AP 295b **Problem Set 4** **Due: Thursday, November 14th, 2002**

Problem 1

In certain materials a narrow energy band, due to the d orbitals of the atoms, lies within a broad energy band, originating from s-type atomic orbitals (For example Cu, Ni). A simple one-dimensional model for these systems is:

$$\mathcal{H}_\circ \;=\; -t\sum_{i\sigma}(c^+_{i\sigma}\,c_{i+1\sigma} + c^+_{i+1\sigma}\,c_{i\sigma}) + E_d\sum_{i\sigma} d^+_{i\sigma}d_{i\sigma} - \Delta\sum_{i\sigma}(c^+_{i\sigma}\,d_{i\sigma} \;+\; d^+_{i\sigma}\,c_{i\sigma})$$

Here $c_{i\sigma}$ annihilate s-type electrons in unit cell i, $d_{i\sigma}$ annihilate localized d-electrons. The electron operators obey the usual anticommutation relations.

a) Calculate the energy spectrum of the electrons for $\Delta = 0$ and $\Delta \neq 0$. Discuss the density of states for the hybridized band.

b) The Anderson Hamiltonian, that describes electrons in a transition metal, also includes the interactions between the electrons

$$\mathcal{H} = \mathcal{H}_0 \;+\; U\sum_i n_{id\uparrow}n_{id\downarrow}$$

where $n_{id\sigma} \;=\; d^+_{i\sigma}d_{i\sigma}$

Discuss the magnetic properties of the system if E_d is less than or greater than E_F, and $E_d + U$ is less than or greater than E_F.

c) In the mean field analysis of the Anderson model one replaces the Anderson Hamiltonian with

$$H_\uparrow \;=\; \sum \varepsilon_c(k)\,c^+_{k\uparrow}\,c_{k\uparrow} \;+ E_d\sum_i n_{id\uparrow} - \Delta\sum_i(c^+_{i\uparrow}\,d_{i\uparrow} \;+\; d^+_{i\uparrow}\,c_{i\uparrow}) + U\sum_i < n_{id\downarrow} > \cdot\, n_{id\uparrow}$$

and a similar one for $H_\downarrow$.

Write the self-consistency condition for the expectation values of the spin occupation of the d states $< n_{d\sigma} >$.

d*) Show that under certain conditions the mean-field approximation predicts the existence of the magnetically ordered state. Calculate the magnitude of the localized moment

$$\mu \;=\; \mu_B \,(< n_{d\uparrow} > - < n_{d\downarrow} >).$$

Note: Experimental realization of the Anderson model with tunable parameters may be possible in artificial semiconductor structures. (C. Marcus, private communication)

Problem 2

The Hamiltonian for the system consisting of the conduction electrons and a localized spin-$\frac{1}{2}$ (the s-d Hamiltonian) is given by:

$$\mathcal{H} \;=\; \sum \varepsilon_k \, a^+_{k\sigma}\, a_{k\sigma} \;+\; \frac{J}{2N} \sum_{kk\prime} \vec{S}\, a^+_{k\alpha}\, \vec{\sigma}_{\alpha\beta}\, a_{k\prime\beta}$$

Here $a^+_{k\alpha}$ are the creation operators for the conduction electrons and $\vec{S}$ is the spin operator for the localized spin. At temperatures below T_k there is a bound state of the impurity spin with the conduction electrons. In the simplest approximation the variational wavefunction for such bound state can be written as:

$$\psi >= \sum_{k>k_f} (\Gamma^{\alpha}_{k\uparrow}\, a^+_{k\uparrow} \;+\; \Gamma^{\alpha}_{k\downarrow}\, a^+_{k\downarrow}) \times |FS > |\alpha >$$

$$+(\Gamma^{\beta}_{k\uparrow}\, a^+_{k\uparrow} \;+\; \Gamma^{\beta}_{k\downarrow}\, a^+_{k\downarrow}) \times |FS > |\beta >$$

where $|FS>$ denotes the wavefunction for the Fermi sea and α and β denote, respectively, the eigen functions for $\uparrow$ and $\downarrow$ spin states of the localized spin. The energy of the bound state ε_B can be defined as:

$$\varepsilon_B \;=\; \frac{< \psi|H|\psi >}{< \psi|\psi >} \;-\; 2 \sum_{k<k_F} \varepsilon_k \;-\; \varepsilon_F$$

a) Show that the energies of the triplet and singlet bound states are given by

$$1 \;+\; \frac{J}{4N} \sum_{k>k_F} \frac{1}{\varepsilon_k \;-\; (\varepsilon_B \;+\; \varepsilon_F)} \;=\; 0$$

$$1 - \frac{3J}{4N} \sum_{k>k_F} \frac{1}{\varepsilon_k - (\varepsilon_B + \varepsilon_F)} = 0$$

b) Show that for $J > 0$ we have a singlet bound state with:

$$\varepsilon_B = -D \left[exp\left(\frac{4n}{3\nu(0)J}\right) - 1\right]^{-1} \simeq -D\, exp\left(-\frac{4n}{3\nu(0)J}\right)$$

where n and $\nu(0)$ are the electron concentration and density of states, respectively.

c) Demonstrate that the wavefunction of the localized state decays as $\cos k_F r/r^2$ for large distances from the impurity atom.

d*) Discuss shortcomings of the variational wavefunction used in this problem and suggest ways to improve it.

Problem 3

Many properites of the collossal magneto resistance (CMR) materials ($e.g.(La,Sr)MnO_3$) and magnetic semiconductors ($e.g.(Ga,Mn)As$) may be understood using Kondo lattice type model

$$\mathcal{H} = \mathcal{H}_{DE} \;+\; \mathcal{H}_{AF}$$

$$\mathcal{H}_{DE} = -\sum_{ij\sigma} t_{ij}(c^{+}_{i\sigma}\, c_{j\sigma} + h.c.) - J_H \sum \vec{\sigma}_i\, \vec{S}_i$$

$$H_{AF} \;=\; J_{AF} \sum_{if} \vec{S}_i\, \vec{S}_j$$

Here $\vec{S}_i$ is the spin of the localized electron orbitals for the Mn atoms on site i (typically $S = \frac{3}{2}$), and $\vec{\sigma}_i \;= \frac{1}{2}\, c^{+}_{i\alpha}\, \vec{\sigma}_{\alpha\beta}\, c_{i\beta}$ is the spin of the conduction electrons on site i (which may vary between $\sigma = 0$ and $\sigma = \frac{1}{2}$. In most situations J_H may be taken to be infinity, so locally the spins are perfectly aligned.

a) For $J_{AF} \;= 0$ and finite density of conduction electrons, show that $\mathcal{H}_{DE}$ favors ferromagnetic ordering of the localized spins $\vec{S}_i$.

Hint: Compare the kinetic energy of conduction electrons when the neighboring $\vec{S}_i$'s are aligned and antialigned.

b) When $J_{AF} > 0$ de Gennes suggested that the ground state will be a canted phase shown in the picture: S^z components of all spins are the same but S^x alternate between the neighboring sites. Explain why this state may have lower energy than the ferro or antiferro ordered states.

c) In the mean-field approximation (i.e. treating spins $\vec{S}_i$ as classical vectors) calculate θ ($tan\theta = \frac{S^x}{S^z}$) as a function of concentration of conduction electrons.

d*) Show that the canted phase has a negative compressibility κ. What does $\kappa < 0$ mean for the stability of the system?

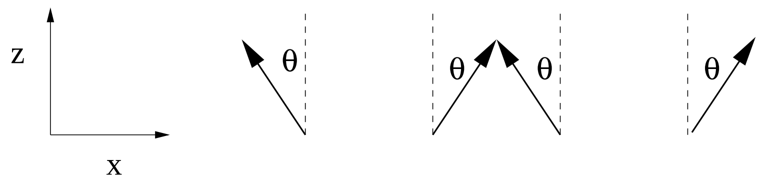

FIG. 1: Problem 3