PHY 555 Problem set #7 Due Wednesday Nov. 9, 2011

1. In class, we did a "microscopic" mean field theory, starting with the Heisenberg Hamiltonian $H = -J\sum \vec{\sigma}_i \cdot \vec{\sigma}_j$, where the sum is over all nearest neighbor pairs (each pair counted once. The result is a mean field formula for the temperature dependence of the "order parameter" <M>, or its dimensionless form m=M/M_0, where M_0 = nμ_B and n is the density of spins. The formula is $m = \tanh(m/t)$.

(a) Rederive this formula, starting with the Heisenberg Hamiltonian, and the replacement $\vec{\sigma}_i \to \langle\vec{\sigma}_i\rangle + (\vec{\sigma}_i - \langle\vec{\sigma}_i\rangle)$, where the second term is the fluctuation around the mean value, and the first term is the mean value. Show that the mean-field result follows from dropping the term quadratic in fluctuations. Show that the formula is insensitive to the spatial dimensionality of the spin lattice.

(b) By solving $m = \tanh(m/t)$ graphically for *m(t)* at a few values of *t*, make a graph that shows all the roots for *t>0*.

(c) Using the fact that Fe (iron) has the bcc structure and has Curie temperature T_c = 1043K, what value of exchange constant *J* is expected in the mean field theory? Do the same for CrO2 (rutile structure, T_c = 386K.)

2. Kittel problem 8, p. 320 **Paramagnetism of S=1 system**. From the clue "paramagnetism" you should deduce that this problem is about non-interacting spins. These spins occur on objects whose dynamics is irrelevant to the magnetization – such as oxygen atoms in vapor.

(a) Find the magnetization as a function of magnetic field B and temperature T for a system of N spins in volume V, with S = 1 (quantized with S_z = 1,0,-1). Their moment is μ, and concentration n=N/V.

(b) In the limit μB << k_BT, obtain the constant C of the Curie law χ=M/H=C/T.

(c) Find the coefficient C of the Curie Law for the same type of system in the classical limit (the spin is distributed with equal probability at any angle – the high S case).

3. The magnetic instability of the interacting electron gas. "Interacting" means that electrons feel each other via the repulsive 1/r Coulomb potential. Overall charge neutrality is achieved by a rigid compensating background charge. As discussed in class, the Hartree-Fock equations have a self-consistent solution when the occupied Hartree-Fock orbitals are plane waves $\psi = \exp(i\vec{k}\cdot\vec{r})/\sqrt{V}$, *V* being the volume of the sample. It was not done in class, but this solution still works if the number of occupied spin-up states differs from the number of occupied spin-down states. The self-consistent computation of the energies is done in a parallel way. This permits a net ferromagnetic spin density $m = n_\uparrow - n_\downarrow$, where the density of electrons *n = N/V* is separated into unequal up and down densities, with $n = n_\uparrow + n_\downarrow$. It then needs to be examined whether the polarized solution or the unpolarized solution has lower energy. The total energy equals $E_{tot} = E_K + E_X$, where the separate kinetic and exchange terms are

$$E_K = \sum_{\vec{k}}^{\text{spins}\uparrow\text{ occupied}} \frac{\hbar^2 k^2}{2m} + \sum_{\vec{k}}^{\text{spins}\downarrow\text{ occupied}} \frac{\hbar^2 k^2}{2m}$$

$$E_X = -\frac{e^2}{2} \sum_{\vec{k},\vec{k}'}^{\text{both spins}\uparrow\text{ occupied}} \frac{1}{|\vec{k}-\vec{k}'|} - \frac{e^2}{2} \sum_{\vec{k},\vec{k}'}^{\text{both spins}\downarrow\text{ occupied}} \frac{1}{|\vec{k}-\vec{k}'|}.$$

For the unpolarized gas, we did the integrals in class, finding the result $E_{tot}/N = (3/5)\varepsilon_F - (3/4\pi)e^2 k_F$. For the polarized gas, this can be generalized to

$$\frac{E_{tot}}{N} = \frac{3}{5}\left(\frac{n_\uparrow}{n}\varepsilon_{F\uparrow} + \frac{n_\downarrow}{n}\varepsilon_{F\downarrow}\right) - \frac{3e^2}{4\pi}\left(\frac{n_\uparrow}{n}k_{F\uparrow} + \frac{n_\downarrow}{n}k_{F\downarrow}\right).$$

where $k_{F\uparrow} = (6\pi^2 n_\uparrow)^{1/3}$, and the other notation follows logically.

(a) Express the total energy in terms of the electron density *n* and the spin density *m*. Evaluate your answer in the limiting cases m=0 and m=n. Also give the Taylor expansion for small m/n to second order.

(b) The magnetization M is $M = m \cdot (g_0 \mu_B / 2) \approx \mu_B m$. The energy per unit volume, $u = nE_{tot}/N$, can be written as $u = \mu_0 \chi^{-1} M^2/2$. This defines the dimensionless susceptibility (SI units.) Use your Taylor series to derive the Pauli susceptibility of the non-interacting gas.

(c) Find the correction to the Pauli susceptibility from E_X. Is there a divergence at some density? What density, and what does it mean?

(d) Find the density at which the total energy of the fully polarized gas (*m=n*) equals that of the unpolarized gas (*m=0*). For what densities is the polarized solution stable?