Spring 2005 - Entrance Examination: Condensed Matter

Solve al least one of the following problems. Write out solutions clearly and concisely. State each approximation used. Diagrams welcome. Number page, problem, and question clearly. Do not write your name on the problem sheet, but use extra envelope.

Problem 1: Electrons in a wire

Consider an electron quantized inside an infinitely long hard wire of square cross section:

$$V(x, y, z) = \begin{cases} 0, & \text{if } -\frac{a}{2} < x < \frac{a}{2}, \quad -\frac{a}{2} < y < \frac{a}{2} \\ +\infty & \text{otherwise} \end{cases} \tag{1}$$

1. Based on the symmetry of the problem, write out the general form for the eigenstates.

2. Using that form, solve Schrödinger's equation and show that the motion along z is free, while discrete eigenvalues are found in the (x, y) plane. Find the six lowest eigenvalues in the plane, their eigenfunctions and their respective degeneracies.

Consider filling these eigenstates with n non-interacting electrons per unit length.

3. Calculate the increase of the Fermi energy E_F and the evolution of the Fermi surface (more precisely of the Fermi points) as n increases. In particular, identify and describe the singularities that will occur in $\frac{dE_F}{dn}$.

4. Concentrate now on the electron density n_2 corresponding to the *second* singularity. Describe qualitatively the change of the total electron energy obtained by deforming the square section (a, a) to a rectangle $(a - \delta, a + \delta)$ with $\delta << a$.

Problem 2: Atomic/molecular long-range interaction with a metallic surface

Consider an atom or a molecule at a distance z, large compared with its linear dimensions, from a flat metallic surface that can be considered "ideal" in the sense that it screens completely and instantaneously any electric field in its interior.

1. Consider an ion of net charge $+Q$ and write the leading term in the force acting on it. Is the ion attracted or repelled from the surface?

2. Write the corresponding ion-surface interaction energy.

Consider now a neutral bi-atomic molecule with a *permanent dipole* $\mathbf{d}$ that forms an angle θ with the surface normal.

3. Write the leading term in the molecule-surface interaction energy. Does the molecule prefer to be oriented parallel or orthogonal to the surface?

Consider then a neutral atom with no permanent dipole and frequency-dependent atomic polarizability, $\alpha(\omega)$.

4. Write the expression for the leading term in the atom-surface interaction energy in terms of the ground-state expectation value of a suitable operator.

5. Re-express the above result in terms of the frequency-dependent atomic polarizability.

6. Give an explicit expression of the interaction energy in the case of a hydrogen atom.

Hints:

1. The frequency-dependent atomic polarizability is given by:

$$\alpha(\omega) = -\sum_{i>0} \left[\frac{\langle \phi_0|\mathbf{d}|\phi_i\rangle\langle\phi_i|\mathbf{d}|\phi_0\rangle}{\hbar\omega - (\epsilon_i - \epsilon_0) + i0^+} - \frac{\langle \phi_0|\mathbf{d}|\phi_i\rangle\langle\phi_i|\mathbf{d}|\phi_0\rangle}{\hbar\omega + (\epsilon_i - \epsilon_0) + i0^+} \right]$$

where ϕ_i are the eigenstates of the atom with eigenvalues ϵ_i in ascending order.

2. The ground state wavefunction of the hydrogen atom is

$$\phi_{1s}(\mathbf{r}) = \frac{1}{\sqrt{\pi a_0^3}} \exp(-r/a_0)$$

where $a_0 = \hbar^2/me^2$ is the Bohr radius.

Problem 3: Spin-orbit splitting in a laterally confined two-dimensional electron gas

Let's consider a gas of electrons with effective mass m^* moving in a plane. The Hamiltonian is:

$$H = \frac{1}{2m^*}(p_x^2 + p_y^2),\tag{2}$$

where $p_x = -i\hbar\frac{\partial}{\partial x}$ and $p_y = -i\hbar\frac{\partial}{\partial y}$ are the Cartesian components of the momentum operator.

1. Write the energy levels of the electrons confined in this plane assuming that the plane is finite with dimensions L_x and L_y and that the wave-functions are zero for $|y| > L_y/2$, while they obey to periodic boundary conditions along x. Show that the energy levels can be labeled by a vector (k_x, k_y) and find the allowed values of k_x and k_y. Discuss also the limit $L_x \to \infty$ and $L_y \to 0$.

Now consider an electric field perpendicular to the plane. This field can act on the electron spin through the spin-orbit interaction. Suppose that you can describe this effect by adding to the free electron Hamiltonian a spin-orbit term:

$$H_{so} = \alpha\left(\sigma_y p_x - \sigma_x p_y\right),\tag{3}$$

where α is a number, proportional to the intensity of the electric field, and to the magnitude of the spin-orbit coupling. σ_x and σ_y are the Pauli matrices. Suppose also $L_x \gg L_y$ so that electrons are free to move along x, while they are confined along y where you can assume that only the lowest energy wave function is occupied.

2. The eigenfunctions of $H + H_{so}$ are spinors with two components. The electron energy levels of H are two-fold degenerate due to the spin degrees of freedom. Using degenerate static perturbation theory show that H_{so} removes this degeneracy for each $k_x \neq 0$. Determine the perturbed energy levels and plot them as a function of k_x.

3. Determine the perturbed wave-functions to zeroth order and calculate the expectation value of the spin angular momentum $\mathbf{S} = \frac{\hbar}{2}(\sigma_x, \sigma_y, \sigma_z)$ on these states.

Hint: The Pauli matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Problem 4: A particle in a box

A particle of mass m is confined bewteen two infinite plane walls separated by a distance d. The particle is in its lowest possible energy state.

1. Which is the quantum-mechanical energy of this state?

Let the separation between the walls slowly (adiabatically) increase from d to $2d$.

2. How does the expectation value of the energy change?

3. Compare the quantum mechanical energy change with the results obtained classically from the mean force exerted on the wall by a bouncing ball of velocity v.

Now assume that the separation between the walls is increased from d to $2d$ at a speed much larger that the average speed of the particle. Classically there is no change in the particle energy since the wall is moving faster than the particle.

4. How does the expectation value of the quantum mechanical energy change?

5. Calculate the probability that the particle is in the new ground state.

Problem 5: Nuclear spin of molecular hydrogen

1. Calculate the probability that the total nuclear spin of a hydrogen molecule, H_2, in the gas phase is equal to 0, in the two distinct low- and high-temperature limits.

   Hints: Neglect the magnetic interaction between nuclear spins. Do not be mislead by the above hint and look for an effect which lifts the degeneracy between states of different total nuclear spin. The equilibrium internuclear distance of H_2 is $d_{eq} = 1.40$ Bohr radii, the mass of a proton is $M_p = 1836 \, m_e$, m_e being the electron mass, and the Boltzmann's constant is $K_B = 8.62 \times 10^{-5}$ eV/K. Think why the above information is relevant.

2. Can you tell why when hydrogen is cooled from above room temperature the fraction of molecules which have 0 nuclear spin tends to stay the same as it is at high temperature, contrary to the results of your calculations (if they are correct)?