SISSA ISAS

SCUOLA INTERNAZIONALE SUPERIORE DI STUDI AVANZATI - INTERNATIONAL SCHOOL FOR ADVANCED STUDIES
I-34014 Trieste ITALY - Via Beirut 4 - Tel. [+]39-40-37871 - Telex:460269 SISSA I - Fax: [+]39-40-3787528

Fall 2007 – 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. Spin, orbital and total angular momentum.

Consider an electron with spin $1/2$, described by a two-component spinor wavefunction

$$\Psi(\mathbf{r}) = \begin{pmatrix} \psi_+(\mathbf{r}) \\ \psi_-(\mathbf{r}) \end{pmatrix} \tag{1}$$

with $\psi_+(\mathbf{r}) = \sqrt{2/3}R(r)Y_1^0(\theta,\phi)$ and $\psi_-(\mathbf{r}) = \sqrt{1/3}R(r)Y_1^1(\theta,\phi)$, where $\mathbf{r} = (r,\theta,\phi)$ are the spherical coordinates of the position vector $\mathbf{r}$ and $Y_l^m(\theta,\phi)$ are the spherical harmonics, eigenvectors of the orbital angular momentum operators L^2 and L_z with $L^2Y_l^m = \hbar^2 l(l+1)Y_l^m$ and $L_zY_l^m = \hbar m Y_l^m$. The radial function $R(r)$ is supposed to be normalized in such a way that $\Psi(\mathbf{r})$ is normalized to one.

1. Calculate the mean value of the orbital angular momentum L_z and of the spin angular momentum S_z on $\Psi(\mathbf{r})$.

2. Show that $\Psi(\mathbf{r})$ is an eigenvector of the total angular momentum operators J^2 and J_z (where $\mathbf{J} = \mathbf{L}+\mathbf{S}$) and find the corresponding eigenvalues.

3. Find the subspace of degenerate eigenvectors of J^2 with the same eigenvalue of the state (1). Describe this subspace with eigenvectors of J_z and find their eigenvalues. **Hint**: Use the operators $J_+ = J_x + iJ_y$ and $J_- = J_x - iJ_y$.

4. Calculate the mean value of S_z in the states found at point 3.

5. Consider now an atom with a single p electron outside closed shells. Without calculating explicitly the radial part, write the ground state one-electron wavefunctions. Write also the wavefunctions of the first excited state. **Hint**: The ground state wavefunctions are eigenvectors of J^2 with eigenvalue $\frac{3}{4}\hbar^2$.

Problem 2. Electron emission.

Non-interacting electrons in a metal with surface can schematically be seen as trapped inside a (semi-infinite sized) potential well of depth $-|V_0|$. Here they fill with Fermi statistics all states between $-|V_0|$ and $-|V_0| + E_F = -W$ (at T=0), where $E_F > 0$ and $W > 0$ are the Fermi energy and the work function, respectively. Note that all electrons possess negative energies, the energy zero being associated to the vacuum. Call $z = 0$ the metal surface plane. In order to be emitted, an electron must have a nonzero probability to be found far outside of the surface, $z \to \infty$.

1) What is the emission probability when the metal is in its ground state?

Temperature. The metal can emit electrons at finite temperature T, through thermal excitation to a positive energy state.

2) Describe qualitatively the temperature dependence to be expected for the probability of thermal emission (this is called thermionic emission).

Electric field. An electric field normal to the surface will greatly affect electron emission. Assume a uniform electric field F for $z > 0$, and call $F > 0$ the field direction pointing out of the surface (force on an electron pointing into the surface).

3) Describe what happens to thermal emission when $F > 0$.

Consider the potential profile seen by an electron when $F < 0$, and take for simplicity $T = 0$. Describe a possible electron escape process, through the effective barrier of fixed heigth W but field dependent thickness.

4) Draw the potential, and find the field dependent barrier thickness $d(F)$ at the Fermi energy.

5) Treat this as a square barrier, and find the approximate field dependence and work function dependence of the electron emission probability for increasing field F from a state at the Fermi energy $E = -W$.

Electric field plus interaction. Consider finally the effect of coulomb interaction between the electrons. In particular, consider the fact that when an electron exits the surface and sits at $z > 0$, things go roughly as though it was leaving behind a mirror image, a “hole” with positive charge and z¡0.

6) Work out the effect that this will have on the field emission probability. In particular, does it enhance or suppress emission?

Problem 3. An electronic monocromator.

Consider the scattering of an electron from a single one dimensional barrier.

1) By using the fact that the form of a wavefunction ψ_+ on the left of the barrier is $e^{ikx} + r(k)e^{-ikx}$, and on the right $t(k)e^{ikx}$, and that ψ_+^* is also a possible wavefunction with the same energy, show that the most general wavefunction has the form

$$\psi(x) \;=\; \begin{cases} A_{L,+}e^{ikx} + A_{L,-}e^{-ikx} & \text{(Left of barrier)} \\ A_{R,+}e^{ikx} + A_{R,-}e^{-ikx} & \text{(Right of barrier)} \end{cases} , \tag{1}$$

where $\begin{pmatrix} A_{R,+} \\ A_{R,-} \end{pmatrix} = \mathbf{M} \cdot \begin{pmatrix} A_{L,+} \\ A_{L,-} \end{pmatrix}$, determining the coefficients of the 2×2 transfer matrix $\mathbf{M}$ in terms of the reflection and transmission amplitudes $r(k)$ and $t(k)$.

2) Consider explicitly a square barrier in $x \in [-a/2, a/2]$, of width a and height V_0. Denoting, for $E > V_0$, by $q = \sqrt{2m(E - V_0)}/\hbar$ the wavevector in the barrier region, and knowing that the transmission coefficient can be expressed as:

$$|t(k)|^2 = \left[1 + \frac{(k^2 - q^2)^2}{4k^2q^2} \sin^2 qa\right]^{-1} , \tag{2}$$

determine the values of the energy $E = \hbar^2k^2/2m$ of the impinging particle for which the transmission coefficient $|t(k)|^2 = 1$. Explain physically this result. What is the form of the matrix $\mathbf{M}$ for such values of E?

3) Suppose you have solved the transmission problem for a given barrier $V(x)$ centered around the origin $x = 0$, determining the matrix $\mathbf{M}^{(0)}$, and you are now asked to solve the same problem when the barrier is translated and centered around $x = b$, i.e., it is $V(x - b)$. Show that the matrix $\mathbf{M}^{(b)}$ describing the transmission of the wave to the right is now given by:

$$\mathbf{M}^{(b)} = \mathbf{D}_b \cdot \mathbf{M}^{(0)} \cdot \mathbf{D}_b^{-1} . \tag{3}$$

What is the expression of the matrix $\mathbf{D}_b$?

4) Imagine now a sequence of N identical barriers, like the ones considered in 2), where the the separation between the centers of the nth and $(n+1)$th barrier is a random number $d_n > a$ (no need to specify better the distribution of d_n, for our scope). How would you express the coefficients $\begin{pmatrix} A_{R,+} \\ A_{R,-} \end{pmatrix}$ of the wave in the region to the right of all barriers, with respect to the coefficients to the left of all barriers $\begin{pmatrix} A_{L,+} \\ A_{L,-} \end{pmatrix}$. What happens to the global transmission at the energies E determined at point 2) above?
DIFFICULT (optional): What do you think will happen when the energy E differs from the one of point 2)?

Problem 4. Finite linear harmonic chain.

Consider a system of three point particles of mass M, constrained on a circle of radius R, and let us indicate with φ_i the angular coordinate of each particle. Suppose that the particles interact among each other through the potential:

$$V(x_1, x_2, x_3) = \frac{1}{2}k\left((x_1 - x_2)^2 + (x_2 - x_3)^2 + (x_3 - x_1)^2\right) \ , \tag{1}$$

where $x_i = R\varphi_i$.

1. Write down the Hamiltonian of the system.

2. Verify that the ground-state wavefunction of the system is symmetric under permutation of the three particles. **HINT**: this question can be answered either explicitly, by constructing the wavefunction (see point 4), or by invoking some more or less general arguments.

3. Write down the Hamiltonian in terms of the normal coordinates that diagonalize the quadric form, Eq. (1). **HINT**: it may be useful to note that the present problem is analogous to finding the normal modes of a *finite* linear harmonic chain with periodic boundary conditions, and use the Bloch theorem to find such normal modes.

4. Calculate the ground-state energy and wave-function.

5. Find the excited-state spectrum and discuss it in terms of the symmetry properties of the system.

6. **DIFFICULT**, optional. Suppose now that the three particles are spin-less fermions. Find the ground-state energy and wavefunction. **HINT**: the fermion ground-state can be considered as an excited state of the Hamiltonian for distinguishable particles. Any excited-state wavefunction of a harmonic system is given by the product of a homogeneous polynomial with the ground-state wavefunction. What is in this case the minimum degree of the polynomial that would make the wavefunction totally antisymmetric? What can be said of the normal modes that are excited in this wavefunction?

Problem 5. Simple model of electron solvation in a polar medium.

Consider the situation of an electron dissolved in a polar medium, such as water or ammonia.

In a very simplified model of electron solvation the electron can be viewed as self-trapped by the polarization induced in the medium inside a spherical cavity of radius R, created in the solvent that is approximated as a continuum of large and homogeneous dielectric constant ($\epsilon_{H_2O} \approx 80$, $\epsilon_{NH_3} \approx 20$).

1. Calculate the total electrostatic potential generated by the the electron in the solvent (outside the cavity) and separate the direct term coming from the electron and the one coming from the polarization of the medium.

2. Calculate the potential induced by the polarization charge inside the cavity and show that this leads to a stabilizing (negative) interaction energy of the electron-solvent system.

3. Calculate the minimum kinetic energy of the electron in the cavity assuming that the electron is completely confined inside the cavity. (i.e. solve the Schroedinger equation in polar coordinates for the lowest state of s-symmetry).

4. Combining the above results, calculate the binding energy of the electron in the cavity and its radius, neglecting any effect associated to the surface tension of the solvent.

5. (Optional) Knowing that the experimental values for the binding energies and cavity radius in ammonia are $\approx 0.8eV$ and $\approx 7\AA$, discuss whether allowing for an imperfect confinement of the electron in the cavity would improve or worsen the agreement of this simple model with experiment.