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 2002 – 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: Two level system

In many compounds and also molecules, a single hydrogen atom bridges between two oxygens, in a "double well" situation: Its energy is a little lower when the hydrogen is a little closer to one oxygen, or to the other. The energy barrier U between the two configurations (a distance d apart) is nevertheless very small; the proton, whose mass m is small can easily tunnel and ends up oscillating between the two positions even at zero temperature. Assuming a one-dimensional motion of the proton in the rigid double well:

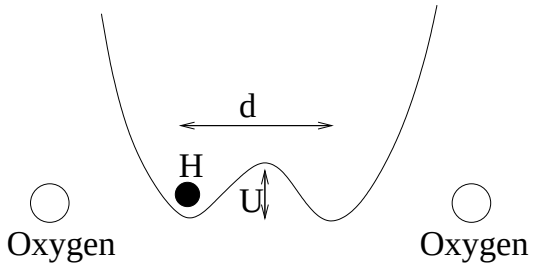

Figure 1: The double well potential.

1. Give a rough estimate of the frequency $\hbar\omega$ of this oscillation, in terms of the parameters.

2. Give a similar rough estimate of the (normalized) probability $P(\delta x)$ to find the proton in a small region δx around the central position.

3. Describe the change of $\hbar\omega$ and of $P(\delta x)$ that will occur when hydrogen is replaced with deuterium.

4. Now suppose, as is the case in real life, that only when the hydrogen sites neare the center, it will give rise to a force drawing the two oxygens together. What do you think will happen to the geometry of real compounds when hydrogen is replaced with deuterium?

Problem 2: Spin polarization of a Fermi gas

Consider a gas of free electrons in three dimension, at zero temperature, and under an external magnetic field B. Assume, if you like, to have N electrons in a cubic box of volume V, with the usual periodic boundary conditions.

1. Taking into account, in the Hamiltonian, only the usual kinetic energy in absence of field, $\sum_i p_i^2/2m$, and the interaction between the external field and the *spin* of the electrons, $2\mu_B B \sum_i S_i^z$, determine the density of electrons below which all the electron spins are fully polarized along the field.

2. Give an estimate of this critical density for a field $B = 10$Tesla. (Use that $\mu_B \approx 5.8 \times 10^{-5}$ eV/Tesla.) Do you think such a critical density is relevant for any 3-dimensional metal ?

3. Repeat the calculation for a two-dimensional electron gas.

Problem 3: One dimensional harmonic chain

Consider a one dimensional harmonic chain with Hamiltonian

$$\hat{H} = \sum_{i=-N}^{N} \frac{p_i^2}{2M} + \frac{K}{2}\left(u_i - u_{i+1}\right)^2, \tag{1}$$

where u_i is the displacement of the i-th atom from its equilibrium position ia, a being the lattice spacing, and p_i the conjugate momentum, satisfying the canonical commutation relations ($\hbar = 1$)

$$[u_n, p_m] = \mathrm{i}\delta_{nm}.$$

Periodic boundary conditions are assumed, namely $u_{N+1} = u_{-N}$.

1. Diagonalize the Hamiltonian (1).

2. Discuss the low temperature behavior of the specific heat.

3. At time $t = 0$ the chain is prepared in a state $|\Psi(0)\rangle$ in which all diplacements are zero apart from $\langle u_0\rangle = q$. For $t > 0$ this state is let propagate with the Hamiltonian (1), namely

   $$|\Psi(t)\rangle = \mathrm{e}^{-i\hat{H}t}|\Psi(0)\rangle.$$

   Find the expression of the average value of the displacement at any given site i at any time $t > 0$, i.e.

   $$\langle u_i(t)\rangle = \langle\Psi(t)|u_i|\Psi(t)\rangle,$$

   and discuss qualitatively its behavior for $|i| \gg 1$.

(**Not compulsory.**) Suppose now that a force is applied to the atom at site 0, so that the following perturbation has to be added to the Hamiltonian

$$\delta\hat{H} = g\left(u_0 - u_{-1}\right) + g\left(u_1 - u_0\right). \tag{2}$$

4. Diagonalize the Hamiltonian (1) in the presence of the perturbation (2).

5. Calculate the average value on the ground state of the displacement at any given site, namely $\langle 0|u_i|0\rangle$.

Problem 4: Heisenberg Ferromagnet

Consider a Heisenberg ferromagnet in an external magnetic field:

$$\begin{aligned} H &= -J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j - h\sum_i S_i^z = -J\sum_{\langle i,j\rangle}(S_i^xS_j^x + S_i^yS_j^y + S_i^zS_j^z) - h\sum_i S_i^z \\ &= -J\sum_{\langle i,j\rangle}\left[S_i^zS_j^z + \frac{1}{2}\left(S_i^+S_j^- + S_i^-S_j^+\right)\right] - h\sum_i S_i^z, \end{aligned} \tag{3}$$

where $J > 0$ is the magnetic coupling between nearest neighbor spins S of a D-dimensional hypercubic lattice of N sites, and $h > 0$ is the external magnetic field in the z direction.

1. Denoting by $|S\rangle_i$ the eigenstate of S_i^z on site i with the maximum spin value $S_i^z|S\rangle_i = S|S\rangle_i$ and $S_i^+|S\rangle_i = 0$, prove that the *classical* state

$$|F\rangle = |S\rangle_1|S\rangle_2...|S\rangle_N, \tag{4}$$

   is an eigenstate of the Hamiltonian (3) and calculate its eigenvalue E_0. Quite obviously $|F\rangle$ corresponds to total $S_{tot}^z = NS$.

2. Show that for any pair of sites and for any wave function $|\Psi\rangle$ we have $\langle\Psi|\mathbf{S}_i\cdot\mathbf{S}_j|\Psi\rangle \leq S^2$, and, using that, prove that the state $|F\rangle$ is indeed the ground state.

3. Now, we try to construct the low-lying energy states. Let us introduce the one-magnon state as:

$$|\mathbf{k}\rangle = N^{-1/2}\sum_j e^{i\mathbf{k}\cdot\mathbf{R_j}}|\mathbf{j}\rangle, \tag{5}$$

   where $|\mathbf{j}\rangle$ is the (normalized) state with S^z lowered by 1 at site j, i.e., $|\mathbf{j}\rangle = (2S)^{-1/2}S_j^-|F\rangle = |S\rangle_1|S\rangle_2...|S-1\rangle_j...|S\rangle_N$. This state has $S_{tot}^z = NS - 1$. Show that $|\mathbf{k}\rangle$ is also an eigenstate of the Hamiltonian (3), i.e., $(H - E_0)|\mathbf{k}\rangle = \omega(\mathbf{k})|\mathbf{k}\rangle$, and calculate $\omega(\mathbf{k})$. (It is useful to evaluate the following matrix elements: $\langle\mathbf{k}|S_i^zS_j^z|\mathbf{k}\rangle$, $\frac{1}{2}\langle\mathbf{k}|(S_i^-S_j^+ + \text{h.c.})|\mathbf{k}\rangle$.)

4. What is the meaning of the fact that for $h = 0$ we have $\omega(\mathbf{k}) = 0$?

5. Discuss why the two-magnon state $|\mathbf{k_1}\rangle|\mathbf{k_2}\rangle$ is not an eigenstate of the Hamiltonian (3).

6. Suppose now that instead of having a ferromagnetic interaction $J > 0$, we have an antiferromagnetic interaction $J < 0$. Show that, in this case, the classical ground state is *not an eigenstate* of the Heisenberg Hamiltonian.

Problem 5: Van der Waals forces between hydrogen atoms

Two hydrogen atoms in their ground state, at a distance $R = |\mathbf{R}|$ much larger that the Bohr radius a_0, attract each other. The total energy of the system E depends on R^{-6}. The effect is due to the electrostatic attraction between the fluctuating dipole moment of the two neutral atoms. This is the well known Van der Waals interaction. In this problem we study what happens when one hydrogen is in an exited $n = 2$ state (n is the main quantum number) and the other is in the ground state.

- 1) Let's call $\mathbf{r}_A$ the coordinates of the electron of atom A with respect to the nucleus A and $\mathbf{r}_B$ the coordinates of the electron of atom B with respect to the nucleus B. Then $q\mathbf{r}_A$ is the dipole moment of atom A and $q\mathbf{r}_B$ the one of atom B (q is the electron charge). Let's assume $|\mathbf{R}| \gg |\mathbf{r}_A|, |\mathbf{r}_B|$. The electric field created by atom A at the position of atom B is

$$\mathbf{E} = -\frac{q}{4\pi\epsilon_0}\frac{1}{R^3}\left[\mathbf{r}_A - 3(\mathbf{r}_A \cdot \mathbf{n})\mathbf{n}\right], \tag{6}$$

  where $\mathbf{n} = \mathbf{R}/|\mathbf{R}|$. Calculate the electrostatic interaction energy $H^{(1)}$ between the two dipoles.

This interaction acts as a perturbation on the Hamiltonian of the two isolated hydrogen atoms.

- 2) Consider the eigenstates of the unperturbed Hamiltonian which correspond to one electron in the $n = 1$ state and one electron in a $n = 2$ state. These eigenstates are degenerate. Count the number of degenerate states (neglecting spin-orbit and other relativistic effects, and assuming that the nuclei are infinitely heavy fixed particles).

- 3) Now assume that $H^{(1)}$ acts as a perturbation which splits the degeneracy of the states found at point 2). Calculate the interaction energy at first order in perturbation theory. Show that this energy goes as R^{-3}. Is the force attractive or repulsive? (Hint: note that if the z axis joins the two nuclei, $H^{(1)}$ commutes with $L_{Az}+L_{Bz}$, where L_{Az} is the projection along the z axis of the angular momentum of electron A, and L_{Bz} the one of electron B)

- 4) Explain qualitatively why the interaction energy is proportional to $-R^{-6}$ when the hydrogen atoms are in the ground state.