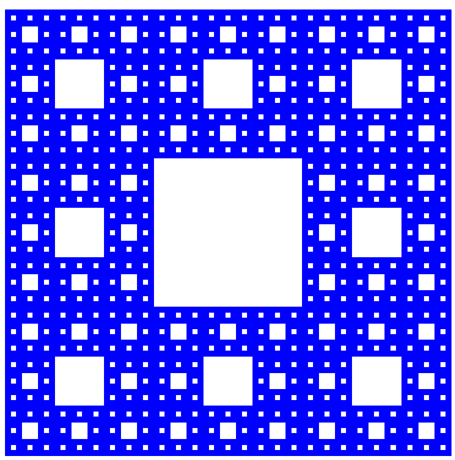
Tuesday 8th October 2013

Hand in to UG office by 14:00 on Monday 14th October
Marked work available in UG office by 12:00 on Wednesday 16th October
RF class at 12:00 on Wednesday 16th October

Statistical Mechanics Problem Sheet 1

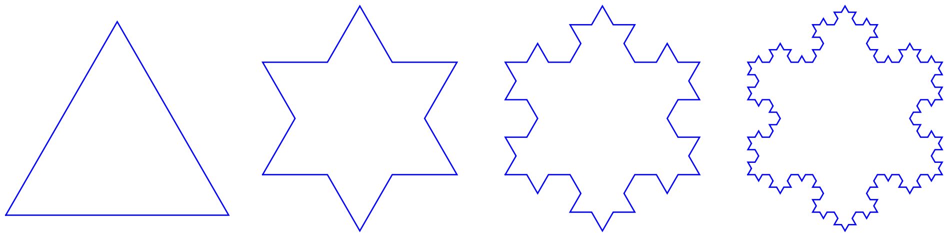
Regular Fractals

1. Sierpinski carpet
   The Sierpinski carpet is constructed by an iterative process akin to that used to build a Sierpinski gasket. Take a square, divide it into $3 \times 3 = 9$ squares and remove the central square. Then, repeat the procedure on the remaining squares.



   Calculate the fractal dimension of this object.

2. Koch curve
   The Koch curve is a line fractal constructed from an equilateral triangle. Take each side of the triangle L, remove the middle third of each side and join up the remaining sides with a triangular kink with sides $L/3$.



The figure above shows the first three iterations.

(a) The Koch curve resembles the perimeter of a snowflake. By deducing a scaling form for the length of the perimeter, calculate the fractal dimension of this curve.

(b) It is said that, if we continue this iteration indefinitely, we will generate a curve that has an infinite perimeter even though it obviously encloses a finite area. Consider the Koch curve obtained by starting with a triangle of side L and applying n iterations of the algorithm described above to obtain a snowflake with line segments of length a. Find a scaling expression for the perimeter of this curve as a function of L and a. Hence show that the perimeter does indeed diverge as $n \to \infty$.

(c) [*Optional.*] Suppose the Koch curve is generated from a triangle of side L with area $\Sigma_0 = \sqrt{3}L^2/4$. Let the area enclosed by the curve generated after n iterations be denoted by Σ_n. Deduce the recurrence relation:

$$\Sigma_n = \Sigma_{n-1} + \left(\frac{4}{9}\right)^{n-1} \frac{\Sigma_0}{3}\,.$$

Hence show that the area enclosed tends to $8\Sigma_0/5$ after many iterations. You may find the geometric series useful: $1 + x + x^2 + \ldots = 1/(1-x)$ for $|x| < 1$.

Random Fractals

3. 1D random walk

Consider a random walk of N steps in one dimension, where each step x_i ($i = 1, \ldots, N$) follows an exponential distribution $p(x) \propto e^{-|x|/a}$ and there is no correlation between different steps. After N steps, the total displacement is $X = \sum_{i=1}^{N} x_i$.

(a) What is the mean displacement $\langle X \rangle$?

(b) Show that the root-mean-square displacement is $\sqrt{2N}\,a$.

(c) Using the central limit theorem (see *Appendix: Probability Basics* in the lecture notes), argue that, for $N \gg 1$, the total displacement X obeys the following distribution:

$$P(X) = \frac{1}{\sqrt{4\pi N a^2}} e^{-X^2/4Na^2}\,.$$

4. Ideal polymer

   The random walk can be used as a model of a polymer molecule in a polymer melt. In this question, we see how entropy plays an important part in the elastic properties of materials such as rubber. (*If you cannot do a part of the question, you can skip to the next part.*)

   (a) Consider a three-dimensional random walk of N uncorrelated steps. For each step $\boldsymbol{r}_i = (x_i, y_i, z_i)$, the component in each direction follows an exponential distribution as for the 1D walk in the previous question:

   $$p(x, y, z) \propto e^{-(|x|+|y|+|z|)/a}.$$

   Let us denote the total displacement by $\boldsymbol{R} = \sum_{i=1}^{N} \boldsymbol{r}_i$.

   (i) Using the results from the 1D random walk in the previous question, write down the mean displacement $\langle \boldsymbol{R} \rangle$ and root-mean-square displacement $\langle \boldsymbol{R}^2 \rangle^{1/2}$ of this walk. Give reasoning.

   (ii) Argue using the central limit theorem that, for $N \gg 1$, the probability density function for $\boldsymbol{R}$ is given by

   $$P(\boldsymbol{R}) = \frac{1}{(4\pi N a^2)^{3/2}} \exp\left(-\frac{\boldsymbol{R}^2}{4Na^2}\right).$$

   (iii) It is important to check results by dimensional analysis. Check that $P(\boldsymbol{R})$ has the correct dimensions.

   (b) [*Harder but contains the interesting physics!*] If monomer-monomer repulsion is ignored, we can assume that $P(\boldsymbol{R})$ describes the end-to-end displacement of an ideal polymer chain with N monomers in three dimensions. More precisely, $P(\boldsymbol{R})d^3R$ is proportional to the probability of finding the end in a small element of volume d^3R centered at $\boldsymbol{R}$. Speaking more loosely, we can say that $P(\boldsymbol{R})$ is proportional to the "number of ways", $W(\boldsymbol{R})$, in which the polymer chain can start at the origin and end up at $\boldsymbol{R}$.

   (i) Using Boltzmann's formula, show that the entropy of the ideal polymer chain for a given displacement $\boldsymbol{R}$ is

   $$S(\boldsymbol{R}) = -k_B \boldsymbol{R}^2/4Na^2 + \text{constant},$$

   where k_B is the Boltzmann constant.

(ii) Suppose a constant force $\boldsymbol{f}$ is applied to the other end of the polymer. Explain why the probability distribution $P(\boldsymbol{R})$ at temperature T in the presence of this applied force is

$$P(\boldsymbol{R}) \propto \exp\left(-\frac{\boldsymbol{R}^2}{4Na^2} + \frac{1}{k_B T}\boldsymbol{f} \cdot \boldsymbol{R}\right).$$

(iii) Show that, in the presence of the applied force, the mean of the end-to-end displacement $\boldsymbol{R}$ becomes

$$\langle \boldsymbol{R} \rangle = \frac{\langle \boldsymbol{R}^2 \rangle_0}{3k_B T}\,\boldsymbol{f},$$

where $\langle \boldsymbol{R}^2 \rangle_0^{1/2}$ is the rms end-to-end distance in the absence of the force as computed in part (a)(i). In other words, the polymer chain obeys Hooke's law — extension $\propto$ tension. [*Hint: by completing the square you can show that the new distribution $P(\boldsymbol{R})$ is also Gaussian but with a non-zero mean.*]

(iv) A rubber band is suspended vertically from the ceiling with a heavy weight hanging from its end. It is a hot day and the room heats up. Does the weight rise or fall?

Tuesday 15th October 2013

Hand in to UG office by 14:00 on Monday 21st October
Marked work available in UG office by 12:00 on Wednesday 23rd October
RF class at 12:00 on Wednesday 23rd October

Statistical Mechanics Problem Sheet 2

Percolation in One Dimension

1. Scaling form of order parameter
   Consider one-dimensional site percolation on a finite chain of L sites subject to periodic boundary conditions.

   (a) Find $n(s,p)$ when (i) $s \leq L-2$, (ii) $s = L-1$, and (iii) $s = L$.

   (b) Explain why the probability that a site belongs to a finite cluster is $\sum_{s=1}^{L-1} sn(s,p)$ rather than $\sum_{s=1}^{L} sn(s,p)$.

   (c) By calculating the right-hand side of the identity

   $$P_\infty(p,L) = p - \sum_{s=1}^{L-1} sn(s,p)\,,$$

   confirm that the probability $P_\infty(p,L)$ of a site belonging to the percolating 'infinite' cluster is p^L.

   (d) (i) Using the identity

   $$\xi(p) = s_\xi(p) = -\frac{1}{\ln p}\,,$$

   which is valid for one-dimensional percolation, express the order parameter $P_\infty(p,L)$ as a function of the system size L and the correlation length ξ.

   (ii) Write the order parameter in the scaling form

   $$P_\infty(\xi,L) = \xi^{-\beta/\nu}\mathcal{P}(L/\xi)$$

   and identify the ratio of critical exponents β/ν and the associated scaling function $\mathcal{P}$. How does $\mathcal{P}(x)$ behave for $x \ll 1$ and $x \gg 1$? [The reason for expressing the exponent as the ratio $-\beta/\nu$ will become clear later in the course.]

2. Moments and moment ratio of the cluster number density
   Consider one-dimensional site percolation on an infinite lattice with site occupation probability p.

   (a) The kth moment $M_k(p)$ of the cluster number density $n(s,p)$ is defined by

   $$M_k(p) = \sum_{s=1}^{\infty} s^k n(s,p)\,.$$

   Using the formula $n(s,p) = (1-p)^2 p^s$ from lectures, show that, in the limit as $p \to p_c^- = 1^-$, where the characteristic cluster size $s_\xi = -1/\ln p$ diverges,

   $$M_k(p) \approx (1-p)^2 s_\xi^{k+1} \int_{1/s_\xi}^{\infty} u^k \exp(-u) du.$$

   (b) Hence show that

   $$M_k(p) \to \Gamma_k (p_c - p)^{-\gamma_k} \quad \text{as} \quad p \to p_c^- = 1^-\,.$$

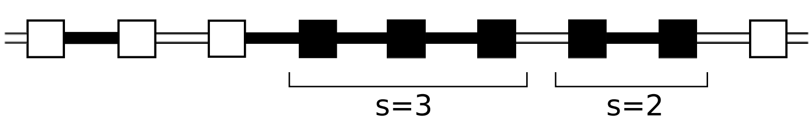
   Identify the critical exponent γ_k and the critical amplitude Γ_k.

   (c) Express the moment ratio

   $$g_k = \frac{M_k M_1^{k-2}}{M_2^{k-1}} \quad \text{for} \quad p \to p_c^-\,, \quad k \geq 2\,,$$

   in terms of the critical amplitudes and hence find the value of g_k.

3. Site-bond percolation in $d = 1$ **(Rapid Feedback question)**
   Consider one-dimensional site-bond percolation on an infinite lattice. Sites are occupied with probability p while bonds are occupied with probability q (see the figure below). A cluster of size s is defined as having s consecutive occupied sites with $s-1$ intermediate occupied bonds. In the figure below, for example, the left-most cluster has size $s = 3$: it terminates to the right because a bond is empty and to the left because a site is empty.



   (a) What is the critical point (p_c, q_c) for site-bond percolation in one dimension?

(b) Show that the cluster number density $n(s, p, q)$ is given by the equation

$$n(s, p, q) = p^s q^{s-1}(1 - pq)^2 \, .$$

(c) Calculate the average cluster size

$$\chi(p, q) = \frac{\sum_{s=1}^{\infty} s^2 n(s, p, q)}{\sum_{s=1}^{\infty} s n(s, p, q)} \, .$$

Comment on the result.

Tuesday 22nd October 2013

Hand in to UG office by 14:00 on Monday 28th October
Marked work available in UG office by 12:00 on Wednesday 30th October
RF class at 12:00 on Wednesday 30th October

Statistical Mechanics Problem Sheet 3

Site Percolation on a Bethe Lattice

1. Correlation function
   Consider site percolation on a Bethe lattice of coordination number z with an occupation probability of p for each site. Starting at a given site i, we can define a distance l_{ij} to another site j using the number of steps needed to reach site j from site i.

   (a) The correlation function $g(i,j)$ is defined as the probability that site j is in the same cluster as site i. Show that $g(i,j) = p^{l_{ij}}$.

   (b) Argue that the mean cluster size $\chi(p)$ is

   $$\chi(p) = \sum_{\text{all sites } j} g(i,j)\,.$$

   (c) Using the expression above for $g(i,j)$, show that, for $p(z-1) < 1$,

   $$\chi(p) = \frac{1+p}{1-p(z-1)}\,.$$

   [Hint: Group together all sites at the same distance from i and sum up the contribution from each group.]

   (d) Hence, write down the percolation threshold p_c for this system.

2. Order parameter **(Rapid Feedback question)**
Consider site percolation on a Bethe lattice of coordination number z, with occupation probability p for each site.

(a) Show that the percolation threshold is $p_c = 1/(z-1)$.

(b) Consider the tree-like structure starting at a given site A and its neighbouring sites, each of which is the root of a branch of this tree. Show that the probability that site A is part of the infinite percolating cluster is given by $P_\infty = p(1 - Q^z)$, where Q is the probability that a branch is *not* connected to infinity.

(c) Explain why the above formula does not work for percolation on a square lattice.

(d) Returning to the Bethe lattice, show that $1 - Q = p(1 - Q^{z-1})$. [Hint: see course notes.]

(e) Hence show that either $Q = 1$ or $1 + Q + \ldots Q^{z-2} = 1/p$.

(f) Consider p just above the percolation threshold p_c and assume that the phase transition is continuous with P_∞ as the order parameter. What can we assume about $P_\infty(p)$ and $Q(p)$ as $p \to p_c^+$?

(g) Using an appropriate Taylor expansion, derive an expression for $Q(p)$ as $p \to p_c^+$. Hence show that

$$P_\infty(p) \simeq \frac{2z}{z-2}\,(p - p_c)$$

as $p \to p_c^+$.

(h) If Q is not equal to 1, we showed in part (e) that it must satisfy a polynomial equation of order $(z-2)$. In part (g) we derived an approximation for one of the roots of this equation in the regime immediately above the percolation threshold. By the fundamental theorem of algebra, however, a polynomial equation of order $(z-2)$ always has $(z-2)$ roots. What about the other $(z-3)$ solutions? Since Q is a probability, physically relevant solutions must satisfy $0 \le Q \le 1$. Show that the polynomial equation has only one real positive solution and that this solution is only ≤ 1 (and hence acceptable) if $p > 1/(z-1)$. What happens otherwise?

Tuesday 29th October 2013

Hand in to UG office by 14:00 on Monday 4th November
Marked work available in UG office by 12:00 on Wednesday 6th November
RF class at 12:00 on Wednesday 6th November

Statistical Mechanics Problem Sheet 4

Questions from 2011 Exam

1. Consider the site percolation problem on a Bethe lattice (Fig. 1) with occupation probability p at each site. The occupation of different sites is independent of each other.

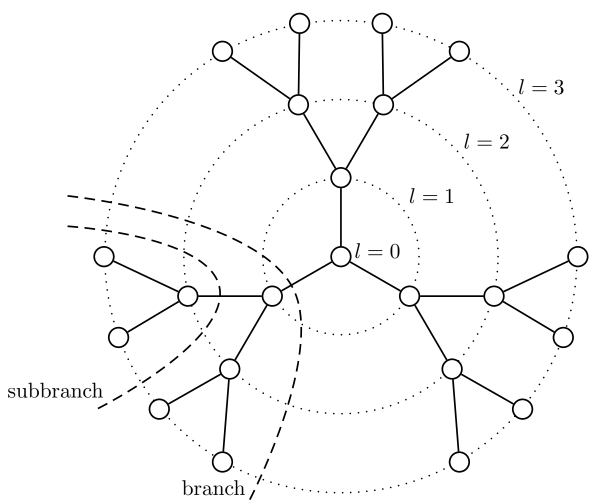


Figure 1: Bethe lattice for the example of coordination number $z = 3$. On a Bethe lattice, each site is connected to z neighbours. It has a tree-like structure. Consider the tree-like structure starting at a given site ($l = 0$). This site has z neighbouring sites (at generation $l = 1$), each of which is the root of a branch of the tree. Each branch has further subbranches (starting at $l = 2, 3, \ldots$).

   (a) The mean cluster size $\chi(p)$ is the expected number of sites in the cluster to which a randomly chosen occupied site belongs. It can be shown that, for

$(z-1)p < 1$,

$$\chi(p) = \frac{1+p}{1-(z-1)p}. \tag{1}$$

(i) How do you expect the mean cluster size $\chi(p)$ to behave as the system approaches the percolation threshold p_c? Hence, identify p_c as a function of the coordination number z of the Bethe lattice.

(ii) Show that, as $p \to p_c^-$ (*i.e.*, from below), the mean cluster size is well approximated by a power law: $\chi(p) \sim (p_c - p)^{-\gamma}$. Identify the exponent γ.

(b) Let $N(l, p)$ be the expected number of occupied sites at generation l that belong to the same cluster as an occupied site at generation 0. It can be shown that

$$N(l,p) = \frac{z}{z-1}\left[(z-1)p\right]^l \qquad \text{for } (z-1)p < 1. \qquad \text{[DO NOT PROVE]} \tag{2}$$

(i) Show that $N(l, p)$ decays exponentially as a function of l: $N(l, p) \sim e^{-l/l_\xi}$, where the characteristic scale for the decay is given by $l_\xi(p) = \frac{1}{|\ln[(z-1)p]|}$.

(ii) How do you expect $l_\xi(p)$ to behave as p approaches the percolation threshold p_c from below? Identify p_c using what you expect for l_ξ as a criterion. Check that this agrees with the threshold you identified in part (a)(i).

(iii) Show that, as $p \to p_c^-$, the characteristic scale l_ξ is well approximated by a power law: $l_\xi \sim (p_c - p)^{-\nu}$. Identify the exponent ν.
You may find it useful to write $p = p_c(1-\delta)$ and consider approximations valid for small δ.

(c) (i) Using the definitions of χ and N, explain why $\chi(p) = 1 + \sum_{l=1}^{\infty} N(l, p)$.

(ii) Using the above relationship between $N(l, p)$ and $\chi(p)$ and the expression (2) for $N(l, p)$, prove that $\chi(p)$ is indeed given by equation (1).

You will need to relate the relevant sum to a geometric series. Recall that: $\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$ for $|x| < 1$. (Note the limits of the sum.)

2. In the site percolation problem, sites on an infinite cubic lattice are occupied independently with probability p. The cluster size distribution $n(s,p)$ gives the density of (non-percolating) clusters of size s, *i.e.*, containing s sites. It can be written in the scaling form:

$$n(s,p) = \frac{1}{s^\tau}\,\mathcal{G}\left(\frac{s}{s_\xi(p)}\right) \qquad \text{with } s_\xi(p) \sim \frac{1}{|p-p_c|^{1/\sigma}} \text{ as } p \to p_c, \tag{1}$$

where p_c is the percolation threshold. Numerical results for the cubic lattice show that $\tau = 2.19$ and $\sigma = 0.45$. Also, it was found that $\mathcal{G}(0)$ is finite and non-zero.

(a) (i) Sketch the cluster size distribution at the percolation threshold ($p = p_c$) on a log-log scale, *i.e.*, $\ln n(s,p_c)$ *vs.* $\ln s$. Discuss the physical significance of this distribution.

(ii) Give a physical interpretation of the quantity $s_\xi(p)$. Sketch on the same diagram as above the distribution $n(s,p)$ at $p = 0.9p_c$ and at $p = 0.95p_c$.

(b) Show that, below the percolation threshold ($p \le p_c$),

$$\sum_{s=1}^{\infty} s\,n(s,p) = p. \tag{2}$$

(c) The mean cluster size diverges as $\chi(p) \sim 1/|p-p_c|^\gamma$ near the percolation threshold. It can be shown that

$$\chi(p) = \frac{1}{p}\sum_{s=1}^{\infty} s^2 n(s,p). \qquad \text{[DO NOT PROVE]}$$

(i) Using the scaling form (1), show that, as $p \to p_c^-$,

$$\chi(p) \sim s_\xi^{3-\tau}\int_{1/s_\xi}^{\infty} u^{2-\tau}\mathcal{G}(u)du.$$

(ii) Using an appropriate approximation for the lower limit of the integral, show that $\chi(p) \sim s_\xi^{3-\tau}$ as $p \to p_c^-$. You should justify the approximation using the information provided at the start of the question.

(iii) Hence, find a numerical value for the exponent γ.

(d) Consider equation (2) with $p = p_c$. Using the scaling form (1), show that the exponent τ is greater than 2 for the site percolation problem on any lattice. (Do not worry about the special case of $\tau = 2$.)

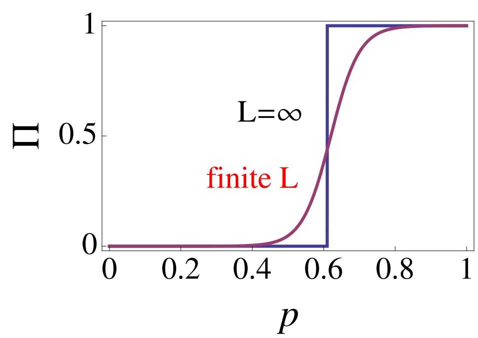
Tuesday 5th November 2013

Hand in to UG office by 14:00 on Monday 11th November
Marked work available in UG office by 12:00 on Wednesday 13th November
RF class at 12:00 on Wednesday 13th November

Statistical Mechanics Problem Sheet 5

Finite-Size Scaling

1. Percolation probability
   Consider the probability $\Pi(p, L)$ of having a percolating cluster in a system of linear size L with site occupation probability p. For an infinite system, $\Pi(p, \infty)$ is zero below the percolation threshold and unity above the threshold. For a system of finite size, Π is smoothed out so that both Π and $d\Pi/dp$ are continuous functions of p.



   (a) Consider first one-dimensional site percolation. Show that $\Pi(p, L)$ can be written in the scaling form

   $$\Pi(p, L) = g_{1\mathrm{D}}(L/\xi(p)).$$

   Identify the function $g_{1\mathrm{D}}$ and the correlation length ξ as a function of p.

   (b) In higher dimensions we can also identify a scaling form

   $$\Pi(p, L) = g_{\pm}(L/\xi(p)),$$

   with $\xi(p) \sim |p - p_c|^{-\nu}$ as $p \to p_c^{\pm}$. Note that we need different g functions for different sides of the transition because Π is not symmetric around p_c.

   (i) Show that the scaling form can be rewritten as

   $$\Pi(p, L) = G((p - p_c)L^{1/\nu}),$$

   and define the single function G in terms of the two functions $g_{\pm}$. [Note that G depends on the signed quantity $p - p_c$ while g_+ and g_- depend on $|p - p_c|$ only.]

(ii) Sketch $d\Pi/dp$ for different system sizes. How does the width of this function evolve with system size?

2. Mean cluster size

   In an infinite system, the mean cluster size near the percolation threshold is given by $\chi(p, L = \infty) \sim |p - p_c|^{-\gamma}$ as $p \to p_c$. The cluster length scale diverges as $\xi(p) \sim |p - p_c|^{-\nu}$.

   (a) A finite-size scaling form for the mean cluster size $\chi(p, L)$ for a finite system of size L can be written using $\chi(p, \infty)$ as a starting point:

   $$\chi(p, L) = \chi(p, \infty) f(\xi/L)\,.$$

   Explain the assumptions in arriving at this expression.
   Assuming that p is very close to p_c, express the scaling form in terms of the lengths ξ and L only.

   (b) Deduce the form of $f(x)$ in the two asymptotic regimes when $x \gg 1$ and when $x \ll 1$. Give your reasoning.

   (c) Hence, show that

   $$\chi(p_c, L) \sim L^{\gamma/\nu}\,. \tag{1}$$

   (d) Explain how you would use numerical data on $\chi(p, L)$ at different p and L to measure the exponents γ and ν.

Scaling Relations

3. Cluster size distribution and mean cluster size **(Rapid Feedback question)**

   (a) The cluster number density for the infinite system follows the scaling form:

   $$n(s, p, L \to \infty) \sim s^{-\tau}\mathcal{G}(s/s_\xi) \quad \text{for} \quad s \gg 1,$$

   with the cluster size diverging like $s_\xi(p, L \to \infty) \sim |p - p_c|^{-1/\sigma}$ as $p \to p_c$. The characteristic length scale of the clusters diverges as $\xi(p) \sim |p - p_c|^{-\nu}$. This question extends this form to finite-size systems.

   (i) Using $s_\xi(p, \infty)$ as a starting point, write down a finite-size scaling form for the characteristic cluster size $s_\xi(p, L)$ for a system with finite size L. This scaling form should be a function of the system size L and characteristic length ξ only. Hence, deduce the behaviour of $s_\xi(p, L)$ for $L \ll \xi(p)$.

   (ii) Using the scaling hypothesis, show that the cluster size distribution at the percolation threshold for a system of finite size L should be given by

   $$n(s, p_c, L) \sim s^{-\tau}\mathcal{G}(s/L^D)\,. \tag{2}$$

   Identify the exponent D in terms of σ and ν.

(b) The mean cluster size $\chi(p)$ is the expectation value of the cluster size to which an occupied site belongs.

(i) Derive the relationship between the mean cluster size $\chi(p)$ and the cluster size distribution $n(s,p)$.

(ii) Use this relationship to link the form (1) for the mean cluster size at $p = p_c$ and the form (2) for $n(s, p_c, L)$. Hence, derive the scaling relation

$$\gamma = (3 - \tau)/\sigma.$$

You may assume that $\mathcal{G}(0)$ is non-zero, $\mathcal{G}(x)$ decays exponentially at large x, and $\tau < 3$.

Tuesday 12th November 2013

Hand in to UG office by 14:00 on Monday 18th November
Marked work available in UG office by 12:00 on Wednesday 20th November
RF class at 12:00 on Wednesday 20th November

Statistical Mechanics Problem Sheet 6

Real space renormalisation group transformation

1. *Site percolation on a one-dimensional lattice (Exam 2010).*

   Consider the site percolation problem on a one-dimensional chain where each site is occupied independently with probability p. In this question, we discuss a real-space renormalisation group (RSRG) scheme where each step involves renormalising a block of b adjacent sites, b being an integer greater than 1.

   (a) Describe briefly the three main steps of the RSRG scheme.

   (b) Show that, after one RSRG step, the site occupation probability p should be renormalised to $p' = R_b(p) = p^b$. Hence, identify the stable and unstable fixed points of this transformation.

   (c) The system has a characteristic cluster length $\xi(p)$ which is a function of the probability p. Show that this RSRG scheme implies that

   $$\left[\xi(p^b)\right]^{-1} = b\,[\xi(p)]^{-1} \tag{1}$$

   for any integer b.

   (d) In renormalisation group theory, it can be shown that $\xi(p) \sim (p_c - p)^{-\nu}$ when p is near the percolation threshold p_c with

   $$\nu = \frac{\ln b}{\ln\left(\left.\frac{dR_b}{dp}\right|_{p=p_c}\right)}. \tag{2}$$

   Without proof, use this formula, find the value of ν for this RSRG scheme.

   (e) It can be shown that, if a function $F(x)$ obeys the relationship

   $$F(bx) = bF(x) \tag{3}$$

for any integer b, then $F(x) = ax$ for some real constant a.[Do not prove] Hence or otherwise, show that the property given by Eq. (1) implies that

$$\xi(p) \propto \frac{1}{\ln p}. \tag{4}$$

Hint: consider $x = \ln p$.

(f) Do the results for $\xi(p)$ from parts (d) and (e) agree? Explain your reasoning.

2. *Bond percolation on a square lattice in two dimensions.* (**RF Question**)

In bond percolation, each bond between neighbouring lattice sites is occupied with probability p and empty with probability $(1-p)$. The bond percolation threshold for a square lattice $p_c = 0.5$. In a real-space renormalisation group transformation on the square lattice with unit lattice spacing, the lattice is replaced by a new renormalised lattice, with super-bonds of length $b = 2$ occupied with probability $R_b(p)$, following the procedure shown in Figure 1

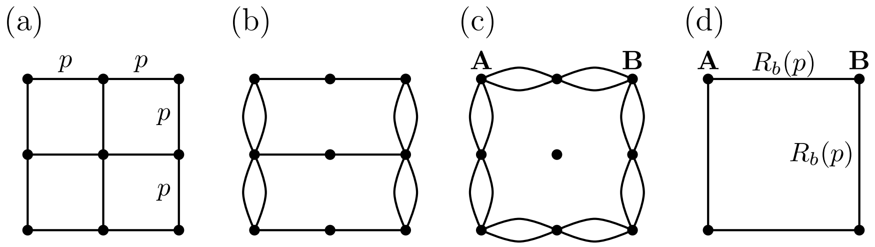


Figure 1: (a) Original lattice with unit lattice spacing where each bond is occupied with probability p. (b) Lattice where every second column in the original lattice is moved one lattice unit to the left. (c) Lattice where, in addition, every second row in the original lattice is moved one lattice unit upwards. In this lattice, there are two bonds between each site. (d) Renormalised lattice with lattice spacing $b = 2$ where each super-bond is occupied with probability $R_b(p)$.

(a) Assuming that the super-bond between **A** and **B** in the renormalised lattice is occupied if there exists a connected path from **A** to **B** along the four bonds in lattice (c), show that

$$R_b(p) = p^4 - 4p^3 + 4p^2. \tag{5}$$

(b) (i) Solve graphically the fixed point equation for the renormalisation group transformation in Equation (5).

(ii) Describe the flow in p-space and the renormalisation of the correlation length when applying the renormalisation group transformation repeatedly.

(iii) Identify clearly the correlation lengths associated with the fixed points $p^\star$ of the renormalisation group transformation and hence explain why fixed points are associated with scale invariance.

(c) (i) Derive a form for the critical exponent ν in terms of the renormalisation group transformation.

(ii) Hence, identify the critical occupation probability p_c, and determine the correlation length exponent ν predicted by the renormalisation group transformation in Equation (5).

Ising Model.

3. *The entropy and the free energy of a system at equilibrium.* (**RF Question)**

The entropy S of a thermal system at equilibrium is defined as

$$S = -k_B \sum_r p_r \ln p_r, \tag{6}$$

where k_B is Boltzmann's constant and p_r is the probability of the system being in a microstate r.

(a) Use the Boltzmann's distribution for p_r to show that

$$S = k_B \ln Z + \langle E \rangle / T. \tag{7}$$

(b) The total free energy

$$F = -k_B T \ln Z. \tag{8}$$

Show that

$$F = \langle E \rangle - TS. \tag{9}$$

4. *Fluctuation-dissipation theorem.*

Consider the Ising model with N spins. The susceptibility per spin, χ, is related to the variance of the total magnetisation by

$$k_B T \chi = \frac{1}{N}\left(\langle M^2 \rangle - \langle M \rangle^2\right), \tag{10}$$

as proved in Section 2.1.2 in the Lecture Notes. Using a similar strategy, prove that the specific heat c is related to the variance of the total energy by

$$k_B T^2 c = \frac{1}{N}\left(\langle E^2 \rangle - \langle E \rangle^2\right). \tag{11}$$

Numerical Answers

1. (b) Stable fixed point $p^\star = 0$. Unstable fixed point $p^\star = 1$. (d) $\nu = 1$.
2. (b)(i) $p^\star = 0, 0.38, 1$. (c)(ii) Predictions by RSRG transformation: $p_c \approx 0.38$ and $\nu \approx 1.63$. Exact valued for $d = 2$: $p_c = 1/2$ and $\nu = 4/3$.

Problem sheet 7 issued: Tuesday 19th November 2013
Solutions available from: Wednesday 27th November 2013

Statistical Mechanics Answer Sheet 7

1. *The spin-spin correlation function and scaling relations.* (**RF Question**)

   (a) The spin-spin correlation function

$$\begin{aligned} g(\mathbf{r}_i, \mathbf{r}_j) &= \langle\ (s_i - \langle s_i\rangle)\ (s_j - \langle s_j\rangle)\ \rangle \\ &= \langle\ s_i s_j - \langle s_i\rangle s_j - s_i\langle s_j\rangle + \langle s_i\rangle\langle s_j\rangle\ \rangle \\ &= \langle s_i s_j\rangle - \langle s_i\rangle\langle s_j\rangle - \langle s_i\rangle\langle s_j\rangle + \langle s_i\rangle\langle s_j\rangle \\ &= \langle s_i s_j\rangle - \langle s_i\rangle\langle s_j\rangle, \end{aligned} \tag{1}$$

   where we use that the ensemble average operation $\langle\cdot\rangle$ is a linear operation and that the ensemble average of a constant is the constant itself.

   (b) Assuming that the system is translationally invariant, we substitute $m = \langle s_i\rangle = \langle s_j\rangle$ and find

$$\begin{aligned} g(\mathbf{r}_i, \mathbf{r}_j) &= \langle s_i s_j\rangle - m^2 \\ &= \langle s_j s_i\rangle - m^2 \\ &= g(\mathbf{r}_j, \mathbf{r}_i) \end{aligned} \tag{2}$$

   from which it follows that the correlation function is symmetric and thus a function of the relative distance between the spins at positions $\mathbf{r}_i$ and $\mathbf{r}_j$ only, that is,

$$g(\mathbf{r}_i, \mathbf{r}_j) = g(|\mathbf{r}_i - \mathbf{r}_j|). \tag{3}$$

   (c) (i) When $|\mathbf{r}_i - \mathbf{r}_j| \to \infty$, the spins become uncorrelated, assuming that we are not at the critical point that is! Thus

$$\begin{aligned} g(\mathbf{r}_i, \mathbf{r}_j) &= \langle s_i s_j\rangle - \langle s_i\rangle\langle s_j\rangle \\ &\to \langle s_i\rangle\langle s_j\rangle - \langle s_i\rangle\langle s_j\rangle \quad \text{for } |\mathbf{r}_i - \mathbf{r}_j| \to \infty \\ &= 0. \end{aligned} \tag{4}$$

   (ii) By definition the spin-spin correlation function of spin i with itself

$$g(\mathbf{r}_i, \mathbf{r}_i) = \langle s_i s_i\rangle - \langle s_i\rangle\langle s_i\rangle = \langle s_i^2\rangle - \langle s_i\rangle^2. \tag{5}$$

Because $s_i = \pm 1 \Leftrightarrow s_i^2 = 1$ we have $\langle s_i^2 \rangle = \langle 1 \rangle = 1$. Also $\langle s_i \rangle = m$, so

$$g(\mathbf{r}_i, \mathbf{r}_i) = 1 - m^2. \tag{6}$$

We assume the external magnetic field $H = 0$ so we can replace m with $m_0(T)$. If $T \geq T_c$, the magnetisation $m_0 = 0$ so that

$$g(\mathbf{r}_i, \mathbf{r}_i) = \begin{cases} 1 & \text{for } T \geq T_c \\ 1 - m_0^2(T) & \text{for } T < T_c. \end{cases} \tag{7}$$

The zero-field magnetisation per spin $m_0(T) \to \pm 1$ for $T \to 0$, implying

$$g(\mathbf{r}_i, \mathbf{r}_i) \to 0 \quad \text{for } T \to 0. \tag{8}$$

This result emphasises that the correlation function measures the fluctuations of the spins *away* from the average magnetisation as is clear from the original definition

$$g(\mathbf{r}_i, \mathbf{r}_i) = \langle\ (s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle)\ \rangle. \tag{9}$$

(iii) In the limit $J/(k_B T) \ll 1$ (high temperatures relative to the coupling constant), the spins will be orientated randomly, that is, there are no correlations between the spins, so we expect $g(\mathbf{r}_i, \mathbf{r}_j) \to 0$.

In the limit $J/(k_B T) \gg 1$ (low temperatures relative to the coupling constant), the spins will be aligned, that is, there are no fluctuations away from the average spin, so we expect $g(\mathbf{r}_i, \mathbf{r}_j) \to 0$.

(d) Because the susceptibility per spin diverges at the critical temperature in zero external field

$$\chi(T, 0) \propto |T - T_c|^{-\gamma} \quad \text{for } T \to T_c, H = 0 \tag{10}$$

the volume integral of the correlation function must also diverge at the critical temperature. Defining $r = |\mathbf{r}_i - \mathbf{r}_j|$, we have

$$\int_V g(\mathbf{r}_i, \mathbf{r}_j) d^d\mathbf{r}_j \propto \int_a^\infty g(r) r^{d-1}\, dr \to \infty \quad \text{for } T \to T_c, H = 0, \tag{11}$$

where a is a lower cutoff = lattice constant. This implies that $g(r)$ cannot decay exponentially with distance r at the critical point $(T, H) = (T_c, 0)$ since this would make the integral convergent in the upper limit. However, the divergence is consistent with an algebraic decay. Assuming

$$\begin{aligned} g(\mathbf{r}_i, \mathbf{r}_j) &\propto |\mathbf{r}_i - \mathbf{r}_j|^{-(d-2+\eta)} \\ &= r^{-(d-2+\eta)} \quad \text{for } T = T_c, H = 0, \text{ and all } r = |\mathbf{r}_i - \mathbf{r}_j| \end{aligned} \tag{12}$$

then

$$\begin{aligned}
\int_V g(\mathbf{r}_i, \mathbf{r}_j) d^d\mathbf{r}_j &\propto \int_a^\infty g(r) r^{d-1}\, dr \\
&\propto \int_a^\infty r^{-(d-2+\eta)} r^{d-1}\, dr \\
&= \int_a^\infty r^{1-\eta}\, dr \\
&= \begin{cases} \left[\frac{1}{2-\eta} r^{2-\eta}\right]_a^\infty & \text{if } \eta \neq 2 \\ [\ln(r)]_a^\infty & \text{if } \eta = 2 \end{cases}
\end{aligned}$$

that is, the integral will only diverge if the critical exponent $\eta \leq 2$. The divergence is logarithmic if $\eta = 2$ and algebraic if $\eta < 2$.

(e) (i) The correlation length diverges as $\xi(T, 0) \propto |T_c - T|^{-\nu}$ for $T \to T_c, H = 0$. The critical exponent ν is independent of whether T_c is approached from below or above, however, the amplitude might differ, as indicated in Figure 1 below.

For $T > T_c$, the correlation length sets the upper linear distance over which spins are correlated. It is also identified as the linear size of the typical (characteristic) largest cluster of correlated spins and measures the typical largest fluctuation away from states with randomly oriented spins.

For $T < T_c$, the correlation length measures the fluctuations away from the fully ordered state, that is, the upper linear size of the holes in the cluster of aligned spins. There will be holes on all scales up to the correlation length.

(ii) When $T \neq T_c$ a finite correlation length ξ is introduced and

$$g(|\mathbf{r}_i - \mathbf{r}_j|) \propto |\mathbf{r}_i - \mathbf{r}_j|^{-(d-2+\eta)} \mathcal{G}_\pm(|\mathbf{r}_i - \mathbf{r}_j|/\xi) \quad \text{for } T \to T_c, \tag{13}$$

where

$$\xi(T, 0) \propto |T_c - T|^{-\nu} \quad \text{for } T \to T_c, H = 0. \tag{14}$$

Consider the relation between the susceptibility per spin and the correlation function

$$k_B T \chi \propto \int_V g(\mathbf{r}_i, \mathbf{r}_j) d^d\mathbf{r}_j. \tag{15}$$

The left-hand side (LHS):

$$k_B T \chi(T, 0) \propto |T - T_c|^{-\gamma} \quad \text{for } T \to T_c, H = 0. \tag{16}$$

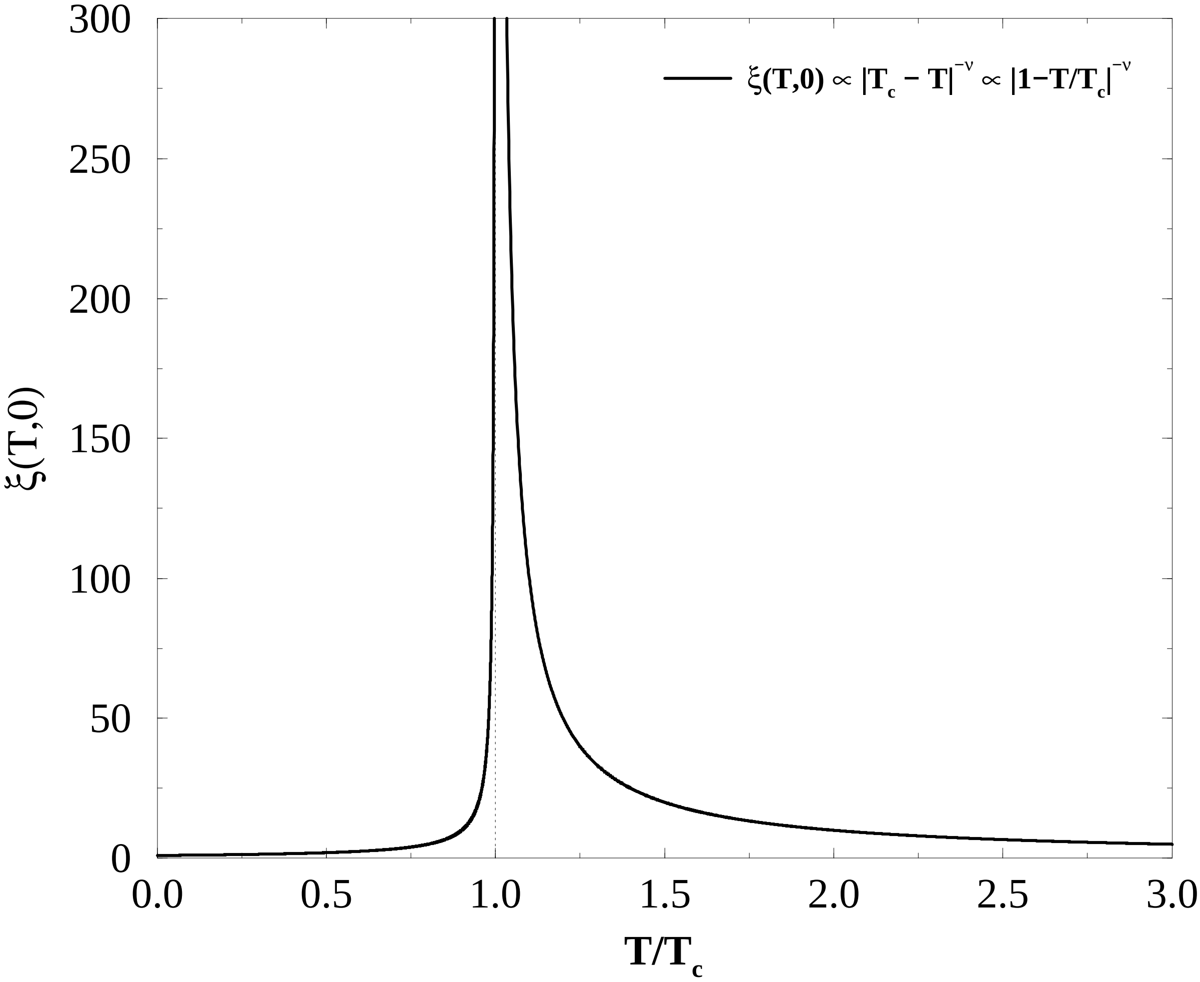


Figure 1: Sketch of the correlation length $\xi(T,0)$ as a function of the temperature T in units of the critical temperature T_c.

The right-hand side (RHS):

$$\begin{aligned}
\int_V g(\mathbf{r}_i, \mathbf{r}_j) d^d\mathbf{r}_j &\propto \int_a^\infty r^{-(d-2+\eta)} \mathcal{G}_\pm(r/\xi) r^{d-1}\, dr \\
&= \int_a^\infty r^{1-\eta} \mathcal{G}_\pm(r/\xi)\, dr \\
&= \int_a^\infty (\tilde{r}\xi)^{1-\eta} \mathcal{G}_\pm(\tilde{r})\, d\tilde{r}\xi \quad \text{with } r = \tilde{r}\xi \\
&= \xi^{2-\eta} \int_a^\infty \tilde{r}^{1-\eta} \mathcal{G}_\pm(\tilde{r})\, d\tilde{r} \\
&= |T - T_c|^{-\nu(2-\eta)} \int_a^\infty \tilde{r}^{1-\eta} \mathcal{G}_\pm(\tilde{r})\, d\tilde{r} \quad \text{for } T \to T_c^\pm. \qquad (17)
\end{aligned}$$

The integral is just a number (which numerical value, however, depends on from which side T_c is approached due to the two different scaling functions $\mathcal{G}_\pm$), so we can conclude by comparing the LHS with the RHS that

$$\gamma = \nu(2 - \eta). \qquad (18)$$

(iii) We assume $T \leq T_c$ and consider the situation in zero external field $H = 0$ with m_0 replacing m. We define

$$\tilde{g}(r) = g(r) + m_0^2 = \langle s_i s_j \rangle. \qquad (19)$$

For $T < T_c$, the correlation length $\xi < \infty$. As the correlation length sets the upper limit of the linear scale over which spins are correlated, the spins will be uncorrelated in the limit $r \to \infty$ as $r \gg \xi$. Thus

$$\tilde{g}(r) = \langle s_i s_j \rangle \to \langle s_i \rangle \langle s_j \rangle = m_0^2 \propto (T_c - T)^{2\beta} \quad \text{for } T \to T_c^-. \qquad (20)$$

This is the reason for considering the function $\tilde{g}(r)$ and not $g(r)$ since the latter will approach zero for $r \gg \xi$.

At $T = T_c$ where the correlation length in infinite, the magnetisation is zero in zero external field, i.e., $m_0(T_c) = 0$. Thus

$$\tilde{g}(r) = g(r) \propto r^{-(d-2+\eta)} \quad \text{at } T = T_c. \qquad (21)$$

One would thus expect, à la finite-size scaling in percolation theory, that

$$\tilde{g}(r) \propto \begin{cases} r^{-(d-2+\eta)} & \text{for } r \ll \xi \\ \xi^{-(d-2+\eta)} & \text{for } r \gg \xi. \end{cases} \qquad (22)$$

Thus for $T < T_c$ where the correlation length is finite, we expect

$$\tilde{g}(r) \propto \xi^{-(d-2+\eta)} \propto |T - T_c|^{\nu(d-2+\eta)} \quad \text{for } r \gg \xi. \qquad (23)$$

Comparing Eq.(23) and Eq.(20) we identify the scaling relation

$$2\beta = \nu(d - 2 + \eta) \Leftrightarrow d - 2 + \eta = 2\beta/\nu. \qquad (24)$$

2. *Critical exponents inequality.*
Given the thermodynamic relation

$$\chi\,(C_H - C_M) = T\left(\frac{\partial\langle M\rangle}{\partial T}\right)_H^2 \tag{25}$$

As $C_M \geq 0$ and $\chi \geq 0$ it follows that

$$\chi\, C_H \geq T\left(\frac{\partial\langle M\rangle}{\partial T}\right)_H^2 . \tag{26}$$

Using the scaling of the different quantities close to the critical point

$$\begin{aligned}
\chi(T,0) &\propto |T-T_c|^{-\gamma} && \text{for } T \to T_c, H=0,\\
C_H &\propto |T-T_c|^{-\alpha} && \text{for } T \to T_c, H=0,\\
\langle M\rangle &\propto (T_c-T)^{\beta} && \text{for } T \to T_c^-, H=0 \text{ implying},\\
\frac{\partial\langle M\rangle}{\partial T} &\propto -(T_c-T)^{\beta-1} && \text{for } T \to T_c^-, H=0
\end{aligned}$$

so by substituting into Equation (26) we find

$$\begin{aligned}
(T_c-T)^{-\gamma}\;(T_c-T)^{-\alpha} &\geq T_c\;\left(-(T_c-T)^{\beta-1}\right)^2 && \text{for } T \to T_c^-\\
(T_c-T)^{-\gamma-\alpha} &\geq T_c\;(T_c-T)^{2\beta-2} && \text{for } T \to T_c^-
\end{aligned}$$

from which we can conclude that

$$\begin{aligned}
-\gamma-\alpha &\leq 2\beta-2 \Leftrightarrow\\
\gamma+\alpha &\geq 2-2\beta \Leftrightarrow\\
\alpha+2\beta+\gamma &\geq 2.
\end{aligned} \tag{27}$$

Notice that the inequality can be repalced by an *equality* for $d = 1, 2, 3$, and 4 and the mean-field exponents for the Ising Model.

3. *Eigenvalues, eigenvectors and diagonalisation.*

   (a) Assume $\mathbf{x} \neq \mathbf{0}$ is an eigenvector for f with eigenvalue λ, that is

   $$f(\mathbf{x}) = \lambda\mathbf{x}. \tag{28}$$

   Since f is linear,

   $$f(\alpha\mathbf{x}) = \alpha f(\mathbf{x}) = \alpha\lambda\mathbf{x} = \lambda(\alpha\mathbf{x}) \tag{29}$$

   so $\alpha\mathbf{x}$ is also an eigenvector with the same eigenvalue λ when $\alpha \neq 0$ (ensuring $\alpha\mathbf{x} \neq \mathbf{0}$.

(b) Assume $\mathbf{x} \neq \mathbf{0}$ is an eigenvector for f with eigenvalue λ. If $\mathbf{A}$ is the associated matrix for the linear function f then

$$\mathbf{A}\mathbf{x} - \lambda\mathbf{x} = (\mathbf{A} - \lambda\mathbf{I})\mathbf{x} = \mathbf{0}, \tag{30}$$

where $\mathbf{I}$ is the identity matrix. If $\det(\mathbf{A} - \lambda\mathbf{I}) \neq 0$ the matrix $\mathbf{A} - \lambda\mathbf{I}$ would be invertible and the only solution to the Equation (30) would be the trivial solution $\mathbf{x} = \mathbf{0}$. Equation (30) can only have non-trivial solutions $\mathbf{x} \neq \mathbf{0}$ if the matrix $\mathbf{A} - \lambda\mathbf{I}$ is not invertible. Therefore, we have

$$\det(\mathbf{A} - \lambda\mathbf{I}) = 0. \tag{31}$$

Equation (31) is called the characteristic equation or the secular equation for the matrix $\mathbf{A}$ and the solutions λ are the eigenvalues of $\mathbf{A}$ (or f).

(c) We need to show that $\mathbf{x}_1 \cdot \mathbf{x}_2 = 0$ assuming that

$$f(\mathbf{x}_1) = \lambda_1\mathbf{x}_1 \quad \text{and} \quad f(\mathbf{x}_2) = \lambda_2\mathbf{x}_2 \qquad \text{with } \lambda_1 \neq \lambda_2. \tag{32}$$

$$f(\mathbf{x}_1) \cdot \mathbf{x}_2 = \lambda_1\mathbf{x}_1 \cdot \mathbf{x}_2 \tag{33a}$$
$$\mathbf{x}_1 \cdot f(\mathbf{x}_2) = \lambda_2\mathbf{x}_1 \cdot \mathbf{x}_2. \tag{33b}$$

Since f is symmetric

$$\lambda_1\mathbf{x}_1 \cdot \mathbf{x}_2 = \lambda_2\mathbf{x}_1 \cdot \mathbf{x}_2. \tag{34}$$

However, $\lambda_1 \neq \lambda_2$ from which we conclude

$$\mathbf{x}_1 \cdot \mathbf{x}_2 = 0. \tag{35}$$

(d) (i) Consider the real and symmetric matrix

$$\mathbf{T} = \begin{pmatrix} \exp(\beta J + \beta H) & \exp(-\beta J) \\ \exp(-\beta J) & \exp(\beta J - \beta H) \end{pmatrix}. \tag{36}$$

The eigenvalues $\lambda_\pm$ of $\mathbf{T}$ are the solutions to the characteristic equation

$$\det(\mathbf{T} - \lambda\mathbf{I}) = 0. \tag{37}$$

The determinant

$$\begin{aligned} \det(\mathbf{T} - \lambda\mathbf{I}) &= \begin{vmatrix} \exp(\beta J + \beta H) - \lambda & \exp(-\beta J) \\ \exp(-\beta J) & \exp(\beta J - \beta H) - \lambda \end{vmatrix} \\ &= \lambda^2 - [\exp(\beta J + \beta H) + \exp(\beta J - \beta H)]\,\lambda + \exp(2\beta J) - \exp(-2\beta J) \\ &= \lambda^2 - 2\exp(\beta J)\cosh(\beta H)\lambda + \exp(2\beta J) - \exp(-2\beta J), \end{aligned} \tag{38}$$

so the solutions to the characteristic Equation (37) are

$$\begin{aligned}
\lambda_\pm &= \frac{2\exp(\beta J)\cosh(\beta H) \pm \sqrt{4\exp(2\beta J)\cosh^2(\beta H) - 4[\exp(2\beta J) - \exp(-2\beta J)]}}{2} \\
&= \exp(\beta J)\left(\cosh(\beta H) \pm \sqrt{\cosh^2(\beta H) - 1 + \exp(-4\beta J)}\right) \\
&= \exp(\beta J)\left(\cosh(\beta H) \pm \sqrt{\sinh^2(\beta H) + \exp(-4\beta J)}\right). \qquad (39)
\end{aligned}$$

(ii) Since $\lambda_+ > \lambda_-$, the associated eigenvectors must be orthogonal. To determine the eigenvectors for $\mathbf{T}$ we must solve the equations

$$\mathbf{T}\mathbf{x}_+ = \lambda_+\mathbf{x}_+ \qquad (40a)$$

$$\mathbf{T}\mathbf{x}_- = \lambda_-\mathbf{x}_- \qquad (40b)$$

or equivalently

$$(\mathbf{T} - \lambda_+\mathbf{I})\mathbf{x}_+ = \mathbf{0} \qquad (40c)$$

$$(\mathbf{T} - \lambda_-\mathbf{I})\mathbf{x}_- = \mathbf{0} \qquad (40d)$$

Then we construct the matrix of eigenvectors

$$\mathbf{U} = (\mathbf{x}_+ \ \mathbf{x}_-) \qquad (41)$$

that will satisfy

$$\mathbf{U}^{-1}\mathbf{T}\mathbf{U} = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}. \qquad (42)$$

Tuesday 19th November 2013

Hand in to UG office by 14:00 on Monday 25th November 2013
Marked work available in UG office by 12:00 on Wednesday 27th November 2013
RF class at 12:00 on Wednesday 27th November 2013

Statistical Mechanics Problem Sheet 7

1. *The spin-spin correlation function and scaling relations.* (**RF Question**)
   The spin-spin correlation function

$$g(\mathbf{r}_i, \mathbf{r}_j) = \langle (s_i - \langle s_i \rangle)\, (s_j - \langle s_j \rangle) \rangle, \tag{1}$$

   measures the correlations in the fluctuations of spins s_i and s_j at positions $\mathbf{r}_i$ and $\mathbf{r}_j$ around their average values $\langle s_i \rangle$ and $\langle s_j \rangle$.

   (a) Show that

$$g(\mathbf{r}_i, \mathbf{r}_j) = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle. \tag{2}$$

   (b) Assume the system is translationally invariant, that is, $\langle s_i \rangle = \langle s_j \rangle = m$. Discuss why this implies that the correlation function can only be a function of the relative distance, that is, $g(\mathbf{r}_i, \mathbf{r}_j) = g(|\mathbf{r}_i - \mathbf{r}_j|)$.

   (c) (i) Discuss the behaviour of the correlation function $g(\mathbf{r}_i, \mathbf{r}_j)$ in the limit $|\mathbf{r}_i - \mathbf{r}_j| \to \infty$ assuming $T \neq T_c$ and zero external field $H = 0$.

   (ii) Discuss the behaviour of the correlation function $g(\mathbf{r}_i, \mathbf{r}_i)$ of spin i with itself (i.e., in the limit $|\mathbf{r}_i - \mathbf{r}_j| \to 0$) as a function of temperature T in zero external field $H = 0$.

   (iii) Discuss the behaviour of the correlation function $g(\mathbf{r}_i, \mathbf{r}_j)$ in the limits of $J/(k_B T) \ll 1$ and $J/(k_B T) \gg 1$ in zero external field $H = 0$.

   The volume integral in d dimensions of the correlation function is related to the susceptibility per spin χ, by

$$k_B T \chi = \sum_j g(\mathbf{r}_i, \mathbf{r}_j) \propto \int_V g(\mathbf{r}_i, \mathbf{r}_j) d^d \mathbf{r}_j. \tag{3}$$

   (d) Convince yourself that the divergence of the susceptibility per spin at the critical point $(T, H) = (T_c, 0)$ is achieved with an algebraically decaying correlation function

$$g(\mathbf{r}_i, \mathbf{r}_j) \propto |\mathbf{r}_i - \mathbf{r}_j|^{-(d-2+\eta)} \quad \text{for } T = T_c, |\mathbf{r}_i - \mathbf{r}_j| \gg 1, \tag{4}$$

defining a new critical exponent, η, and prove that $\eta \leq 2$.
Hint: Assume Equation (4) is valid for all $r = |\mathbf{r}_i - \mathbf{r}_j|$ and recall that for a function depending only on the distance r but not the direction $\int_V f(\mathbf{r}_i, \mathbf{r}_j)\, d^d\mathbf{r}_j \propto \int_0^\infty f(r) r^{d-1} dr$ in d dimensions.

For $T \neq T_c$, the correlation function will have a cutoff, defining implicitly the correlation length ξ, by

$$g(\mathbf{r}_i, \mathbf{r}_j) \propto |\mathbf{r}_i - \mathbf{r}_j|^{-(d-2+\eta)} \mathcal{G}_\pm(r/\xi) \quad \text{for } T \to T_c^\pm, |\mathbf{r}_i - \mathbf{r}_j| \gg 1, \tag{5a}$$

$$\xi \propto |T_c - T|^{-\nu} \quad \text{for } T \to T_c, H = 0, \tag{5b}$$

and the scaling functions

$$\mathcal{G}_\pm(x) = \begin{cases} \text{constant} & \text{for } x \ll 1 \\ \text{decays rapidly} & \text{for } x \gg 1. \end{cases} \tag{6}$$

(e) (i) Sketch the correlation length as a function of temperature T, and discuss the physical interpretation of the correlation length ξ.

(ii) Use Equation (3) and assume Equation (5) is valid for all $r = |\mathbf{r}_i - \mathbf{r}_j|$ to show the scaling relation

$$\gamma = \nu(2 - \eta). \tag{7}$$

(iii) Prove that

$$d - 2 + \eta = 2\beta/\nu. \tag{8}$$

Hint: Assume $T \leq T_c$. Define $\tilde{g}(r) = g(r) + m^2$ and consider the limit $r \to \infty$, that is, $r \gg \xi$.

2. *Critical exponents inequality.*

The critical exponent β characterises the pick-up of the magnetisation per spin, that is, $m(T, 0) \propto \pm (T_c - T)^\beta$ for $T \to T_C^-$. The critical exponent γ characterises the divergence of the susceptibility per spin, that is, $\chi(T, 0) \propto |T - T_c|^{-\gamma}$ for $T \to T_C$. The critical exponent α characterises the divergence of the specific capacity, that is, $c(T, 0) \propto |T - T_c|^{-\alpha}$ for $T \to T_C$.
Given the thermodynamic relation

$$\chi(C_H - C_M) = T \left(\frac{\partial m}{\partial T} \right)_H^2, \tag{9}$$

where T is temperature, χ is the susceptibility per spin, C_H and C_M are the specific heat at constant external field and magnetisation and $m(T, H) = \langle M \rangle / N$ the average magnetisaion per spin, respectively, show that as $C_M \geq 0$ it follows generally that the critical exponents satisfy the inequality

$$\alpha + 2\beta + \gamma \geq 2. \tag{10}$$

3. *Eigenvalues, eigenvectors and diagonalisation.*

Let f be a linear function from $\mathbb{R}^n$ into $\mathbb{R}^n$. If there is a non-zero vector $\mathbf{x} \in \mathbb{R}^n$ and a number λ such that $f(\mathbf{x}) = \lambda\mathbf{x}$, then $\mathbf{x}$ is called an eigenvector of the linear function f, and λ is called its associated eigenvalue.

(a) Show that if $\mathbf{x}$ is an eigenvector for f so is $\alpha\mathbf{x}$ for any number $\alpha \neq 0$.

(b) Let A be the associated matrix for the linear function f. Argue that the eigenvalues for the function f are the solutions to the characteristic equation

$$\det(\mathsf{A} - \lambda\mathsf{I}) = 0. \tag{11}$$

(c) Assume that f is symmetric, that is,

$$f(\mathsf{x}) \cdot \mathsf{y} = \mathsf{x} \cdot f(\mathsf{y}) \quad \text{for all } \mathsf{x}, \mathsf{y} \in \mathbb{R}^n, \tag{12}$$

or, if A is the associated symmetric matrix,

$$(\mathsf{A}\mathsf{x}) \cdot \mathsf{y} = \mathsf{x} \cdot (\mathsf{A}\mathsf{y}) \quad \text{for all } \mathsf{x}, \mathsf{y} \in \mathbb{R}^n. \tag{13}$$

Show that if $\mathbf{x}_1$ and $\mathbf{x}_2$ are eigenvectors of f corresponding to distinct eigenvalues λ_1 and λ_2, then $\mathbf{x}_1$ and $\mathbf{x}_2$ are orthogonal, that is, $\mathbf{x}_1 \cdot \mathbf{x}_2 = 0$.

(d) Consider the real and symmetric 2×2 matrix T in Section 2.4, Equation (2.61) on page 141 in the lecture notes.

(i) Find the eigenvalues $\lambda_\pm$ for T.

(ii) Outline explicitly the procedure to construct a matrix U such that

$$\mathsf{U}^{-1}\mathsf{T}\mathsf{U} = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}. \tag{14}$$

Note that there is no need to perform the procedure unless you feel the urge to do so.

Problem sheet 8 issued: Tuesday 26th November 2013
Solutions available from: Wednesday 4th December 2013

Statistical Mechanics Answer Sheet 8

1. *Second-order PT in a mass-spring system: Landau theory.* (**RF Question**)

   (a) The total energy of the mass-spring system

$$\begin{aligned} U(\theta) &= \text{elastic potential energy} + \text{gravitational potential energy} \\ &= \frac{1}{2}k(a\theta)^2 + mg(a\cos\theta - a) \\ &= \frac{1}{2}ka^2\theta^2 + mga(\cos\theta - 1). \end{aligned} \tag{1}$$

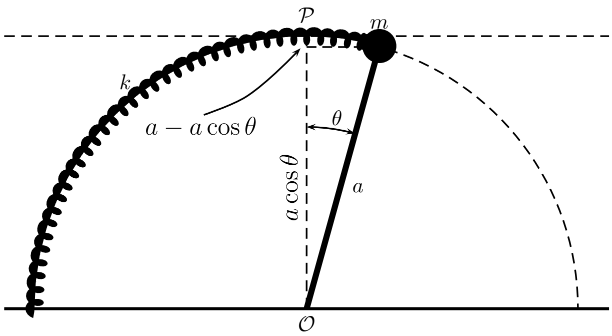


Figure 1: The projection of the rod of length a onto the vertical dashed line has length $a\cos\theta$ where the angle θ is measured (positive clockwise) from the vertical. Hence, the position of the center of mass of the variable mass m is $a - a\cos\theta = a(1-\cos\theta)$ below the zeroth-level of the gravitational potential energy indicated by the horizontal dashed line.

   (b) (i) We expand the cosine to fourth order to find

$$\begin{aligned} U(\theta) &= \frac{1}{2}ka^2\theta^2 + mga(1 - \frac{\theta^2}{2!} + \frac{\theta^4}{4!} - \cdots - 1) \\ &= \frac{a}{2}(ka - mg)\theta^2 + \frac{mga}{24}\theta^4 + \mathcal{O}(\theta^6), \end{aligned} \tag{2}$$

   where the coefficient of the fourth-order term is positive while the coefficient of the second-order term is zero for $ka = mg$ and changes sign from positive when $ka > mg$ to negative when $ka < mg$.

(ii) As the total energy $U(\theta)$ is an even function in θ (reflecting the symmetry of the problem), all the odd terms in the Taylor expansion around $\theta = 0$ are zero.

(iii) We denote the angle of equilibrium with θ_0. When $ka > mg$, the unique minimum is at $\theta_0 = 0$. When $ka = mg$, the unique minimum is at $\theta_0 = 0$. When $ka < mg$, there are two minima at $\pm\theta_0 \neq 0$.

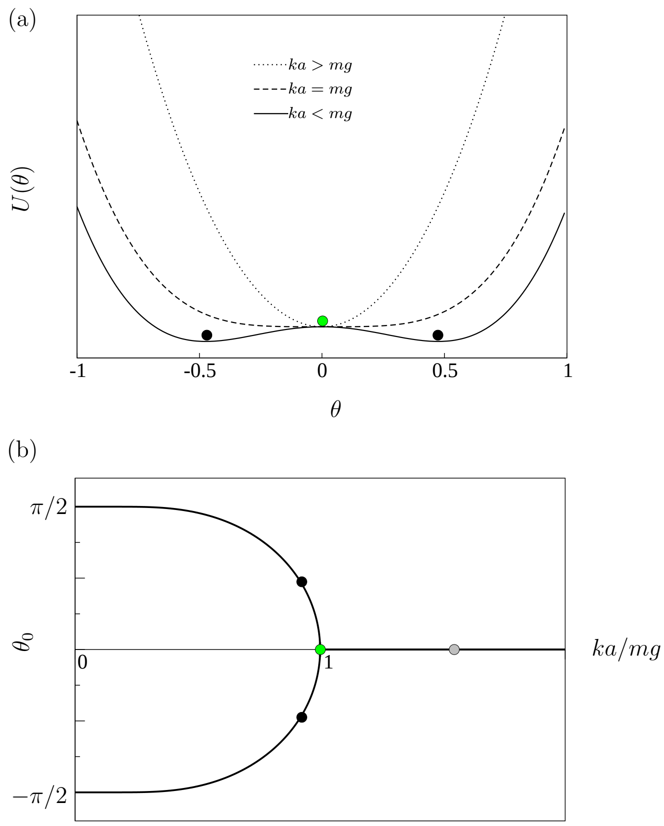


Figure 2: (a) The energy, $U(\theta)$, versus the angle θ. The solid circles show the position of the minima of the energy of the corresponding graph. For $ka > mg$, the minimal energy implies $\theta = 0$. For $ka = mg$, the trivial solution $\theta = 0$ is marginally stable However, for $ka < mg$, the minimal energy implies $\theta = \pm\theta_0 \neq 0$. (b) The angle of equilibrium, θ_0 as a function of the ratio ka/mg.

(iv) The system is in equilibrium when $dU/d\theta = 0$. Hence

$$\begin{aligned} \frac{dU}{d\theta} &= a(ka - mg)\theta + \frac{mga}{6}\theta^3 \\ &= mga\theta\left(\frac{ka}{mg} - 1 + \frac{1}{6}\theta^2\right) \\ &= 0 \end{aligned} \tag{3}$$

with solutions

$$\theta_0 = \begin{cases} 0 & \text{for } \frac{ka}{mg} \geq 1 \\ \pm\sqrt{6(1 - ka/mg)} & \text{for } \frac{ka}{mg} < 1 \end{cases}$$
$$= \begin{cases} 0 & \text{for } \frac{m_c}{m} \geq 1 \\ \pm\sqrt{6[(m - m_c)/m]} & \text{for } \frac{m_c}{m} < 1, \end{cases} \tag{4}$$

where $m_c = ka/g$.

(v) See Figure 4.

(vi) Landau suggested a simplistic general theory of second-order phase transitions based on expanding the free energy in powers of the order parameter. In the absence of a magnetic-like field, symmetry dictates that only even powers of the order parameter appear in the expansion. For example, in the Ising model

$$f - f_0 = a_2(T - T_c)m^2 + a_4 m^4 \quad \text{with } a_2, a_4 > 0,$$

where an expansion up to fourth order is sufficient to give a qualitative description of second-order phase transitions occurring at temperature T_c. The term f_0 is an unimportant constant, while $a_4 > 0$ in order for the free energy to be physically realistic, i.e. not minimised by extreme values of the order parameter. As written, the left-hand side is given by a quartic polynomial which always has one trivial solution, $m = 0$, and two non-trivial solutions, $m = \pm m_0(T)$, so long as $T < T_c$. As T passes through T_c from above, the trivial solution becomes unstable and two stable non-trivial solutions appear. Below T_c, therefore, the order parameter of the system is non-zero.

(vii) The order parameter of the mass-spring system is the equilibrium angle θ_0 which is zero for $m \leq m_c$ and non-zero for $m > m_c$. The critical value of the variable mass $m_c = ka/g$.

2. *Diluted Ising model.*

(a) A spin s_i is situated on each lattice site $\mathbf{r}_i$. However, the spin only interacts with with the nearest neighbours with probability p. Identifying a nonzero coupling constant $J_{ij} = J > 0$ as an occupied bond and $J_{ij} = 0$ as an empty bond, we have an exact mapping onto a bond percolation theory problem.

(b) (i) At $T = 0$, the total free energy $F = \langle E \rangle - TS = \langle E \rangle$. Because an equilibrium system will minimise the free energy, at $T = 0$ it will minimise its energy. In order to minimise the energy, all spins within a given cluster will point in the same direction. However, spins belonging to different clusters need not point in the same direction.

(ii) Within a cluster, $s_i = s_j$ so $s_i s_j = s_i^2 = 1$ implying $\langle s_i s_j \rangle = 1$ if the spins belong to the same cluster. If the spins i and j belong to different clusters, they are not correlated at all, that is, given, e.g., that $s_i = 1$ then $s_j = 1$ with probability 0.5 and $s_j = -1$ with probability 0.5 leaving $\langle s_i s_j \rangle = 0.5 \cdot 1 + 0.5 \cdot (-1) = 0$. Hence

$$\langle s_i s_j \rangle = \begin{cases} 1 & i, j \text{ in the same percolation cluster} \\ 0 & \text{otherwise.} \end{cases} \tag{5}$$

(iii) For $p < p_c$ all clusters are finite. Since the clusters are not correlated, the average magnetisation must be zero.
For $p > p_c$, we can argue that all the finite clusters do not contribute to the magnetisation as their magnetisation would average out to zero. Hence, the magnetisation then becomes equal to $P_\infty(p)$, the density of the infinite cluster. In zero external field, the orientation of the spins in the infinite cluster is either up $+$ or down $-$.
For $p = p_c$ the argument is the same as for $p > p_c$ with the additional information that the density of the infinite cluster $P_\infty(p)$ is zero at $p = p_c$ and hence there is no net magnetisation.
In summary

$$m_0(p) = \pm P_\infty(p) = \begin{cases} 0 & \text{for } p \leq p_c \\ \neq 0 & \text{for } p > p_c. \end{cases} \tag{6}$$

(c) (i) $P_\infty(p)$ is the probability for a spin to belong to the percolating infinite cluster. As $\tanh(sH/k_B T) \to 0$ for $H \to 0^{\pm}$, the last term will vanish and

$$m_0(p) = \lim_{H \to 0^{\pm}} m(p, H) = \pm P_\infty(p)$$

consistent with the result of (b)(iii).

(ii) The susceptibility per spin in zero external field

$$\chi(T, 0) = \left(\frac{\partial m}{\partial H} \right)_T \bigg|_{H=0}.$$

Assuming $H \ll k_B T$ we use the Taylor expansion $\tanh(sH/k_B T) \approx sH/k_B T + \mathcal{O}\left((sH/k_B T)^3\right)$. Since $P_\infty(p)$ does not depend on the external field, we find,

$$\chi(T, 0) = \left(\frac{\partial m}{\partial H} \right)_T \bigg|_{H=0} = \sum_{s=1}^{\infty} \frac{s^2 n(s, p)}{k_B T} = \beta \chi(p) \propto |p - p_c|^{-\gamma} \tag{7}$$

as the divergence of the second moment of the cluster number density $n(s, p)$ is characterized by the exponent γ when $p \to p_c$.

(d) When $p < p_c$, the magnetisation in zero external field $m_0(p) = 0$. We are at low temperature, so we may assume that within a cluster $\langle s_i s_j \rangle = 1$. In a cluster of size s there are a total of s^2 different pairs, so $\frac{1}{k_B T} \sum_i \sum_j \langle s_i s_j \rangle = \frac{1}{k_B T} s^2$. We can calculate the average susceptibility per spin by summing over all possible cluster sizes weighted by the cluster number density, that is,

$$\chi(T, 0) = \sum_{s=1}^{\infty} \left(\frac{1}{k_B T} \sum_i \sum_j \langle s_i s_j \rangle \right) n(s, p) = \frac{1}{k_B T} \sum_{s=1}^{\infty} s^2 n(s, p). \tag{8}$$

3. (a) *Landau theory for the Ising model.*

(i) On each site $\mathbf{r}_i$, there is a spin variable $s_i = \pm 1$ that can take on only two values: spin up $(+1)$ or spin down (-1).

(ii) It is energetically favorable for neighbouring spins to be parallel. So, $J > 0$ so that a pair of parallel spins where $s_i s_j = +1$ has energy $-J$ and a pair of anti-parallel spins where $s_i s_j = -1$ has energy $+J$.

(iii) The first sum runs over distinct nearest neighbour pairs (i.e., we assume that the spin-spin interaction J_{ij} fall off so rapidly that only nn interactions are present). If z denotes the coordination number, then

$$\sum_{\langle ij \rangle} 1 = \frac{z}{2} \sum_{i=1}^{N} 1 = \frac{1}{2} N z, \tag{9}$$

where the factor of 1/2 ensures that we are counting *distinct* nearest-neighbour pairs only.

(b) See Figure 3.

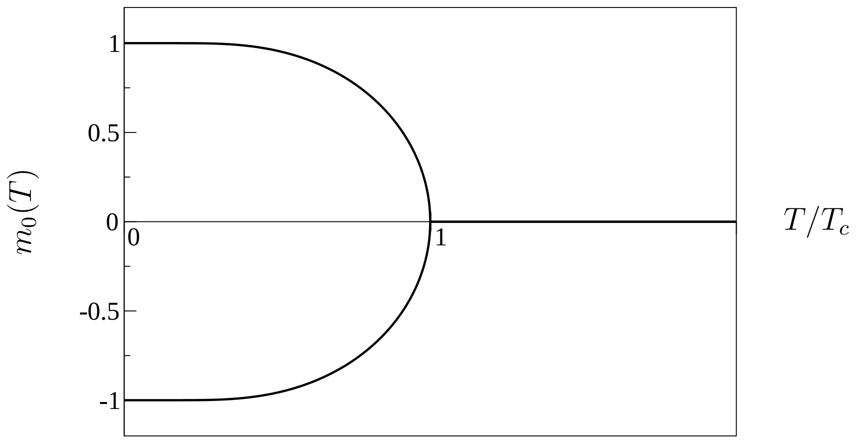


Figure 3: When $T \to 0$, then $m_0(T) \to \pm 1$. When $T \to T_c^-$, the magnetisation decreases sharply but continuously to zero at $T = T_c$. For all $T \geq T_c$, the magnetisation per spin in zero external field $m_0(T) = 0$.

(c) See Figure 4.

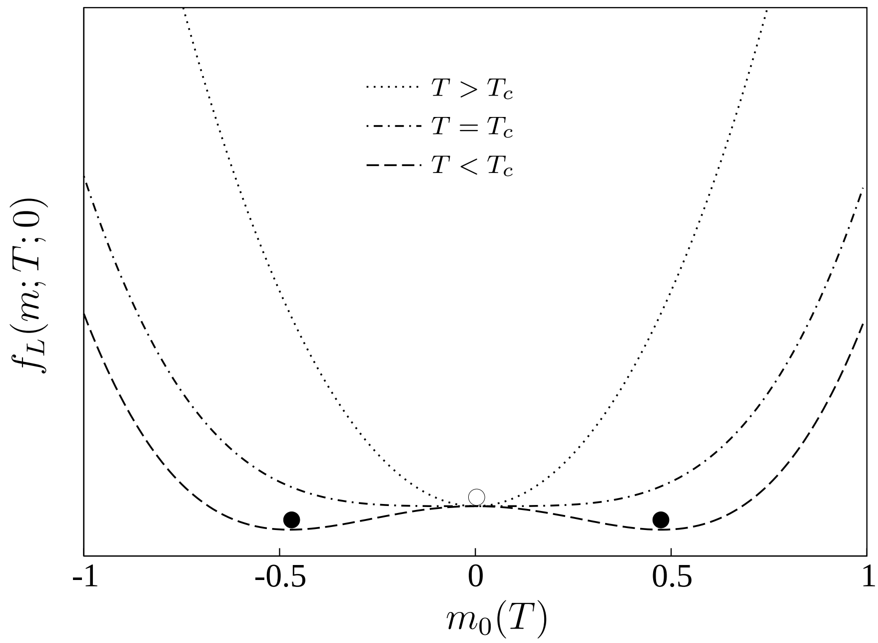


Figure 4: The Landau free energy per spin $f_L(m;T;0)$ vs. the average magnetisation per spin in zero external field $m_0(T)$. The solid circles show the position of the minima of the free energy of the corresponding graph. For $T \geq T_c$, unique minimum at $m_0(T) = 0$. For $T < T_c$, double minima at $m_0(T) = \pm m_0 \neq 0$.

Minimise f_L with respect to m:

$$\left(\frac{\partial f}{\partial m}\right)_{T,H} = 0 \Leftrightarrow 2a_2(T - T_c)m + 4a_4 m^3 - H = 0. \tag{10}$$

In zero external field, we have

$$2m_0(T)\left[a_2(T - T_c) + 2a_4 m_0^2(T)\right] = 0. \tag{11}$$

For $T \geq T_c$ this implies $m_0(T) = 0$ because $a_4 > 0$.
For $T < T_c$ this implies $m_0(T) = \pm\left[a_2(T_c - T)/2a_4\right]^{1/2} \propto \pm\left(T_c - T\right)^{1/2}$.
In summary

$$\begin{aligned} m_0(T) &= \begin{cases} 0 & \text{for } T \geq T_c \\ \pm\left[a_2(T_c - T)/2a_4\right]^{1/2} & \text{for } T \to T_c^- \end{cases} \\ &\propto \begin{cases} 0 & \text{for } T \geq T_c \\ \pm(T_c - T)^{1/2} & \text{for } T \to T_c^-. \end{cases} \end{aligned} \tag{12}$$

(d) See Figure 5.

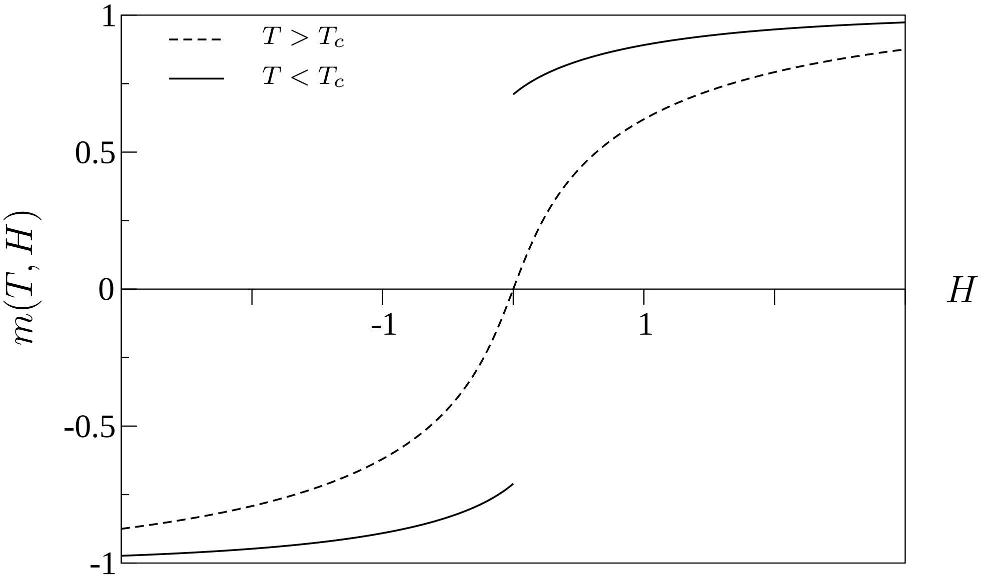


Figure 5: Sketch of the magnetisation per spin $m(T, H)$ versus the external field H for two different temperatures $T > T_c$ and $T < T_c$. For large external fields, the magnetisation saturates to $m = \pm 1$ for both graphs. When $H = 0$: For $T > T_c$ graph is continuous and it crosses the point $(0, 0)$ because $m(T, 0) = 0$. For $T < T_c$, the graph have a discontinuous jump at $H = 0$ because $\lim_{H \to 0^{\pm}} m(T, H) = \pm m(T, 0) \neq 0$.

(e) (i) I have been quite 'naughty' posing you this question as it is tempting you to make wrong conclusions in order to reach an almost (a factor of 2 will be missing) correct answer. Of course, I would never do that in an exam situation. However, it might be very instructive because it exposes two types of wrong-doing (that are intimately linked) that are found quite frequently in literature on the Ising model.

Case 1 – wrong mean-field theory:

First, we derive the result for non-interacting spins in an external field H (Sec. 2.2 in notes). The total energy is

$$E_{\{s_i\}} = -H \sum_{i=1}^{N} s_i. \tag{13}$$

The partition function is

$$\begin{aligned}
Z(T,H) &= \sum_{\{s_i\}} \exp\left(-\beta E_{\{s_i\}}\right) = \sum_{\{s_i\}} \exp\left(\beta H \sum_{i=1}^{N} s_i\right) \\
&= \sum_{\{s_i\}} \prod_{i=1}^{N} \exp\left(\beta H s_i\right) = \left(2\cosh\beta H\right)^N . \qquad (14)
\end{aligned}$$

The free energy per spin

$$f(T,H) = -k_B T \ln\left(2\cosh\beta H\right), \qquad (15)$$

and hence, the magnetisation per spin is given by

$$m(T,H) = -\left(\frac{\partial f}{\partial H}\right)_T = k_B T \frac{2\sinh\beta H}{2\cosh\beta H}\,\beta = \tanh\beta H. \qquad (16)$$

The total energy of the Ising model in this version of the mean-field model:

$$\begin{aligned}
E_{\{s_i\}} &= -J\sum_{\langle ij\rangle} s_i s_j - H\sum_{i=1}^{N} s_i \\
&\approx -J\sum_{\langle ij\rangle} s_i m - H\sum_{i=1}^{N} s_i \\
&= -Jm\frac{z}{2}\sum_{i=1}^{N} s_i - H\sum_{i=1}^{N} s_i \quad \text{each site } i \text{ has } \frac{z}{2} \text{ distinct nn} \\
&= -\left(Jm\frac{6}{2} + H\right)\sum_{i=1}^{N} s_i \quad z = 6 \text{ in } d = 3 \text{ cubic lattice} \\
&= -\left(3Jm + H\right)\sum_{i=1}^{N} s_i \\
&= -H_{\text{eff}}\sum_{i=1}^{N} s_i, \qquad (17)
\end{aligned}$$

where we have introduced an effective external field

$$H_{\text{eff}} = 3Jm + H. \qquad (18)$$

So far nothing illegal has taken place. However, now the argument (wrongly) states that using Eq. (16), we find that the magnetisation must satisfy the equation

$$m(T,H) = \tanh\beta H_{\text{eff}} = \tanh\left(\beta 3Jm + \beta H\right). \qquad (19)$$

To see that this is indeed a conclusion that **cannot** be drawn, we need to go through the second case that is often presented in the literature.

Case 2 - wrong mean-field theory:
We start with the mean-field energy

$$E_{\{s_i\}} \approx -\left(3Jm + H\right)\sum_{i=1}^{N} s_i. \tag{20}$$

The associated partition function is

$$\begin{aligned} Z &= \sum_{\{s_i\}} \exp\left(\left(\beta 3Jm + \beta H\right)\sum_{i=1}^{N} s_i\right) \\ &= \sum_{\{s_i\}} \prod_{i=1}^{N} \exp\left[\left(\beta 3Jm + \beta H\right) s_i\right] \\ &= \left[2\cosh\left(\beta 3Jm + \beta H\right)\right]^N . \end{aligned} \tag{21}$$

The free energy per spin is

$$\begin{aligned} f &= -\frac{1}{N} k_B T \ln\left[\left[2\cosh\left(\beta 3Jm + \beta H\right)\right]^N\right] \\ &= -k_B T \ln\left[2\cosh\left(\beta 3Jm + \beta H\right)\right]. \end{aligned} \tag{22}$$

Hence, the magnetisation per spin is

$$\begin{aligned} m &= -\left(\frac{\partial f}{\partial H}\right)_T \\ &= k_B T \frac{2\sinh(\beta 3Jm + \beta H)}{2\cosh(\beta 3Jm + \beta H)}\left(\beta 3J\left(\frac{\partial m}{\partial H}\right)_T + \beta\right) \\ &= \tanh(\beta 3Jm + \beta H)\left(3J\left(\frac{\partial m}{\partial H}\right)_T + 1\right). \end{aligned} \tag{23}$$

However it is common to use a dirty trick and (wrongly) briefly assume that m is independent of H. In doing so, we arrive at the following equation for determining m in the mean-field picture

$$\begin{aligned} m &= -\left(\frac{\partial f}{\partial H}\right)_T \\ &= k_B T \frac{2\sinh(\beta 3Jm + \beta H)}{2\cosh(\beta 3Jm + \beta H)} \\ &= \tanh(\beta 3Jm + \beta H). \end{aligned} \tag{24}$$

This is in effect what is tacitly done in case 1 also. Indeed, Eq.(16) states

$$m(T,H) = k_B T \frac{2\sinh\beta H}{2\cosh\beta H}\left(\frac{\partial \beta H}{\partial H}\right)_T \tag{25}$$

and substituting in this equation $H_{\text{eff}} = 3Jm + \beta H$ we arrive at the same result.

Case 3 - correct mean-field theory:
Following the derivation in the notes (Sec. 2.5), we find that the correct equation for determining m in the mean-field picture is, in fact

$$m = \tanh(\beta 6Jm + \beta H), \tag{26}$$

that is, there is an extra factor of 2 in the contribution to the 'internal field'.

Also, cases 1 and 2 would also fail to yield an equation for the magnetisation m using the equation

$$\left(\frac{\partial f}{\partial m}\right)_{T,H} = 0 \tag{27}$$

(ii) Mean field theory result:

$$m = \tanh(\beta 6Jm + \beta H) = \tanh\left[(6Jm + H)/(k_B T)\right]. \tag{28}$$

Uncorrelated spins in an effective field $H_{\text{eff}} = H + 6Jm$. Each spin feels the external field H. Also, each spin feels the average magnetisation m of each of its 6 ($d = 3$ cubic lattice) neighbouring spins. In the exchange interaction: $-Js_is_j$ this corresponds to an effective internal field of $6Jm$.

As you can see from the discussion above, this interpretation is strictly speaking, not scientifically sound but nevertheless frequently used in the literature.

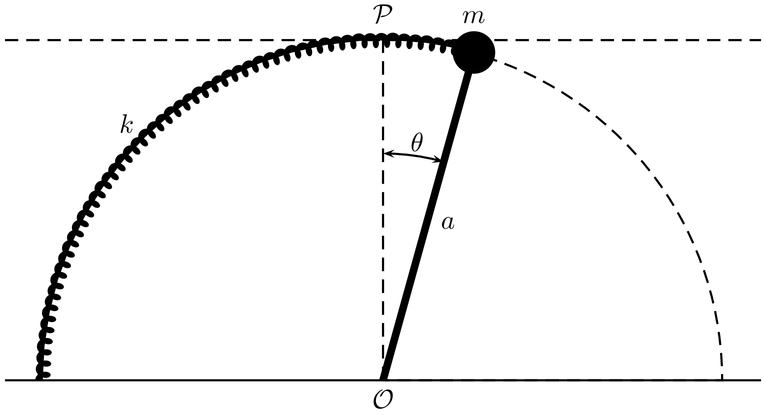
Tuesday 26th November 2013

Hand in to UG office by 14:00 on Monday 2nd December
Marked work available in UG office by 12:00 on Wednesday 4th December
RF class at 12:00 on Wednesday 4th December

Statistical Mechanics Problem Sheet 8

1. *Second order PT in a mass-spring system: Landau theory.* (**RF Question**)

   A rigid massless rod of length a can rotate around a fixed point $\mathcal{O}$ in the vertical plane only. The orientation of the rod is given by its angle θ to be measured positive clockwise from the vertical. At the top of the rod is placed a *variable* mass m which is linked to a circular harmonic spring of radius a and spring constant k. When the rod is vertical, the length of the spring equals its natural length, $\pi a/2$.



   (a) Show that the total energy of the mass-spring system is

   $$U(\theta) = \frac{1}{2}ka^2\theta^2 + mga(\cos\theta - 1), \tag{1}$$

   where the zeroth-level of the gravitational potential energy is defined as the horizontal dashed line passing through the point $\mathcal{P}$, the position of the mass when the rod is vertical.

   (b) (i) Expand the function $U(\theta)$ in Eq. (1) around $\theta = 0$ up to fourth order, to show that

   $$U(\theta) = \frac{a}{2}(ka - mg)\theta^2 + \frac{mga}{24}\theta^4. \tag{2}$$

(ii) Explain why only terms of even order appear in the expansion in Eq. (2).

(iii) Sketch the function $U(\theta)$ in Eq. (2) for $ka > mg, ka = mg$, and $ka < mg$.

(iv) Using Eq. (2), find an explicit expression for the angle of equilibrium $\theta_0(m)$ when $ka > mg$ and $ka < mg$.

(v) Sketch the solution of the angle of equilibrium $\theta_0(m)$ as a function of the ratio ka/mg. Relate the graph to the sketches from question (iii).

(vi) Briefly outline the Landau theory of second-order phase transitions in general.

(vii) What is the order parameter of the mass-spring system? What is the critical value m_c of the variable mass m? Explain your answers.

2. *Diluted Ising model.*

Consider the diluted Ising model in zero external field with the energy

$$E_{\{s_i\}} = -\sum_{\langle ij \rangle} J_{ij} s_i s_j, \tag{3}$$

where $s_i = \pm 1$ is the spin at lattice position i, the sum runs over different pairs of nearest neighbour sites, and the coupling constants

$$J_{ij} = \begin{cases} J > 0 & \text{with probability } p \\ 0 & \text{with probability } (1-p). \end{cases} \tag{4}$$

(a) Discuss how this problem is related to percolation theory.

(b) In the following, assume the temperature $T = 0$.

(i) What is the ground state of the diluted Ising model?

(ii) Show that

$$\langle s_i s_j \rangle = \begin{cases} 1 & i, j \text{ in the same percolation cluster} \\ 0 & \text{otherwise.} \end{cases} \tag{5}$$

(iii) Argue why the average magnetisation per spin $m_0(p) = 0$ for $p \leq p_c$. Based on your knowledge of percolation, find an expression for $m_0(p)$ when $p > p_c$.

You may assume that for small non-zero external field H and low temperatures $k_B T \ll J$, the magnetisation per spin

$$m(p, H) = \pm P_\infty(p) + \sum_{s=1}^{\infty} s n(s, p) \tanh(sH/k_B T), \tag{6}$$

where $n(s, p)$ is the cluster number density.

(c) (i) What does the term $P_\infty(p)$ represent? Find the magnetisation $m_0(p)$ in the limit of $H \to 0$.

(ii) Define the susceptibility χ per spin. Assuming $H \ll k_B T$, show that the susceptibility per spin diverges when $p \to p_c$.

(d) A version of the fluctuation-dissipation theorem states that

$$\chi = \frac{1}{k_B T} \sum_i \sum_j \left(\langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \right) \tag{7}$$

where $\langle s_i \rangle = \langle s_j \rangle = m_0$. Assume p approaches p_c from below and $k_B T \ll J$. Calculate the susceptibility using this formula and show it is consistent with the result derived in (c)(ii).

3. *Landau theory for the Ising model.*

Consider an Ising ferromagnet with spins on a three-dimensional cubic lattice. The total energy $E_{\{s_i\}}$ of the system in an applied external field H is given by

$$E_{\{s_i\}} = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_{i=1}^{N} s_i. \tag{8}$$

(a) (i) Explain the variable s_i of the Ising model.

(ii) Give and explain the sign of J suitable for a ferromagnet.

(iii) Explain what the first sum runs over, that is, what does $\langle ij \rangle$ signify?

For an Ising ferromagnet at temperature T in an external applied field H, the Landau free energy density (per spin) is given by

$$f_L(m; T; H) = f_0(T) + a_2(T - T_c)m^2 + a_4 m^4 - mH \tag{9}$$

where $m = \langle s_i \rangle$ is the average magnetisation per spin and T_c, a_2 and a_4 (all positive) are phenomenological parameters. Consider first the ferromagnet in the absence of an applied magnetic field, $H = 0$.

(b) Sketch the magnetisation per spin of the Ising ferromagnet as a function of temperature. Indicate clearly the behaviour at temperatures $T \to 0$, near $T = T_c$, and at high temperatures $T \gg T_c$.

(c) Sketch the Landau free energy density f_L at $H = 0$ as a function of m for the three temperatures: $T > T_c$, $T = T_c$ and $T < T_c$. Hence, deduce the equilibrium magnetisation $m_0(T)$ as a function of temperature T, as predicted by Landau theory.

An external field $H \neq 0$ is applied to the ferromagnet parallel to the spin axis.

(d) Sketch the magnetisation per spin m as a function of the applied field H in the range $-\infty < H < \infty$ for two temperatures: $T > T_c$ and $T < T_c$. Indicate clearly the behaviour near zero field and at high fields. Hint: make sure your answer here is consistent with your answer to part (b).

One version of a mean-field theory for the Ising model approximate the total energy

$$E_{\{s_i\}} \approx -J \sum_{\langle ij \rangle} s_i m - H \sum_{i=1}^{N} s_i, \tag{10}$$

where $m = \langle s_j \rangle$.

(e) (i) Using this approach, write down the self-consistent equation given by mean-field theory for the magnetisation per spin m at temperature T in non-zero external field H in a three-dimensional cubic lattice.

(ii) Give a physical picture to explain your equation and its relationship with the magnetisation of a single spin in a field H:

$$m = \tanh\left(\frac{H}{k_B T}\right) \tag{11}$$

where H is expressed in the same units as in Eq. (8).

Problem sheet 9 issued: Tuesday 3rd December 2013
Solutions available from: Wednesday 11th December 2013

Statistical Mechanics Answer Sheet 9

1. *Scaling ansatz of free energy per spin and scaling relations.* (**RF Question**)

   (a) Consider the Ising model on a d-dimensional lattice in an external field H.

   (i) The total energy for a system of N spins $s_i = \pm 1$ with constant nearest-neighbour interactions $J > 0$ placed in a uniform external field H is

   $$E_{\{s_i\}} = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_{i=1}^{N} s_i, \tag{1}$$

   where the notation $\langle ij \rangle$ restricts the sum to run over all distinct nearest-neighbour pairs.

   (ii) Let $M_{\{s_i\}} = \sum_{i=1}^{N} s_i$ denote the total magnetisation and $\langle M \rangle$ the average total magnetisation. The order parameter for the Ising model is defined as the magnetisation per spin

   $$m(T, H) = \lim_{N \to \infty} \frac{\langle M \rangle}{N}. \tag{2}$$

   Consider the free energy $F = \langle E \rangle - TS$. The ratio of the average total energy, $\langle E \rangle$, to the temperature times entropy, TS, defines a dimensionless scale $J/(k_B T)$. A competition exists between the tendency to randomise the orientation of spins for $J \ll k_B T$, and a tendency to align spins for $J \gg k_B T$. In the former case, the free energy is minimised by maximising the entropic term: the magnetisation is zero because the spins point up and down randomly. In the latter case, the free energy is minimised by minimising the total energy: the magnetisation is non-zero because the spins tend to align. Since the entropy in the free energy is multiplied by temperature, for sufficiently low temperatures, the minimisation of the free energy is dominated by the minimisation of the total energy. Therefore, at least qualitatively, there is a possibility of a phase transition from a phase with zero magnetisation at relatively high temperatures, to a phase with non-zero magnetisation at relatively low temperatures.

We assume that the singular part of free energy per spin is a generalised homogeneous function,

$$f(t,h) = b^{-d} f(b^{y_t} t, b^{y_h} h) \quad \text{for } t \to 0^{\pm}, h \to 0, \forall\, b > 0. \tag{3}$$

(b) Below, we use the notation $\frac{\partial f}{\partial t} = f'_t$ and $\frac{\partial^2 f}{\partial t^2} = f''_{tt}$ and similar for partial derivatives w.r.t. h.

(i) The critical exponent α associated with the specific heat in zero external field characterises its divergence as $t \to 0$ and is defined by

$$c(t,0) \propto |t|^{-\alpha} \quad \text{for } t \to 0. \tag{4}$$

The specific heat is related to the free energy per spin:

$$c(t,h) \propto \left(\frac{\partial^2 f}{\partial t^2}\right) \propto b^{2y_t - d} f''_{tt}(b^{y_t} t, b^{y_h} h). \tag{5}$$

Choosing $b = |t|^{-1/y_t}$ and setting $h = 0$ we find

$$c(t,0) \propto |t|^{-\frac{2y_t - d}{y_t}} f''_{tt}(\pm 1, 0) \quad \text{for } t \to 0^{\pm}, \tag{6}$$

and since $f''_{tt}(\pm 1, 0)$ are just numbers, we identify

$$\alpha = \frac{2y_t - d}{y_t}. \tag{7}$$

(ii) The critical exponent β associated with the order parameter (magnetisation per spin) in zero external field characterises the pick up of the order parameter as $t \to 0^-$ and is defined by

$$m(t,0) \propto |t|^{\beta} \quad \text{for } t \to 0^-. \tag{8}$$

The magnetisation per spin is related to the free energy per spin:

$$m(t,h) \propto -\left(\frac{\partial f}{\partial h}\right) \propto b^{y_h - d} f'_h(b^{y_t} t, b^{y_h} h). \tag{9}$$

Choosing $b = |t|^{-1/y_t}$ and setting $h = 0$ we find

$$m(t,0) \propto |t|^{\frac{d - y_h}{y_t}} f'_h(-1, 0) \quad \text{for } t \to 0^-, \tag{10}$$

and since $f'_h(-1,0)$ is just a number, we identify

$$\beta = \frac{d - y_h}{y_t}. \tag{11}$$

(iii) The critical exponent γ associated with the susceptibility in zero external field characterises its divergence when $t \to 0$ and is defined by

$$\chi(t,0) \propto |t|^{-\gamma} \quad \text{for } t \to 0. \tag{12}$$

The susceptibility is related to the free energy per spin:

$$\chi(t,h) \propto -\left(\frac{\partial^2 f}{\partial h^2}\right) \propto b^{2y_h-d} f''_{hh}(b^{y_t}t, b^{y_h}h). \tag{13}$$

Choosing $b = |t|^{-1/y_t}$ and setting $h = 0$ we find

$$\chi(t,0) \propto |t|^{-\frac{2y_h-d}{y_t}} f''_{hh}(\pm 1, 0) \quad \text{for } t \to 0 \tag{14}$$

and since $f''_{hh}(\pm 1, 0)$ are just numbers, we identify

$$\gamma = \frac{2y_h - d}{y_t}. \tag{15}$$

(iv) The critical exponent δ associated with the order parameter at the critical temperature characterises how the magnetisation per spin vanishes for small external fields and is defined by

$$m(0,h) \propto \text{sign}(h)|h|^{1/\delta} \quad \text{for } h \to 0^{\pm}. \tag{16}$$

The magnetisation per spin is related to the free energy per spin:

$$m(t,h) \propto -\left(\frac{\partial f}{\partial h}\right) \propto b^{y_h-d} f'_h(b^{y_t}t, b^{y_h}h). \tag{17}$$

Choosing $b = |h|^{-1/y_h}$ and setting $t = 0$ we find

$$m(0,h) \propto |h|^{\frac{d-y_h}{y_h}} f'_h(0, \pm 1) \quad \text{for } h \to 0 \tag{18}$$

and since $f'_h(0, \pm 1)$ are just numbers, we identify

$$\delta = \frac{y_h}{d - y_h}. \tag{19}$$

(v) We find

$$\begin{aligned}\alpha + 2\beta + \gamma &= \frac{2y_t - d + 2d - 2y_h + 2y_h - d}{y_t} \\ &= 2\end{aligned}$$

and

$$\begin{aligned}\beta(\delta-1) &= \frac{d-y_h}{y_t}\left(\frac{y_h}{d-y_h}-1\right)\\ &= \frac{d-y_h}{y_t}\left(\frac{2y_h-d}{d-y_h}\right)\\ &= \frac{2y_h-d}{y_t}\\ &= \gamma.\end{aligned}$$

2. *One-dimensional Ising model with periodic boundary conditions* (Exam 2007)

   (a) The total energy for a system of N spins $s_i = \pm 1$ with constant nearest-neighbour interactions $J > 0$ placed in a uniform external field H is

$$\begin{aligned}E_{\{s_i\}} &= -J\sum_{\langle ij\rangle} s_i s_j - H\sum_{i=1}^{N} s_i,\\ &= -J\sum_{i=1}^{N} s_i s_{i+1} - H\sum_{i=1}^{N} s_i.\end{aligned} \tag{20}$$

   The sum over all distinct nearest-neighbour pairs $\langle ij\rangle$ reduces to the sum over all spins in $d=1$ with $s_{N+1} = s_1$.

   (b) (i) At $T = 0$ all spins are aligned. Hence there are 2 microstates with all spins pointing up or all spins pointing down.

   (ii) When $T \to \infty$ all spins are pointing up and down at random without any correlations. Hence there are a total of 2^N microstates.

   (iii) The total energy $E_{\{s_i\}} = -J\sum_{i=1}^{N} s_i s_{i+1}$ in zero external field. At $T = 0$ all spins are aligned. At $T = \infty$ spins are pointing up and down at random. Hence, the energy per spin

$$\epsilon(T,0) = \frac{\langle E\rangle}{N} = \begin{cases}-J & \text{at } T=0,\\ 0 & \text{for } T\to\infty.\end{cases} \tag{21}$$

   (iv) The magnetisation per spin

$$m(T,0) = \frac{\langle M\rangle}{N} = \begin{cases}\pm 1 & \text{at } T=0,\\ 0 & \text{for } T\to\infty\end{cases} \tag{22}$$

   since at $T = 0$ all spins are aligned while at $T = \infty$ spins are pointing up and down at random.

(v) The entropy $S = k_B \ln \Omega$ where Ω is the number of microstates. Hence

$$S(T,0) = \begin{cases} k_B \ln 2 & \text{for } T = 0, \\ N k_B \ln 2 & \text{for } T \to \infty. \end{cases} \tag{23}$$

You may also arrive at the same result using

$$S(T,0) = -k_B \sum_{\{s_i\}} p_{\{s_i\}} \ln p_{\{s_i\}}, \tag{24}$$

where $p_{\{s_i\}}$ is given by the Boltzmann distribution

$$p_{\{s_i\}} = \frac{\exp\left(-\beta E_{\{s_i\}}\right)}{\sum_{\{s_i\}} \exp\left(-\beta E_{\{s_i\}}\right)}, \tag{25}$$

with $\beta = 1/(k_B T)$ the 'inverse temperature'.

For $T \to 0$, only the two ground states will have a non-zero probability and $p_{\{s_i=+1\forall i\}} = p_{\{s_i=-1\forall i\}} = 1/2$. Hence

$$S(0,0) = -k_B \sum_{\{s_i\}} p_{\{s_i\}} \ln p_{\{s_i\}} = -k_B \left(\frac{1}{2}\ln\frac{1}{2} + \frac{1}{2}\ln\frac{1}{2}\right) = k_B \ln 2. \tag{26}$$

For $T \to \infty$, $\beta \to 0$ and all 2^N microstates have equal probability with $p_{\{s_i\}} = 2^{-N}$. Hence

$$S(\infty,0) = -k_B \sum_{\{s_i\}} p_{\{s_i\}} \ln p_{\{s_i\}} = -k_B 2^N 2^{-N} \ln 2^{-N} = N k_B \ln 2. \tag{27}$$

(vi) The total free energy $\langle F \rangle = \langle E \rangle - TS$. Hence, using the results of (iii) and (v) we find that the free energy per spin

$$f(T,0) = \frac{F}{N} = \begin{cases} -J - \frac{1}{N} k_B T \ln 2 & \text{for } T = 0, \\ -k_B T \ln 2 & \text{for } T \to \infty. \end{cases} \tag{28}$$

(c) The magnetisation per spin

$$m(T,H) = \frac{\sinh \beta H}{\sqrt{\sinh^2 \beta H + \exp(-4\beta J)}}, \tag{29}$$

where $\beta = 1/(k_B T)$ and $J > 0$ the coupling constant. We note that $\sinh \beta H \to 0$ for $H \to 0^{\pm}$.

When $T > 0$, the term $\exp(-4\beta J)$ is finite and hence $\lim_{H\to 0} m(T,H) = 0$.

When $T = 0$, the term $\exp(-4\beta J)$ is zero and hence $\lim_{H\to 0^{\pm}} m(0,H) = \pm 1$.

Hence there is no phase-transition in the Ising model in zero external field at any finite temperature.

3. *One-dimensional Ising model with periodic boundary conditions* (Exam 2010)

   (a) The partition function for the $d = 1$ Ising model:

$$Z_{\text{ring}} = \sum_{\{s_i\}} e^{-\beta E_{\{s_i\}}} = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} e^{\beta J s_1 s_2} e^{\beta J s_2 s_3} \ldots e^{\beta J s_{N-1} s_N} e^{\beta J s_N s_1} \tag{30}$$

   where $\beta = 1/(k_B T)$ with k_B the Boltzmann constant and T the temperature.

   (b) Using the notation of the transfer matrix, we find

$$\begin{aligned}
Z_{\text{ring}} &= \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} e^{\beta J s_1 s_2} e^{\beta J s_2 s_3} \ldots e^{\beta J s_{N-1} s_N} e^{\beta J s_N s_1} \\
&= \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} T_{s_1 s_2} T_{s_2 s_3} \ldots T_{s_{N-1} s_N} T_{s_N s_1} \\
&= \sum_{s_1=\pm 1} \sum_{s_3=\pm 1} \cdots \sum_{s_{N-1}=\pm 1} \left(\sum_{s_2=\pm 1} T_{s_1 s_2} T_{s_2 s_3} \right) \cdots \left(\sum_{s_N=\pm 1} T_{s_{N-1} s_N} T_{s_N s_1} \right) \\
&= \sum_{s_1=\pm 1} \sum_{s_3=\pm 1} \cdots \sum_{s_{N-1}=\pm 1} T^2_{s_1 s_3} T^2_{s_3 s_5} \ldots T^2_{s_{N-3} s_{N-1}} T^2_{s_{N-1} s_1} \\
&= \sum_{s_1=\pm 1} \sum_{s_5=\pm 1} \cdots \sum_{s_{N-3}=\pm 1} T^4_{s_1 s_5} T^4_{s_5 s_9} \ldots T^4_{s_{N-3} s_1} \\
&= \sum_{s_1=\pm 1} T^N_{s_1 s_1} \\
&= \operatorname{Tr}\left(\mathbf{T}^N\right),
\end{aligned} \tag{31}$$

   where we use the (general) fact of matrix multiplication

$$\sum_{s_k} T_{s_i s_k} T_{s_k s_j} = T^2_{s_i s_j}. \tag{32}$$

   (c) The transfer matrix in zero external field ($H = 0$) is

$$\mathbf{T} = \begin{pmatrix} T_{+1+1} & T_{+1-1} \\ T_{-1+1} & T_{-1-1} \end{pmatrix} = \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix}. \tag{33}$$

   The eigenvalues $\lambda_\pm$ of $\mathbf{T}$ are the solutions to the characteristic equation

$$\det(\mathbf{T} - \lambda \mathbf{I}) = 0. \tag{34}$$

   The determinant

$$\det(\mathbf{T} - \lambda \mathbf{I}) = \begin{vmatrix} e^{\beta J} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} - \lambda \end{vmatrix} = \lambda^2 - 2e^{\beta J}\lambda + e^{2\beta J} - e^{-2\beta J} \tag{35}$$

so the solutions to the characteristic Equation (34) are

$$\begin{aligned}\lambda_\pm &= \frac{2e^{\beta J} \pm \sqrt{4e^{2\beta J} - 4[e^{2\beta J} - e^{-2\beta J}]}}{2} \\ &= e^{\beta J} \pm e^{-\beta J} \\ &= \begin{cases} 2\cosh\beta J, \\ 2\sinh\beta J. \end{cases}\end{aligned} \tag{36}$$

Hence, the partition function

$$\begin{aligned}Z_{\text{ring}} &= \lambda_+^N + \lambda_-^N \\ &= (2\cosh\beta J)^N + (2\sinh\beta J)^N \\ &= (2\cosh\beta J)^N \left[1 + \tanh^N \beta J\right].\end{aligned} \tag{37}$$

(d) In the high-temperature limit

$$\beta J \ll 1. \tag{38}$$

Taylor expansion to first order yields $\cosh\beta J \approx 1$ and $\tanh\beta J \approx \beta J$ so that the partition function

$$\begin{aligned}Z_{\text{ring}} &= (2\cosh\beta J)^N \left[1 + \tanh^N \beta J\right] \\ &\approx 2^N \left[1 + (\beta J)^N\right] \\ &\approx 2^N\end{aligned} \tag{39}$$

because $(\beta J)^N \ll 1$. Hence, the total free energy of the system

$$\begin{aligned}F_{\text{ring}} &= -k_B T \ln Z_{\text{ring}} \\ &\approx -k_B T \ln 2^N \\ &= -TNk_B \ln 2 \\ &= -TS,\end{aligned} \tag{40}$$

where the entropy is given by

$$S = k_B \ln 2^N, \tag{41}$$

and also given by

$$S = -k_B \sum_{\{s_i\}} p_{\{s_i\}} \ln p_{\{s_i\}}, \tag{42}$$

with

$$\lim_{T\to\infty} p_{\{s_i\}} = \lim_{T\to\infty} \frac{e^{-\beta E_{\{s_i\}}}}{\sum_{\{s_i\}} e^{-\beta E_{\{s_i\}}}} = \frac{1}{2^N}. \tag{43}$$

The N spins are effectively free spins because the thermal energy k_BT is much larger than the energy $2J$ it costs to one flip from a $\uparrow\uparrow$ to a $\uparrow\downarrow$ local configuration. Therefore the free energy is just entropic with $-Tk_B \ln 2$ per spin.

(e) (i) Assume extremely low temperature with $\beta J \gg 1$. Using that

$$2\cosh x = e^x + e^{-x} \approx e^x \quad \text{for } x \gg 1, \tag{44a}$$
$$2\sinh x = e^x - e^{-x} \approx e^x \quad \text{for } x \gg 1, \tag{44b}$$

we find that the partition function

$$\begin{aligned} Z_{\text{ring}} &= (2\cosh\beta J)^N + (2\sinh\beta J)^N \\ &\approx e^{N\beta J} + e^{N\beta J} \\ &= 2e^{N\beta J}. \end{aligned} \tag{45}$$

Hence the total free energy

$$\begin{aligned} F_{\text{ring}} &= -k_BT\ln Z_{\text{ring}} \\ &\approx -k_BTN\beta J - k_BT\ln 2 \\ &= -NJ - k_BT\ln 2. \end{aligned} \tag{46}$$

(ii) Recall that $F = \langle E\rangle - TS$. Hence, we identify the first term, $-NJ$ as the energy of the ground state where all spins are aligned at $T = 0$. The second term, $-k_BT\ln 2$, tells us that the entropy is $k_B \ln 2$ at low temperatures. This is because there are two degenerate ground states, all spins pointing up or all spins pointing down.

4. *Ising model in* $d > 1$ (Exam 2006)

(a) (i) The total energy for a system of N spins $s_i = \pm 1$ with constant nearest-neighbour interactions $J > 0$ placed in a uniform external field H is

$$E_{\{s_i\}} = -J\sum_{\langle ij\rangle} s_i s_j - H\sum_{i=1}^{N} s_i, \tag{47}$$

where the notation $\langle ij\rangle$ restricts the sum to run over all distinct nearest-neighbour pairs.

(ii) Spins interact only with their nearest neighbours. The interaction strength is assumed to be a constant. The spins can only take one of two values $s_i = \pm 1$. Finally, the external field H is constant.

(b) (i) The free energy per spin

$$f(T, H) = -\frac{1}{N}k_BT\ln Z. \tag{48}$$

(ii) The average magnetisation per spin

$$m(T,H) = \left\langle \frac{1}{N}\sum_{i=1}^{N} s_i \right\rangle . \quad (49)$$

The statistical mechanical definition of the free energy yields

$$\begin{aligned}
-\left(\frac{\partial f}{\partial H}\right)_T &= \frac{1}{N}k_B T \frac{\partial}{\partial H}\ln Z \\
&= \frac{1}{N}k_B T \frac{1}{Z}\frac{\partial}{\partial H} Z \\
&= \frac{1}{N}k_B T \frac{1}{Z}\frac{\partial}{\partial H}\sum_{\{s_i\}}\exp(-\beta E_{\{s_i\}}) \\
&= \frac{1}{Z}\sum_{\{s_i\}}\exp(-\beta E_{\{s_i\}})\frac{1}{N}\sum_{i=1}^{N} s_i \\
&= \frac{1}{Z}\sum_{\{s_i\}}\exp(-\beta E_{\{s_i\}}) m_{\{s_i\}} \quad (50)
\end{aligned}$$

which is indeed the average magnetisation per spin.

(c) For $T \geq T_c$, the spins are equally likely to be pointing up and down on average so the magnetisation per spin is zero. The magnetisation picks up abruptly at $T = T_c$ and for $T < T_c$ a finite fraction of the spins are aligned. At $T = 0$, all spins point in the same direction. Hence, $m(0,0) = \pm 1$.

(d) (i) The average magnetisation per spin is

$$m(T,H) = -\left(\frac{\partial f}{\partial H}\right)_T . \quad (51)$$

Hence, for fixed temperature, T, the magnetisation per spin is the negative slope of the free energy per spin as a function of the external field H.

(ii) Clearly $T > T_c$ has zero slope at $H = 0$. For $T < T_c$ the slope is finite and take the same numerical value for $H \to 0^{\pm}$ but with different sign. At $T = T_c$, the slope is also zero but the second derivative (susceptibility) diverges, that is, the rate of change in the slope is infinite.

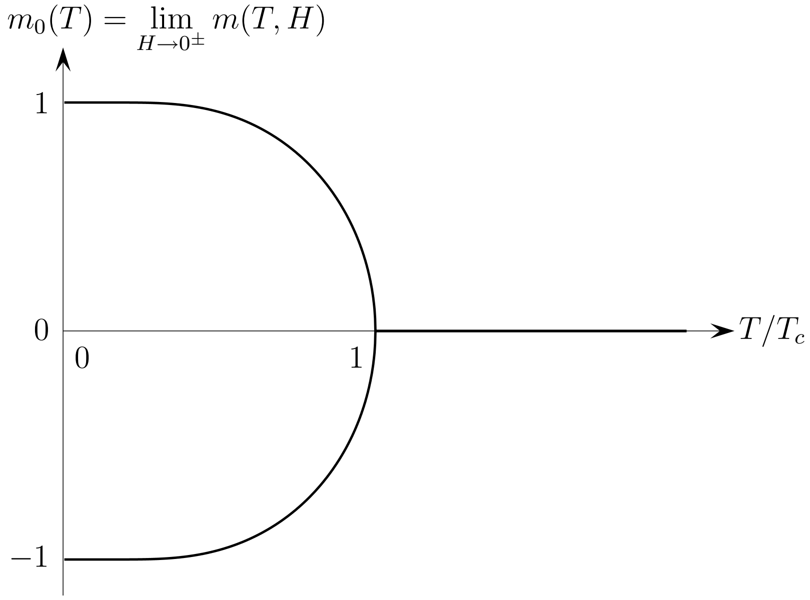


Figure 1: A sketch of the magnetisation per spin $m_0(T) = \lim_{H \to 0^\pm} m(T,H)$ versus the relative temperature T/T_c for the Ising model.

Tuesday 3rd December 2013

Hand in to UG office by 14:00 on Monday 9th December
Marked work available in UG office by 12:00 on Wednesday 11th December
RF class at 12:00 on Wednesday 11th December

Statistical Mechanics Problem Sheet 9

1. *Scaling ansatz of free energy per spin and scaling relations.* (**RF Question**)
   Consider the Ising model on a d-dimensional lattice in an external field H.

   (a) (i) Write down the energy $E_{\{s_i\}}$ for the Ising model. Clearly identify all symbols.

   (ii) Identify the order parameter for the Ising model and discuss qualitatively its behaviour as a function of temperature T in zero external field.

   Let $t = (T - T_c)/T_c$ and $h = H/(k_B T)$ denote the reduced temperature and external field, respectively. Assume that the singular part of free energy per spin is a generalised homogeneous function,

   $$f(t,h) = b^{-d} f(b^{y_t} t, b^{y_h} h) \quad \text{for } t \to 0^{\pm}, h \to 0, \forall\, b > 0, \tag{1}$$

   where d is the dimension and y_t, y_h are positive exponents.

   (b) (i) Define the critical exponent α associated with the specific heat in zero external field and show that Equation (1) implies

   $$\alpha = \frac{2y_t - d}{y_t}. \tag{2}$$

   (ii) Define the critical exponent β associated with the order parameter in zero external field and show that Equation (1) implies

   $$\beta = \frac{d - y_h}{y_t}. \tag{3}$$

   (iii) Define the critical exponent γ associated with the susceptibility in zero external field and show that Equation (1) implies

   $$\gamma = \frac{2y_h - d}{y_t}. \tag{4}$$

(iv) Define the critical exponent δ associated with the order parameter at the critical temperature and show that Equation (1) implies

$$\delta = \frac{y_h}{d - y_h}. \tag{5}$$

(v) Hence confirm the two scaling relations

$$\alpha + 2\beta + \gamma = 2, \tag{6a}$$
$$\gamma = \beta(\delta - 1). \tag{6b}$$

2. *One-dimensional Ising model with periodic boundary conditions* (Exam 2007)
Consider the $d = 1$ Ising model with N spins in an external field H.

(a) Write down the total energy $E_{\{s_i\}}$ for the one-dimensional Ising model with periodic boundary conditions. Identify clearly all the terms and discuss briefly the approximations entering into the Ising model.

Now consider the one-dimensional Ising model in zero external field $H = 0$.

(b) (i) Describe the microstates at zero temperature, $T = 0$. How many different microstates are there at $T = 0$?

(ii) Describe the microstates in the limit of infinite temperature, $T \to \infty$. How many different microstates are there when $T \to \infty$?

(iii) What is the energy per spin

$$\frac{\langle E \rangle}{N} = \begin{cases} ? & \text{at } T = 0 \\ ? & \text{for } T \to \infty \end{cases} \tag{7}$$

of the one-dimensional Ising model? Explain your answers.

(iv) What is the magnetisation per spin

$$m(T, 0) = \frac{\langle M \rangle}{N} = \begin{cases} ? & \text{at } T = 0 \\ ? & \text{for } T \to \infty \end{cases} \tag{8}$$

of the one-dimensional Ising model? Explain your answers.

(v) What is the (total) entropy

$$S(T, 0) = \begin{cases} ? & \text{at } T = 0 \\ ? & \text{for } T \to \infty \end{cases} \tag{9}$$

of the one-dimensional Ising model? Explain your answers.

(vi) What is the free energy per spin

$$f(T,0) = \frac{F}{N} = \begin{cases} ? & \text{at } T = 0 \\ ? & \text{for } T \to \infty \end{cases} \tag{10}$$

of the one-dimensional Ising model? Explain your answers.

(c) Exact solution of the one-dimensional Ising model in a non-zero external field yields

$$m(T,H) = \frac{\sinh \beta H}{\sqrt{\sinh^2 \beta H + \exp(-4\beta J)}}, \tag{11}$$

for the magnetisation per spin where $\beta = 1/(k_B T)$ and $J > 0$ the coupling constant. Discuss the possibility of a phase-transition in the one-dimensional Ising model in zero external field.

3. *One-dimensional Ising model with periodic boundary conditions* (Exam 2010)

Consider the Ising model for a ring of N sites with periodic boundary conditions. Because $s_{N+1} = s_1$, then in the absence of an external field, the total energy of the system is given by:

$$E_{\{s_i\}} = -J \sum_{i=1}^{N-1} s_i s_{i+1} - J s_N s_1 \tag{12}$$

where the spin s_i at site $\mathbf{r}_i$ may take on the values ± 1.

(a) Write down the partition function Z_{ring} of this system at temperature T as a sum over all possible spin configurations of the chain of N spins.

(b) Show that this partition function can be written in the form $Z_{\text{ring}} = \operatorname{Tr}\left(\mathbf{T}^N\right)$ with the transfer matrix $\mathbf{T}$ whose elements are:

$$T_{s,s'} = e^{\beta J s s'} \tag{13}$$

where $s, s' = \pm 1$ and $\beta = 1/(k_B T)$ with k_B being the Boltzmann constant.

(c) Show that the partition function is given by:

$$Z_{\text{ring}} = (2\cosh \beta J)^N \left[1 + \tanh^N(\beta J)\right]. \tag{14}$$

You may use the fact that $\operatorname{Tr}\left(\mathbf{T}^N\right) = \lambda_+^N + \lambda_-^N$ where $\lambda_+ > \lambda_-$ are the two eigenvalues of the transfer matrix $\mathbf{T}$.

(d) The total free energy of the system is given by $F_{\text{ring}} = -k_B T \ln Z_{\text{ring}}$. Derive the total free energy F_{ring} in the high-temperature regime. You only need to give the leading term for F_{ring} in this regime. You should give an inequality defining the high-temperature regime and give a physical interpretation.

(e) Consider the system at a fixed and finite N in the regime of extremely low temperatures: $\beta J \gg 1$ and $N \ll 1/\ln(\tanh \beta J)$.

(i) Show that

$$F_{\text{ring}} \approx -NJ - k_B T \ln 2 \tag{15}$$

in this low-temperature regime.

(ii) Give a physical interpretation of the two terms in the form of the free energy given by Eq. (15)

4. *Ising model in $d > 1$* (Exam 2006)

Consider an Ising model in dimension $d > 1$.

(a) (i) Write down the total energy $E_{\{s_i\}}$ for the Ising model with N spins in an external field H. Clearly identify all symbols.

(ii) Discuss the simplifications entering into the Ising model.

(b) The partition function is given by $Z = \sum_{\{s_i\}} \exp\left(-\beta E_{\{s_i\}}\right)$ where $\beta = 1/(k_B T)$ is the inverse temperature.

(i) Express the free energy per spin $f(T, H)$ in terms of the partition function.

(ii) Define the average magnetisation per spin $m(T, H)$ for the Ising model and prove that

$$m(T, H) = -\left(\frac{\partial f}{\partial H}\right)_T . \tag{16}$$

(c) Make a sketch of the average magnetisation per spin in zero external field, $m_0(T) = \lim_{H \to 0^\pm} m(T, H)$ as a function of temperature, T. Comment on your sketch to emphasize relevant and characteristic features.

(d) Figure 1 below displays the free energy per spin, $f(T, H)$, as a function of external field for, H, for three temperatures $T > T_c$, $T = T_c$ and $T < T_c$.

(i) How can you determine the average magnetisation per spin graphically from Fig. 1?

(ii) Consider the average magnetisation per spin in the limit $H \to 0^\pm$. Explain whether your sketch in sub-question (c) is qualitatively consistent with the average magnetisation per spin $\lim_{H \to 0^\pm} m(T, H)$ determined from Fig. 1.

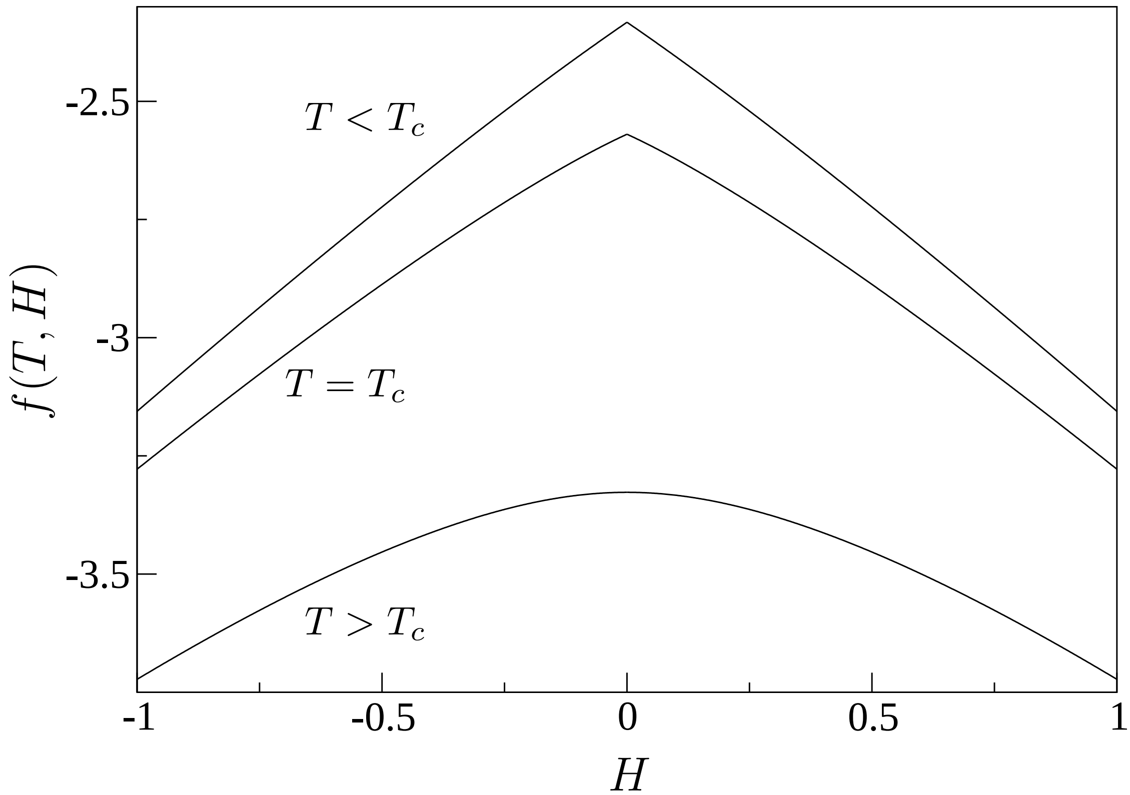


Figure 1: The free energy per spin, $f(T, H)$, versus the external field, H, for temperatures $T > T_c$ (lower graph) $T = T_c$ (middle graph) and $T < T_c$ (upper graph).