Short summary week 1

One-electron (H-like) system:

Bohr: Classical orbitals, quantized size of orbital angular momentum

$$r_n = a_0 \frac{n^2}{Z}, \quad a_0 = 0{,}53 \text{ Å}.$$

$$v_n = \alpha \cdot c \cdot \frac{Z}{n}, \quad \alpha \approx \frac{1}{137}.$$

$$E_n = -R \cdot \frac{Z^2}{n^2}, \quad R = 10766 \text{ cm}^{-1} \text{ for H}$$

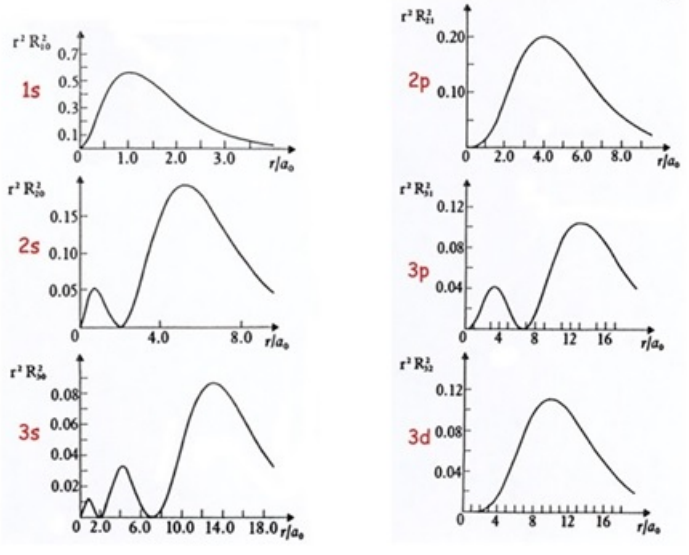
$$\frac{1}{\lambda} = R \cdot Z^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

QM:

Same energies as Bohr, probability distribution of electron position

$$\Psi_{\ell,m}(r,\theta,\varphi) = R_{n,\ell}(r) Y_{\ell,m}(\theta,\varphi)$$

$$R(\rho) = \rho^{\ell} \cdot e^{-\rho} \cdot c_0 \cdot \left(1 + \sum_{k=1}^{n-\ell-1} \frac{c_k}{c_0} \cdot \rho^k\right), \quad \rho = \frac{Z}{n a_0} \cdot r$$



General Angular Momentum Operators.

Orbital, spin, nuclear, sums of momenta....

Defined from the commutator relations derived for the orbital case.

$$\left[\hat{J}_x, \hat{J}_y\right] = i\hbar\hat{J}_z, \quad \left[\hat{J}_y, \hat{J}_z\right] = i\hbar\hat{J}_x, \quad \left[\hat{J}_z, \hat{J}_x\right] = i\hbar\hat{J}_y.$$

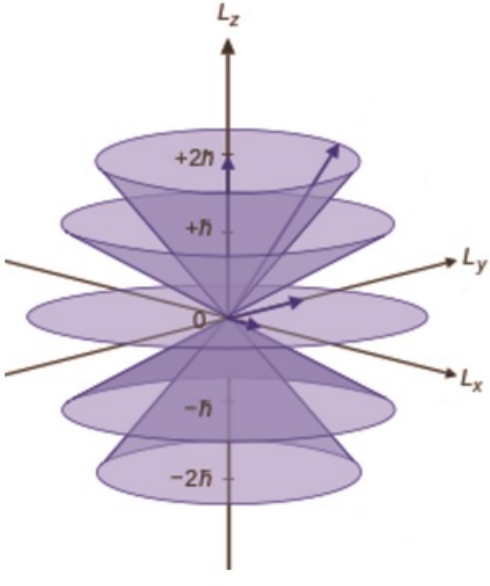
$$\left[\hat{J}^2, \hat{J}_i\right] = 0, i = x, y, z$$

Orbital angular momentum

$$\hat{L}^2 Y_{\ell,m_\ell}(\theta,\varphi) = \hbar^2 \ell(\ell+1) \cdot Y_{\ell,m_\ell}(\theta,\varphi)$$

$$\hat{L}_z Y_{\ell,m_\ell}(\theta,\varphi) = m \cdot \hbar \cdot Y_{\ell,m_\ell}(\theta,\varphi).$$

ℓ integer and $m_\ell = -\ell, -\ell+1, ..., \ell-1, \ell$



Spin angular momentum

$$\hat{S}^2 \chi_{j,m_s} = \hbar^2 s(s+1) \cdot \chi_{j,m_s}$$

$$\hat{S}_z \chi_{j,m_s} = m_s \cdot \hbar \cdot \chi_{j,m_s}.$$

For one electron:

$s = 1/2, m_s = \pm\ 1/2$

Coupling of two angular momenta

Let χ_{j_i,m_i} be eigenfunctions of $\hat{j}_i^2$ and $\hat{j}_{iz}$ for $i=1$ and 2, and $\hat{J}=\hat{j}_1+\hat{j}_2$.

$$J=\left|j_1-j_2\right|,\left|j_1-j_2\right|+1,\ldots\ldots,j_1+j_2$$

The eigenfunctions of $\hat{J}^2$ and $\hat{J}_z$ are then obtained through:

$$\psi_{j_1,j_2,J,M}=\sum_{m_1}C(j_1,m_1,j_2,M-m_1:J,M)\cdot\chi_{j_1,m_1}\cdot\chi_{j_2,M-m_1}.$$

where the *C*-factors are called Clebsch-Gordan coefficients.

$\psi_{j_1,j_2,J,M}$ is an eigenfunction of $\hat{j}_1^2$, $\hat{j}_2^2$, $\hat{J}$, and $\hat{J}_z$

Clebsch-Gordan coefficients, both in exact analytical form and also numerically, may be found in tables or obtained from the net, e.g at:
http://personal.ph.surrey.ac.uk/~phs3ps/cgjava.html