Particle in 3D box : x, y, z variables

$$V(x,y,z) = \begin{cases} 0 & \text{if } 0<x<L_x,\ 0<y<L_y,\ 0<z<L_z \\ \infty & \text{otherwise} \end{cases}$$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}$$

$$= -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) = -\frac{\hbar^2}{2m}\nabla^2$$

(Laplacian)

Laplace operator $\rightarrow$ $\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$

$$\nabla^2 = \nabla \cdot \nabla \cdot$$

SE $$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z) = E\psi(x,y,z)$$

4-D representations (visualize) $\longrightarrow$

Contour surface

$$\psi(x,y,z) \equiv \underbrace{\psi_{n_x n_y n_z}(x,y,z)}$$

$$E_n = E_{n_x} + E_{n_y} + E_{n_z}$$

$$= \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{l_z}\right)\frac{\hbar^2}{2m}$$

cubic box $\underline{L_x = L_y = L_z}$

Degeneracy

max possible $= \underline{6}$

Shorthand

$$\boxed{\langle E_i \rangle = \langle i|\hat{H}|i\rangle}$$

$$\int \psi_i^* \cdot \psi_i \, d\tau = 1$$

$$i \quad j \qquad = 0$$

$$\langle i|j\rangle = \int \psi_i^* \psi_j \, d\tau = \begin{cases} 1, & i=j \\ 0, & i\neq j \end{cases}$$

$$\longleftrightarrow$$

Bra ; Ket

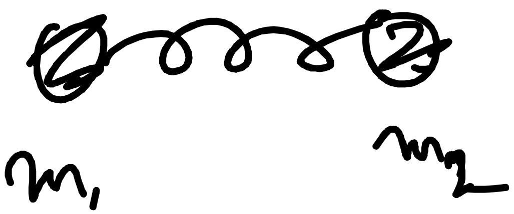
$$\langle i|E|i\rangle = E$$

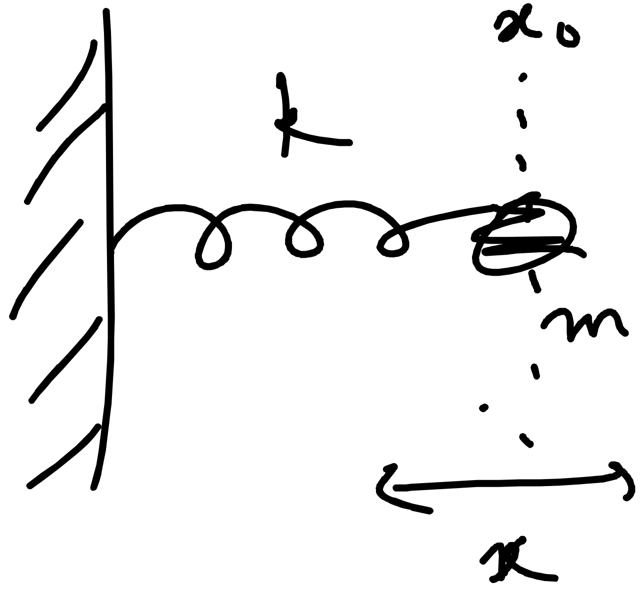
$$\langle i|i\rangle = 1$$

Complex conjugate

Complex #

Simple Harmonic Oscillator $\longleftrightarrow$ Vibrations





$$V(x) = \frac{1}{2} k x^2 = \frac{1}{2} m \omega^2 x^2$$

$$\hat{H}\psi = E\psi$$

$$\hat{H} = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \underbrace{\frac{1}{2} k x^2} \right]$$

SE $\quad -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}kx^2\psi(x) = E\psi$

Solve using "Power Series" method : solutions are quantized

zero point energy $\frac{\hbar\omega}{2}$ $\longrightarrow$ $E_n = \left(n + \frac{1}{2}\right)\hbar\omega\,, \quad n = 0, 1, 2, \ldots$

$$\omega = \sqrt{\frac{k}{m}}$$

$V(x) \longrightarrow \infty$ only when $x \to \pm\infty \Rightarrow \psi(x) \longrightarrow 0$

$$\psi_n(x) = N_n H_n(\alpha x)\exp\left(-\alpha^2 x^2/2\right)$$

$$\psi_n(x) = N_n H_n(\alpha x) \exp\left(-\frac{\alpha^2 x^2}{2}\right)$$

$$\alpha = \left(\frac{mk}{\hbar^2}\right)^{1/4} \quad \& \quad N_n = \left(\frac{\alpha}{2^n n! \, \pi^{1/2}}\right)^{1/2}$$

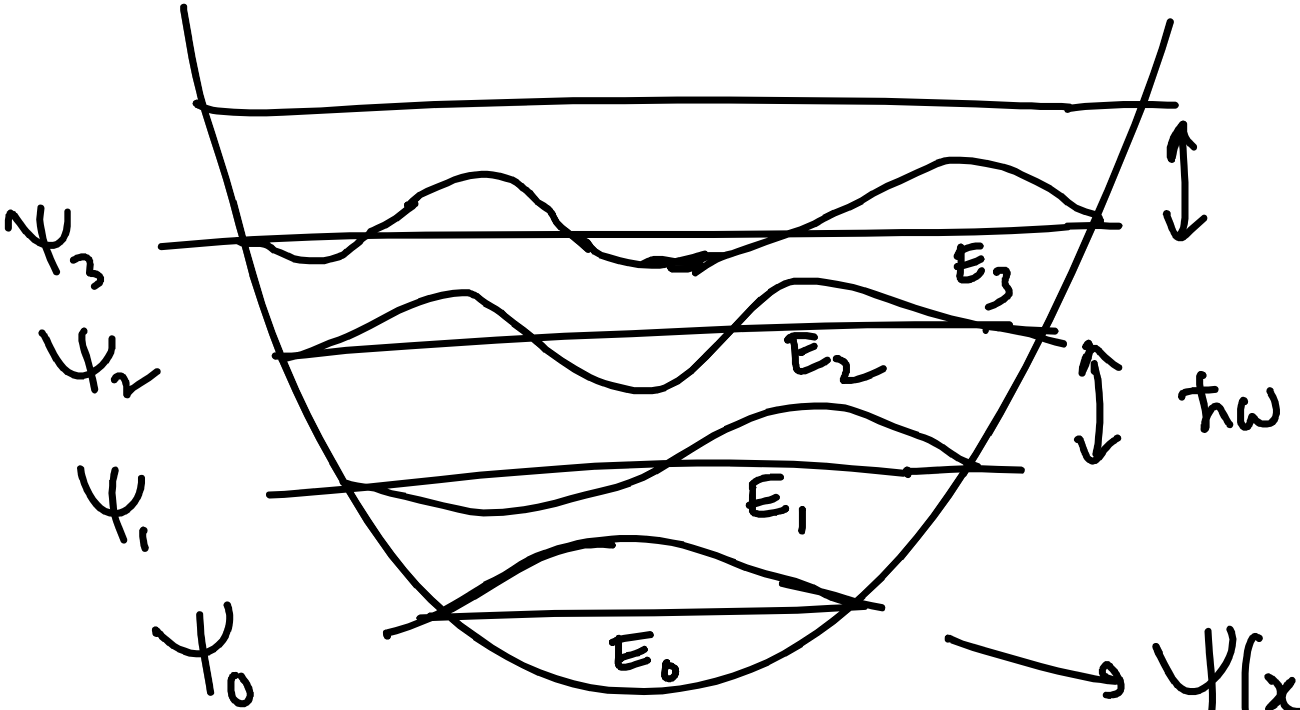
H_n is Hermite polynomials of order "n".

Say $\boxed{\alpha x = t}$ $\quad H_0(t) = 1 \; ; \; H_1(t) = 2t \; ;$

$H_2(t) = 4t^2 - 2 \; ; \; H_3(t) = 8t^3 - 12t$

$H_n(t) \longrightarrow f(t^n)$

$\exp\left(-\frac{\alpha^2 x^2}{2}\right) \rightarrow$ Gaussian f^n



$$\psi_0(x) = \left(\frac{\alpha}{\pi^{1/2}}\right)^{1/2} e^{-\alpha^2 x^2/2}$$

1-D SHO