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

$$\langle\psi|\phi\rangle = \int \psi^*\phi\,\mathrm{d}x$$

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:

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

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

Quantum Numbers

$$l = 0,1,2,3...n$$

$$m_l = l, l-1, ..., -l$$

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

$$s = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, ...$$

$$m_s = s, s-1, ..., -s$$

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

$$j = l+s, l+s-1, ..., |l-s+1|, |l-s|$$

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

Total angular momentum:

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

Matrix Elements:

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

$$\langle s,m'|\hat{S_\pm}|s,m\rangle = \sqrt{s(s+1)-m(m\pm1)}\hbar\delta_{m',m\pm1}$$

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:

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

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

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:

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

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

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

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