Physics 661 **Homework 6** **Due Tuesday, March 4, 2025**

Reading assignment: sections 18.2-18.4, 20.1, and 20.2 of the text.

Problem 1. Compute the direct and exchange integrals $I_{2,0,0}$ and $J_{2,0,0}$, as defined in eqs. (18.3.4) and (18.3.5), for the $(1s)(2s)$ excited states of the helium atom. Note that from eqs. (11.1.42) and (11.1.43), the one-electron wavefunctions with $Z = 2$ are $\phi_{1,0,0}(r) = e^{-2r/a_0}\sqrt{8/\pi a_0^3}$ and $\phi_{2,0,0}(r) = e^{-r/a_0}(1 - r/a_0)/\sqrt{\pi a_0^3}$. Check that $0 < J_{2,0,0} < I_{2,0,0}$. Use these results to estimate the energies of the ${}^1S_0$ and ${}^3S_1$ states, and their energy splitting $\Delta E = 2e^2 J_{2,0,0}$, at first order in perturbation theory. Compare to the results quoted in Figure 18.3.1.

Hints: you should find

$$E = \left(-5 + \frac{N_{\text{direct}}}{81} \pm \frac{N_{\text{exchange}}}{729}\right)\frac{e^2}{2a_0},$$

where N_{direct} and N_{exchange} are each certain integers between 60 and 70, which you will discover. To set up the integrals, follow the example of the method used in eqs. (15.3.8)-(15.3.18). Before integrating, you are encouraged to change to dimensionless variables $u = r_1/a_0$ and $v = r_2/a_0$. The result for ΔE is far from a triumph, as you should find that it is numerically about a factor of 3 larger than the experimental value. The important things are that it has the correct sign, and that it is much smaller than the energy shift from the direct integral.

Problem 2. Consider three **identical** spin-1/2 fermions bound in a 3-d isotropic harmonic oscillator potential characterized by frequency ω. The fermions do not interact with each other. You may want to review the results found in section 10.5 of the class text for a single particle in a 3-d isotropic harmonic oscillator, in particular, eq. (10.5.23), and note that in that equation l is the orbital angular momentum quantum number, and $k = 0, 1, 2, 3, \ldots$ is another integer.

(a) Use the Pauli exclusion principle to find the energies and the degeneracies of the ground state energy level and the first excited energy level. Give the spectroscopic term notation ${}^{2S+1}L_J$ for the allowed states in each case. [Hint: you may find it good to think of combining two of the fermions first, then add the third, somewhat similar to how you might treat Lithium in the atomic shell model. For the ground state energy level, you should find that the degeneracy is greater than 5 and less than 10, and consists of two distinct spectroscopic terms. For the first excited state energy level, you should find that the degeneracy is greater than 30 and less than 50, and consists of 11 spectroscopic terms, some of which are repeated.]

(b) If a spin-orbit perturbation Hamiltonian is added, $W = a\vec{L}\cdot\vec{S}$, where $\vec{L}$ and $\vec{S}$ are the total orbital and spin angular momenta of the fermions, then what are the energies and spectroscopic term notations of the lowest three energy eigenstates states if a is positive? Answer the same question if a is negative. [Hint: to avoid excess work, think carefully about what the "lowest three" energy eigenstates are after the perturbation is included.]

(c) Now suppose that in addition to the perturbation W, there is a much weaker perturbation $W' = bL_z$. Use degenerate perturbation theory to find the energy splitting of the lowest level you found in part (b), by finding the the matrix representation for W' and finding its eigenvalues. The cases of positive a and negative a are different, so treat them separately. [Hint: you may find eqs. (12.3.16)-(12.3.21) useful. Note that these give the total angular momentum orthobasis kets (on the left) in terms of the product basis kets (on the right).]

Problem 3. For each of the cases of Calcium ($Z = 20$), Scandium ($Z = 21$), Titanium ($Z = 22$), Nickel ($Z = 28$), Germanium ($Z = 32$) and Selenium ($Z = 34$), use the shell model to find the electronic configuration. Recall that the shell filling order is:

$$1s, \quad 2s, \quad 2p, \quad 3s, \quad 3p, \quad \begin{pmatrix} 4s \\ 3d \end{pmatrix}, \quad 4p, \quad \begin{pmatrix} 5s \\ 4d \end{pmatrix}, \quad 5p, \quad \begin{pmatrix} 6s \\ 4f \\ 5d \end{pmatrix}, \quad 6p, \quad \begin{pmatrix} 7s \\ 5f \\ 6d \end{pmatrix}$$

You should assume that the $4s$ shell fills before the $3d$ shell; although this is not always the case, it is true for these examples. Assume the Russell-Saunders approximation is good to find the spectroscopic term notation for all of the states with the electronic configuration you found, and apply Hund's rules to select the ground state in each case. (Note: it is possible to look up the answers, of course. Show your reasoning and process, not just the answer.)