Spring 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: Electrons in a box

A single free electron is constrained inside a hard-walled box of square parallelepiped shape, of sides a, b, c.

1. Solve Schrödinger's equation, find the spectrum of eigenvalues and eigenvectors, and describe the electron ground state energy E_0 and wavefunction Ψ_0.

2. Calculate the forces exerted on the three faces of the box in directions a, b, c when the electron is in the ground state, and from these the corresponding pressures P_a, P_b, P_c. Comment the result.

3. Keeping a fixed box volume V, determine for what values of a, b, c, E_0 is minimum. Comment the result.

4. Now consider two electrons instead of one, initially with a, b, c determined at point [3]. Ignoring their Coulomb interaction, determine their ground state energy for total spins $S = 0$ and $S = 1$.

5. Suppose the box sides to be expandable, so that a, b, c can change, while keeping the volume V fixed. Determine the values of a, b, c which minimize the ground state energy respectively for total spins $S = 0$ and $S = 1$. Comment the result.

6. *(Optional)* Finally, turn on a weak delta-function repulsion between the two electrons $U = vV\delta(x_1 - x_2)\delta(y_1 - y_2)\delta(z_1 - z_2)$ where v is an energy parameter measuring the repulsion strength and V is the volume. Use first-order perturbation theory to estimate the value of v for which the ground state energy is $E_{S=0} = E_{S=1}$.

Problem 2: Simple model for a H_2 molecule

Let us consider a very crude approximation for the H_2 molecule, in which the electrons can only occupy the $1s$ orbital $|R\rangle$ of the hydrogen atom and the distance D_0 between the atoms is fixed. The Hamiltonian H is such that if this orbital is empty the energy is zero, if it is singly occupied (with spin up or down) the energy is ϵ, and if it is doubly occupied the energy is $2\epsilon + U$. Moreover, there is a finite amplitude $\langle R|H|R'\rangle = -t$ for hopping one electron from one atom to the other. Finally, for simplicity, consider the case in which the overlap between the two $1s$ orbitals centered around different hydrogen atoms is vanishing, namely $\langle R'|R\rangle = 0$.

1. Calculate the energy levels and the eigenfunctions for the case of the H_2^+ molecule.

2. Consider now the case of the H_2 molecule and enumerate the number of singlets and triplets.

   2a. Calculate the variational energy for the "molecular orbital" state in which both electrons occupy the lowest energy level found for H_2^+ (with opposite spins) and write down this state as a function of the singlets states. In this state, what is the probability to find both electrons on the same atom as a function of U?

   2b. The opposite "Heitler-London" approximation consists in writing the orbital part of the ground-state wave function like:

   $$|\Psi_{HL}\rangle = \frac{1}{\sqrt{2}}(|R'\rangle|R\rangle + |R\rangle|R'\rangle). \tag{1}$$

   Calculate the variational energy for this state and discuss the differences with respect to the one of [2a]. What is now the probability to find the electrons on the same site?

   2c. Abandoning now the above approximations, carry out the exact calculation for the energy spectrum (both for singlets and triplets) and plot schematically the energy levels as a function of U. Discuss the validity of the approximations [2a] and [2b] for weak and strong interaction U.

3. Now introduce the possibility that the distance between the two atoms could change, namely $D = D_0 + \delta$. In this case, the hopping amplitude changes into $t \to t(1-\delta)$; an elastic cost is also added, $K\delta^2/2$. Find the equilibrium value for δ in the two limiting cases $U = 0$ and $U \gg t$.

Problem 3: Electron transmission through a spin-dependent potential step

Consider the one dimensional motion of an electron with spin 1/2 in a spin dependent potential energy: $V(z) = 0$ for $z < 0$ and $V(z) = V_0 + V_1\sigma_z$ for $z > 0$ (σ_z is the Pauli matrix, both V_0 and V_1 are positive and $V_1 < V_0$).

1. Find the transmission coefficient for an electron with spin-up (parallel to the z axis) moving rightward with energy E to be transmitted from the region $z < 0$ to the region $z > 0$.

2. Solve the problem at point [1] for an electron with spin down (parallel to the z axis).

3. Solve the problem at point [1] for an electron with spin along the $+x$ axis. Discuss the three cases $0 < E < V_0 - V_1$, $V_0 - V_1 < E < V_0 + V_1$, $E > V_0 + V_1$.

4. Find the average value of the spin operator $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$ for the electron at point [3] reflected in the region $z < 0$ and for the electron transmitted in the region $z > 0$. Discuss the results as a function of energy.

Problem 4: Spin-orbit coupling for one electron in a box

Consider one electron described by the following Hamiltonian (atomic units are considered) with a simple spin-orbit interaction:

$$H = -\frac{1}{2}\nabla^2 + i\gamma\left[\sigma_y\partial_x - \sigma_x\partial_y\right] \tag{2}$$

where $\gamma > 0$ is a (spin-orbit coupling) parameter, whereas σ_x and σ_y are Pauli matrices acting on the electron spin $\sigma = \pm 1/2$. Periodic boundary conditions for the electronic wave function are assumed in a finite cube with side L and volume L^3.

1. Consider a spin dependent wave function $\psi(\sigma, x, y, z)$ with given momentum k_x, k_y, k_z, quantized in unit of $2\pi/L$. Determine the eigenvalue spectrum as a function of γ and the momentum.

2. For what values of the box side L there exist zero energy eigenstates with non vanishing momentum?

Problem 5: Configurations of dimers on a checkerboard

Consider a $2 \times L$ rectangular checkerboard, and L domino pieces, each occupying 2 squares of the checkerboard.

1a. How many inequivalent configurations of domino pieces, N_L, can you form?
(**Hint:** Try to find out a recursive relation between N_L and $N_{L'}$ for $L' < L$.)

1b. Calculate the configuration entropy per site $s_L = k_B(\log N_L)/L$ as $L \to \infty$.

Imagine now that spin-1/2 Pauli matrices are placed at the centers of each square of the checkerboard. Let nearest-neighbor spins be paired into singlets, for instance, on sites 1-2:

$$|1-2\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\right)$$

2. How many configurations can you form where all the spins are paired into nearest-neighbor singlets?

Let the Hamiltonian governing the system be:

$$H = J\sum_{\langle i,j\rangle} \underbrace{\left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4}\right)}_{P_{ij}} = J\sum_{\langle i,j\rangle} P_{ij}$$

Prove that for any singlet configuration:

3a. $P_{12}|1-2\rangle = -|1-2\rangle$.

3b. $P_{23}|1-2\rangle|3-4\rangle = \frac{1}{2}|2-3\rangle|1-4\rangle$.

Restricting your analysis to a $L = 3$ checkerboard, show that starting from the nearest-neighbor singlets configurations the Hamiltonian generates configurations with singlets between non-nearest neighbors.

4. Indicating by $|\Psi_i\rangle$ the necessary singlet configurations, set-up the Hamiltonian action in the form $H|\Psi_i\rangle = \sum_j h_{ij}|\Psi_j\rangle$ (the solution is not required).