86(11): Exchange Integral in Helium

In note 86(10) the Coulomb integral for He was evaluated for the repulsion between two 1s electrons. The same type of analysis could be carried out for (ns, n's) interactions (e.g. 1s to 2s electron - electron repulsion), but when the wavefunction has an angular dependence, e.g. for 2s to 2p electron to electron interaction, there are more terms in the expansion of $1/r_{12}$.

The exchange integral occurs when configurations are considered in which one electron occupies $n_1 l_1 m_{l1}$ and the other a different orbital $n_2 l_2 m_{l2}$. The unperturbed wavefunction is degenerate:

$$\psi_0 = \psi_{n_1 l_1 m_{l1}}(\underline{r}_1)\psi_{n_2 l_2 m_{l2}}(\underline{r}_2) = \psi_{n_1 l_1 m_{l1}}(\underline{r}_2)\psi_{n_2 l_2 m_{l2}}(\underline{r}_1) \quad -(1)$$

i.e.:

$$\psi_0 = a(1)b(2) = a(2)b(1) \quad -(2)$$

The unperturbed energy is $E_a + E_b$. The perturbed energy is calculated using the degenerate form of first order perturbation theory. The <u>exchange integral</u> is then defined as:

$$K = \frac{e^2}{4\pi\epsilon_0}\int (a(1)b(1))\frac{1}{r_{12}}(a(2)b(2))\, d\tau_1 d\tau_2 \quad -(3)$$

The exchange ...

2) but the corresponding wave-functions are:

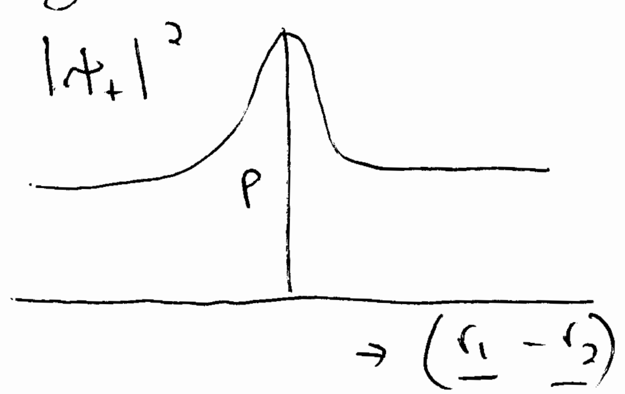
$$\psi_{\pm}(1,2) = \left(\frac{1}{2}\right)^{1/2}\left(a(1)b(2) \pm b(1)a(2)\right) \quad -(4)$$

$$= \left(\frac{1}{2}\right)^{1/2}\left(\psi_{n_1 l_1 m_{l1}}(\underline{r}_1)\psi_{n_2 l_2 m_{l2}}(\underline{r}_2) \pm \psi_{n_2 l_2 m_{l2}}(\underline{r}_1)\psi_{n_1 l_1 m_{l1}}(\underline{r}_2)\right) \quad -(5)$$

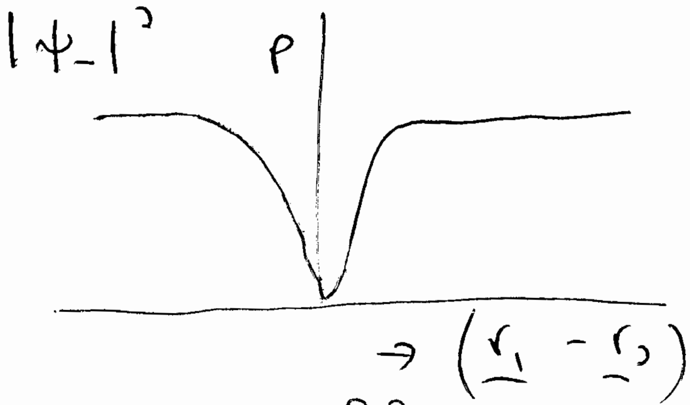
where the individual wave-functions are <u>hydrogen-like</u>. So radiative corrections can be applied to these wavefunctions straightforwardly. The energy levels are:

$$E = E_a + E_b + J \pm K, \quad -(6)$$

so the electron-electron repulsion separates the degenerate energy levels by $2K$.



<u>Fermi Heap</u>



<u>Fermi Hole</u>

So we may now compute radiative corrections to Fermi Hole and Fermi Heap theory.