Phys 511: HOMEWORK ASSIGNMENT No (1)

January 22nd 2007

DUE DATE: Monday 5th February 2007.
(Please note that late assignments may not receive a full mark.)

QUESTION (1): EXCHANGE

(i) Hund's rules: Using all 3 of Hund's rules, give the spin and orbital states of:
(a) an Fe^{+3} ion; (b) a Cu^{+2} ion; (c) the Mn^{+4} and Mn^{+3} ions; and (d) the Er^{+2} and Ho^{+2} ions.

(ii) Direct Hund Exchange: Consider an atom with 2 electrons, which are able to go in one of 2 orbital states $|\phi_\alpha\rangle$ and $|\phi_\beta\rangle$, so that with the 2 possible available spin states for each, one can make Slater determinants involving 4 different spin states.

Show that if we now add an interaction $U(|\mathbf{r}_1 - \mathbf{r}_2|)$ between the 2 electrons, then we can derive an effective Hamiltonian for the 2 spins, with an exchange interaction as well as a spin-independent Coulomb interaction; and derive the strength of this interaction.

(iii) 'Kinetic' intersite exchange: Consider a toy model for intersite exchange in which we start with a Hamiltonian

$$H_{toy} \;=\; -t\sum_\sigma (c^\dagger_{A,\sigma} c_{B,\sigma} + H.c.) \;+\; \frac{U}{2}\sum_{j=A,B}\sum_\sigma n_{j,\sigma}n_{j,-\sigma} \tag{1}$$

We assume 2 fermions in the problem. The 6 possible 2-fermion states split into 3 triplet and 3 singlet states. Find the eigenfunctions and eigenenergies of this system as a function of t and U. Calculate also the probability of double occupation of one of the sites as a function of $g = U/4t$.

(iv) Superexchange: Suppose we have 2 TM ions with a p-orbital between them. The p-orbital has 2 unfilled states, whereas the relevant d-orbital on each TM ion has a single unfilled state. The effective Hamiltonian for the system is assumed to be

$$\begin{aligned} H_{eff} \;&=\; E^d_1 d^\dagger_{1\sigma} d_{1\sigma} + E^d_2 d^\dagger_{2\sigma} d_{2\sigma} + \epsilon_p p^\dagger_\sigma p_\sigma \\ &+\; (t_1 d^\dagger_{1\sigma} p_\sigma + t_2 d^\dagger_{2\sigma} p_\sigma \; + H.c.) \;+\; \frac{1}{2}\sum_\sigma (U_1 n^d_{1\sigma} n^d_{1,-\sigma} + U_2 n^d_{2\sigma} n^d_{2,-\sigma} + U_p n^p_\sigma n^p_{-\sigma}) \end{aligned} \tag{2}$$

in which we see that the hopping amplitudes between the p-site and the 2 d-sites are different, as are the local d-site energies and Hubbard U's. In terms of U_1, U_2, U_p, t_1, t_2 and the charge transfer energies $\Delta_1 = \epsilon_p - E^d_1$ and $\Delta_2 = \epsilon_p - E^d_2$, find the superexchange coupling for this system.

QUESTION (2): DIPOLAR INTERACTIONS

Consider the dipolar interaction with spin Hamiltonian

$$H_{dd} \;=\; \frac{1}{2}\sum_{i\neq j}\frac{1}{r^3_{ij}}\left[\mathbf{m}_i\cdot\mathbf{m}_j \;-\; 3\frac{(\mathbf{m}_i\cdot\mathbf{r}_{ij})(\mathbf{m}_j\cdot\mathbf{r}_{ij})}{r^2_{ij}}\right] \tag{3}$$

where $\mathbf{r}_{ij}$ is the radius vector between the 2 spins, which we will assume to have angular coordinates (θ, ϕ) with respect to the z-axis. We assume the moments $\mathbf{m}_j = -2\mu_B \mathbf{S}_j$.

(i) Consider the problem for 2 spins only, and assume they are spin- 1/2. Then this Hamiltonian can be rewritten in the basis of the 4 available spin states $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$. Rewrite H_{dd} in this representation, in terms of the spin operators $\hat{S}_i^z, \hat{S}_j^z$ and $\hat{S}_i^\pm, \hat{S}_j^\pm$.

(ii) Find the eigenvalues of this Hamiltonian

(iii) Now suppose that we apply a transverse field to the problem, so that an extra term

$$\delta H \ = \ -\gamma H_\perp(\hat{S}_i^x \ + \ \hat{S}_j^x) \tag{4}$$

is added to the problem. What are the eigenvalues of the problem now? Plot a graph of eigenvalues of this system, showing in particular the limiting behaviour when the applied field is much weaker/stronger than the dipolar interaction.

QUESTION (3): LANDAU LEVELS

Consider the Hamiltonian

$$H_{LL} \ = \ \frac{1}{2m}[\mathbf{p} + e\mathbf{A}(\mathbf{r})]^2 \ = \ \frac{1}{2m}\pi^{\mathbf{2}}(\mathbf{r}) \tag{5}$$

where for an electron, e is negative, and we assume the electron is moving in the xy plane, with a uniform static field $\mathbf{B} = \nabla \times \mathbf{A}$ oriented along the z-axis.

(i) find the commutation relation between $\hat{\pi}_x$ and $\hat{\pi}_y$, in terms of fundamental constants and the magnetic length $l_o = \sqrt{\hbar/eB}$.

(ii) Show that if we define an operator $a^\dagger = \frac{l_o}{\hbar\sqrt{2}}(\hat{\pi}_x + i\hat{\pi}_y)$, then we can rewrite the Hamiltonian in the form of a simple Harmonic oscillator system.

(iii) Write down a set of coherent states for this oscillator system, and find their overlap.

END OF ASSIGNMENT (1)