Spring 2004 – Entrance Examination: Condensed Matter

Solve at 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: Free electrons in d=1,2, and 3 dimensions

Consider N free electrons contained in a space of "volume" L^d, with $d = 1, 2$, and 3, respectively. Assuming periodic boundary conditions at the box boundaries, determine for each dimension d:

1. the allowed one-electron eigenfunctions, their quantum numbers, and their energy.
2. the Fermi momentum k_F and Fermi energy E_F, obtained by occupying each one-electron state with 2 electrons of opposite spin.
3. the density of electronic states per spin, $n(E) = \sum_{\mathbf{k}} \delta(E - E_{\mathbf{k}})$, to be calculated both at the Fermi energy E_F and at $E \to 0$.
4. the value (even approximate) of the free electron heat capacity $C_v = \partial E_{tot}(T)/\partial T$, where E_{tot} is the total internal energy of the electron gas at temperature T.

Problem 2. Orbital wavefunction of Helium atom

Consider the orbital part of the two-electron ground state $\Phi(\vec{r}_1, \vec{r}_2)$ of the Helium atom, satisfying the following Schrödinger equation in atomic units:

$$\left[-\frac{1}{2}(\nabla_1 + \nabla_2) - \frac{Z}{|\vec{r}_1|} - \frac{Z}{|\vec{r}_2|} + \frac{1}{|\vec{r}_1 - \vec{r}_2|}\right] \Phi(\vec{r}_1, \vec{r}_2) = E_0 \Phi(\vec{r}_1, \vec{r}_2) \tag{1}$$

where $\vec{r}_i$, for $i = 1, 2$, are the positions of the two electrons, the ion position being considered fixed at the origin $x = y = z = 0$, E_0 is the ground state energy and $Z = 2$ is the atomic number. The orbital wavefunction Φ is symmetric under particle interchange $\Phi(\vec{r}_1, \vec{r}_2) = \Phi(\vec{r}_2, \vec{r}_1)$, because the ground state is a spin singlet.

1. Show that if an electron position $\vec{r}_i$ is very close to the ion, namely that $|\vec{r}_i| << 1$, the following electron-ion "cusp condition" is verified *exactly* for Φ, e.g. for $i = 1$:

   $$|\vec{r}_1| \nabla_1 \Phi(\vec{r}_1, \vec{r}_2) = -2Z\Phi(\vec{r}_1, \vec{r}_2) \tag{2}$$

   for $|\vec{r}_1| \to 0$.

   Hint: Neglect the angular dependence in the Laplacian , so that:

   $$\nabla_1 \Phi(\vec{r}_1, \vec{r}_2) = \frac{1}{|\vec{r}_1|^2} \frac{d^2 |\vec{r}_1|^2 \Phi}{d^2 |\vec{r}_1|}$$

   for $|\vec{r}_1| << 1$.

2. What happens when the two electrons are very close ?

   Hint: change variables $\vec{r} = \vec{r}_1 - \vec{r}_2$ and $\vec{R} = \vec{r}_1 + \vec{r}_2$, and study the case $|r| << 1$, at fixed non zero $|\vec{R}|$. Find therefore the analogous electron-electron cusp condition in this limit:

   $$|\vec{r}| \nabla \Phi(\vec{r}, \vec{R}) = \Phi(\vec{r}, \vec{R}) \tag{3}$$

   for $|\vec{r}| \to 0$.

3. Does a Hartee-Fock wavefunction $\Phi(\vec{r}_1, \vec{r}_2) = \phi(\vec{r}_1)\phi(\vec{r}_2)$ satisfy the above cusp conditions (ion-electron and electron-electron) for some orbital $\phi(\vec{r})$? (Consider for instance a simple exponential for $\phi(r) = \exp(-B|\vec{r}|)$, where B is a suitable constant).

Problem 3. A simple system with three spins

Consider a quantum system made of three spin $\frac{1}{2}$ particles interacting through the Hamiltonian:

$$H = K\mathbf{s}_1 \cdot \mathbf{s}_2 + J(\mathbf{s}_2 \cdot \mathbf{s}_3 + \mathbf{s}_1 \cdot \mathbf{s}_3).$$

1. Show that $\mathbf{S}_{12} = \mathbf{s}_1 + \mathbf{s}_2$ and $\mathbf{S} = \mathbf{s}_1 + \mathbf{s}_2 + \mathbf{s}_3$ are constants of motions, whereas $\mathbf{S}_{13} = \mathbf{s}_1 + \mathbf{s}_3$ and $\mathbf{S}_{23} = \mathbf{s}_2 + \mathbf{s}_3$ are not.

2. Find the eigenvalues of the Hamiltonian as functions of J and K and of the conserved quantum numbers.

3. Discuss the energy and the symmetry of the ground state for $K = J > 0$ and for $K = J < 0$.

4. (More difficult, optional) Draw a 'phase diagram' for the ground state as a function of J and K. That is, partition the KJ plane in regions, each characterized by different symmetries (*i.e.* quantum numbers) of the ground state.

Problem 4. Eigenstates of one-dimensional potentials

You certainly remember that the gaussian wavefunction $\psi_0(x) = Ce^{-x^2/(2\sigma^2)}$ is the ground state solution of the harmonic potential.

1. Consider now the wavefunction

$$\psi_0(x) = Ce^{-\frac{1}{n}\left(\frac{x}{\sigma}\right)^n} , \tag{4}$$

   where σ is a quantity with dimension of a length, and n is a positive integer. For what class of integers n is ψ_0 an acceptable wavefunction? For each acceptable n, what is the corresponding potential $V_n(x)$ for which ψ_0 is an eigenstate with energy eigenvalue $E_0 = 0$? Plot the resulting potential for $n = 4$.

2. Generalize the previous construction, i.e., find out the general form of the potential $V(x)$ such that the following wavefunction

$$\psi_0(x) = Ce^{-\frac{W(x)}{W_0}} , \tag{5}$$

   is an eigenfuction with energy eiegenvalue $E_0 = 0$. (Here $W(x)$ is an arbitrary function, such that the resulting ψ_0 is normalizable, and W_0 is a constant with dimension of energy.) Can ψ_0 be an excited eigenstate? If not, why?

3. Consider now states of the form:

$$\psi(x) = P(x)e^{-\frac{1}{n}\left(\frac{x}{\sigma}\right)^n} , \tag{6}$$

   where $P(x)$ is a polynomial of degree ≥ 1 in x. Discuss why, on general grounds, ψ cannot be the ground state of a regular potential. By writing the Schrödinger equation explicitly, prove that ψ is a candidate *excited state* of the potential $V_n(x)$ found in point 1) only for $n = 2$.

Problem 5. Electrons in a magnetic wire with a domain wall

Let us consider an electron in a wire which is infinite along the z direction and has a square cross section with edge length L. The wire is composed of a magnetic material whose magnetization has, in each point, the direction of the unit vector $\hat{\mathbf{M}}(\mathbf{r})$. The Hamiltonian of the electron is:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{\Delta}{2}\,\hat{\mathbf{M}} \cdot \sigma \tag{7}$$

where σ is the vector of the Pauli matrices, and Δ is the spin splitting of the electron due to the coupling with the magnetization, and it is constant. An infinite potential constrains the electron to remain inside the wire, while motion along z is free.

- Find the energy spectrum of an electron with spin up and of an electron with spin down inside a wire with uniform magnetization ($\hat{\mathbf{M}} = (0,0,1)$) and write the eigenfunctions of the Hamiltonian. Hint: separate motion transverse and parallel to the wire.

- For a fixed energy E, count the number of different eigenfunctions of the Hamiltonian at that energy.

Now consider a wire where the direction of the magnetization is $\hat{\mathbf{M}} = (0,0,1)$ for $z < 0$ and $\hat{\mathbf{M}} = (0,0,-1)$ for $z > 0$. The position $z = 0$ where the magnetization changes sign is called a domain wall.

- Find the reflection and transmission coefficient of an electron with energy E and spin up which propagates from the region $z < 0$ toward the region $z > 0$ and is scattered by the domain wall. Study only the energy region $E < \frac{5\hbar^2}{2m}(\pi/L)^2 - |\Delta|/2$ and assume $|\Delta| << \frac{\hbar^2}{2m}(\pi/L)^2$.

Problem 6. Scattering through a localized spin in 1-D

Consider an electron which moves in one-dimension. In general its wave-function can be described by a spinor

$$\Psi(x) = \begin{pmatrix} \psi_\uparrow(x) \\ \psi_\downarrow(x) \end{pmatrix}.$$

$\psi_\uparrow(x)$ and $\psi_\downarrow(x)$ are, respectively, the spin up and spin down components of the wave-function.

At the origin $x = 0$ the electron scatters through a δ-like potential $-U\,\delta(x)$, with $U > 0$. In addition a spin-1/2 impurity $\vec{S}$, sits at the origin and is coupled to the electron spin through the exchange term

$$2\,J\,\delta(x)\,\vec{S}\cdot\vec{\sigma}, \tag{8}$$

with $J > 0$ and where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, σ_x, σ_y and σ_y being the Pauli matrices which act on the spin components of the electron wave-function. The localized-spin wave-function (fixed at $x = 0$) may also be represented by a two-component spinor

$$\chi = \begin{pmatrix} \chi_\uparrow \\ \chi_\downarrow \end{pmatrix},$$

so that

$$S_z\,\chi = \frac{1}{2}\begin{pmatrix} \chi_\uparrow \\ -\chi_\downarrow \end{pmatrix}, \quad S^+\,\chi = \begin{pmatrix} \chi_\downarrow \\ 0 \end{pmatrix}, \quad S^-\,\chi = \begin{pmatrix} 0 \\ \chi_\uparrow \end{pmatrix}.$$

The total wave-function (electron plus localized spin) has therefore four components $\psi_\alpha(x)\,\chi_\beta$, with $\alpha, \beta = \uparrow, \downarrow$. The Hamiltonian is therefore

$$\begin{aligned} \mathcal{H}(x)\;\psi_\alpha(x)\,\chi_\beta \;&=\; -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_\alpha(x)\,\chi_\beta - U\,\delta(x)\,\psi_\alpha(x)\,\chi_\beta \\ &\quad +2\,J\,\delta(x)\,\left(\vec{\sigma}\,\Psi(x)\right)_\alpha \cdot \left(\vec{S}\,\chi\right)_\beta. \end{aligned} \tag{9}$$

Suppose that the electron arrives from $x = -\infty$ in a plane-wave state with momentum k and spin up, namely with the initial wavefunction

$$\Psi_{in}(x) = \begin{pmatrix} \mathrm{e}^{i\,k\,x} \\ 0 \end{pmatrix}.$$

At the same time the localized spin is initially down, *i.e.*

$$\chi_{in} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

After the electron scatters through the localized potential and spin, it will be partly reflected and partly transmitted. Moreover the exchange term (**??**) may also induce spin-flips of the electron and localized spin. Therefore the scattering process is characterized by two transmission amplitudes $t_\uparrow$ and $t_\downarrow$ as well as by two reflection amplitudes, $r_\uparrow$ and $r_\downarrow$, where $\uparrow$ and $\downarrow$ refer to the spin components of the electron wave-function.

- Question: Calculate $t_\uparrow$, $t_\downarrow$, $r_\uparrow$ and $r_\downarrow$.

Hints: At $x = 0$, use the continuity of the wave-function and the appropriate jump of its derivative to reproduce the δ-function singularity.