Phase Transitions

Homework Sheet 4
Due 10am Mon Mar 13th 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 4–1.

This is a review of the Van der Waals equation of state, with the goal of calculating its critical point. The Van der Waals equation is

$$\left(p + \frac{a}{V^2}\right)(V - b) = Nk_BT$$

(a) Derive heuristically the Van der Waals equation by considering how the ideal gas equation of state is modified by the two key features of interparticle interactions: (i) short-range hard core repulsion and (ii) long-range attractive interactions. You do not need to do any formal calculations such as virial and cluster expansion, but you should explain where the term proportional to V^{-2} comes from, and why the power law is -2 in that term. (*Hint: I find it easiest to approach this by writing the ideal gas equation of state in the form* $p = Nk_BT/V$). Where did you make a mean field approximation?

(b) Sketch the isotherms we expect to see experimentally for a real physical fluid in the $p - V$ plane for several temperatures above, below and at the critical temperature.

(c) On the same diagram sketch the isotherms for the Van der Waals fluid, and explain why at the critical point, all solutions v_i $(i = 1 \ldots 3)$ to the equation $p = p(v)$ become degenerate at the critical point: $v_i = v_c$. The Van der Waals isotherms differ from your answer to (b): in what part of the Van der Waals isotherm is the behavior not just different from (b) but completely unphysical? Here $v \equiv V/N$.

(d) By writing the Van der Waals equation as a cubic in v, and equating it to $(v - v_c)^3 = 0$, calculate the critical values of p_c, v_c and T_c in terms of the coefficients a and b introduced above.

(e) Show that near the critical point, the Van der Waals equation of state has the same equation of state that we derived in class for the Ising model in the mean field approximation. Hence calculate the critical exponents of the liquid-gas transition in the mean field approximation.

Question 4–2.

In HW 2, you studied the infinite range Ising model, and showed how a phase transition can occur in the thermodynamic limit. Your results were very similar to those of the Weiss model of ferromagnetism, because in a mean field description such as the Weiss model, every spin is interacting with every other spin. In this question, we will look at the nearest neighbour Ising model, and systematically derive mean field theory by the method of steepest descents. This approach, based on the Hubbard-Stratonovich transformation is probably the most general method for turning statistical mechanics problems into field theories. We will see that mean field theory just comes from taking the maximum term in the partition function. The Hamiltonian is

$$H_\Omega\{S\} = -\frac{1}{2}\sum_{i\neq j} J_{ij}S_iS_j - \sum_i H_iS_i$$

where $J_{ij} = J > 0$ if i and j are nearest neighbours and $J_{ij} = 0$ otherwise. In this question, we will use Einstein's summation convention: repeated indices are to be summed over, *i.e.* $A_{ij}x_j \equiv \sum_j A_{ij}x_j$.

(a) Prove the identity

$$\int_{-\infty}^{\infty}\prod_{i=1}^{N}\left(\frac{dx_i}{\sqrt{2\pi}}\right)\exp\left(-\frac{1}{2}x_iA_{ij}x_j + x_iB_i\right) = \frac{1}{\sqrt{\det \mathrm{A}}}e^{\frac{1}{2}B_i(A^{-1})_{ij}B_j}$$

where A is a real symmetric positive matrix, and $\mathbf{B}$ is an arbitrary vector. [*Hint: Make change of variables* $y_i = x_i - (A^{-1})_{ij}B_j$.]

(b) We want to use the above identity to make the term in the Hamiltonian with S_iS_j linear in S_i, just as you did for the infinte range model. Why can you not do that straight away? Show that this technical point is easily dealt with by a trivial redefinition of the zero of energy.

(c) Apply the identity of part (a), making the identification $A^{-1}_{ij} = J_{ij}$ and $B_i = S_i$. Show that (apart from an unimportant constant of proportionality)

$$Z = \int_{-\infty}^{\infty}\prod_{i=1}^{N} d\psi_i e^{-\beta S(\{\psi_i\},\{H_i\},\{J_{ij}\})}$$

where

$$S = \frac{1}{2}(\psi_i - H_i)J^{-1}_{ij}(\psi_j - H_j) - \frac{1}{\beta}\sum_i \log(2\cosh\beta\psi_i).$$

This form for the partition function is really what is meant by the term functional integral. The dummy variable ψ_i is like a function $\psi(\mathbf{r})$ in the limit that the lattice spacing $a \to 0$ and $N \to \infty$.

(d) Assume that we can approximate Z by the maximum term in the functional integral: $Z \approx \exp -S(\bar{\psi}_i)$ where $\bar{\psi}_i$ is the value of the field ψ_i which minimises S. Find the equation satisfied by $\bar{\psi}_i$, and show that the magnetisation at site i,

$$m_i \equiv \langle S_i\rangle = -\partial F/\partial H_i \approx -\partial S/\partial H_i$$

is given by $m_i = \tanh\beta\bar{\psi}_i$. Hence find $H_i(\{m_j\})$.

(e) Let $\bar{S}$ be the value of S at $\psi_i = \bar{\psi}_i$. The mean field approximation is that the free energy $F \approx \bar{S}$. Show that

$$\bar{S}(\{m_i\}) = \frac{1}{2}J_{ij}m_im_j - \frac{1}{\beta}\sum_i \log\left(\frac{2}{\sqrt{1-m_i^2}}\right).$$

Hence calculate the mean field approximation to the Gibbs free energy from the Legendre transform

$$\Gamma\{m_i\} = \bar{S} + \sum_i H_i(\{m_j\})m_i.$$

Verify that the equation of state is correctly given by $H_i = \partial\Gamma/\partial m_i$.

Question 4–3.

(a) There is a well-known thermodynamic relation for fluids connecting the heat capacity at constant pressure with that at constant volume. Show that there is an analogous result for magnetic systems: $C_H - C_M = \frac{T}{\chi_T}\left(\frac{\partial M}{\partial T}\right)_H^2$. Hence show that $C_H \geq \frac{T}{\chi_T}\left(\frac{\partial M}{\partial T}\right)_H^2$.

(b) Using the definitions of the critical exponents, show that the inequality you have found can only be satisfied if $\alpha + 2\beta + \gamma \geq 2$.

(c) We will see later that the RG implies that the singular part of the bulk free energy per site $f(t, H)$ must have the so-called *scaling form*

$$f(t, H) = Ht^\beta F_f\left(\frac{H}{t^{2-\alpha-\beta}}\right),$$

where the so-called *scaling function* F_f has only one argument, and possesses certain analytical properties as its argument tends to zero or infinity. Show that the scaling form implies that the exponents actually satisfy $\alpha + 2\beta + \gamma = 2$. What did you need to assume about F_f?

(c) A consequence of the RG is that for $H = 0$, near the critical point, the (connected) two-point correlation function $G(r, t)$ has the scaling form

$$G(r, t) = \frac{1}{r^{d-2+\eta}} F_G(rt^\nu)$$

with the scaling function F_G satisfying certain analytical properties as its argument tends to zero or infinity. Using the static susceptibility sum rule show that $\gamma = \nu(2-\eta)$. What did you need to assume about F_G?

(d) Assuming that the static scaling hypothesis is valid, derive the relation

$$\delta = \frac{d + 2 - \eta}{d - 2 + \eta}.$$

Question 4–4.

This problem applies the ideas of critical point scaling and data collapse to fully-developed fluid turbulence. You do not need to know anything about turbulence or fluid dynamics to do this problem.

On the web page I have deposited a data file for the dependence of the friction factor $f(Re, r/D)$ of a turbulent fluid as it flows through a pipe. The friction factor is basically the drag on the wall of the pipe exerted by the fluid, normalized by ρU^2 where ρ is the density and U is the mean speed along the pipe. The Reynolds number is a dimensionless measure of speed and is $Re \equiv UD/\nu$ where D is the pipe diameter and ν is the kinematic viscosity of the fluid. The roughness ratio r/D describes the radius r of small sand grains that were glued to the side of the pipe by Nikuradse, normalised by D. In this question, you will analyze these data assuming that turbulence is some sort of stochastic motion governed by a non-equilibrium critical point.

(a) Plot the data on a log-log plot. The data show a hump at $\log(\mathrm{Re}) = 3.6$ and thereafter decline with Re (for most values of roughness). The decline is basically a straight line on the log-log plot of the data. Estimate the exponent α where $f \sim Re^{-\alpha}$. Notice that the range over which the power law works depends on the roughness.

(b) For large Re, the data become independent of Re, but depend on the roughness ratio as $f \sim (r/D)^{\beta}$. Estimate β.

(c) The two facts in parts (a) and (b) can be combined into one scaling law, by analogy with what happens in critical phenomena. You should think of Re as being like the inverse of t in the magnet problems, and r/D as being like the external field H. Deduce a scaling law for the friction factor, and verify your prediction by making an appropriate plot of the data.