

3 topics

- a) QM in 3-D focus on atomic systems
use series sol's of SHO
- b) Exploit & understand symmetry in QM. Focus on rotational systems
ladder structure for angular momentum
new QM element: spin
addition of angular momentum uses heavily tensor product construction
apply to atomic systems
- c) Approx. methods: dimensional analysis, uncertainty principle, variational method, & perturbation theory

$D=3$

$$H = \frac{\vec{p}^2}{2m} + V(\vec{x})$$

$$\vec{p} = -i\hbar \vec{\nabla} = -i\hbar \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) = (p_x, p_y, p_z) = (p_1, p_2, p_3)$$

$$\vec{x} = (x, y, z) = \vec{r} = (x_1, x_2, x_3)$$

$$[x_i, p_j] = i\hbar \delta_{ij}$$

$$\text{energy eigenstates: } H \Phi_E(\vec{x}) = E \Phi_E(\vec{x})$$

$$\Psi_E(t, \vec{x}) = e^{-iEt/\hbar} \Phi_E(\vec{x})$$

$$\sum_E C_E \Phi_E(\vec{x}) \longrightarrow \sum_E C_E e^{-i\frac{E}{\hbar}t} \Phi_E(\vec{x})$$

normalizable:

$$\underbrace{\int dx \int dy \int dz}_{\int d^3x \rightarrow \int d^3r} |\Phi_E(\vec{x})|^2 = \text{finite}$$

einstein summation convention

$$\vec{x} \cdot \vec{x} = \sum_i^3 x_i x_i$$

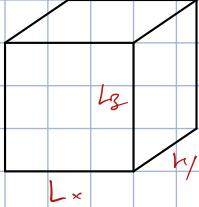
$$(\vec{x} \cdot \vec{x}, \vec{p} \cdot \vec{p}) = \sum_i x_i x_i \sum_j p_j p_j \stackrel{\text{einstein}}{\equiv} x_i x_i p_j p_j \neq x_i x_i p_i p_i$$

in $D=3$, SE

- ① is a PDE vs ODE
- ② requires using a coord. system adapted to symmetry of problem
 $(x, y, z) \rightarrow (r, \theta, \phi)$
- ③ soln's involve new, special f^k 's

Bessel f^k's, Laguerre poly, spherical harmonics

Particle in a box



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

$$-\frac{\hbar^2}{2m} \vec{\nabla} \cdot \vec{\nabla} \phi_E(\vec{x}) = E \phi_E(\vec{x})$$

$$\begin{aligned} \phi_E(\text{side of box}) &= 0 \\ \phi_E(0, y, z) &= \phi_E(L_x, y, z) = 0 \\ \dots & \dots \\ \phi_E(L_x, L_y, z) &= 0 \end{aligned}$$

$$\phi_E(\vec{x}) = \phi_1(x) \phi_2(y) \phi_3(z)$$

$$-\frac{\hbar^2}{2m} \left(\underbrace{\frac{\partial^2}{\partial x^2}}_{\phi_1(x)} + \underbrace{\frac{\partial^2}{\partial y^2}}_{\phi_2(y)} + \underbrace{\frac{\partial^2}{\partial z^2}}_{\phi_3(z)} \right) \phi_1(x) \phi_2(y) \phi_3(z) = E \phi_1(x) \phi_2(y) \phi_3(z)$$

$$\overline{\phi_1(x) \phi_2(y) \phi_3(z)}$$

$$-\frac{\hbar^2}{2m} \left(\underbrace{\frac{1}{\phi_1(x)} \frac{\partial^2}{\partial x^2}}_{f^k \text{ of } x} + \underbrace{\frac{1}{\phi_2(y)} \frac{\partial^2}{\partial y^2}}_{f^k \text{ of } y} + \underbrace{\frac{1}{\phi_3(z)} \frac{\partial^2}{\partial z^2}}_{f^k \text{ of } z} \right) = E$$

constant

$$-\frac{\hbar^2}{2m} \frac{1}{\phi_1} \cdot \frac{d^2\phi_1}{dx^2} = E_1$$

$$-\frac{\hbar^2}{2m} \frac{1}{\phi_2} \cdot \frac{d^2\phi_2}{dy^2} = E_2$$

$$-\frac{\hbar^2}{2m} \frac{1}{\phi_3} \cdot \frac{d^2\phi_3}{dz^2} = E_3$$

$$\phi_1(x) = C_1 \sin\left(\frac{n_x \pi x}{L}\right) \quad n_x = 1, 2, 3, \dots$$

$$\phi_2(y) = C_2 \sin\left(\frac{n_y \pi y}{L}\right) \quad n_y = 1, 2, 3, \dots$$

$$\phi_3(z) = C_3 \sin\left(\frac{n_z \pi z}{L}\right) \quad n_z = 1, 2, 3, \dots$$

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

$$\phi_E(\vec{x}) = \phi_{n_x}(x) \cdot \phi_{n_y}(y) \cdot \phi_{n_z}(z)$$

$$\chi(\vec{x}) = \sum_{n_x n_y n_z} C_{n_x n_y n_z} \phi_E^{n_x n_y n_z}(\vec{x})$$