

## October 2009 - 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.: Hydrogenic atom in a magnetic field

Let us consider an atom composed by a nucleus of charge  $-Ze$  and one electron. Indicating with  $\mathbf{L}$  and  $\mathbf{S}$  the orbital and spin angular momentum, the Hamiltonian of the electron in a magnetic field  $\mathbf{B} = (0, 0, B)$  can be written as:

$$H = H_0 + \zeta(r)\mathbf{L} \cdot \mathbf{S} + \frac{\mu_B}{\hbar}B(L_z + 2S_z),$$

where  $H_0$  is the Hamiltonian in absence of spin-orbit coupling (the second term) and in zero magnetic field (the third term). Here  $\mu_B$  is the Bohr magneton and  $\zeta(r)$  is a radial function independent from the angular and spin variables.

1. Indicate with  $|n, l, s, j, m_j\rangle$  the eigenstates of  $H_0$ ,  $\mathbf{L}^2$  and  $\mathbf{S}^2$  with total angular momentum (orbital plus spin)  $\mathbf{J}^2$  and  $J_z$  equal to  $\hbar^2 j(j+1)$  and  $\hbar m_j$  respectively.  $n$  is the main quantum number and  $l$  and  $s$  label the orbital and spin angular momentum. Are  $|n, l, s, j, m_j\rangle$  eigenstates of  $H$  when  $B = 0$  and why?
2. Indicate with  $|n, l, s, m_l, m_s\rangle$  the eigenstates of  $H_0$ , with orbital  $\mathbf{L}^2$ ,  $L_z$ , and spin  $\mathbf{S}^2$  and  $S_z$  angular momentum equal to  $\hbar^2 l(l+1)$ ,  $\hbar m_l$ ,  $\hbar^2 s(s+1)$ , and  $\hbar m_s$ , respectively. Show that when the spin-orbit term can be neglected,  $|n, l, s, m_l, m_s\rangle$  are eigenstates of  $H$ .
3. Use now perturbation theory for the general case of an electron in a  $p$  state ( $l = 1$ ). The six states  $|n, l, s, m_l, m_s\rangle$  with  $l = 1$ ,  $m_l = 0, \pm 1$ ,  $s = 1/2$ ,  $m_s = \pm 1/2$  are degenerate eigenstates of  $H_0$ . Write the matrix elements of  $H$  between these six states.
4. Diagonalize the matrix obtained at point [3.] and plot the scaled eigenvalues  $E' = E/\hbar^2\zeta_{n,1}$  as a function of  $x = \mu_B B/\hbar^2\zeta_{n,1}$ , where  $\langle n, 1, 1/2, m_l, m_s | \zeta(r) | n, 1, 1/2, m'_l, m'_s \rangle = \zeta_{n,1} \delta_{m_l, m'_l} \delta_{m_s, m'_s}$ .
5. (Optional) Repeat points [3.] and [4.] for a  $d$  electron ( $l = 2$ ).

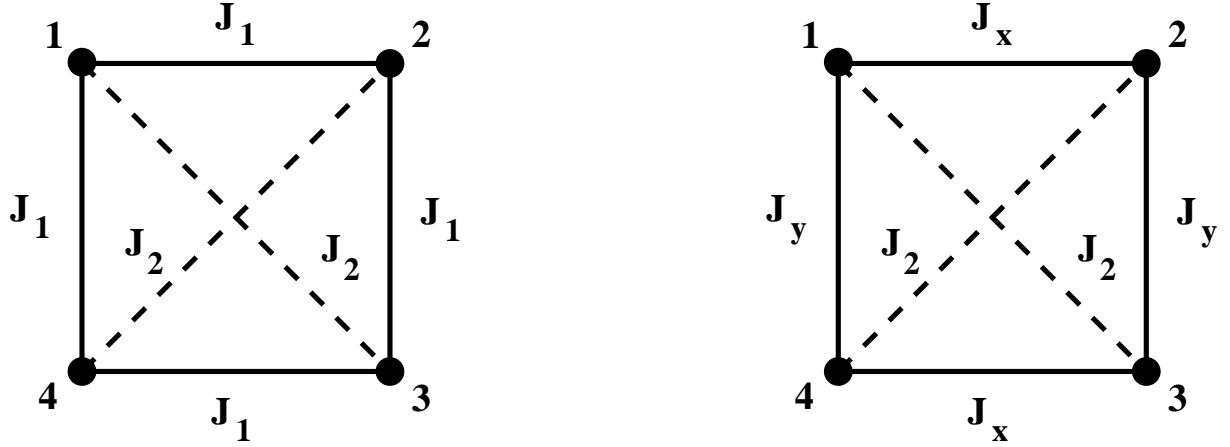


Figure 1: Four-site spin cluster before (left panel) and after (right panel) the deformation.

## Problem 2.: Spin-lattice coupling in a spin cluster

Consider the four-site square cluster in the left panel of Fig. 1. At each site there is a spin  $S = 1/2$ , labeled from 1 to 4 in the figure. The spins are coupled among each other by antiferromagnetic exchange couplings according to the bonds shown in the figure. For instance, spin 1 is coupled to spin 2 by the term  $J_1 \mathbf{S}_1 \cdot \mathbf{S}_2$  and to spin 3 by  $J_2 \mathbf{S}_1 \cdot \mathbf{S}_3$ , with both  $J_1$  and  $J_2$  positive.

1. Calculate the spectrum of the cluster, namely all eigenvalues, as function of  $J_2/J_1$  [Hints: Identify proper quantum numbers, i.e. total spin etc., and re-write the Hamiltonian in terms of them.];
2. Discuss qualitatively the low temperature behavior of the entropy and magnetic susceptibility as function of  $J_2/J_1$ .

Now suppose that the cluster can deform in two possible ways: either the square changes into a rectangle, deformation  $q_1$ , or sites 1 and 3 move up while 2 and 4 down, deformation  $q_2$ . The elastic energy cost of the deformation is

$$\mathcal{K} = \frac{K}{2} (q_1^2 + q_2^2). \quad (1)$$

Assume that, without deformation,  $J_1 = J_2 = J > 0$ , while, after it, the exchange constants change as in the right panel of Fig. 1, with

$$\begin{aligned} J_x &= J \left( 1 + \frac{g}{\sqrt{3}} q_1 + \frac{g}{3} q_2 \right), \\ J_y &= J \left( 1 - \frac{g}{\sqrt{3}} q_1 + \frac{g}{3} q_2 \right), \\ J_2 &= J \left( 1 - \frac{2g}{3} q_2 \right). \end{aligned}$$

- 3.** Including the elastic cost Eq. (1), calculate the ground state energy of the cluster  $E(q_1, q_2)$  and find the minimum with respect to the classical variables  $q_1$  and  $q_2$ . [*Hints:* The perturbation preserves total spin, so its effect is to split and couple among each other states with the same total spin.]

### Problem 3.: Two hydrogen atoms at large distance

Consider two hydrogen atoms placed at a sufficiently large distance, for example 10 Angstrom, an order of magnitude larger than the equilibrium H-H distance in the  $\text{H}_2$  molecule. Assume each proton to give rise to only one bound state electron level, i.e. focus just on the hydrogenic  $1s$  orbitals, of binding energy  $E_0$  (in real H,  $E_0 = 13.6$  eV). Assume next that an electron bound to one proton can “hop” to the other proton bound state with a hopping energy  $-t$ , very small because of the large distance. Finally, assume that if a single proton bound state is occasionally occupied by two opposite spin electrons, their mutual repulsion will reduce the total energy of the two electrons from  $-2 E_0$  to  $-2 E_0 + U$ .

1. Find the total number of two-electron states and classify them according to the total spin quantum number.
2. Calculate eigenstates and eigenvalues as function of  $U$  and  $t$ .
3. Calculate the probability in the ground state to find zero, one or two electrons on a single proton.
4. (Optional) Because the hopping  $t$  will decay exponentially with the H-H distance, this treatment would predict an exponential interaction of the two atoms at large distance. This is well known to be wrong, and the true interaction decays as a power law (nothing to do with the Coulomb interaction of the nuclei, though). Explain why, and identify the crucial missing ingredient in the above model.

## Problem 4.: One-dimensional bound state

One electron moves in one dimension and it is confined to the right half-space ( $x > 0$ ) where it feels a potential energy  $V(x)$ . The Schrödinger equation reads:

$$-\frac{d^2\Psi(x)}{dx^2} - \frac{|g|}{x}\Psi(x) = E\Psi(x)$$

1. What is the ground-state solution of the Schrödinger equation at large  $x$ ?
2. What is the boundary condition at  $x = 0$ ?
3. Find the ground-state wave function and its energy.
4. Calculate the expectation value  $\langle x \rangle$  and  $\langle x^2 \rangle$  in the ground state.
5. Guess the form of the first excited state, determine its energy, and check the orthogonality with respect to the ground state.
6. (Optional) Try to generalize the expression of the eigenvalues of all bound states.