Particle in a Box

1) $$H\Psi = E\Psi$$

$$-\frac{1}{2m}\frac{d^2}{dx^2}\Psi = (E-V)\Psi$$

$$V = \begin{cases} 0, & 0 \le x \le L \\ \infty, & \text{otherwise} \end{cases}$$

for $x \in (-\infty, 0) \cup (L, \infty)$, $V = \infty$

$$\Psi = 0$$

for $x \in [0, L]$, $V = 0$.

$$\frac{1}{2m}\frac{d^2\Psi}{dx^2} = -E\Psi \Rightarrow \frac{d^2\Psi}{dx^2} = -2mE\Psi$$

$$\Psi = Ae^{i\sqrt{2mE}x} + Be^{-\sqrt{2mE}ix}$$

Ψ is continuous

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

$$A + B = 0. \quad \Rightarrow A = -B.$$

$$Ae^{\sqrt{2mE}Li} + Be^{-\sqrt{2mE}Li} = 0.$$

$$\Rightarrow e^{\sqrt{2mE}Li} - e^{-\sqrt{2mE}Li} = 0$$

$$\Rightarrow \cos(\sqrt{2mE}L) + i\sin(\sqrt{2mE}L) - \cos(\sqrt{2mE}L) + i\sin(\sqrt{2mE}L) = 0$$

$$\Rightarrow 2i\sin(\sqrt{2mE}L) = 0 \Rightarrow \sqrt{2mE}L = n\pi, \quad n \in \mathbb{Z}$$

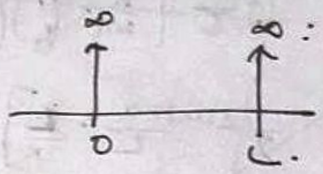
$$\Rightarrow \boxed{E = \frac{n^2\pi^2}{2mL^2}}$$

$$\frac{n^2h^2}{8mL^2} \rightarrow \frac{n^2h^2}{\pi^2 8mL^2}\pi^2 = n^2\left(\frac{h}{2\pi}\right)^2 \cdot \frac{\pi^2}{2mL^2}$$

2) $\psi = A\cos Kx + B\sin Kx$

$x = 0, L \to \psi = 0$

(it is bound)



$\Rightarrow A = 0$

$B\sin KL = 0$

$K = \frac{n\pi}{L}$

$H_{1n} = \frac{-1}{2m}\frac{d^2}{dx^2} + V(x)$

$-\cancel{B} K^2 \cancel{\sin Kx} = -2mE\cancel{\sin Kx}$

$K = \sqrt{2mE} \qquad \Rightarrow E = \frac{n^2\pi^2}{2mL^2}$

$$\boxed{\langle\phi_m|H|\phi_n\rangle = \int dx\, \phi_m^* H \phi_n}$$

$\psi = B\sin Kx$

$\int_0^L |\psi|^2 dx = 1$

$\Rightarrow \int_0^L B^2 \sin^2 Kx\, dx = 1$

$\Rightarrow B^2 \int_0^L \left(\frac{1}{2} - \frac{\cos 2Kx}{2}\right) dx = 1 \Rightarrow B^2\left[\frac{x}{2} - \frac{\sin 2Kx}{4K}\right]_0^L = 1$

$\Rightarrow B^2\left[\frac{L}{2} - \frac{\sin 2KL}{4K}\right] = 1 \qquad (\sin KL = 0 \Rightarrow \sin 2KL = 0)$

$\Rightarrow B^2\left[\frac{L}{2}\right] = 1 \Rightarrow B = \sqrt{\frac{2}{L}}$

$\Rightarrow \psi = \sqrt{\frac{2}{L}}\sin Kx \qquad (K = \sqrt{2mE})$

$\Rightarrow \psi = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}$ $\longrightarrow$ this is $\phi(x)$.

$\phi_1(x) = \sqrt{\frac{2}{L}}\sin\frac{\pi x}{L} \qquad (n=1)$

$\phi_2(x) = \sqrt{\frac{2}{L}}\sin\frac{2\pi x}{L} \qquad (n=2)$

$\langle\phi_1|H|\phi_1\rangle = \int dx\, \phi_1 H \phi_1$

$= \int dx \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)\cdot\left[-\frac{1}{2m}\left(-\frac{\pi^2}{L^2}\cdot\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)\right) + \alpha x\right]$

$= \left[\frac{\pi^2}{mL^3}\int \sin^2\left(\frac{\pi x}{L}\right)dx + \alpha\sqrt{\frac{2}{L}}\int x\sin\frac{\pi x}{L}\right]_0^L$

2) $\langle \phi_1 | H_{in} | \phi_1 \rangle =$

If $\hat{x} = x$ is an operator then $\hat{x} f(x) = x f(x)$ (FFS!)

$$\int_0^L dx \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)\cdot\left[-\frac{1}{2m}\frac{d^2}{dx^2} + \alpha x\right]\left(\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)\right)$$

$$= \int_0^L \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) \cdot \left[+\frac{1}{2m}\sin\left(\frac{\pi x}{L}\right)\left(\frac{\pi^2}{L^2}\right)\cdot\sqrt{\frac{2}{L}} + \alpha\sqrt{\frac{2}{L}}\, x \sin\left(\frac{\pi x}{L}\right)\right] dx$$

$$= \left(\frac{1}{\cancel{2}m}\right)\left(\frac{\cancel{2}}{L}\right)\left(\frac{\pi^2}{L^2}\right)\int_0^L \sin^2\left(\frac{\pi x}{L}\right)dx + \alpha\left(\frac{2}{L}\right)\int_0^L x\sin^2\left(\frac{\pi x}{L}\right)dx$$

$$= \frac{\pi^2}{mL^3}\int_0^L \frac{1}{2}\left(1-\cos\left(\frac{2\pi x}{L}\right)\right)dx + \alpha\left(\frac{2}{L}\right)\int_0^L x\cdot\frac{1}{2}\left(1-\cos\left(\frac{2\pi x}{L}\right)\right)dx$$

$$= \frac{\pi^2}{2mL^3}\left[x - \sin\left(\frac{2\pi x}{L}\right)\cdot\frac{L}{\pi}\right]_0^L + \alpha\left(\frac{\cancel{2}}{L}\right)\frac{1}{\cancel{2}}\int_0^L \left(x - x\cos\left(\frac{2\pi x}{L}\right)\right)dx$$

$$= \frac{\pi^2}{2mL^3}\left[x - \sin\left(\frac{2\pi x}{L}\right)\cdot\frac{L}{\pi}\right]_0^L + \alpha\left(\frac{1}{L}\right)\left[\frac{x^2}{2} - \left[x\sin\left(\frac{2\pi x}{L}\right)\cdot\frac{L}{2\pi} + \cos\left(\frac{2\pi x}{L}\right)\cdot\frac{L^2}{4\pi^2}\right]\right]_0^L$$

$$= \frac{\pi^2}{2mL^3}\left[L - \sin\left(\frac{2\pi L}{L}\right)\cdot\frac{L}{\pi} - 0\right] + \alpha\left(\frac{1}{L}\right)\left[\frac{L^2}{2} - \left(L\sin\left(\frac{2\pi L}{L}\right)\cdot\frac{L}{2\pi} + \cos\left(\frac{2\pi L}{L}\right)\frac{L^2}{4\pi^2}\right) - 0 + \left[0 + \frac{L^2}{4\pi^2}\right]\right]$$

$$= \frac{\pi^2}{2mL^3}\left[L\right] + \alpha\left(\frac{1}{L}\right)\left[\frac{L^2}{2} - \cancel{\frac{L^2}{4\pi^2}} + \cancel{\frac{L^2}{4\pi^2}}\right]$$

$$= \frac{\pi^2}{2mL^2} + \frac{\alpha L}{2}.$$

$\langle \phi_1 | H_{in} | \phi_2 \rangle =$

$$\int_0^L dx \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)\left[-\frac{1}{2m}\frac{d^2}{dx^2} + \alpha x\right]\left(\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)\right)$$

$$= \int_0^L \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)\cdot\left[+\frac{1}{2m}\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)\cdot\frac{4\pi^2}{L^2} + \alpha\sqrt{\frac{2}{L}}\cdot x\sin\left(\frac{2\pi x}{L}\right)\right]dx$$

$$= \frac{1}{2m}\left(\frac{2}{L}\right)\left(\frac{4\pi^2}{L^2}\right)\int_0^L \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)dx + \alpha\left(\frac{2}{L}\right)\int_0^L x\sin\left(\frac{\pi x}{L}\right)\cdot\sin\left(\frac{2\pi x}{L}\right)dx$$

$$= \frac{\cancel{4}^{2}\pi^2}{mL^3}\int_0^L \frac{1}{\cancel{2}}\left(\cos\left(\frac{\pi x}{L}\right) - \cos\left(\frac{3\pi x}{L}\right)\right)dx + \alpha\left(\frac{\cancel{2}}{L}\right)\int_0^L \frac{x}{\cancel{2}}\left(\cos\left(\frac{\pi x}{L}\right) - \cos\left(\frac{3\pi x}{L}\right)\right)dx$$

$$= \frac{2\pi^2}{mL^3}\left[\sin\left(\frac{\pi x}{L}\right)\cdot\frac{L}{\pi} - \sin\left(\frac{3\pi x}{L}\right)\cdot\frac{L}{3\pi}\right]_0^L + \alpha\left(\frac{1}{L}\right)\left[\left(x\sin\left(\frac{\pi x}{L}\right)\cdot\frac{L}{\pi} + \cos\left(\frac{\pi x}{L}\right)\cdot\frac{L^2}{\pi^2}\right) - \left(x\sin\left(\frac{3\pi x}{L}\right)\cdot\frac{L}{3\pi} + \cos\left(\frac{3\pi x}{L}\right)\cdot\frac{L^2}{9\pi^2}\right)\right]_0^L$$

$$= \frac{2\pi^2}{mL^3}\left[\sin\left(\frac{\pi L}{L}\right)\cdot\frac{L}{\pi} - \sin\left(\frac{3\pi L}{L}\right)\cdot\frac{L}{3\pi} - 0\right] + \alpha\left(\frac{1}{L}\right)\left[\left(L\sin\left(\frac{\pi L}{L}\right)\cdot\frac{L}{\pi} + \cos\left(\frac{\pi L}{L}\right)\cdot\frac{L^2}{\pi^2}\right) - \left(L\sin\left(\frac{3\pi L}{L}\right)\cdot\frac{L}{3\pi} + \cos\left(\frac{3\pi L}{L}\right)\cdot\frac{L^2}{9\pi^2}\right) - \left(0 + \frac{L^2}{\pi^2}\right) + \left(0 + \frac{L^2}{9\pi^2}\right)\right]$$

$$= \alpha\left(\frac{1}{L}\right)\left[-\frac{L^2}{\pi^2} + \frac{L^2}{9\pi^2} - \frac{L^2}{\pi^2} + \frac{L^2}{9\pi^2}\right] = \alpha\left(\frac{1}{L}\right)\left[-\frac{16L^2}{9\pi^2}\right]$$

$$= \frac{-16\alpha L}{9\pi^2}$$

$\langle \phi_2 | H_{in} | \phi_1 \rangle =$

$$\int_0^L dx \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)\left[-\frac{1}{2m}\frac{d^2}{dx^2} + \alpha x\right]\left(\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)\right)$$

$$= \int_0^L \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)\left[+\frac{1}{2m}\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)\cdot\frac{\pi^2}{L^2} + \alpha\sqrt{\frac{2}{L}}x\sin\left(\frac{\pi x}{L}\right)\right]dx$$

$$= \frac{1}{2m}\left(\frac{2}{L}\right)\left(\frac{\pi^2}{L^2}\right)\int_0^L \sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{\pi x}{L}\right)dx + \alpha\left(\frac{2}{L}\right)\int_0^L x\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)dx$$

$$= \frac{\pi^2}{mL^3}\int_0^L \frac{1}{2}\left(\cos\left(\frac{\pi x}{L}\right) - \cos\left(\frac{3\pi x}{L}\right)\right)dx + \alpha\left(\frac{\cancel{2}}{L}\right)\int_0^L \frac{x}{\cancel{2}}\left(\cos\left(\frac{\pi x}{L}\right) - \cos\left(\frac{3\pi x}{L}\right)\right)dx$$

$$= \frac{\pi^2}{2mL^3}\left[\sin\left(\frac{\pi x}{L}\right)\cdot\frac{L}{\pi} - \sin\left(\frac{3\pi x}{L}\right)\cdot\frac{L}{3\pi}\right]_0^L + \alpha\left(\frac{1}{L}\right)\left[\left(x\sin\left(\frac{\pi x}{L}\right)\cdot\frac{L}{\pi} + \cos\left(\frac{\pi x}{L}\right)\cdot\frac{L^2}{\pi^2}\right) - \left(x\sin\left(\frac{3\pi x}{L}\right)\cdot\frac{L}{3\pi} + \cos\left(\frac{3\pi x}{L}\right)\cdot\frac{L^2}{9\pi^2}\right)\right]_0^L$$

$$= \frac{\pi^2}{2mL^3}\left[\sin\left(\frac{\pi \cancel{L}}{\cancel{L}}\right)\cdot\frac{L}{\pi} - \sin\left(\frac{3\pi \cancel{L}}{\cancel{L}}\right)\cdot\frac{L}{3\pi} - 0\right] + \alpha\left(\frac{1}{L}\right)\left[\begin{array}{l}\left(L\sin\left(\frac{\pi L}{L}\right)\cdot\frac{L}{\pi} + \cos\left(\frac{\pi L}{L}\right)\cdot\frac{L^2}{\pi^2}\right) - \\ \left(L\sin\left(\frac{3\pi L}{L}\right)\cdot\frac{L}{3\pi} + \cos\left(\frac{3\pi L}{L}\right)\cdot\frac{L^2}{9\pi^2}\right) - \\ \left(0 + \frac{L^2}{\pi^2}\right) + \left(0 + \frac{L^2}{9\pi^2}\right)\end{array}\right]$$

$$= \alpha\left(\frac{1}{L}\right)\left[-\frac{L^2}{\pi^2} + \frac{L^2}{9\pi^2} - \frac{L^2}{\pi^2} + \frac{L^2}{9\pi^2}\right] = \alpha\left(\frac{1}{\cancel{L}}\right)\left(\frac{-16 L^{\cancel{2}}}{9\pi^2}\right)$$

$$= -\frac{16\alpha L}{9\pi^2}$$

$$\langle \phi_2 | H_{in} | \phi_2 \rangle =$$

$$\int_0^L dx \cdot \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)\cdot\left[\frac{-1}{2m}\frac{d^2}{dx^2} + \alpha x\right]\left(\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)\right)$$

$$= \int_0^L \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)\cdot\left[+\frac{1}{2m}\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)\cdot\frac{4\pi^2}{L^2} + \alpha\sqrt{\frac{2}{L}}\cdot x\sin\left(\frac{2\pi x}{L}\right)\right]dx$$

$$= \frac{1}{\cancel{2}m}\left(\frac{\cancel{2}}{L}\right)\left(\frac{4\pi^2}{L^2}\right)\int_0^L \sin^2\left(\frac{2\pi x}{L}\right)dx + \alpha\left(\frac{2}{L}\right)\int_0^L x\sin^2\left(\frac{2\pi x}{L}\right)dx$$

$$= \frac{\overset{2}{\cancel{4}}\pi^2}{mL^3}\int_0^L \frac{1}{\cancel{2}}\left(1 - \cos\left(\frac{4\pi x}{L}\right)\right)dx + \alpha\left(\frac{\cancel{2}}{L}\right)\int_0^L \frac{x}{\cancel{2}}\left(1 - \cos\left(\frac{4\pi x}{L}\right)\right)dx$$

$$= \frac{2\pi^2}{mL^3}\left[x - \sin\left(\frac{4\pi x}{L}\right)\cdot\frac{L}{4\pi}\right]_0^L + \alpha\left(\frac{1}{L}\right)\left[\frac{x^2}{2} - \left[x\sin\left(\frac{4\pi x}{L}\right)\cdot\frac{L}{4\pi} + \cos\left(\frac{4\pi x}{L}\right)\cdot\frac{L^2}{16\pi^2}\right]\right]_0^L$$

$$= \frac{2\pi^2}{mL^3}\left[L - \sin\left(\frac{4\pi \cancel{L}}{\cancel{L}}\right)\cdot\frac{L}{4\pi} - 0\right] + \alpha\left(\frac{1}{L}\right)\left\{\begin{array}{l}\frac{L^2}{2} - \left[L\sin\left(\frac{4\pi L}{L}\right)\cdot\frac{L}{4\pi} + \cos\left(\frac{4\pi L}{L}\right)\cdot\frac{L^2}{16\pi^2}\right] \\ -0 + \left[0 + \frac{L^2}{16\pi^2}\right]\end{array}\right\}$$

$$= \frac{2\pi^2}{mL^{\cancel{3}2}}\left[\cancel{L}\right] + \alpha\left(\frac{1}{\cancel{L}}\right)\left[\frac{L^{\cancel{2}}}{2} - \cancel{\frac{L^2}{16\pi^2}} + \cancel{\frac{L^2}{16\pi^2}}\right]$$

$$= \frac{2\pi^2}{mL^2} + \frac{\alpha L}{2}.$$

$$\Rightarrow \langle \phi_1 | H_{in} | \phi_1 \rangle = \frac{\pi^2}{2mL^2} + \frac{\alpha L}{2}$$

$$\langle \phi_1 | H_{in} | \phi_2 \rangle = \frac{-16\alpha L}{9\pi^2}$$

$$\langle \phi_2 | H_{in} | \phi_1 \rangle = \frac{-16\alpha L}{9\pi^2}$$

$$\langle \phi_2 | H_{in} | \phi_2 \rangle = \frac{2\pi^2}{mL^2} + \frac{\alpha L}{2}$$

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3) $\phi_p = \sqrt{\frac{2}{L}} \sin\left(\frac{p\pi x}{L}\right)$ $\quad p, q \in N$

$\phi_q = \sqrt{\frac{2}{L}} \sin\left(\frac{q\pi x}{L}\right)$.

$\langle \phi_p | H_{in} | \phi_q \rangle =$

$$\int_0^L dx \sqrt{\frac{2}{L}} \sin\left(\frac{p\pi x}{L}\right) \left[\frac{-1}{2m}\frac{d^2}{dx^2} + \alpha x\right] \left(\sqrt{\frac{2}{L}} \sin\left(\frac{q\pi x}{L}\right)\right).$$

$$= \int_0^L \sqrt{\frac{2}{L}} \sin\left(\frac{p\pi x}{L}\right) \left[\frac{+1}{2m}\sqrt{\frac{2}{L}} \sin\left(\frac{q\pi x}{L}\right) \cdot \frac{q^2\pi^2}{L^2} + \alpha \sqrt{\frac{2}{L}} \cdot x \sin\left(\frac{q\pi x}{L}\right)\right] dx$$

$$= \frac{1}{\cancel{2}m}\left(\frac{\cancel{2}}{L}\right)\left(\frac{q^2\pi^2}{L^2}\right) \int_0^L \sin\left(\frac{p\pi x}{L}\right) \sin\left(\frac{q\pi x}{L}\right) dx + \alpha\left(\frac{2}{L}\right) \int_0^L x \sin\left(\frac{p\pi x}{L}\right) \sin\left(\frac{q\pi x}{L}\right) dx$$

$$= \frac{q^2\pi^2}{mL^3} \int_0^L \frac{1}{2}\left(\cos\left(\frac{(p-q)\pi x}{L}\right) - \cos\left(\frac{(p+q)\pi x}{L}\right)\right) dx + \alpha\left(\frac{\cancel{2}}{L}\right) \int_0^L \frac{x}{\cancel{2}}\left(\cos\left(\frac{(p-q)\pi x}{L}\right) - \cos\left(\frac{(p+q)\pi x}{L}\right)\right) dx$$

for $i=j$,
$p=q$

$\Rightarrow \langle \phi_p | H_{in} | \phi_q \rangle =$

$$\frac{q^2\pi^2}{2mL^3}\int_0^L \left(1-\cos\left(\frac{2q\pi x}{L}\right)\right)dx + \alpha\left(\frac{1}{L}\right)\int_0^L x\left(1-\cos\left(\frac{2q\pi x}{L}\right)\right)dx$$

$$= \frac{q^2\pi^2}{2mL^3}\left[x - \sin\left(\frac{2q\pi x}{L}\right)\cdot\frac{L}{2q\pi}\right]_0^L + \alpha\left(\frac{1}{L}\right)\left[\frac{x^2}{2} - \left(x\sin\left(\frac{2q\pi x}{L}\right)\cdot\frac{L}{2q\pi} + \cos\left(\frac{2q\pi x}{L}\right)\cdot\frac{L^2}{4q^2\pi^2}\right)\right]_0^L$$

$$= \frac{q^2\pi^2}{2mL^3}\left[L - \sin\left(\frac{2q\pi L}{L}\right)\cdot\frac{L}{2q\pi} - 0\right] + \alpha\left(\frac{1}{L}\right)\left[\frac{L^2}{2} - \left(L\sin\left(\frac{2q\pi L}{L}\right)\cdot\frac{L}{2q\pi} + \cos\left(\frac{2q\pi L}{L}\right)\cdot\frac{L^2}{4q^2\pi^2}\right) + \left(0 + \frac{L^2}{4q^2\pi^2}\right)\right]$$

$$= \frac{q^2\pi^2}{2mL^2} + \frac{\alpha}{L}\left[\frac{L^2}{2} - \cancel{\frac{L^2}{4q^2\pi^2}} + \cancel{\frac{L^2}{4q^2\pi^2}}\right]$$

$$= \frac{q^2\pi^2}{2mL^2} + \frac{\alpha L}{2}$$

for $i \neq j$,
$p \neq q$.

$\langle \phi_p | H_{in} | \phi_q \rangle =$

$$\frac{q^2\pi^2}{2mL^3}\int_0^L \left(\cos\left(\frac{(p-q)\pi x}{L}\right) - \cos\left(\frac{(p+q)\pi x}{L}\right)\right)dx + \alpha\left(\frac{1}{L}\right)\int_0^L x\left(\cos\left(\frac{(p-q)\pi x}{L}\right) - \cos\left(\frac{(p+q)\pi x}{L}\right)\right)dx$$

$$= \frac{q^2\pi^2}{2mL^3}\left[\sin\left(\frac{(p-q)\pi x}{L}\right)\cdot\frac{L}{\pi(p-q)} - \sin\left(\frac{(p+q)\pi x}{L}\right)\cdot\frac{L}{\pi(p+q)}\right]_0^L$$
$$+\alpha\left(\frac{1}{L}\right)\left[\left(x\sin\left(\frac{(p-q)\pi x}{L}\right)\cdot\frac{L}{\pi(p-q)} + \cos\left(\frac{(p-q)\pi x}{L}\right)\cdot\frac{L^2}{\pi^2(p-q)^2}\right) - \left(x\sin\left(\frac{(p+q)\pi x}{L}\right)\cdot\frac{L}{\pi(p+q)} + \cos\left(\frac{(p+q)\pi x}{L}\right)\cdot\frac{L^2}{\pi^2(p+q)^2}\right)\right]_0^L$$

$$= \frac{q^2\pi^2}{2mL^3}\left[\sin\left(\frac{(p-q)\pi L}{L}\right)\cdot\frac{L}{\pi(p-q)} - \sin\left(\frac{(p+q)\pi L}{L}\right)\cdot\frac{L}{\pi(p+q)} - 0\right]$$
$$+\alpha\left(\frac{1}{L}\right)\left[\left(L\sin\left(\frac{(p-q)\pi L}{L}\right)\cdot\frac{L}{\pi(p-q)} + \cos\left(\frac{(p-q)\pi L}{L}\right)\cdot\frac{L^2}{\pi^2(p-q)^2}\right) - \left(L\sin\left(\frac{(p+q)\pi L}{L}\right)\cdot\frac{L}{\pi(p-q)} + \cos\left(\frac{(p+q)\pi L}{L}\right)\cdot\frac{L^2}{\pi^2(p+q)^2}\right) - \left(0 + \frac{L^2}{\pi^2(p-q)^2}\right) + \left(0 + \frac{L^2}{\pi^2(p+q)^2}\right)\right]$$

$$= \alpha \left(\frac{1}{L}\right)\left[\frac{L^2}{\pi^2(p-q)^2}\cos((p-q)\pi) - \frac{L^2}{\pi^2(p+q)^2}\cos((p+q)\pi) - \frac{L^2}{\pi^2(p-q)^2} + \frac{L^2}{\pi^2(p+q^2)^2}\right]$$

$$= \alpha\left(\frac{1}{\cancel{L}}\right)\left[\frac{L^{\cancel{2}}}{\pi^2(p-q)^2}\left(\cos((p-q)\pi) - 1\right) + \frac{L^{\cancel{2}}}{\pi^2(p+q)^2}\left(1 - \cos((p+q)\pi)\right)\right]$$

$$= \frac{\alpha L}{\pi^2}\left[\frac{1}{(p-q)^2}\left(\cos((p-q)\pi) - 1\right) - \frac{1}{(p+q)^2}\left(\cos((p+q)\pi) - 1\right)\right]$$

~~if $p-q$ = even $\Rightarrow$ $p+q$ is also even~~

$\cancel{\langle\phi_p|H_{in}|\phi_q\rangle = \frac{\alpha L^2}{\pi}\left(\frac{1}{(p-q)^2}(1\right.}$

For $i=j$ (diagonal)

$$\langle \phi_p | H_{in} | \phi_q \rangle = \frac{q^2 \pi^2}{2mL^2} + \frac{\alpha L}{2}$$

For $i \neq j$ (off-diagonal)

$$\langle \phi_p | H_{in} | \phi_q \rangle =$$

$$\frac{\alpha L}{2\pi^2}\left[\frac{1}{(p-q)^2}\left(\cos((p-q)\pi) - 1\right) - \frac{1}{(p+q)^2}\left(\cos(p+q)\pi - 1\right)\right]$$

5) (i) $\psi(x) = \sum_n c_n \phi_n(x)$.

$\psi(x) = c_1\phi_1(x) + c_2\phi_2(x) + \dots\dots c_n\phi_n(x)$

Expectation value of energy is

$\langle E \rangle = \langle \psi | H_{in} | \psi \rangle$

$\Rightarrow \langle E \rangle = \int dx\, \psi^*(x)\, H_{in}\, \psi(x)$.

$= \int dx\, (c_1^*\phi_1^*(x) + c_2^*\phi_2^*(x) + \dots\dots c_n^*\phi_n^*(x))\, H_{in}\, (c_1\phi_1(x) + c_2\phi_2(x) + \dots\dots c_n\phi_n(x))$

$= \int dx\, (c_1^*\phi_1^*(x)) H_{in} (c_1\phi_1(x)) + \int dx\, (c_1^*\phi_1^*(x)) H_{in} (c_2\phi_2(x)) + \dots\dots$

here we are considering only 2 states

$\Rightarrow n = 2$

$= \int dx\, (c_1^*\phi_1^*(x)) H_{in}(c_1\phi_1(x)) + \int dx\, (c_1^*\phi_1^*(x)) H_{in}(c_2\phi_2(x)) +$
$\int dx\, (c_2^*\phi_2^*(x)) H_{in}(c_1\phi_1(x)) + \int dx\, (c_2^*\phi_2^*(x)) H_{in}(c_2\phi_2(x))$

$= |c_1|^2 \langle \phi_1 | H_{in} | \phi_1 \rangle + c_1^* c_2 \langle \phi_1 | H_{in} | \phi_2 \rangle + c_2^* c_1 \langle \phi_2 | H_{in} | \phi_1 \rangle +$
$|c_2|^2 \langle \phi_2 | H_{in} | \phi_2 \rangle$

$$\Rightarrow \langle E\rangle = |c_1|^2\left(\frac{\pi^2}{2mL^2}+\frac{\alpha L}{2}\right) + c_1^* c_2\left(\frac{-16\alpha L}{9\pi^2}\right) + c_2^* c_1\left(\frac{-16\alpha L}{9\pi^2}\right)$$
$$+ |c_2|^2\left(\frac{2\pi^2}{mL^2}+\frac{\alpha L}{2}\right)$$

(ii) here, we are dealing with real values

$$\Rightarrow \langle E\rangle = c_1^2\left(\frac{\pi^2}{2mL^2}+\frac{\alpha L}{2}\right) + c_1 c_2\left(\frac{-32\alpha L}{9\pi^2}\right) + c_2^2\left(\frac{2\pi^2}{mL^2}+\frac{\alpha L}{2}\right)$$

$$\frac{\partial\langle E\rangle}{\partial c_K} = 0 \text{ for all } K$$

$$\frac{\partial\langle E\rangle}{\partial c_1} = 0$$

$$\Rightarrow \cancel{2}c_1\left(\frac{\pi^2}{2mL^2}+\frac{\alpha L}{2}\right) + c_2\left(\frac{-\cancel{32}^{\,16}\alpha L}{9\pi^2}\right) = 0$$

$$\Rightarrow c_1\left(\frac{\pi^2}{2mL^2}+\frac{\alpha L}{2}\right) + c_2\left(\frac{-16\alpha L}{9\pi^2}\right) = 0 \longrightarrow (1)$$

$$\frac{\partial\langle E\rangle}{\partial c_2} = 0$$

$$\Rightarrow c_1\left(-\frac{\cancel{32}^{\,16}\alpha L}{9\pi^2}\right) + \cancel{2}c_2\left(\frac{2\pi^2}{mL^2}+\frac{\alpha L}{2}\right) = 0$$

$$\Rightarrow c_1\left(\frac{-16\alpha L}{9\pi^2}\right) + c_2\left(\frac{2\pi^2}{mL^2}+\frac{\alpha L}{2}\right) = 0 \longrightarrow (2)$$

5)(i)

$\int |\psi|^2 dx = 1$

for $\psi = c_1 \phi_1(x) + c_2 \phi_2(x) + \ldots$

$\int |\psi|^2 = c_1^2 + c_2^2 + \ldots$

so, to make the above condition true,

take $\psi = \dfrac{c_1\phi_1(x) + c_2\phi_2(x) + \ldots}{\sqrt{|c_1|^2 + |c_2|^2 + \ldots}}$

here we are dealing with 2 states

$\Rightarrow \psi(x) = \dfrac{c_1\phi_1(x) + c_2\phi_2(x)}{\sqrt{|c_1|^2 + |c_2|^2}}$

Expectation value of energy is

$\langle E \rangle = \langle \psi | H | \psi \rangle$

$\Rightarrow \langle E \rangle = \int dx\, \psi^* H \psi$

$= \int dx \left(\dfrac{c_1^*\phi_1^*(x) + c_2^*\phi_2^*(x)}{\sqrt{|c_1|^2 + |c_2|^2}} \right) H_{in} \left(\dfrac{c_1\phi_1(x) + c_2\phi_2(x)}{\sqrt{|c_1|^2 + |c_2|^2}} \right)$

$= \dfrac{1}{(|c_1|^2 + |c_2|^2)} \left[\int c_1^*\phi_1^*(x) H c_1 \phi_1(x) + \int c_1^* \phi_1^*(x) H c_2 \phi_2(x) + \int c_2^* \phi_2^*(x) H c_1 \phi_1(x) + \int c_2^* \phi_2^*(x) H c_2 \phi_2(x) \right]$

$\Rightarrow \langle E \rangle = \dfrac{|c_1|^2 \langle \phi_1 | H_{in} | \phi_1 \rangle + c_1^* c_2 \langle \phi_1 | H | \phi_2 \rangle + c_2^* c_1 \langle \phi_2 | H_{in} | \phi_1 \rangle + |c_2|^2 \langle \phi_2 | H_{in} | \phi_2 \rangle}{(|c_1|^2 + |c_2|^2)}$

here we are dealing with only real values.

$\Rightarrow \langle E \rangle = \dfrac{c_1^2 \left(\frac{\pi^2}{2mL^2} + \frac{\alpha L}{2} \right) + 2c_1c_2 \left(\frac{-16\alpha L}{9\pi^2} \right) + c_2^2 \left(\frac{2\pi^2}{mL^2} + \frac{\alpha L}{2} \right)}{(c_1^2 + c_2^2)}$

$$\frac{\partial \langle E\rangle}{\partial c_k} = 0 \quad \text{for all } c_k$$

$$\frac{\partial \langle E\rangle}{\partial c_1} = 0$$

$$\Rightarrow \frac{(c_1^2+c_2^2)\left[\cancel{2}c_1\left(\frac{\pi^2}{2mL^2}+\frac{\alpha L}{2}\right)+\cancel{2}c_2\left(\frac{-16\alpha L}{9\pi^2}\right)\right] - \left(c_1^2\left(\frac{\pi^2}{2mL^2}+\frac{\alpha L}{2}\right)+2c_1c_2\left(\frac{-16\alpha L}{9\pi^2}\right)+c_2^2\left(\frac{2\pi^2}{mL^2}+\frac{\alpha L}{2}\right)\right)(\cancel{2}c_1)}{(c_1^2+c_2^2)^2} = 0$$

$$\Rightarrow \frac{\left[\cancel{c_1^3\left(\frac{\pi^2}{2mL^2}+\frac{\alpha L}{2}\right)} + c_1^2c_2\left(\frac{-16\alpha L}{9\pi^2}\right) + c_1c_2^2\left(\frac{\pi^2}{2mL^2}+\frac{\alpha L}{2}\right) + c_2^3\left(\frac{-16\alpha L}{9\pi^2}\right) - \cancel{c_1^3\left(\frac{\pi^2}{2mL^2}+\frac{\alpha L}{2}\right)} - 2c_1^2c_2\left(\frac{-16\alpha L}{9\pi^2}\right) - c_1c_2^2\left(\frac{2\pi^2}{mL^2}+\frac{\alpha L}{2}\right)\right]}{(c_1^2+c_2^2)^2} = 0$$

$$\Rightarrow \frac{\left[c_1c_2^2\left(-\frac{3\pi^2}{2mL^2}\right) + c_2^3\left(\frac{-16\alpha L}{9\pi^2}\right) - c_1^2c_2\left(\frac{-16\alpha L}{9\pi^2}\right)\right]}{(c_1^2+c_2^2)^2} = 0 \longrightarrow (1)$$

$$\frac{\partial \langle E\rangle}{\partial c_2} = 0$$

$$\Rightarrow \frac{(c_1^2+c_2^2)\left[\cancel{2}c_1\left(\frac{-16\alpha L}{9\pi^2}\right)+\cancel{2}c_2\left(\frac{2\pi^2}{mL^2}+\frac{\alpha L}{2}\right)\right] - \left(c_1^2\left(\frac{\pi^2}{2mL^2}+\frac{\alpha L}{2}\right)+2c_1c_2\left(\frac{-16\alpha L}{9\pi^2}\right)+c_2^2\left(\frac{2\pi^2}{mL^2}+\frac{\alpha L}{2}\right)\right)(\cancel{2}c_2)}{(c_1^2+c_2^2)^2} = 0$$

$$\Rightarrow \frac{\left[c_1^3\left(\frac{-16\alpha L}{9\pi^2}\right) + c_1^2c_2\left(\frac{2\pi^2}{mL^2}+\frac{\alpha L}{2}\right) + c_1c_2^2\left(\frac{-16\alpha L}{9\pi^2}\right) + \cancel{c_2^3\left(\frac{2\pi^2}{mL^2}+\frac{\alpha L}{2}\right)} - c_1^2c_2\left(\frac{\pi^2}{2mL^2}+\frac{\alpha L}{2}\right) - 2c_1c_2^2\left(\frac{-16\alpha L}{9\pi^2}\right) - \cancel{c_2^3\left(\frac{2\pi^2}{mL^2}+\frac{\alpha L}{2}\right)}\right]}{(c_1^2+c_2^2)^2} = 0$$

$$\Rightarrow \frac{c_1^3\left(-\frac{16\alpha L}{9\pi^2}\right) + c_1^2c_2\left(\frac{3\pi^2}{2mL^2}\right) - c_1c_2^2\left(-\frac{16\alpha L}{9\pi^2}\right)}{(c_1^2+c_2^2)^2} = 0 \longrightarrow (2)$$

$$c_1^2 + c_2^2 = 1 \longrightarrow (3)$$

(1) $\Rightarrow$ divide by c_2 on both sides

$$\frac{1}{(c_1^2+c_2^2)^2}\left[c_2^2\left(\frac{-16\alpha L}{9\pi^2}\right) + c_1c_2\left(\frac{-3\pi^2}{2mL^2}\right) - c_1^2\left(\frac{-16\alpha L}{9\pi^2}\right)\right] = 0 \longrightarrow (4)$$

(2) $\Rightarrow$ divide by c_1 on both sides

$$\frac{1}{(c_1^2+c_2^2)^2}\left[c_1^2\left(\frac{-16\alpha L}{9\pi^2}\right) + c_1c_2\left(\frac{3\pi^2}{2mL^2}\right) - c_2^2\left(\frac{-16\alpha L}{9\pi^2}\right)\right] = 0 \longrightarrow (5)$$

divide (5) by c_2^2 on both sides

$$\Rightarrow \frac{1}{(c_1^2+c_2^2)^2}\left[\left(\frac{c_1}{c_2}\right)^2\left(\frac{-16\alpha L}{9\pi^2}\right) + \left(\frac{c_1}{c_2}\right)\left(\frac{3\pi^2}{2mL^2}\right) - \left(\frac{-16\alpha L}{9\pi^2}\right)\right] = 0 .$$

$$\Rightarrow \left(\frac{c_1}{c_2}\right) = \frac{-\left(\frac{3\pi^2}{2mL^2}\right) \pm \sqrt{\frac{9\pi^4}{4m^2L^4} + 4\left(\frac{256\alpha^2L^2}{81\pi^4}\right)}}{2\left(\frac{-16\alpha L}{9\pi^2}\right)}$$

$$= -\left(\frac{3\pi^2}{2mL^2}\right)$$

$$a c_1 + b c_2 = 0$$
$$c c_1 + d c_2 = 0$$

$$\begin{vmatrix} H_{11} - E & H_{12} \\ H_{21} & H_{22} - E \end{vmatrix} = 0$$

$$E = \langle E \rangle$$

Secular determinant

$$\begin{vmatrix} H_{11}-E & H_{12} \\ H_{21} & H_{22}-E \end{vmatrix} = 0$$

$$\Rightarrow (H_{11}-E)(H_{22}-E) - H_{12}H_{21} = 0$$

$$\Rightarrow H_{11}H_{22} - E(H_{11}+H_{22}) + E^2 - H_{12}H_{21} = 0$$

$$\Rightarrow E^2 - E(H_{11}+H_{22}) + (H_{11}H_{22} - H_{12}H_{21}) = 0$$

$$H_{11} = \frac{\pi^2}{2mL^2} + \frac{\alpha L}{2}$$

$$H_{22} = \frac{2\pi^2}{mL^2} + \frac{\alpha L}{2}.$$

$$H_{12} = \frac{-16\alpha L}{9\pi^2}$$

$$H_{22} = -\frac{16\alpha L}{9\pi^2}$$

$$\cancel{\Rightarrow E = \frac{\left(\frac{5\pi^2}{mL^2} + \alpha L\right) \pm \sqrt{\left(\frac{\pi^2}{2mL^2} + \frac{\alpha L}{2}\right)\left(\frac{2\pi^2}{mL^2} + \frac{\alpha L}{2}\right) - \frac{256\alpha^2 L^2}{81\pi^4}}}{2}}$$

$$\cancel{E\left(\frac{5\pi^2}{mL^2} + \alpha L\right) \pm \sqrt{\frac{2\pi^2}{mL^2} + \frac{\alpha L}{2}}}$$

$$\Rightarrow E = \frac{\left(\frac{5\pi^2}{2mL^2} + \alpha L\right) \pm \sqrt{\left(\frac{\pi^2}{2mL^2} + \frac{\alpha L}{2} + \frac{2\pi^2}{mL^2} + \frac{\alpha L}{2}\right)^2 - 4\left(\frac{\pi^2}{2mL^2} + \frac{\alpha L}{2}\right)\left(\frac{2\pi^2}{mL^2} + \frac{\alpha L}{2}\right) + 4\left(-\frac{16\alpha L}{9\pi^2}\right)^2}}{2}$$

$$\Rightarrow E = \frac{\left(\frac{5\pi^2}{2mL^2} + \alpha L\right) \pm \sqrt{\left(\frac{2\pi^2}{mL^2} + \cancel{\frac{\alpha L}{2}} - \frac{\pi^2}{2mL^2} - \cancel{\frac{\alpha L}{2}}\right)^2 + \left(\frac{32\alpha L}{9\pi^2}\right)^2}}{2}$$

$$\Rightarrow E = \frac{\left(\frac{5\pi^2}{2mL^2} + \alpha L\right) \pm \sqrt{\left(\frac{3\pi^2}{2mL^2}\right)^2 + \left(\frac{32\alpha L}{9\pi^2}\right)^2}}{2}$$

for $\alpha = -0.1$, $m = 1$, $L = 10$.

$$\langle E \rangle = \frac{\left(\frac{5\pi^2}{2\times 100} - 1\right) \pm \sqrt{\frac{9\pi^4}{4\times 10^4} + \left(\frac{32}{9\pi^2}\right)^2}}{2}$$

$$= \frac{(-0.753) \pm \sqrt{0.022 + 0.129}}{2}$$

$$= \frac{-0.753 \pm 0.389}{2} = -0.182, -0.571$$