Three Dimensions

Schrodinger Eqn

$$i\hbar \frac{d}{dt} |\psi\rangle = \hat{H} |\psi\rangle$$

Hamiltonian

$$\hat{H} = \frac{\vec{\hat{P}} \cdot \vec{\hat{P}}}{2m} + V(\vec{R}) \qquad \text{quantum}$$

$$H = \frac{p^2}{2m} + V(\vec{r}) \qquad \text{classical}$$

$$\vec{\hat{P}} = (\hat{P}_x, \hat{P}_y, \hat{P}_z)$$

In position basis,

$$\hat{P}_x = \frac{\hbar}{i} \frac{\partial}{\partial x} \qquad \hat{P}_y = \frac{\hbar}{i} \frac{\partial}{\partial y}$$

$$\hat{P}_z = \frac{\hbar}{i} \frac{\partial}{\partial z}$$

So

$$\vec{\hat{p}} = \frac{\hbar}{i} \nabla$$

and the SE becomes

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(\vec{r})\psi$$

$$\psi(x, y, z) = \langle \vec{r} | \psi \rangle$$

<u>Normalization</u>

$$1 = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \; \psi^*(x, y, z)\, \psi(x, y, z)$$

We have a differential equation, so try separation of variables.

$$\psi(\vec{r},t) = R(\vec{r})T(t)$$

$$i\hbar\, R(\vec{r})\frac{\partial T}{\partial t} = T\left[\frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]R(\vec{r})$$

$$i\hbar\,\frac{1}{T}\frac{\partial T}{\partial t} = \frac{1}{R}\underbrace{\left[\frac{-\hbar^2}{2m}\nabla^2 R + V(\vec{r})R\right]}_{H}$$

$$= \text{constant} \equiv E$$

Note, $\hat{H}R = ER \implies E$ is the energy

$$\frac{dT}{dt} = \frac{E}{i\hbar}T$$

$$T(t) = e^{-i\frac{Et}{\hbar}}$$

$$\psi(\vec{r},t) = \phi_E(\vec{r})\, e^{-iEt/\hbar}$$

Time Independent Schrodinger Equation (TISE)

$$\frac{-\hbar^2}{2m}\nabla^2\phi_E + V(\vec{r})\,\phi_E = E\,\phi_E$$

General Solution

$$\psi(\vec{r},t) = \sum_n c_n \phi_n(\vec{r})\, e^{-iEt/\hbar}$$

Our ability to solve the TISE will depend on V

Consider potentials of the form

1. Separable $\quad V(\vec{r}) = V_x(x) + V_y(y) + V_z(z)$

2. Radial $\quad V(\vec{r}) = V(r) \qquad r = \sqrt{x^2+y^2+z^2}$

3. Cylindrical $\quad V(\vec{r}) = V(\rho) \qquad \rho = \sqrt{x^2+y^2}$

<u>Separable Potentials</u>

$$V(\vec{r}) = V_x(x) + V_y(y) + V_z(z)$$

<u>TISE</u>

$$-\frac{\hbar^2}{2m}\nabla^2\phi + V(\vec{r})\phi = E\phi$$

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_x(x)\right]\phi + \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + V_y(y)\right]\phi$$

$$+ \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + V_z(z)\right]\phi = E\phi$$

More separation of variables

$$\phi(\vec{r}) = \phi_x(x)\,\phi_y(y)\,\phi_z(z)$$

$$\underbrace{\frac{1}{\phi_x}\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V_x(x)\right]\phi_x}_{E_x} + \underbrace{\frac{1}{\phi_y}\left[\frac{-\hbar^2}{2m}\frac{d^2}{dy^2} + V_y(y)\right]\phi_y}_{E_y}$$

$$+ \underbrace{\frac{1}{\phi_z}\left[\frac{-\hbar^2}{2m}\frac{d^2}{dz^2} + V_z(z)\right]\phi_z}_{E_z} = E$$

If each depend on different variables and are equal to a constant, each must be individually constant.

$$E = E_x + E_y + E_z$$

Examples of Separable Potentials

3D Infinite Square Well (Box)

$$V(\vec{r}) = \begin{cases} 0 & x \in [0, L_x] \quad y \in [0, L_y] \\ & z \in [0, L_z] \\ \infty & \text{otherwise} \end{cases}$$

Anisotropic Harmonic Oscillator

$$V(\vec{r}) = \frac{1}{2} k_x x^2 + \frac{1}{2} k_y y^2 + \frac{1}{2} k_z z^2$$

Note if $k_x = k_y = k_z \equiv k$

Isotropic Harmonic Oscillator

$$V(\vec{r}) = \frac{1}{2} k r^2$$

What can we ask is 3D?

1. Outcomes + Probability

2. $|\psi(t)\rangle$

3. Time evolution of averages

4. Uncertainty relations

$$\sigma_x \sigma_{p_x} \geq$$

5. $P(x \in [a,b])$ Probability

$$= \int_a^b dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \; \psi^* \psi$$

6. $P(x \in [a,b],\ y \in [c,d],\ z \in [e,f])$

$$= \int_a^b dx \int_c^d dy \int_e^f dz \; \psi^* \psi$$

Ex A particle is confined to an two-dimensional infinite square well. Find ground state energy and

$$P(x \in [0, a/2], y \in [0, a/2])$$

Sln

$$V(x,y) = \begin{cases} 0 & x \in [0,a], y \in [0,a] \\ \infty & \text{otherwise} \end{cases}$$

$$\phi(x,y) = \phi_x(x)\, \phi_y(y)$$

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin k_n x$$

$$\phi_n(y) = \sqrt{\frac{2}{a}} \sin k_n y$$

$$k_n = \frac{n\pi}{a}$$

Normalization

$$1 = \int_0^a dx \int_0^a dy \; \phi^* \phi$$

$$= \underbrace{\left[\int_0^a dx \; \phi_n^*(x)\, \phi_n(x)\right]}_{= 1} \underbrace{\left[\int_0^a dy \; \phi_n^*(y)\, \phi_n(y)\right]}_{= 1}$$

$\Rightarrow$ It will often be useful to independently normalize the parts of a separable wave function

$$E = E_x + E_y = \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m}$$

$$= \frac{\hbar^2}{2m}\left(\frac{n_x^2 \pi^2}{a^2} + \frac{n_y^2 \pi^2}{a^2}\right)$$

$$= \frac{\hbar^2 \pi^2}{2ma^2}\left(n_x^2 + n_y^2\right) \qquad \begin{array}{l} n_x > 0 \\ n_y > 0 \end{array}$$

Ground State $n_x = 1$ $n_y = 1$

$$E_0 = E_{n_x=1} + E_{n_y=1}$$

$$= \frac{2\hbar^2\pi^2}{2ma^2} = \frac{\hbar^2\pi^2}{ma^2}$$

$$P\left(x \in [0, a/2],\ y \in [0, a/2]\right)$$

$$= \int_0^{a/2} dx \int_0^{a/2} dy\ \phi_0^* \phi_0$$

$$= \int_0^{a/2} dx \int_0^{a/2} dy \left(\sqrt{\frac{2}{a}} \sin k_1 x\right)^2 \left(\sqrt{\frac{2}{a}} \sin k_1 y\right)^2$$

$$= \underbrace{\left[\int_0^{a/2} dx \left(\sqrt{\frac{2}{a}} \sin k_1 x\right)^2\right]}_{= \frac{1}{2}} \underbrace{\left[\int_0^{a/2} dy \left(\sqrt{\frac{2}{a}} \sin k_1 y\right)^2\right]}_{= \frac{1}{2}}$$

$= 1/4$ which it had to be.