PHYSICS 219

Homework 6

Hand in to me or my mailbox on or before the final exam on Monday June 12.

1. *Neutron scattering cross section due to magnetic scattering.*
   Neutrons have a magnetic moment, $\vec{\mu}$, which interacts with the magnetic moment of the spins in the system, $\vec{\mu}_i = g\mu_B \mathbf{S}_i$, where g is the Landé g-factor and μ_B is the Bohr magneton, through the dipole-dipole interaction. Determine the inelastic scattering cross section for magnetic scattering in the Born approximation. You may assume that the neutron beam is unpolarized. Show that only the spin components transverse to the momentum transfer contribute.
   Hint: If you have difficulty you should find help in W. Marshall and S. W. Lovesey, "Theory of Thermal Neutron Scattering" or S. W. Lovesey "Theory of neutron scattering from condensed matter", Vol. 2. Neglect any orbital contribution to the magnetic moment of the solid. The main thing you need to know is what the magnetic dipole-dipole interaction looks like in $\mathbf{q}$-space. This is discussed in E & M textbooks like Jackson. See also my notes from another class that I taught `http://apyoung.com/232/rpa2.pdf`, Eq. (41). (Remember that the interaction of two magnetic dipoles $\mathbf{m}_1$ and $\mathbf{m}_2$ can be obtained from $-\mathbf{m}_1 \cdot \mathbf{B}(\mathbf{r}_1)$, where $\mathbf{B}(\mathbf{r}_1)$ is the magnetic field at dipole 1 due to dipole 2.)

   Note: Neutron scattering measurements are generally performed with an unpolarized beam, in which case the cross section involves the nuclear scattering, as well as the magnetic scattering. However, additional information can be obtained if the the beam is spin-polarized (though at the price of some loss of intensity). In particular one can separate out magnetic scattering from other forms of scattering by measuring the *difference* in scattering cross section for different polarizations.

2. *An expression for the susceptibility*
   Consider a system with Hamiltonian $\mathcal{H}$ to which we add a small static perturbation f which couples to some variable in the system, A say, *i.e.* the total Hamiltonian is

   $$\mathcal{H} - fA .$$

   We have already seen that a *classical* expression for the zero field linear response function (susceptibility), χ, defined by

   $$\langle A \rangle = \chi f + \cdots ,$$

   is

   $$\chi = \frac{1}{k_B T} \langle AA \rangle ,$$

   where, in this expression and in the rest of the problem (unless otherwise stated), averages are evaluated with $f = 0$. We will also assume throughout this question that $\langle A \rangle = 0$ if $f = 0$.

   Here we consider the quantum case, for which we may *not* assume that A and $\mathcal{H}$ commute.

   (a) Show, using the cyclic invariance of the trace, that the non commutativity of A and $\mathcal{H}$ does *not* matter for the *first* derivative of the free energy with respect to f, and that the obvious expression for $\langle A\rangle$,

$$\langle A\rangle = \frac{\text{Tr } Ae^{-\beta[\mathcal{H}-fA]}}{\text{Tr } e^{-\beta[\mathcal{H}-fA]}} \ ,$$

is also equal to $-\partial F/\partial f$, where F is the free energy.

(b) Show that the non-commutativity does, however, matter for the second derivative and that the susceptibility can be written as

$$\chi = \int_0^\beta d\tau \langle A(\tau)A\rangle \ ,$$

where

$$A(\tau) = e^{\tau\mathcal{H}} A e^{-\tau\mathcal{H}} \ .$$

Hint: In order to carry the second derivative of the free energy with respect to f, write

$$\exp(-\tau[\mathcal{H} - fA]) = \exp(-\tau\mathcal{H}) \ S(\tau) \ ,$$

where $0 \le \tau \le \beta$, and find $dS/d\tau$. Simplify this expression to first order in f and integrate (what is $S(0)$?)

(c) Write out the answer to part (b) explicitly in terms of exact eigenstates $|n\rangle$ and eigenvalues E_n of $\mathcal{H}$, and the probability of occupancy of these states, P_n, and do the integral. Show that there are two types of terms (i) those with an overall factor of $1/T$ (which by themselves give a Curie law, $\chi \sim 1/T$ at low temperature) and those without such a factor (which are purely quantum mechanical and have no classical analogue, and by themselves give a temperature independent susceptibility at low T). The latter are often called Van Vleck terms.

Note: The expression for $A(\tau)$ looks similar to that of a time dependent operator in the Heisenberg picture of quantum mechanics but at *imaginary time*. This is not a coincidence, and results from the similarity between the time evolution operator in quantum mechanics, $\exp(it\mathcal{H}/\hbar)$, and the statistical operator in statistical mechanics, $\exp(-\beta\mathcal{H})$. This analogy is heavily exploited in many body theory.

3. *A trivial application of the equations of motion method.*
Consider a spin $\mathbf{S}$ in a magnetic field H. Compute the the spin Green functions from their equations of motion (no approximations are needed for this simple example) and show that they have poles at the Larmor frequency for spin precession.

4. *A non-trivial application of the equations of motion method.*
Consider the spin-1/2 Ising model in a transverse field, whose Hamiltonian is given by

$$\mathcal{H} = -\sum_{\langle i,j\rangle} J_{ij} S_i^z S_j^z - \Gamma \sum_i S_i^x ,$$

where the $\mathbf{S}_i$ are spin-1/2 operators. From the equations of motion technique and using the random phase approximation (RPA), compute the Green function $\langle\langle S^z; S^z\rangle\rangle_{k,\omega}$. You should give the result both above T_c, where $\langle S^z\rangle = 0$, and also below T_c. From this, show that the RPA predicts that there is an elementary excitation at wavevector $\mathbf{k}$ of frequency, $\omega_{\mathbf{k}}$, given by

$$\omega_k^2 = \Gamma\left(\Gamma - J(\mathbf{k})\langle S^x\rangle\right) + J(0)\langle S^z\rangle^2 \ ,$$

where $J(\mathbf{k})$ is the Fourier transform of J_{ij}. Hence show using the mean-field value for $\langle S^x\rangle$, that the frequency of the $\mathbf{k} = 0$ mode goes to zero at the (mean field) transition temperature. (The mean field theory for the statics of this model was done in Problem 1 of homework set 4). This mode with zero frequency is known as a "soft-mode" and is a common feature of second order transitions. Sketch $\omega_{\mathbf{k}=0}$ against T showing both regions, $T > T_c$ and $T < T_c$.

Note: The RPA is an approximation for dynamics which is analogous to the mean field approximation for statics. Note also that a weakness of the RPA is that it predicts no damping of the excitations.