PHYSICS 847

**Home Work Assignment # 5** 5/7/2009

Due: Tuesday, 5/19/2009

**1.** Read the exact solution for the one dimensional (1D) Ising chain from your text.

(i) Work through the derivation of the zero field ($H = 0$) free energy

$$F(T) = -Nk_BT \ln\left[2\cosh(J/k_BT)\right].$$

(ii) Look at the derivation of the Free energy in a finite field and the magnetization $m(T, H)$, even if you do not work through all the details.
(iii) Work through the derivation of the spin-spin correlation function $\langle S_i S_j \rangle$ as a function of separation $r = |i - j|$ for $H = 0$.
(iv) Look carefully at the various plots of thermodynamic functions for the 1D Ising chain shown in your book along with their comparison to mean field approximation results.

Now for the only part that you have to do. Check for $H = 0$ the classical fluctuation-dissipation theorem relating the susceptibility to the correlation function.

**2.** In this problem we will explore First-order or discontinuous transitions in a system described by a Landau Free energy functional of the form

$$\mathcal{F}(\phi) = \frac{1}{2}r\phi^2 - w\phi^3 + u\phi^4 + \ldots$$

The order parameter is a scalar $\phi$ but the symmetries of the problem give rise to a third order term absent in the case of magnetic systems studied in class. Such "cubic invariants" in $\mathcal{F}$ arise in the study of melting (solid-liquid phase transition) and in the study of liquid crystals (nematic-to-isotropic transition) for reasons which we will not go into here.

As usual we will choose $r$ to be positive at high $T$ and negative at low $T$ so that

$$r = a(T - T^*),$$

where $T^*$ is *not* the phase transition temperature and its meaning will be clarified below. We will take $w > 0$ and $u > 0$ to be independent of temperature.

**(a)** Make careful sketches of $\mathcal{F}$ as a function of $\phi$ at various temperatures. Much of the rest of this problem will make use of these plots!

**(b)** Show graphically that, coming down from high $T$, there is a temperature $T^{**}$ at which a new minimum first appears in $\mathcal{F}$ at a non-zero value of $\phi$. Find an expression for $T^{**}$ in terms of the parameters of the model $a, w, u$ and $T^*$.

**(c)** At a temperature $T = T_p$ this second minimum becomes degenerate with minimum at $\phi = 0$, which was stable at high $T$. Argue that there is a first order phase transition at $T_p$. Determine $T_p$ in terms of the parameters $a, w, u$ and $T^*$, and also determine the corresponding value of the order parameter $\phi_p$.

**(d)** From the graphs of $\mathcal{F}(\phi)$ discuss what happens at $T^*$. Specifically what is the key difference between $T > T^*$ and $T < T^*$?

**(e)** A general phenomenon associated with first-order transitions is *hysteresis* when cycling through the transition and the related effects of supercooling and superheating. Discuss the significance of the three temperatures $T^{**}, T_p, T^*$ from this perspective.

**(f)** Although the Landau theory of phase transitions can describe first-order phase transitions in a qualitatively reasonable manner, in general it is much better suited to describe continuous phase transitions. Why? Under what conditions does the description of a first-order transition become more accurate?

**3.** *Ising Model with Vacancies:* Consider a generalization of the Ising model where the spin on each site can take *three* values $S_i = +1, 0, -1$. Sites with $S_i = 0$ may be thought of as vacancies that are free to move. The system is described by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j + \Delta \sum_i S_i^2$$

where $J > 0$ is a ferromagnetic interaction between neighboring sites of a lattice with coordination number $q$ (= number of nearest neighbors).

**(a)** Describe qualitatively the ground state that you expect in in the limit of very large positive $\Delta$, i.e., $T = 0 < J \ll \Delta$. Do you expect a phase transition as $T$ increases? If so, make a crude estimate of $T_c$.

**(b)** Describe qualitatively the ground state that you expect for very large *negative* $\Delta$, i.e., $T = 0 < J \ll |\Delta|$. In this case, do you expect a phase transition as $T$ increases? If so, make a crude estimate of $T_c$.

**(c)** Next, consider this model at zero temperature and determine its phases and the location of phase transition(s) as a function of the parameter $K = \Delta/qJ$ as follows.
Let $N_0$ be the number of vacancies in the ground state. Obtain an expression for the ground state energy $E$ as a function of $N_0$ by arguing that the system *phase separates* into two regions: one with all the (non-zero) spins clumped together and the other with all the vacancies grouped together. In the expression for $E$ ignore the effects along the boundary between the two regions in the thermodynamic limit. Minimize $E(N_0)$. Check that your answer agrees with the $T = 0$ limits discussed qualitatively in (a) and (b).

**(d)** Now consider the effect of finite temperatures within a mean field approach. Denote the mean magnetization per site by $m$, and obtain a mean field Hamiltonian $\mathcal{H}_{\text{mf}}$ for this system by making a mean field approximation for the ferromagnetic coupling term by writing $S_i = m + \delta m_i$, where $\delta m_i = S_i - m$ and ignoring fluctuations. You can treat the $S_i^2$ term exactly.

**(e)** Define the mean field free energy $F_{\text{mf}}(m)$ as

$$\exp\left[-\beta F_{\text{mf}}(m)\right] = \text{Tr}\exp\left(-\beta\mathcal{H}_{\text{mf}}\right)$$

where the "trace" is a sum over all spin configurations $\{S_i = 0, \pm 1\}$.
Show that the dimensionless free energy per site $f(m) \equiv F_{\text{mf}}(m)/NqJ$ is given by

$$f(m) = \frac{m^2}{2} - \tilde{T}\ln\left[1 + 2y^{-1}\cosh\left(\frac{m}{\tilde{T}}\right)\right]$$

with the dimensionless temperature $\tilde{T} \equiv k_B T/qJ$ and the dimensionless coupling $y \equiv \exp(K/\tilde{T})$ where $K = \Delta/qJ$ was defined in part (c) above.

**(f)** The thermal equilibrium value of $m$ is obtained by minimizing the free energy. In general this can be done numerically. Here we will specialize to the case where $m$ is small and consider an expansion of the free energy in powers of $m$:

$$f(m) = \text{const.} + Am^2 + Bm^4 + Cm^6 + \ldots$$

This is the Landau Free energy for this problem and we will see that it is necessary to go to sixth order here.
Determine $A, B, C$ as functions of temperature $\tilde{T}$ and the coupling $y$. (This is straightforward but tedious and you can use Mathematica if you want).

**(g)** Find the condition for $C > 0$ which is required for stability (if we truncate the expansion at sixth order). Then find the condition under which $B$ is also positive. Under these conditions, it is possible to obtain a continuous ("second order") phase transition within the mean field approach. Find the locus in the $(\tilde{T}, K)$-plane where a continuous transition takes place.

**(h)** Find the location of the "tricritical point" in the $(\tilde{T}, K)$-plane at which both $A = 0$ and $B = 0$.

**(i)** For temperatures below the tricritical point, argue from the form of $f(m)$, that that the phase transition becomes discontinuous ("first order"). To make a rough estimate of the first order phase boundary in the $(\tilde{T}, K)$-plane one may use the following argument: (1) the tricritical point value of $K$ is quite close to the $T = 0$ transition found in part (c), and (2) using the Clausius-Clapeyron relation and the third law of thermodynamics the phase boundary must come in with zero slope at $T = 0$.