{L}{2}\right)^2$$

$$= \frac{\pi^2}{4} \frac{V_0}{\left(\frac{\hbar^2 \pi^2}{2mL^2}\right)}$$

$\leftarrow$ Box ground state

then $\quad \xi \tan \xi = \eta$

$$\xi^2 + \eta^2 = a^2$$

odd solutions give $\quad -\xi \cot \xi = \eta$

8-6

Modern Physics 330 January 21, 2020

1D box graphical solution

For 1D box of length L, depth V_0

$k^2 = 2mE/\hbar^2$ and $q^2 = 2m(V_0 - E)/\hbar^2$

Define dimensionless variables $\xi = kL/2$, $\eta = qL/2$ and well strength parameter

$$a^2 = \frac{mV_0L^2}{2\hbar^2}$$

even solutions:

$$\xi \tan \xi = \eta$$

odd solutions:

$$-\xi / \tan \xi = \eta$$

intersects with

$$\xi^2 + \eta^2 = a^2$$

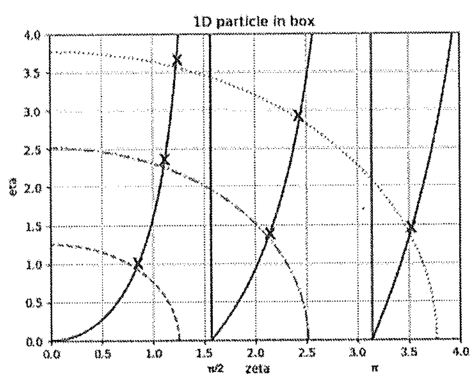


Figure 1: Graphical solution of 1D box. Three different values of a are drawn. The 'x's mark solutions. Ignore vertical lines which are plotting artifacts.

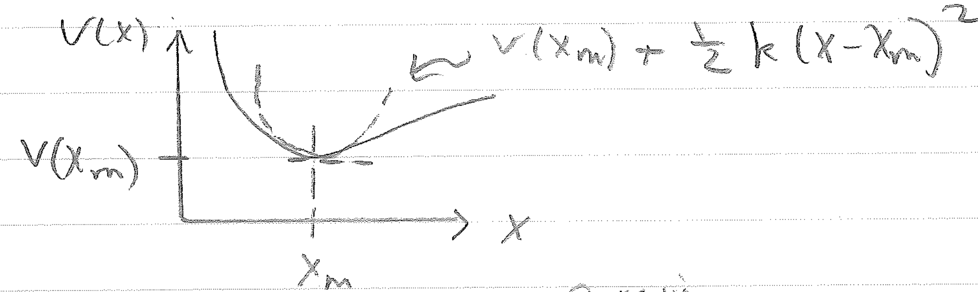
Intersection values ξ_n have energies

$$E_n = 2\xi_n^2 \frac{\hbar^2}{mL^2} = \left(\frac{2\xi_n}{\pi}\right)^2 \frac{\hbar^2\pi^2}{2mL^2} = \left(\frac{2\xi_n}{\pi}\right)^2 E_1^{\text{box}}$$

In 1D there is always at least one solution no matter how small the strength parameter a.

Harmonic Oscillator

Just about any potential is approximately harmonic near a minimum



$$V(x) = V(x_m) + \cancel{\frac{dV}{dx}\Big|_{x_m}}^{\,0 \text{ @ min.}} (x - x_m) + \frac{1}{2} \underbrace{\frac{dV}{dx}\Big|_{x_m}}_{k \,=\, m\omega^2} (x - x_m)^2$$

Gaussian wave packet

$$\phi(x) = \frac{1}{\pi^{1/4} x_0^{1/2}} \exp\left[-\frac{1}{2}\left(\frac{x}{x_0}\right)^2\right]$$

normalized

$$\int_{-\infty}^{\infty} |\phi|^2 dx = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{dx}{x_0} e^{-(x/x_0)^2} = 1$$

comparing to standard form of Gaussian PDF $|\phi|^2$

$$\frac{1}{x_0^2} = \frac{1}{2\sigma^2} \qquad \sigma = \Delta x = \frac{x_0}{\sqrt{2}}$$

$$\Delta x \Delta p = \frac{\hbar}{2} \quad \text{for \underline{Gaussian} PDF}$$

min. uncertainty

$$\Delta p = \frac{\hbar}{\sqrt{2}\, x_0}$$

Gaussian is solution to harmonic potential

$$\frac{d\phi}{dx} = \frac{-x}{x_0^2}\phi$$

$$\frac{d^2\phi}{dx^2} = \left(-\frac{1}{x_0^2} + \frac{x^2}{x_0^4}\right)\phi$$

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} + V\phi = E\phi$$

substituting,

$$-\frac{\hbar^2}{2m}\frac{x^2}{x_0^4} + \frac{\hbar^2}{2m}\frac{1}{x_0^2} + V(x) = E$$

solution with $V(x) = \frac{\hbar^2}{2m}\frac{x^2}{x_0^4} = \frac{1}{2}m\omega^2x^2$

$$E = \frac{\hbar^2}{2mx_0^2} = \frac{1}{2}\hbar\omega$$

$$x_0 = \sqrt{\frac{\hbar}{m\omega}}$$

We can guess (zero nodes in ϕ) that this is the ground state.

x_0 corresponds to classical turning point

$$E = \frac{1}{2}m\omega^2x_0^2$$

General Solution

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} + \frac{1}{2}m\omega^2x^2\phi = E\phi$$

giving $E_n = \hbar\omega\left(\frac{1}{2}+n\right)$ $n=0,1,2,\ldots$

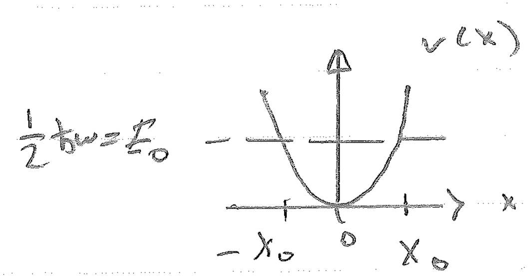
$E_n - E_{n-1} = \hbar\omega$ equally spaced

Wave functions

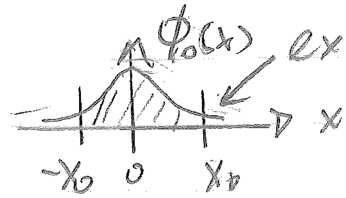
$$\phi_n(x) = \frac{1}{\pi^{1/4}}\frac{1}{x_0^{1/2}}\frac{H_n\left(\frac{x}{x_0}\right)}{\sqrt{2^n n!}}e^{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2}$$

$H_n(y)$ are Hermite polynomials

	parity	# nodes
$H_0 = 1$	even	0
$H_1 = 2y$	odd	1
$H_2 = 4y^2 - 2$	even	2
$H_3 = 8y^3 - 12y$	odd	3
...		



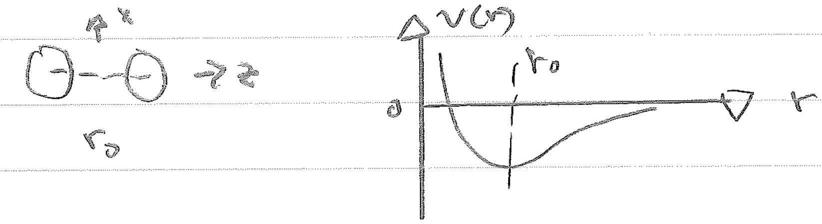
$\pm x_0$ classical turning points



extends beyond classical turning points

$$P_{classical} = \int_{x_0}^{x_0} |\phi_0|^2 dx = \mathrm{erf}(1) \cong 0.84$$

Diatomic Molecule vibrational modes



$V<0$ bound

$$V(r) = V(r_0) + \frac{1}{2} m\omega^2 (r - r_0)^2$$

$$E_n^{vib} = \hbar\omega\left(n + \frac{1}{2}\right)$$

typical $\hbar\omega \approx \left(\frac{1}{3}\right) eV \gg kT\Big|_{300K} = \left(\frac{1}{40}\right) eV$

Frozen at room temperature making rigid rotor approximation valid.

$C_V = \frac{5}{2} R$ molar heat capacity

Rotational mode about symmetry axis (z) also frozen

$$E_i^{rot} = \frac{1}{2}\frac{\langle L^2 \rangle}{I_i} = \frac{1}{2}\frac{\hbar l(l+1)}{I_i} \qquad l = 0, 1, 2, \ldots$$

i axis index

$I_z \ll I_x = I_y$