Phase Transitions

Homework Sheet 2
Due 10am 16th Feb 2017, in the 563 box.

Please attempt these problems without referring to textbooks, although you may use your notes. The most efficient way to learn is to attempt a question and then if you are stuck, read the relevant section of the notes, then close the notes and try again.

Question 2–1.
This question concerns the convexity of the free energy for the nearest neighbour Ising model:

$$-H_\Omega\{S\} = H\sum_i S_i + J\sum_{<ij>} S_i S_j$$

(a) Show that $g(\beta) \equiv \lim_{N(\Omega)\to\infty} \log Z_\Omega(\beta)/N(\Omega)$ is convex down in β.
(b) By considering the second derivative of $g(\beta)$ or otherwise, show that the free energy per unit volume $f(T) = -(1/\beta)g(\beta)$ is convex up in T. Try to be as careful as you can.
(c) The Gibbs free energy is defined as

$$\Gamma_\Omega(M) = F_\Omega(H(M)) + N(\Omega)MH(M)$$

where $H(M)$ is given implicitly by $M(H) = -\partial f/\partial H$. Show that $\Gamma(M)$ is convex down in M.
(d) Sketch the form of $\Gamma(M)$, $f(H)$, $M(H)$, $M(T)$, $H(M)$, for the cases $T > T_c$ and $T < T_c$. Quantities without the subscript Ω are taken in the thermodynamic limit. What is the form of the quantities above for a finite system Ω?

Exercise 2–2. This question concerns the infinite-range Ising model, where the coupling constant $J_{ij} = J$ for all (sometimes abbreviated by the symbol $\forall$) i, j (*i.e.* no restriction to nearest neighbour interactions).

$$-H_\Omega\{S\} = H\sum_i S_i + \frac{J_0}{2}\sum_{ij} S_i S_j$$

You will solve this model using a method referred to as the Hubbard-Stratonovich transformation, or auxiliary fields. Although it is nothing more than completing the square, this technique is one of the most useful tricks in the physicist's arsenal. The virtue of the present example is that you will be able to calculate a partition function in an essentially exact way, and see precisely how it is that the thermodynamic limit or the zero temperature limit are required in order for there to be a phase transition.

This is the first of several similar looking calculations which derive mean field theory in a systematic way. Making the range of the interactions infinite means that each degree of freedom feels every other degree of freedom, so that fluctuations are reduced. The concept of mean field is not an approximation in such a system.

(a) Explain why this model only makes sense if $J_0 = J/N$, where N is the number of spins in the system.

(b) Prove that

$$\exp\left\{\frac{a}{2N}x^2\right\} = \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi/Na}}\, e^{-\frac{Na}{2}y^2 + axy} \qquad \text{Re } a > 0.$$

(c) Hence show that

$$Z_\Omega = \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi/N\beta J}}\, e^{-N\beta L}$$

where

$$L = \frac{J}{2}y^2 - \frac{1}{\beta}\ln\left\{2\cosh(\beta(H + Jy))\right\}.$$

When can this expression become non-analytic?

(d) In the thermodynamic limit, this integral can be evaluated exactly by the method of steepest descents. The method of steepest descents can be crudely thought of as approximating an integral by the value of the integrand evaluated at the point where the integrand has its largest value within the range of integration. A much more detailed account is given in many mathematics books, the best of which is that by C. Bender and S. Orszag, but you do not need such sophistication to solve this homework problem. Show that

$$Z(\beta, H, J) = \sum_i e^{-\beta N L(H,J,\beta,y_i)}$$

and find the equation satisfied by y_i. What is the probability of the system being in the state specified by y_i? Hence show that the magnetisation is given by

$$M \equiv \lim_{N(\Omega)\to\infty} \frac{1}{\beta N(\Omega)} \frac{\partial \ln Z_\Omega}{\partial H} = y_0$$

where y_0 is the position of the global minimum of L.

(e) Now consider the case $H = 0$. By considering how to solve the equation for y_i graphically, show that there is a phase transition and find the transition temperature T_c. Discuss the acceptability of all the solutions of the equation for y_i both above and below T_c.

(f) Calculate the isothermal susceptibility

$$\chi_T \equiv \frac{\partial M}{\partial H}.$$

For $H = 0$, show that χ_T diverges to infinity both above and below T_c, and find the leading and next to leading behaviour of χ_T in terms of the reduced temperature $t = (T - T_c)/T_c$.

Question 2–3.

(a) Review to your own satisfaction the statistical mechanics of fluids as given in §2.11 of my book. (No need to hand anything in.)

(b) Work through the algebra of the Ising model – lattice gas analogue given in §2.12. (No need to hand anything in.)

(c) Consider the following simple model of a β-brass binary alloy. Equal numbers of copper and zinc atoms reside on the sites of a body-centred cubic lattice. At high temperatures, each site is occupied at random by either copper or zinc. At $T = T_c$, it is found that there is a continuous phase transition to a state of order where each atomic species is found preferentially on one of the two sub-lattices of the b.c.c. lattice. The order parameter for this transition may be chosen to be the difference between the expected number of copper and zinc atoms on a chosen sub-lattice. Let the variable $S_i = +1$ if site i is occupied by a copper atom and $S_i = -1$ if it is occupied by a zinc atom. Assume that the interaction between all types of atom is nearest neighbour (i.e. define energies J_{CuCu}, J_{CuZn} etc), write down an appropriate Hamiltonian for a lattice gas model of this alloy. Show that it reduces to the nearest neighbour Ising model Hamiltonian, with an exchange interaction

$$J = \frac{1}{4}(J_{CuCu} + J_{ZnZn} - 2J_{CuZn}).$$

Your result shows that this system is in the same universality class as the Ising ferromagnetic transition. Is there any analogue of the external magnetic field for the alloy system? If so, what would the phase diagram be expected to be?