Lecture 18 Highlights

We continued to discuss the unperturbed eigenenergies and eigenfunctions of the Helium atom. Note that the anti-symmetric space wavefunction:

$$\Psi_A^0(1,2) = \frac{1}{\sqrt{2}}\left(\psi_a(1)\psi_b(2) - \psi_a(2)\psi_b(1)\right)$$

has a peculiar property. If both particles are in the same single-particle state (lists of quantum numbers $a = b$), then the wavefunction is zero. This remarkable property is shared by much more sophisticated multi-identical-particle Fermionic wavefunctions and is called the Pauli Exclusion Principle. It says that no two Fermions in a multi-identical-particle composite Fermion (overall anti-symmetric) wavefunction can occupy the same exact single-particle quantum state.

This principle now constrains the types of He atom wavefunctions we can write down. They can only be of the form:

$$\Psi^0(1,2) \sim \psi_{Symmetric}(1,2)\chi_{Anti-Symmetric}(1,2),$$

or

$$\Psi^0(1,2) \sim \psi_{Anti-Symmetric}(1,2)\chi_{Symmetric}(1,2),$$

where ψ represents the space-part of the wavefunction and χ represents the spin part of the wavefunction (here it is assumed that the He-atom wavefunction can be factorized like this). A symmetric space wavefunction that respects indistinguishability can be written in this way, for example:

$$\Psi_S^0(1,2) = \frac{1}{\sqrt{2}}\left(\psi_a(1)\psi_b(2) + \psi_a(2)\psi_b(1)\right)$$

But what about symmetric and anti-symmetric spin wavefunctions χ? It turns out that we already have them, at least for the combination of two spin-1/2 particles. The spin triplet states ($|11\rangle, |10\rangle, |1-1\rangle$) are symmetric under permutation (also called exchange) of the two particles, while the spin singlet state ($|00\rangle$) is antisymmetric. Fantastic!

We now have 4 candidate He atom wavefunctions:

$$\Psi_{He}^0(1,2) = \frac{1}{\sqrt{2}}\left(\psi_a(1)\psi_b(2) - \psi_a(2)\psi_b(1)\right)|11\rangle$$

or

$$\Psi_{He}^0(1,2) = \frac{1}{\sqrt{2}}\left(\psi_a(1)\psi_b(2) - \psi_a(2)\psi_b(1)\right)|10\rangle$$

or

$$\Psi_{He}^0(1,2) = \frac{1}{\sqrt{2}}\left(\psi_a(1)\psi_b(2) - \psi_a(2)\psi_b(1)\right)|1-1\rangle$$

or

$$\Psi_{He}^0(1,2) = \frac{1}{\sqrt{2}}\left(\psi_a(1)\psi_b(2) + \psi_a(2)\psi_b(1)\right)|00\rangle$$

We then took a detour into 1D infinite square wells again to discuss the correlations built in to multi-particle states by the anti-symmetry constraint. Consider a

1D infinite square well between x = 0 and x = a. Put two non-interacting but identical particles into the well, and ignore the spin part of the wavefunction for now. Suppose they are identical Fermions. Both particles cannot occupy the (n=1) ground state of the well, due to the Pauli exclusion principle. One can write down two possible ground state wavefunctions as follows. The first is anti-symmetric in space and puts one particle in the n=1 ground state and the other in the n=2 first excited state. Notice that it does this in a way that respects the indistinguishability of the two particles:

$$\psi_{12}^{A}(1,2) = \frac{\sqrt{2}}{a}\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) - \sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right],$$

where x_1 refers to the x-coordinate of particle 1, and x_2 to that of particle 2. The second wavefunction is symmetric in space, and also puts the particles into different states:

$$\psi_{12}^{S}(1,2) = \frac{\sqrt{2}}{a}\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) + \sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]$$

Both of these wavefunctions have the same un-perturbed energy of $E_{12}^{A} = E_{12}^{S} = \frac{5\pi^2\hbar^2}{2ma^2}$.

From the plots of $\psi_{12}^{S}(x_1, x_2)$ and $\psi_{12}^{A}(x_1, x_2)$ posted on the web site, one can see that the probability of finding the particles at the same location $x_1 = x_2$ is significantly higher in the symmetric vs. the antisymmetric wavefunctions. This means that when a repulsive perturbing potential is turned on (like a Coulomb potential), it will leave the anti-symmetric space wavefunction at a lower energy than the symmetric space wavefunction. This energy difference is called the “exchange energy” or “exchange splitting.”