Physics 602

Homework Set 2

Due date: Monday, March 21, at the end of the lecture.

Note: you are allowed to use only the textbook (Grosso & Parravicini), lecture notes, materials that I specifically provided, and Mathematica or other similar software to do the homework.

1. Recall that we proved in class the Bohr-van Leeuwen theorem about the absence of magnetism from purely classical arguments. However, we can still treat localized magnetic moments purely classically. Consider a paramagnetic solid that consists of noninteracting magnetic ions with magnetic moment $\vec{\mu}$. Suppose a weak uniform magnetic \vec{B} is applied. Ignore any orbital degrees of freedom, i.e. take the energy to be $E = -\vec{\mu} \cdot \vec{B}$.

- 1. Treating $\vec{\mu}$ as classical vector of fixed length and using classical statistical mechanics, compute the average component of the magnetic moments along the field. Derive the Curie law, $M = C_{cl}/T$ and determine C_{cl} .
- 2. Repeat the same exercise, but for a quantum magnetic moment $\vec{\mu} = -g\mu_B \vec{J}$, where \vec{J} is a quantum spin of magnitude J. In what limit do you expect the quantum Curie constant C_q to agree with its classical counterpart C_{cl} ? Is this the case?

2. N noninteracting spin-1/2s (no orbital degrees of freedom, just spins) are placed in a magnetic field of strength B. Compute the heat capacity of the system $C_V = \partial U/\partial T$, where U is the internal energy of the system.

3. Two-site Hubbard model. Consider the Hubbard Hamiltonian for two sites

$$H = -t\sum_{\sigma} (c_{1\sigma}^{\dagger}c_{2\sigma} + c_{2\sigma}^{\dagger}c_{1\sigma}) + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}), \quad U > 0$$

Assume there are two electrons in the system.

- 1. Find the eigenvalues and eigenvectors of the Hamiltonian. Plot the eigenvalues
- 2. Now let's analyze the large U limit. Observe that for large U the spectrum consists of high and low energy sectors separated by a large gap $\approx U$ (these become the upper and lower Hubbard bands, respectively, for an infinite lattice). Discard the high energy sector. In the low energy sector, determine the eigenstates and eigenvalues to the leading order in 1/U and assign a total spin value to each eigenstate. Show that the low energy sector is that of a two-site antiferromagnetic Heisenberg Hamiltonian $J\vec{s_1} \cdot \vec{s_2}$, where $\vec{s_1}$ and $\vec{s_2}$ are spins of the electrons, and determine J in terms of t and U.