Three-Dimensional Problems   Lecture 24

Cartesian Coordinates

Most useful if $V(\vec{r}) = V_1(x) + V_2(y) + V_3(z)$

$\longrightarrow$ Schrödinger Equation then reads

$$\left\{\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \hat{V}_1(x)\right] + \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \hat{V}_2(y)\right] + \left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \hat{V}_3(z)\right]\right\}\psi(x,y,z) = E\,\psi(x,y,z)$$

$$\psi(x,y,z) = X(x)\,Y(y)\,Z(z)$$

$$\longrightarrow \left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \hat{V}_1(x)\right]X(x) = E_x\,X(x)$$

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dy^2} + \hat{V}_2(y)\right]Y(y) = E_y\,Y(y)$$

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dz^2} + \hat{V}_3(z)\right]Z(z) = E_z\,Z(z)$$

where $E_x + E_y + E_z = E$

The Free Particle

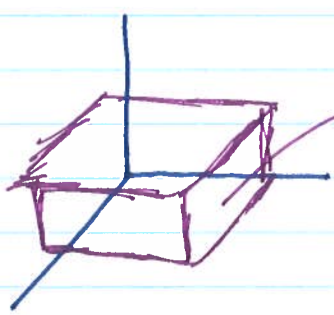
$$X(x) = Ae^{i|k_x|x} + Be^{-i|k_x|x}$$

$|k_x| = \sqrt{\dfrac{2mE_x}{\hbar^2}}$; similar solutions for $Y(y)$, $Z(z)$

$$\psi_{\vec{k}}(\vec{r}) = Ce^{i\vec{k}\cdot\vec{r}}$$

$E = \dfrac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right)$; $\vec{p} = \hbar\vec{k}$

Three Dimensional Box



$V = 0$ inside
$= \infty$ outside

Side lengths are L_1, L_2, L_3

$-\dfrac{\hbar^2}{2m}\nabla^2\psi(x,y,z) = E\psi(x,y,z)$ with B/C $\psi = 0$ at walls and beyond.

Inside the box:

$\hat{x}$: $-\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2}X(x) = E_x X(x)$ with $X(x) = 0$ for $x \leq 0$, $x \geq L_1$

$X(x) = \sqrt{\dfrac{2}{L_1}}\sin\left(\dfrac{n_x\pi}{L_1}x\right)$; $E_{n_x} = \dfrac{\hbar^2}{2m}\dfrac{\pi^2 n_x^2}{L_1^2}$

Thus,

$$\psi_{n_x,n_y,n_z}(x,y,z) = \sqrt{\frac{8}{V}} \sin\left(\frac{n_x \pi x}{L_1}\right) \sin\left(\frac{n_y \pi y}{L_2}\right) \sin\left(\frac{n_z \pi z}{L_3}\right)$$

volume $L_1 \cdot L_2 \cdot L_3$

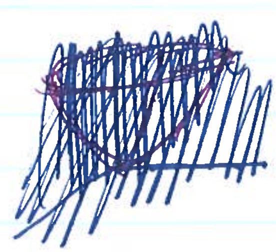
$$E_{n_x,n_y,n_z} = \frac{\hbar^2 \pi^2}{2m}\left(\frac{n_x^2}{L_1^2} + \frac{n_y^2}{L_2^2} + \frac{n_z^2}{L_3^2}\right)$$

- For the specific case of a cube with side length L, we observe degeneracy.

E/E_0	Quantum #'s (n_x, n_y, n_z)	Degeneracy
4	(2,2,2)	1
11/3	(3,1,1) (1,3,1) (1,1,3)	3
3	(2,2,1) (2,1,2) (1,2,2)	3
2	(2,1,1) (1,2,1) (1,1,2)	3
1	(1,1,1)	1
0		

Three Dimensional Harmonic Oscillator

$$V(\vec{r}) = \tfrac{1}{2}k_1 x^2 + \tfrac{1}{2}k_2 y^2 + \tfrac{1}{3}k_3 z^2$$



$$X(x):\ -\frac{\hbar^2}{2m}\frac{d^2 X(x)}{dx^2} + \frac{1}{2}k_1 x^2 X(x) = E_x X(x)$$

$$E_{n_x} = (n_x + 1/2)\hbar\omega_1 \qquad \omega_1 = \sqrt{\frac{k_1}{m}}$$

$$\alpha_1 = \left(\frac{m k_1}{\hbar^2}\right)^{1/4}$$

$$\psi_{n_x}(x) = \left(\frac{\alpha_1}{\sqrt{\pi}\, 2^{n_x} n_x!}\right)^{1/2} e^{-1/2(\alpha_1^2 x^2)} \underbrace{H_{n_x}(\alpha_1 x)}_{\text{Hermite}}$$

In all dimensions,

$$\psi_{n_x n_y n_z}(x,y,z) = \left(\frac{\alpha_1}{\sqrt{\pi}\,2^{n_x} n_x!}\right)^{1/2}\left(\frac{\alpha_2}{\sqrt{\pi}\,2^{n_y} n_y!}\right)^{1/2}\left(\frac{\alpha_3}{\sqrt{\pi}\,2^{n_z} n_z!}\right)^{1/2}$$

$$\times\, e^{-\frac{1}{2}\left[\alpha_1^2 x^2 + \alpha_2^2 y^2 + \alpha_3^2 z^2\right)} \times H_{n_x}(\alpha_1 x)\, H_{n_y}(\alpha_2 y)\, H_{n_3}(\alpha_3 z)$$

$$E = (n_x + \tfrac{1}{2})\hbar\omega_1 + (n_y + \tfrac{1}{2})\hbar\omega_2 + (n_z + \tfrac{1}{2})\hbar\omega_3$$

$$\omega_i = \sqrt{\frac{k_i}{m}}\ , \quad \alpha_i = \left(\frac{m k_i}{\hbar^2}\right)^{1/4}$$

For an isotropic oscillator with $k_1 = k_2 = k_3 = \underline{k}$

$$E_n = (n + 3/2)\hbar\omega\ ; \quad n = n_x + n_y + n_z$$

$E/\hbar\omega$	Quantum #s (n_x, n_y, n_z)	Degeneracy
7/2	(1,1,0) (1,0,1) (0,1,1) (2,0,0) (0,2,0) (0,0,2)	6
5/2	(1,0,0) (0,1,0) (0,0,1)	3
3/2	(0,0,0)	1