

4. (8.4) Schrödinger eqn for free particle ( $U=0$ ) in 3D

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = -\frac{2ME}{\hbar^2} \psi$$

want to show

$$\psi = e^{i\vec{k} \cdot \vec{r}} = e^{i(k_x x + k_y y + k_z z)} \text{ satisfies S eqn}$$

$$\frac{\partial^2 \psi}{\partial x^2} = (+ik_x)^2 e^{i(k_x x + k_y y + k_z z)} = -k_x^2 e^{i\vec{k} \cdot \vec{r}} = -k_x^2 \psi$$

$$\text{similarly, } \frac{\partial^2 \psi}{\partial y^2} = -k_y^2 \psi \quad \& \quad \frac{\partial^2 \psi}{\partial z^2} = -k_z^2 \psi$$

$$\text{substitute in: } -k_x^2 \psi - k_y^2 \psi - k_z^2 \psi = -\frac{2ME}{\hbar^2} \psi$$

$$\Rightarrow -(k_x^2 + k_y^2 + k_z^2) \psi = -\frac{2ME}{\hbar^2} \psi$$

$$\text{so if } E = \frac{\hbar^2}{2M} (k_x^2 + k_y^2 + k_z^2) = \frac{\hbar^2 k^2}{2M} \text{ this is an equality}$$

interpretation of  $\vec{k}$ : for free particle,  $E = \vec{k} = \frac{p^2}{2M}$

$$\text{so } \hbar \vec{k} = \vec{p} \quad \text{or} \quad \vec{k} = \frac{\vec{p}}{\hbar}$$

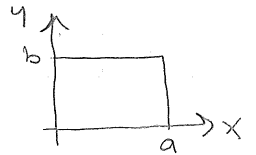
and since (de Broglie)  $p = \frac{h}{\lambda}$ ,  $k = \frac{h}{\lambda \hbar} = \frac{2\pi}{\lambda} = \text{wavenumber}$

5. (8.9) particle of mass  $M$  in 2D rigid box with sides  $a$  &  $b$

$U = 0$  for  $0 \leq x \leq a + 0 \leq y \leq b$ ;  $U = \infty$  otherwise

so  $\psi(x, y) = 0$  outside box

$$\text{inside box, } \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = -\frac{2ME}{\hbar^2} \psi$$



using separation of variables, write  $\psi(x, y) = X(x)Y(y)$

$$\Rightarrow \text{S eqn inside box becomes } X''Y + XY'' = -\frac{2ME}{\hbar^2} XY$$

$$\Rightarrow \frac{X''}{X} + \frac{Y''}{Y} = -\frac{2ME}{\hbar^2}; \text{ separates into } \frac{X''}{X} = -k_x^2, \frac{Y''}{Y} = -k_y^2, k_x^2 + k_y^2 = \frac{2ME}{\hbar^2}$$

$$\text{so } X = B_1 \sin k_x x + B_2 \cos k_x x, \quad Y = C_1 \sin k_y y + C_2 \cos k_y y$$

boundary conditions:

$$\text{at } x=0, \quad X(b) = B_2 \cos k_x x = 0 \Rightarrow B_2 = 0$$

$$\text{at } y=0, \quad Y(0) = C_2 \cos k_y y = 0 \Rightarrow C_2 = 0$$

$$\text{at } x=a, \quad X(a) = B_1 \sin k_x a = 0 \Rightarrow k_x a = n_x \pi \Rightarrow k_x = \frac{n_x \pi}{a} \quad n_x = 1, 2, 3, \dots$$

$$\text{at } y=b, \quad Y(b) = C_1 \sin k_y b = 0 \Rightarrow k_y b = n_y \pi \Rightarrow k_y = \frac{n_y \pi}{b} \quad n_y = 1, 2, 3, \dots$$

$$\text{so } \psi(x, y) = \overset{A}{B_1 C_1} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{b}\right)$$

$$\text{and } k_x^2 + k_y^2 = \frac{2ME}{\hbar^2} \Rightarrow \left(\frac{n_x \pi}{a}\right)^2 + \left(\frac{n_y \pi}{b}\right)^2 = \frac{2ME}{\hbar^2} \Rightarrow E = \frac{\hbar^2 \pi^2}{2M} \left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2}\right)$$