

Reading assignment: sections 16.2-16.4, 17.1, 17.2, and 18.1 of the text.

Problem 1. Two **identical** spin-1/2 fermions are confined to a cubic box of side L . The fermions do not have any Hamiltonian interaction with each other. The sides and exterior of the box have infinite potential. Put one corner of the box at the origin.

(a) For a **one-particle** state, the energy eigenstate wavefunctions are

$$\psi_{n_x, n_y, n_z}(x, y, z) = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right). \quad (1)$$

What are the corresponding **one-particle** energies?

(b) In the remainder of this problem, we will consider two-particle energy eigenstates, organized in terms of the total spin, $S = 0$ or $S = 1$. But notice that in this problem we have cubic symmetry, rather than spherical symmetry, so we *cannot* organize energy eigenstates in terms of orbital angular momentum! This is because the potential, and therefore the Hamiltonian, does not commute with L^2 or L_z . Instead, we want to consider states that are either of the form

$$\chi_{S, m_S} \psi_A(x_1, y_1, z_1) \psi_A(x_2, y_2, z_2), \quad (2)$$

when the two particles have the same spatial wavefunction ψ_A , or

$$\chi_{S, m_S} \frac{1}{\sqrt{2}} [\psi_A(x_1, y_1, z_1) \psi_B(x_2, y_2, z_2) \pm \psi_B(x_1, y_1, z_1) \psi_A(x_2, y_2, z_2)], \quad (3)$$

if they have different spatial wavefunctions, where χ_{S, m_S} is the spin ket for $S = 0$ or $S = 1$, and A or B represents (n_x, n_y, n_z) for a given 1-particle wavefunction. Find the energy eigenvalues and the corresponding degeneracies for the lowest three energy levels of the two-fermion system.

[Hints: the one-particle energies simply add to give the two-particle energies, since we are not including any interactions between the particles. Also, recall that for $S = 0$, the spatial wavefunction is symmetric under interchange of the labels 1 and 2, while for $S = 1$, the spatial wavefunction must be anti-symmetric under interchange of the labels 1 and 2. You should find that the total number of states in the lowest three energy levels is a number greater than 35.]

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 9.5 of the class text for a single particle in a 3-d isotropic harmonic oscillator, in particular, eq. (9.5.24), and note that in that equation l is the orbital angular momentum quantum number, and $k = 0, 1, 2, 3, \dots$ 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 if a is positive? What 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 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. (11.3.16)-(11.3.21) 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.)