Statistical Physics
Section 11: Exact Results for the Ising Model

In one dimension the Ising energy becomes

$$E = -h\sum_{i=1}^{N} S_i - J\sum_{i=1}^{N} S_i S_{i+1} \tag{1}$$

Note that we have assumed periodic boundary conditions which mean we take $S_{N+1} = S_1$ i.e. the spins are on a ring. This is a standard device to make things simple—one can consider other boundary conditions but it won't alter the physics.

11. 1. Solution in $1d$ *for* $h = 0$

$$\uparrow\uparrow \cdots \uparrow\uparrow\downarrow\downarrow \cdots \downarrow\downarrow\uparrow\uparrow \cdots \uparrow\uparrow$$

Example of two domain walls in a one-dimensional assembly of N Ising spins.

As we saw last section a microstate consists of clusters or domains of spins of the same sign separated by 'domain walls'. In the absence of an external field there are two possible ground state which contain no domain walls (the all up and all down configurations of spins). The number of domain walls in a microstate specifies the energy relative to the ground state i.e. each domain wall costs energy $2J$.

Let

$$n_i = \frac{1 - S_i S_{i+1}}{2} = \begin{cases} 1 & \text{if domain wall present} \\ 0 & \text{if no domain wall present} \end{cases} \tag{2}$$

Then

$$S_i S_{i+1} = 1 - 2n_i \tag{3}$$

and

$$E = -NJ + 2J\sum_{i=1}^{N} n_i \tag{4}$$

The first term is just a constant which can be ignored, thus the assembly has been transformed to a non-interacting assembly of domain walls.

The Boltzmann distribution for the single domain wall problem can be written down

$$p(n_i) = \frac{\mathrm{e}^{-2\beta J n_i}}{1 + \mathrm{e}^{-2\beta J n_i}} \tag{5}$$

The probability $p(1) = p$ that a domain wall is present then has the behaviour

$$\begin{array}{llll} \beta \to \infty & (T \to 0) & p \simeq \mathrm{e}^{-2\beta J} \to 0 \\ \beta \to 0 & (T \to \infty) & p \to 1/2 \end{array}$$

So we get the expected limits of no domain walls at $T = 0$ and a disordered state where spins are randomly up or down as $T \to \infty$. However already we can see from (5) that $p(1)$ goes smoothly between these two extremes and there is no phase transition. Thus for $T > 0$ we are always in the paramagnetic phase.

To see this in more detail we should consider the two point correlation function. Let j and k be two sites separated by distance $l = |j - k|$ and let m be the number of domain walls between the two sites.

Then

$$S_j S_k = \begin{array}{ll} +1 & \text{if } m \text{ even} \\ -1 & \text{if } m \text{ odd} \end{array} = (-1)^m$$

and we can average to obtain

$$\langle S_j S_k \rangle = \sum_m p_m (-1)^m \tag{6}$$

where p_m is the probability that there are precisely m domain walls between the two sites. p_m is given by the binomial distribution for having m domain walls in the l possible locations between the two sites with a domain wall present with probability p thus

$$\langle S_j S_k \rangle = \sum_{m=0}^{l} \left(\begin{array}{c} l \\ m \end{array} \right) p^m (1-p)^{l-m} (-1)^m = (1-2p)^l \tag{7}$$

where we have spotted the binomial expansion of $(1-2p)^l$. We can write this as (convince yourself)

$$\langle S_j S_k \rangle = \exp l \ln(1-2p) = \exp -l/\xi \tag{8}$$

where the *correlation length*

$$\xi = \frac{1}{|\ln(1-2p)|} \simeq \frac{1}{2p} \simeq \frac{\mathrm{e}^{2\beta J}}{2} \tag{9}$$

when p is small (low T)

Now we conclude from (8) that

$$\lim_{|j-k| \to \infty} \langle S_j S_k \rangle = 0 \quad \forall T > 0 \tag{10}$$

which implies that we are always in the paramagnetic phase. This is because we expect generally

$$\lim_{|j-k| \to \infty} \langle S_j S_k \rangle = \langle S_i \rangle^2 \tag{11}$$

so for a ferromagnetic phase we would obtain a non-zero limit and there would be *long-range order*.

Thus we have shown that there is no long-range order and no phase transition in the $d = 1$ Ising model. This directly contradicts our mean field prediction of a phase transition (for $z = 2$) at $T_c = 2J/k$. Mean field theory is disastrously wrong in one dimension!

On the other hand we see that ξ diverges as $T \to 0$ so we could think of $T = 0$ as a critical point, but this is a bit of a cheat really.

*11. 2. *General solution of 1d Ising Model (see Advanced Statistical Physics Course)*

For the general case ($h \neq 0$) we wish to calculate the partition function

$$Z = \sum_{\{S_i = \pm 1\}} \mathrm{e}^{-\beta E(\{S_i\})} = \sum_{S_1 = \pm 1} \sum_{S_2 = \pm 1} \cdots \sum_{S_N = \pm 1} \mathrm{e}^{-\beta E(\{S_i\})} \tag{12}$$

Now let us write the energy in the following way

$$E(\{S_i\}) = -\frac{h}{2}\sum_i S_i - \frac{h}{2}\sum_i S_{i+1} - J\sum_i S_i S_{i+1} \tag{13}$$

Then

$$\exp(-\beta E) = \prod_i \exp\left[\frac{\beta h}{2}(S_i + S_{i+1}) + \beta J S_i S_{i+1}\right] \tag{14}$$

and we have

$$Z = \sum_{\{S_i=\pm 1\}} \prod_i T(S_i, S_{i+1}) \tag{15}$$

where

$$T(S_i, S_{i+1}) = \exp\left[\frac{\beta h}{2}(S_i + S_{i+1}) + \beta J S_i S_{i+1}\right] \tag{16}$$

We can write the values $T(S_i, S_{i+1})$ as a 2×2 symmetric matrix known as the **Transfer Matrix**

$$T = \begin{pmatrix} \mathrm{e}^{\beta(J+h)} & \mathrm{e}^{-\beta J} \\ \mathrm{e}^{-\beta J} & \mathrm{e}^{\beta(J-h)} \end{pmatrix} \tag{17}$$

where the first (second) row corresponds to $S_i = +1$ (-1) and the first (second) column corresponds to $S_{i+1} = +1$ (-1)

Now writing out (15), and recalling we are using periodic boundary conditions, we have

$$\begin{aligned} Z &= \sum_{S_1=\pm 1}\sum_{S_2=\pm 1} T(S_1, S_2) \sum_{S_3=\pm 1} T(S_2, S_3) \ldots \sum_{S_N=\pm 1} T(S_{N-1}, S_N) T(S_N, S_1) && (18)\\ &= \mathrm{Trace}\left[T^N\right] && (19)\\ &= \lambda_+^N + \lambda_-^N && (20) \end{aligned}$$

In going from (18) to (19) we have used the usual rules of matrix multiplication and the definition of the trace as the sum of the diagonal elements; in going from (19) to (20) we have used the usual properties of the eigenvalues and trace of a symmetric matrix.

Direct calculation (you are invited to do so in the tutorial) gives $\lambda_\pm$, the eigenvalues of T, as

$$\lambda_\pm = \mathrm{e}^{\beta J}\cosh\beta h \pm \sqrt{\mathrm{e}^{2\beta J}\sinh^2\beta h + \mathrm{e}^{-2\beta J}} \tag{21}$$

Then the free energy per spin

$$f = -\frac{kT}{N}\ln Z \to -kT\ln\lambda_+ \tag{22}$$

for large N.

The thermodynamic properties can be obtained by taking the various derivatives of f with respect to h, β.

11. 3. Absence of long-range order in 1*d*

Let us generally consider two phases of a one dimensional system separated by a domain wall.

$$AA\cdots AABB\cdots BB$$

Domain wall between two phases A and B

and assume the two phases have equal free energies. In the Ising model the two phases are the Ferromagnetic up and down phases. We wish to determine whether a domain wall is favoured thermodynamically.

The energy cost ΔE of the domain wall will be *finite* if the interactions are short-ranged. For example the Ising model we have studied has nearest neighbour interactions and the energy cost is $\Delta = 2J$. We could also consider an Ising model with next nearest neighbour interactions etc. The important point is that the energy cost of a domain wall does not depend on the system size N.

The entropy gain due to the creation of a domain wall can be computed from the Boltzmann entropy

$$\Delta S = k \ln \Omega$$

where here $\Omega = N$ is the number of possible positions for the domain wall. Thus the free energy difference of a state of two domains divided by a domain wall over the ordered state of one phase is

$$\Delta F = \Delta E - T\Delta S = \Delta E - kT \ln N \tag{23}$$

which for all $T > 0$ will be negative for sufficiently large N. Thus entropy wins, domain walls are always created and long range order cannot be maintained in one dimension.

11. 4. Existence of a Phase Transition in $d = 2$

Let us consider the Ising model on a square lattice. A domain wall between the up and down phases is now an extended object: a chain of links.

$$\begin{array}{cccccc} + & + & + & + & + & + \\ + & + & + & + & - & + \\ + & + & + & - & - & + \\ - & - & - & - & - & - \end{array}$$

In $2d$ a Domain wall between up and down domains is an extended object

Let's say the length of the chain is $\tilde{N}$.

Then the energy cost of the whole chain is

$$\Delta E = 2J\tilde{N}$$

since we have $\tilde{N}$ nearest neighbour pairs of spins of opposite signs.

To evaluate the entropy gain due to a domain wall in the system we have to estimate Ω the number of possible paths for the domain wall. If we start at the left hand side and the size of the lattice is $N = L \times L$ then there are L starting positions.

At each step the domain wall can move to the right, move up or move down. This implies that the number of domain walls is approximately

$$\Omega \simeq L3^{\tilde{N}} \tag{24}$$

This may seem a crude estimate (in fact it is an upper bound) but we only need a crude estimate because we take the logarithm

$$\Delta S = k\tilde{N} \ln 3 + k \ln L \simeq k\tilde{N} \ln 3 \tag{25}$$

Then

$$\Delta F \simeq \tilde{N} \left[2J - kT \ln 3\right] \tag{26}$$

Clearly for sufficiently low T, namely

$$T < \frac{2J}{\ln 3} \tag{27}$$

$\Delta F > 0$ and a domain wall is not thermodynamically favoured. Thus the ordered phase is stable for low enough T (but $T > 0$) and long range order is maintained.

However we know that at large T the domain wall must be favoured and we should have a disordered phase. This will occur at a critical temperature T_c. The above domain wall argument can be sharpened (see Huang) so that it actually gives a rigorous lower bound

$$T_c > \frac{2J}{\ln 3} \tag{28}$$

which compares favourably to the exact value determined from the exact solution (Huang chapter 15..... but not for the faint hearted!)

$$T_c = \frac{2J}{\ln(\sqrt{2}+1)} \tag{29}$$

What the crude argument misses is the existence of small 'bubbles' of the minority phase inside the majority phase at finite (but low) T.

11. 5. Mapping to a Lattice Gas

In the lattice gas model each site of a lattice is either occupied by a particle or is empty. Thus each lattice site has associated with it a variable

$$c_i = \begin{array}{c} 1 \\ 0 \end{array} \tag{30}$$

The overall number concentration of the gas is

$$c = \frac{\text{number of particles}}{\text{number of lattice sites}} = \frac{\sum_i c_i}{N} \tag{31}$$

A hardcore repulsion between lattice gas particles is wired in due to the occupancy $c_i = 1.0$. A short-range attractive potential is introduced by an energy $-\epsilon < 0$ associated with a pair of neighbouring particles.

$$E = -\epsilon \sum_{<ij>} c_i c_j \tag{32}$$

Now the *canonical* partition function for the lattice gas should respect the fact that only microstates with precisely Nc particles are allowed:

$$Z_c = \sum_{\{c_i=1,0\}} \mathrm{e}^{-\beta E} \delta(\sum_i c_i - Nc) \tag{33}$$

where the δ–function restricts the sum to the allowed microstates. However it is easier to work on the Grand Canonical Ensemble where we allow the particle number to fluctuate but introduce a chemical potential μ to tune the average number of particles

$$\mathcal{Z}_{LG} = \sum_{\{c_i=1,0\}} \mathrm{e}^{-\beta(E-\mu\sum_i c_i)} = \sum_{\{c_i=1,0\}} \exp\left[+\beta\epsilon \sum_{<ij>} c_i c_j + \beta\mu \sum_i c_i\right] \tag{34}$$

where the sum over $c_i = 1, 0$ is now unrestricted.

The effective energy $E - \mu\sum_i c_i$ can be mapped onto the Ising energy (plus a constant) by the identification

$$S_i = 2c_i - 1 \qquad J = \frac{\epsilon}{4} \qquad h = \frac{\epsilon z + 2\mu}{4} \tag{35}$$

(see tutorial). Therefore

$$\mathcal{Z}_{LG} = \text{Const.} \times Z_{Ising} \tag{36}$$

and the grand potential of the lattice gas and free energy of the Ising model are the same (up to an unimportant constant)

$$\Phi_{LG}(T, \mu) = F_{Ising}(T, h) + \text{constant} \tag{37}$$

The coexistence curve of the lattice gas is then

$$\mu_c = -\epsilon z/2 \tag{38}$$

(which corresponds to $h = 0$) and the critical point will be given by the Ising value $T_c(J) = T_c(\epsilon/4)$

Figure 1: Phase diagram of the lattice gas in the (μ, T) plane

Thus for $T < T_c$ we have a discontinuous transition as μ is increased through μ_c from a liquid phase to the gas phase

$$c_{liq} = \frac{1 + |m|}{2} \quad \rightarrow \quad c_{gas} = \frac{1 - |m|}{2} \tag{39}$$

where $\pm|m|$ is the magnetisation in the ferromagnetic phase of the Ising model.