PHYSICS 219

Homework 5

Due in class, Wednesday May 31

1. *Review question*
   Consider a single spin-1 Ising spin in a field h. The Hamiltonian is given by

   $$\mathcal{H} = \Delta S^2 - hS,$$

   where $\Delta > 0$ and S takes the values ± 1 and 0. The term in S^2 could represent energy level splittings caused by the environment of the magnetic ion in the crystal. These are called "crystal field splittings".

   (a) What are the energy levels?

   (b) Compute the partition function and free energy.

   (c) From part 1b compute the energy and specific heat.

   (d) From part 1b compute the magnetization.

   (e) Hence compute the zero-field susceptibility, χ. Show that χ vanishes both as $T \to \infty$ and as $T \to 0$.

2. *Location of the "tricritical point" of a spin-1 model*
   Consider the spin-1 Ising model of the previous question but with the spins now coupled by interactions, so the Hamiltonian is

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

   where again $\Delta > 0$ and $S_i = 1, 0$ or -1. The interactions J_{ij} are equal to $J\,(> 0)$ if i and j and nearest neighbors and 0 otherwise. (Take the number of nearest neighbors to be z).

   (a) Consider $T = 0$. Show that the ground state has all S_i equal to 0 if $\Delta > zJ/2$ and has either all $S_i = 1$ or all -1 if $\Delta < zJ/2$. Hence there is a first order (discontinuous) transition at $T = 0$ as a function of changing Δ.
   Note: You may assume here that in the ground state all spins are equal.

   (b) Find the self consistent equation determining the magnetization $m \equiv \langle S_i \rangle$ in the mean field approximation.

   (c) Assuming that the transition is continuous (second order) show that the equation which determines T_c for a given value of Δ is

   $$e^{\beta\Delta} = 2(\beta J z - 1)\,.$$

   Hence determine T_c to first order in Δ.
   Note: The transition *is* second order for Δ small.

(d) Although the transition is second order for small Δ, it turns out to be first order for larger Δ. The point where the transition changes from second order to first order is called a "tricritical point". (In the Landau theory description it is where the coefficients of *both* the quadratic and quartic terms vanish.) To locate first order transitions, in general you need to not only determine the value of m in the $m \neq 0$ phase, but also the free energies of the $m \neq 0$ and $m = 0$ phases. The stable phase is the one with lower free energy.

However, we can determine determine the location of the tricritical point here by the following arguments.

The solution to part 2b is of the form

$$m = f(m, \Delta, T) .$$

Expand f in powers of m up to the first two non-vanishing orders

$$f(m, \Delta, T) = mA(\Delta, T) + m^3 B(\Delta, T) + \cdots ,$$

and determine the functions A and B.

(e) Show graphically that you expect a second order transition if $B(\Delta, T) < 0$ at the point where $A(\Delta, T) = 1$ but that you expect it to be be a first order transition if $B(\Delta, T) > 0$. Hence the tricritical point is where

$$A(\Delta, T) = 1, \quad B(\Delta, T) = 0 .$$

(f) Show that the solution is

$$e^{\beta\Delta} = 4, \quad \beta J z = 3 ,$$

see Capel, Physica, **32**, 966, (1966), who, unfortunately, uses a cumbersome version of mean field theory, and non-intuitive notation.

(g) Sketch the phase diagram. You should show the location of the critical point at $\Delta = 0$, the location of the phase transition at $T = 0$, the location of the tricritical point, and the region where the transition is second order and the region where it is first order.

3. *Estimate* $\ln 2$ *by Monte Carlo sampling.*
Determine

$$\int_0^1 \frac{1}{1+x}\, dx ,$$

by Monte Carlo sampling, (i.e. choose n values of x at random and evaluate the integrand for those values of x). Estimate the error by repeating the calculation m times (where m could be 100) for the same number, n, of x-values but with different random numbers. Check that your answer agrees with the exact value to within roughly the expected error. Then repeat this procedure for different values of n and check that the error goes *roughly* as $n^{-1/2}$.

4. *High temperature series expansions.*
From the coefficients given in the handout for the expansion of the susceptibility for the Ising model, i.e.

$$k_B T \chi = \sum_{n=0}^{\infty} a_n \mathrm{v}^n$$

where

$$\mathrm{v} = \tanh(\beta J) \ ,$$

estimate the critical value v_c and the critical exponent γ for (i) the square lattice, (ii) the diamond lattice, (iii) the simple cubic (s.c.) lattice, and (iv) the body centered cubic (b.c.c.) lattice. (Hint: plot successive ratios against $1/n$ and fit.) Check that you obtain universality, i.e. the exponents only depend on dimension, not on the coordination number (in particular the coordination of the square and diamond lattices are the same and the low order terms in the expansion are very similar, yet the exponents are very different.)

Compute the ratio of the transition temperature that you find to the mean field prediction for each lattice. Compare your answer for T_c or v_c for the square lattice with the exact result obtained from duality.