Quantum Physics III (8.06) — Spring 2016

Assignment 8

Readings

- Griffiths, Sections 5.1-5.3.
- Optional: Shankar, Ch. 10; Cohen-Tannoudji, Ch. XIV

Problem Set 8

1. The "Exchange Force" (15 points)

(a) Spatial wavefunctions: Let $|\alpha\rangle$, $|\beta\rangle$ be two orthogonal single-particle states for particles in 1-d. with $\psi_{\alpha}(x) = \langle x | \alpha \rangle$ and $\psi_{\beta}(x) = \langle x | \beta \rangle$. Define the distinguishable, symmetric and antisymmetric states to be

$$|\Psi_D\rangle \equiv |\alpha\rangle \otimes |\beta\rangle \tag{1}$$

$$|\Psi_S\rangle \equiv \frac{|\alpha\rangle \otimes |\beta\rangle + |\beta\rangle \otimes |\alpha\rangle}{\sqrt{2}} \tag{2}$$

$$|\Psi_A\rangle \equiv \frac{|\alpha\rangle \otimes |\beta\rangle - |\beta\rangle \otimes |\alpha\rangle}{\sqrt{2}} \tag{3}$$

Using tensor product notation, the position of the first (resp. second) particle is given by the operator $\hat{x}_1 \equiv \hat{x} \otimes I$ (resp. $\hat{x}_2 \equiv I \otimes \hat{x}$). Define $D_D = \langle \Psi_D | (\hat{x}_1 - \hat{x}_2)^2 | \Psi_D \rangle$, $D_s = \langle \Psi_S | (\hat{x}_1 - \hat{x}_2)^2 | \Psi_S \rangle$ and $D_A = \langle \Psi_A | (\hat{x}_1 - \hat{x}_2)^2 | \Psi_A \rangle$. Calculate $D_S - D_D$ and $D_A - D_D$. Give a brief intuitive explanation of the signs of your answers.

(b) Spins: Now consider two spin-s particles. For a single particle, let $|s, m_a\rangle$ be the $\hbar m_a$ eigenstate of the S_z operator. Suppose $m_a \neq m_b$. Define

$$|\Psi_D\rangle \equiv |s, m_a\rangle \otimes |s, m_b\rangle \qquad D_D \equiv \langle \Psi_D | (\vec{S}_1 - \vec{S}_2)^2 | \Psi_D\rangle \quad (4)$$

$$|\Psi_S\rangle \equiv \frac{|s, m_a\rangle \otimes |s, m_b\rangle + |s, m_b\rangle \otimes |s, m_a\rangle}{\sqrt{2}} \qquad D_S \equiv \langle \Psi_S | (\vec{S}_1 - \vec{S}_2)^2 | \Psi_S \rangle \quad (5)$$

$$|\Psi_A\rangle \equiv \frac{|s, m_a\rangle \otimes |s, m_b\rangle - |s, m_b\rangle \otimes |s, m_a\rangle}{\sqrt{2}} \quad D_A \equiv \langle \Psi_A | (\vec{S}_1 - \vec{S}_2)^2 | \Psi_A\rangle \quad (6)$$

Calculate D_D, D_S, D_A in terms of m_a, m_b . Order them from smallest to largest; i.e. write down an expression of the from $D_X \leq D_Y \leq D_Z$ with $\{X, Y, Z\}$ some permutation of $\{D, S, A\}$.

[*Hint:* You will find it useful to express $\vec{S}_1 \cdot \vec{S}_2$ in terms of the appropriate raising and lowering operators.]

2. Two Electrons: Spin-dependent Interaction and Heisenberg Hamiltonian (20 points)

Consider two electrons with the spatial wave function of one of them given by ψ_1 and that of the other one by ψ_2 . We will first ignore the interactions between the electrons. That is, the Hamiltonian of the system can be written as

$$\mathcal{H} = H_0(\vec{r_1}) + H_0(\vec{r_2}) \tag{7}$$

where H_0 denotes the Hamiltonian for a one-electron system (which is spin-independent). Assume for simplicity that ψ_1 and ψ_2 are distinct (i.e. orthogonal) eigenstates of H_0 of the same energy.

The spatial wave function of the full system may be either symmetric or antisymmetric under the interchange of the electrons' coordinates. Since the electrons are spin- $\frac{1}{2}$ fermions, the overall wave function must be antisymmetric under the simultaneous interchange of both space coordinates and spin.

- (a) Suppose the spatial wave function is antisymmetric, write down the full wave functions for the system. For these states, what are the eigenvectors and eigenvalues of the square and the z-component of the total spin operator $\vec{S}_{tot} = \vec{S}_1 + \vec{S}_2$? $(\vec{S}_{1,2}$ are the spin operator for each electron respectively.)
- (b) Repeat part (a) in the case where the spatial wave function is symmetric.
- (c) So far all the states enumerated in parts (a) and (b) have the same energy. Now add the following term to the Hamiltonian (7):

$$\mathcal{H}' = C\vec{S}_1 \cdot \vec{S}_2 \ . \tag{8}$$

That is, the electrons interact by a spin-spin force due to the interaction of the magnetic moment of each with the magnetic field generated by the other. What are the eigenstates of the system including the interaction \mathcal{H}' ? What are the energies of the states in parts (a) and (b)?

(d) Now suppose we *ignore* the interaction (8) and consider the following Coulomb repulsion between the two electrons

$$\mathcal{H}'' = \frac{e^2}{|\vec{r_1} - \vec{r_2}|} \tag{9}$$

Using perturbation theory, compute the first-order contribution of \mathcal{H}'' to the energy difference ϵ between the states in (a) and (b). You may leave your answer in integral form since the explicit spatial wave functions are not given.

(e) Suppose that the system has no spin-spin interaction \mathcal{H}' but does have the Coulomb repulsion \mathcal{H}'' . Argue that such a two-electron system can be described by an *effective* Hamiltonian of the form

$$\mathcal{H}_{\rm eff} = -J\vec{S}_1 \cdot \vec{S}_2 \tag{10}$$

and express J in terms of ϵ . From your answer to 1(a), what do you think the sign of J will be? [*Note:* You do *not* need to do a detailed calculation or a rigorous proof here. Instead it is enough to give a hand-wavy argument: from 1(a), (anti)symmetric wavefunctions yield particles that are (closer or farther) to each other, which should (increase or decrease) the Coulomb repulsion.]

[Another note: This exercise tells us that the Hamiltonian for a two-electron (or more generally many-electron) system which depends only on space and not on spin variables can in fact be mimicked by an effective spin-spin interaction. This is a direct consequence of the Pauli exclusion principle: spin space and real space are interconnected quantum mechanically. Equation (10) was first realized by Heisenberg who used it to understand the origin of ferromagnetism. Note that in a solid, direct spin-spin interactions (8) are also present, but are much weaker (about one hundred times smaller) than (10) which arises from electrostatic interactions.]

3. Estimating the Properties of Copper (Adapted from Griffiths 5.16 & 5.17, 15 points)

The density of copper is 8.96 gm/cm^3 , its atomic weight is 63.5 gm/mole, and the number of free electrons per copper atom is well-approximated by 1. In this problem you will attempt to model some of the properties of copper, assuming that copper can be described as a non-relativistic free electron gas.

- (a) Calculate the electron Fermi energy for copper in eV.
- (b) Is it safe to assume that the electrons in copper are non-relativistic?
- (c) Calculate the Fermi temperature for copper, namely the temperature at which the characteristic thermal energy $(k_B T)$, where k_B is the Boltzmann constant and T is the Kelvin temperature) equals the Fermi energy for copper. Solid copper has a melting point of 1356 K. Is it safe to assume that the electrons in solid copper are close to the ground state configuration?
- (d) The *bulk modulus* of a material measures how it responds to uniform compression:

$$B = -V \frac{\partial P}{\partial V},\tag{11}$$

where V is the volume of the material and P is the pressure. Show that B = (5/3)P for a free electron gas. How well does the free electron gas model account for the bulk modulus of copper, 1.34×10^{12} Ba? (Barye (Ba) = 1 dyne/cm² is the cgs unit for pressure.) Is this expected?

4. Fermi Surface for a Harmonic Trap (20 points)

The concept of a Fermi surface and a Fermi energy extends beyond just the free electron gas model. Consider a non-interacting electron gas in a two-dimensional harmonic trap, namely N electrons confined to a potential

$$V(x,y) = \frac{1}{2}m_e\omega^2(x^2 + y^2),$$
(12)

ignoring all electron-electron interactions. (The electrons are rigidly confined to the x-y plane.) You may assume that N is very large such that sums can be replaced by the appropriate integrals.

- (a) In a harmonic trap, it is no longer helpful to label the one-particle states by their k_x and k_y values. What are the one-particle states and energies in this two-dimensional harmonic trap?
- (b) Find a graphical way to visualize the one-particle states, and draw the appropriate Fermi surface for N electrons.
- (c) What is the Fermi energy E_F ?
- (d) What is the total energy E_{total} of the ground state?
- (e) Calculate the chemical potential

$$\mu = \frac{\partial E_{\text{total}}}{\partial N},\tag{13}$$

and explain the physical significance of the result.

5. White Dwarfs, Neutron Stars, and Black Holes (15 points)

Note: You can directly use formulae derived in lecture for this problem as far as you state clearly the meaning of those formulae.

- (a) Consider a white dwarf star of the same mass as the Sun. Assume that the star is mainly made of Carbon. What is the radius of the star? Note that the Sun has a mass of $M_{sun} = 2 \times 10^{33}$ g and a radius of $R_{sun} = 7 \times 10^5$ km. Find the ratio of the mass density of the white dwarf and the Sun.
- (b) Calculate the Fermi temperature for the white dwarf in (a). Suppose this white dwarf has a surface temperature of 10^4 K (which then looks white), and a core temperature close to 10^7 K. Is our zero temperature approximation justified?
- (c) In a neutron star, the neutron degeneracy pressure stabilizes the collapse. Calculate the radius of a neutron star with the mass of the Sun. You can assume that the star only consists of neutrons and the neutron gas is free.¹ Find the (neutron) Fermi energy and compare it to the rest energy of a neutron.
- (d) If a star has a mass M that is larger than the Chandrasekhar mass for a neutron star, the degenerate neutron pressure cannot balance the attractive force of the gravity and the star will collapse to form a black hole. A black hole has a "surface of no return", i.e. any object lying within a radius r_s from the center of gravity of the black hole can not escape and will be devoured by the black hole. r_s is called the "Schwarzschild radius". Estimate r_s by combining M with G_N (Newton's constant) and c to obtain a length. Evaluate your r_s for $M = M_{sun}$. Compare the answer with those in (a) and (c).

 $^{^{1}}$ This is not a very good approximation to the realistic situation in which nuclear interactions between neutrons are important.

6. "Free" Electron Gas? (15 points)

In our discussion of electron gases in metals and in white dwarfs, we have made the assumption that Coulomb interactions between electrons are not important.

- (a) Express in words or simple equations, how you would formulate a criterion to check this assumption.
- (b) For a white dwarf of one solar mass, use your criterion to check whether the assumption is valid.

[Hints. 1. Remember that metals and stars are electrically neutral objects. 2. Recall that first-order perturbation theory provides a rigorous bound on the ground-state energy in one direction.]

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