

Basics

Linear superposition of eigenstates:

$$|\psi, t\rangle = \sum_i c_i(t) |u_i\rangle$$

$$\Psi(\vec{r}, t) = \sum_i c_i(t) u_i(\vec{r})$$

Probability of getting result:

$$P(A_i) = |c_i(t)|^2$$

Identity operator in a basis, i :

$$\hat{I} = \sum_i |i\rangle \langle i|$$

Expectation value of observable:

$$\langle \hat{A} \rangle = \langle \psi, t | \hat{A} | \psi, t \rangle$$

Uncertainty relations:

$$\Delta \hat{A}_t \equiv (\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2)^{\frac{1}{2}}$$

$$\Delta \hat{A}_t \Delta \hat{B}_t \geq \frac{1}{2} | \langle [\hat{A}, \hat{B}] \rangle |$$

Schrödinger equation:

$$\hat{H}\psi = i\hbar \frac{\partial}{\partial t} \psi$$

Braket \leftrightarrow Function notation

$$\langle \psi | \phi \rangle = \int \psi^* \phi \, dx$$

Angular Momentum & Spin

Angular Momentum Operators:

$$\hat{L}^2 |l, m\rangle = l(l+1)\hbar^2 |l, m\rangle$$

$$\hat{L}_z^2 |l, m\rangle = m\hbar |l, m\rangle$$

Spherical Polars:

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \left(\frac{\partial^2}{\partial \phi^2} \right) \right]$$

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$$

Quantum Numbers

$$l = 0, 1, 2, 3 \dots n$$

$$m_l = l, l-1, \dots, -l$$

$$m_l \text{ degeneracy} = (2l+1)$$

$$s = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$$

$$m_s = s, s-1, \dots, -s$$

$$m_s \text{ degeneracy} = (2s+1)$$

$$j = l+s, l+s-1, \dots, |l-s+1|, |l-s|$$

Russel Saunders notation labels terms $n^{(2s+1)}l_j$

Total angular momentum:

$$\hat{J} \equiv \hat{L} + \hat{S}$$

$$[\hat{J}_i, \hat{J}_j] = i\hbar \varepsilon_{ijk} \hat{J}_k$$

coupled basis $|l, m_l, s, m_s\rangle$

uncoupled basis $|l, s, j, m_j\rangle$

Matrix Elements:

$$\langle s, m' | \hat{S}_z | s, m \rangle = m\hbar \delta_{m', m}$$

$$\langle s, m' | \hat{S}_{\pm} | s, m \rangle = \sqrt{s(s+1) - m(m \pm 1)} \hbar \delta_{m', m \pm 1}$$

Perturbation Theory

Non Degenerate (Time independent):

$$E_n^{(1)} = \langle n^{(0)} | \hat{H}' | n^{(0)} \rangle \equiv H'_{nn}$$

$$|n^{(1)}\rangle = \sum_{k \neq n} \frac{H'_{kn}}{(E_n^{(0)} - E_k^{(0)})} |k^{(0)}\rangle$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{|H'_{mn}|^2}{(E_n^{(0)} - E_m^{(0)})}$$

Degenerate:

$$\sum_{n=1}^g (H'_{kn} - E^{(1)} \delta_{kn}) b_n = 0, \quad k = 1, \dots, g$$

$$\det(H'_{kn} - E^{(1)} \delta_{kn}) = 0$$

Atoms

General multi-electron Hamiltonian:

$$\hat{H} = \sum_{i=1}^N \left\{ \frac{\hat{p}_i^2}{2m} - \frac{Ze^2}{(4\pi\epsilon_0)r_i} \right\} + \sum_{i>j=1}^N \frac{e^2}{(4\pi\epsilon_0)r_{ij}}$$

Hydrogen fine structure:

$$\Delta_{nj} = E_n^{(0)} \frac{(Z\alpha)^2}{n^2} \left(\frac{n}{j + \frac{1}{2}} - \frac{3}{4} \right)$$

2-Electron wavefunctions:

$$\chi_{1,1} = \alpha_1 \alpha_2$$

$$\chi_{1,0} = \frac{1}{\sqrt{2}} \{ \alpha_1 \beta_2 + \beta_1 \alpha_2 \}$$

$$\chi_{1,-1} = \beta_1 \beta_2$$

$$\chi_{0,0} = \frac{1}{\sqrt{2}} \{ \alpha_1 \beta_2 - \beta_1 \alpha_2 \}$$