Note Title 18-10-2016

Particle in a box

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) \quad \ldots \quad (1)$$

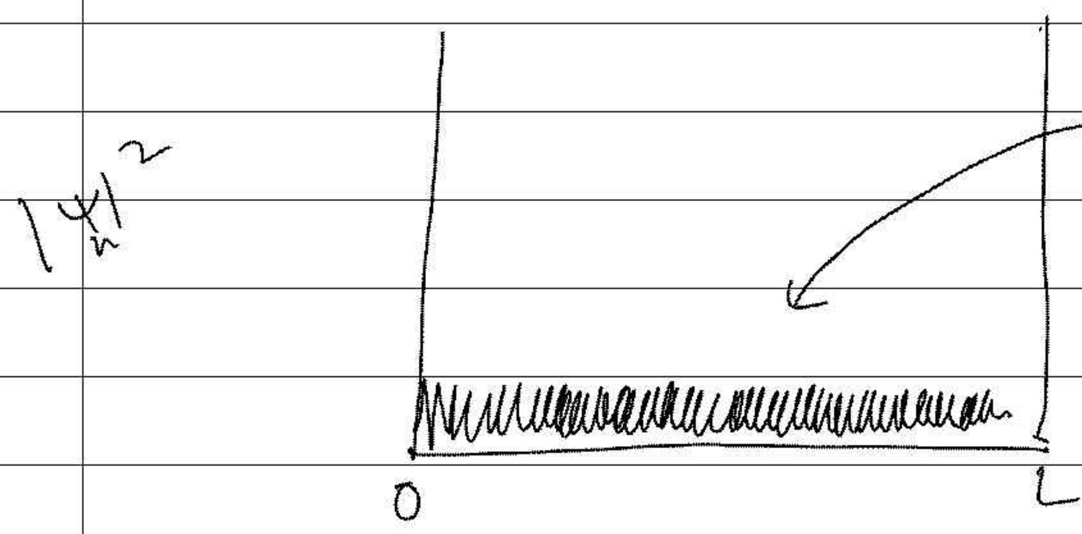
$$E_n = \frac{n^2 h^2}{8 m L^2} \quad \ldots \quad (2)$$

$$\Delta E = E_{n+1} - E_n$$

$$= \frac{(2n+1) h^2}{8 m L^2} \quad \ldots \quad (3)$$

# of nodes (wavefunction) = $\underline{\underline{n-1}}$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E_n \psi_n(x) \quad \ldots \quad (4)$$



for high 'n'
'constant probability'

high 'n'
classical and
quantum pictures
merge!

$\Leftarrow$ 'Bohr's correspondence principle'

Expectation values

$$\langle x \rangle = \int_0^L \psi^*(x)\, x\, \psi(x)\, dx$$

$$= \int_0^L \sqrt{\left(\frac{2}{L}\right)} \sin\left(\frac{n\pi x}{L}\right) x \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) dx$$

$$= \left(\frac{2}{L}\right) \int_0^L x \sin^2\left(\frac{n\pi x}{L}\right) dx$$

$$= \frac{L}{2}$$

$$\langle x^2 \rangle = \left(\frac{2}{L}\right) \int_0^L x^2 \sin^2\left(\frac{n\pi x}{L}\right) dx$$

$$= \frac{L^2}{3} - \frac{L^2}{2n^2\pi^2}$$

$\langle p_x^2 \rangle$ = . - - - -

$$\langle E \rangle = \frac{\langle p^2 \rangle}{2m}$$

$$\langle p_x^2 \rangle = 2m \langle E \rangle = 2m \cdot \frac{n^2 h^2}{8mL^2}$$

$$= \frac{n^2 h^2}{4L^2}$$

$$\langle p_x \rangle = \frac{2}{L}\int_0^L \sin\left(\frac{n\pi x}{L}\right) -i\hbar\frac{d}{dx} \sin\left(\frac{n\pi x}{L}\right) dx$$

$$= -\frac{2}{L}\left(\ \right)\int_0^L \sin\left(\frac{n\pi x}{L}\right)\cos\left(\frac{n\pi x}{L}\right) dx$$

$$= 0$$

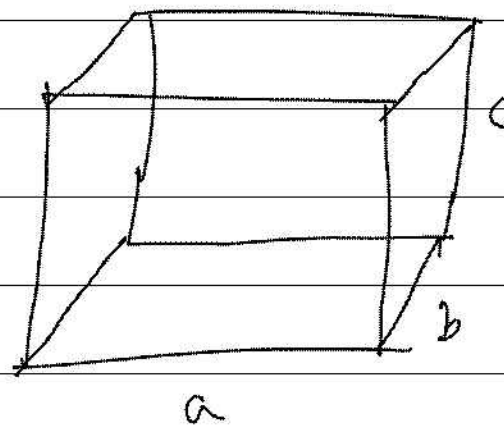
$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left[\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)\right]$$

$$= -\frac{\hbar^2}{2m}\left(-\frac{n^2\pi^2}{L^2}\right)\left[\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)\right]$$

$$= \frac{n^2\pi^2\hbar^2}{2mL^2}\psi_n(x)$$

$$= \underbrace{\frac{n^2h^2}{8mL^2}}_{E_n}\psi_n(x)$$

Particle in a 3-D box



$0 \leq x \leq a$

$0 \leq y \leq b$

$0 \leq z \leq c$

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right] = E\psi \quad \cdots \text{①}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi \, . \qquad \text{②}$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Laplacian

$$E_{n_x, n_y n_z} = E_{n_x} + E_{n_y} + E_{n_z} \quad \cdots \text{③}$$

$$E_{n_x, n_y, n_z} = \frac{n_x^2 h^2}{8ma^2} + \frac{n_y^2 h^2}{8mb^2} + \frac{n_z^2 h^2}{8mc^2}$$

$$= \frac{h^2}{8m}\left[\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right] \quad \cdots \text{④}$$

Cubic box $[a = b = c]$

$$E_{n_x, n_y, n_z} = \frac{h^2}{8ma^2}\left[n_x^2 + n_y^2 + n_z^2\right] \quad \cdots (5)$$

$n_x = 1, 2, 3 \ldots$

$n_y = 1, 2, 3 \ldots$

$n_z = 1, 2, 3, \ldots$

$n_x = 1, \quad n_y = 1, \quad n_z = 1 \qquad (1, 1, 1)$

$$E = \frac{3h^2}{8ma^2}$$

$$\left.\begin{array}{lll} n_x = 1, & n_y = 1, & n_z = 2 \\ 2 & 1 & 1 \\ 1 & 2 & 1 \end{array}\right\} \text{E same}$$

$\Downarrow$

Degenerate!

Degeneracy!				
6	321			
1		222		$\frac{12h^2}{8ma^2}$
3	3,1,1	1,3,1	1,1,3	$\frac{11h^2}{8ma^2}$
3	221	212	122	$\frac{9h^2}{8ma^2}$
3	211	121	112	$\frac{6h^2}{8ma^2}$
1		1,1,1		$\frac{3h^2}{8ma^2}$