8.512 Theory of Solids II HW # 4 Due: 04/04/2022

Due: Monday April 4 by 5pm

Reading: class notes

Quantum magnetism

1. [Magnetism of a single atom]

Quantum Langevin paramagnetism arises when an atom with nonzero magnetic moment interacts with an external magnetic field. This interaction is described by the Hamiltonian

$$H = -\mu_B g J_z B$$
,

where μ_B is Bohr's magneton, g is Lande factor and $J_z = -J, -J + 1, ..., J - 1, J$ is a projection of the total angular momentum of the atom \widehat{J} on the direction of the magnetic field. Write down the partition function for such an atom (an ensemble of non-interacting atoms) at temperature T.

- a) [10 pts] Find an average magnetic moment of an atom from this partition function. Express the result in the form $M = \mu_B L_J(x)$, where we defined a dimensionless strength of magnetic field as $x = \mu_B g J B / T$.
 - b) [10 pts] Write down an explicit expression for the function $L_J(x)$.

What is $L_{1/2}(x)$, $L_{\infty}(x)$? In evaluating $L_{\infty}(x)$ replace the sum over $J_z = -J, ...J - 1, J$ by an integral $\int_{-J}^{J} dJ$.

c) [10 pts] Find the magnetic susceptibility per atom, $\chi = dM/dB$, and compare the result with the Langevin's result for a classical magnetic moment.

2. [Mean-field theory of magnetism in solids]

a) [10 pts] Using classical Weiss equation for spontaneous magnetic moment in ferromagnets

$$M = \mu_B L_J(\mu B_{\rm int}/T),$$

assuming that the magnetic moment M of an atom in a crystal "feels" an internal magnetic field $B_{\rm int} = \lambda M$ find the value of Curie temperature T_c below which magnetic order exists. Find an analytic dependence of magnetization M(T) on temperature T for temperatures very close to the Curie temperature. In the final result replace an unknown constant λ by T_c . Sketch the dependence M vs. T for all temperatures.

Hint: Expand L(x) up to the second nonvanishing term.

- b) [10 pts] Weiss antiferromagnetism is described assuming that the magnetic moment μ of an atom in a crystal "feels" an internal magnetic field $B_{\rm int} = -\lambda M$, where M an average magnetic moment and $\lambda > 0$ is some constant.
 - Derive Curie-Weiss law for antiferromagnets by calucating M(B=0,T) using Langevin formulas at high temperatures.
 - What happens if the temperature is lower than the critical temperature T_c ? What is the value of T_c in terms of λ ?
 - Plot the dependence of M(B=0,T).
 - Find the magnetic susceptibility χ at T=0 for this system. Is it para- or diamagnetic?

Hint: In this question take into account that local magnetic moments will arrange in the direction approximately orthogonal to the direction of an applied uniform magnetic field B (why?).

3. [Band magnetism] Itinerant ferromagnetism in interacting Fermi fluids occurs via the Stoner instability. Consider the following Hamiltonian of interacting Fermions

$$H = \int d^3x \left[\sum_{\sigma=\uparrow,\downarrow} \psi_{\sigma}^{\dagger}(x) \left(\frac{p^2}{2m} - \mu \right) \psi_{\sigma}(x) + g \psi_{\uparrow}^{\dagger}(x) \psi_{\downarrow}^{\dagger}(x) \psi_{\downarrow}(x) \psi_{\uparrow}(x) \right]$$

Here $\psi_{\sigma}(x)$ annihilates a fermion with spin $\sigma = \uparrow, \downarrow$ at point x, μ is the chemical potential and g is the strength of contact (delta function) interaction between fermion densities with opposite spins $n_{\uparrow,\downarrow}$ (there is no contact interaction between fermions with equal spins because of fermion exclusion).

- a) [10 pts] Show that the interaction term can be written as $\frac{g}{4}(n^2 4s^2)$, where $n = n_{\uparrow} + n_{\downarrow}$, $s = n_{\uparrow} n_{\downarrow}$. Argue that, at a constant total density, a spin-polarized state allows to gain the interaction energy.
- b) [10 pts] Show that the kinetic energy (the first term in the Hamiltonian above) increases as a function of spin polarization s.
- c) [10 pts] By comparing the results of questions a) and b) determine the value of interaction g_c above which spontaneous spin polarization occurs.
- d) [10 pts] What is the critical exponent β defined by the singularity of the average magnetization near the transition $s \sim (g g_c)^{\beta}$?

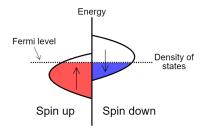


FIGURE 1. Schematic band structure for the Stoner model of band ferromagnetism. An exchange interaction has split the energy of states with different spins, and states near the Fermi energy E_F are spin-polarized.

4. [An exchange interaction mechanism] [10 pts]

This problem illustrates exchange interaction between localized spins mediated by conduction electrons, known as the double exchange mechanism. Consider fermions hoppins between two lattice sites (k = 1, 2) and coupled to localized spins on these sites:

$$H = t(c_{1,\alpha}^{\dagger} c_{2,\alpha} + c_{2,\alpha}^{\dagger} c_{1,\alpha}) - J_H \sum_{k=1,2} \mathbf{S}_k \cdot \frac{1}{2} c_{k,\alpha}^{\dagger} \sigma_{\alpha\beta} c_{k,\beta}$$

where summation over spin indices is assumed. The quantities $\mathbf{S}_{1,2}$ are classical $(S \gg 1)$ core spins at lattice sites 1, 2, respectively. Conduction electrons can hop from one lattice site to another (first term in the Hamiltonian) and interact with core spins by ferromagnetic exchange (Hund's rule) interaction (second term). Assume that there is just one electron on those two sites $\sum_{k=1,2} c_{k,\alpha}^{\dagger} c_{k,\alpha} = 1$. In the limit $J_H \gg t$ find the lowest eigenvalue $E_0(\mathbf{S}_1, \mathbf{S}_2)$ of the electron living at those sites if the core spins do not change in time. Using adiabatic approximation (which is justified by small parameter 1/S) write down an effective Hamiltonian for just core spins ("induced by electron") as

$$H_{eff} = E_0(\mathbf{S}_1, \mathbf{S}_2)$$

Is this interaction ferro- or antiferromagnetic? When can this interaction be replaced by Heisenberg interaction?

- Hint 1. It is convenient to choose orientation of \mathbf{S}_1 along the z-axis.
- Hint 2. Use canonical transformation $c_{2,\alpha} \to U_{\alpha\beta}c_{2\beta}$, such that $U^{-1}\mathbf{S}_2\sigma U = S\sigma_z$.

For original papers on double exchange see:

- 1. C. Zener, Phys. Rev. 82, 403 (1951).
- 2. P. W. Anderson and H. Hasegawa, Phys. Rev. 100, 675 (1955).
- 3. P. G. de Gennes, Phys. Rev. 118, 141 (1960).