

We have shown that, in the absence of spin-spin interactions, the Ising Model does not predict any phase transition.

So, let's study the **interacting case** $J \neq 0$ in one dimension $d = 1$. In this case, the volume V , which coincides with the number of cells (as we have fixed the lattice step a to 1 with a choice of units), is more properly a length $L \equiv V$.

For simplicity, we start from the case of **no external field** $b = 0$ and **open boundary conditions** (fig. ??).

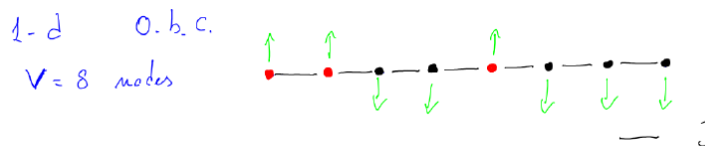


Figure (1) – One-dimensional Ising Model with **open** boundary conditions.

The partition function is given by:

$$\begin{aligned}
 Z_L(K) &\stackrel{(?)}{=} \sum_{\{\sigma\}} \exp \left(K \sum_{\langle x,y \rangle} \sigma_x \sigma_y \right) = \sum_{\sigma_1=\pm 1} \cdots \sum_{\sigma_{L-1}=\pm 1} \sum_{\sigma_L=\pm 1} e^{K\sigma_1\sigma_2} e^{K\sigma_2\sigma_3} \cdots e^{K\sigma_{L-1}\sigma_L} = \\
 &\stackrel{(a)}{=} \sum_{\sigma_1=\pm 1} \cdots \sum_{\sigma_{L-1}=\pm 1} e^{K\sigma_1\sigma_2} \cdots e^{K\sigma_{L-2}\sigma_{L-1}} 2 \cosh(K\sigma_{L-1})
 \end{aligned}$$

where in (a) we summed over the last spin σ_L . Note that \cosh is even, and so (thanks to our choice of *symmetric* spin-like variables):

$$2 \cosh(K\sigma_{L-1}) = 2 \cosh(\pm K) = 2 \cosh(K)$$

and so:

$$Z_L(K) = 2 \cosh K \underbrace{\sum_{\sigma_1=\pm 1} \cdots \sum_{\sigma_{L-1}=\pm 1} e^{K\sigma_1\sigma_2} \cdots e^{K\sigma_{L-2}\sigma_{L-1}}}_{Z_{L-1}(K)} = 2 \cosh(K) Z_{L-1}(K)$$

Reiterating:

$$Z_L(K) = (2 \cosh K)^L \stackrel{(?)}{=} e^{-\beta L f(K)}$$

Taking the logarithm of both sides:

$$L \ln(2 \cosh K) = -\beta L f(K) \Rightarrow -\beta f(K) = \ln(2 \cosh K)$$

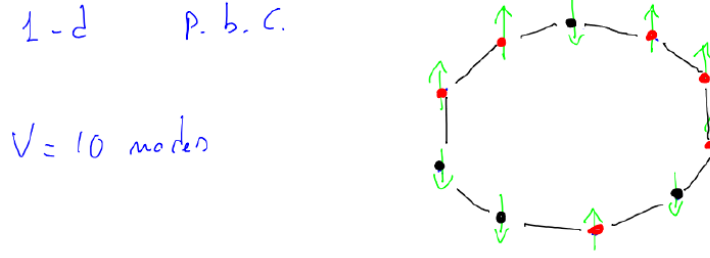


Figure (2) – One-dimensional Ising Model with **periodic** boundary conditions.

If we had chosen **periodic boundary conditions** instead (fig. ??) and $h \neq 0$, the partition function would have been:

$$Z \stackrel{??}{=} \sum_{\{\sigma\}} \exp \left(K \sum_{\langle x,y \rangle} \sigma_x \sigma_y + h \sum_x \sigma_x \right) = \quad (1)$$

$$= \sum_{\sigma_1 = \pm 1} \dots \sum_{\sigma_L = \pm 1} e^{K\sigma_1\sigma_2} \dots e^{K\sigma_{L-1}\sigma_L} e^{K\sigma_L\sigma_1} e^{h\sigma_1} \dots e^{h\sigma_L} \quad (2)$$

Note how the last spin σ_L interacts with the first one σ_1 . We can rewrite the spin-spin interactions more compactly as:

$$e^{K\sigma_1\sigma_2} \dots e^{K\sigma_{L-1}\sigma_L} e^{K\sigma_L\sigma_1} = \prod_{i=1}^L e^{K\sigma_i\sigma_{i+1}} \quad \sigma_{L+1} \equiv \sigma_1 \quad (3)$$

With a trick, we can rewrite also the terms $e^{h\sigma_i}$ as a product over *pairs* (σ_i, σ_{i+1}) . Thanks to p.b.c., each cell is *connected* to exactly 2 neighbouring cells (in $d = 1$) and so a product over pairs contains the product of *squares* of each node - because each cell is multiplied by itself once for every neighbour:

$$\prod_{i=1}^L e^{h\sigma_i} = \prod_{\langle i,j \rangle} \exp \left(h \frac{\sigma_i + \sigma_j}{2} \right) = \prod_{i=1}^L \exp \left(h \frac{\sigma_i + \sigma_{i+1}}{2} \right) \quad \sigma_{L+1} \equiv \sigma_1 \quad (4)$$

Substituting (??) and (??) back in (??) leads to:

$$Z = \sum_{\{\sigma\}} \prod_{i=1}^L \exp \left(K\sigma_i\sigma_{i+1} + h \frac{\sigma_i + \sigma_{i+1}}{2} \right) \quad (5)$$

Let's define a **matrix** **T** with entries equal to the factors in (??):

$$T_{\sigma\sigma'} \equiv \exp \left(K\sigma\sigma' + h \frac{\sigma + \sigma'}{2} \right) \quad (6)$$

As $\sigma, \sigma' \in \{\pm 1\}$, **T** is a 2×2 matrix:

$$\mathbf{T} = \begin{matrix} & \begin{matrix} \sigma' = +1 & \sigma' = -1 \end{matrix} \\ \begin{matrix} \sigma = +1 \\ \sigma = -1 \end{matrix} & \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix} \end{matrix}$$

\mathbf{T} is called the **transfer matrix** for the $d = 1$ Ising Model with periodic boundaries.

Substituting (??) in (??) leads to:

$$\begin{aligned} Z &= \sum_{\{\sigma\}} \prod_{i=1}^L T_{\sigma_i \sigma_{i+1}} = \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \cdots \sum_{\sigma_{L-1}=\pm 1} \sum_{\sigma_L=\pm 1} T_{\sigma_1 \sigma_2} T_{\sigma_2 \sigma_3} \cdots T_{\sigma_{L-1} \sigma_L} T_{\sigma_L \sigma_1} = \\ &\stackrel{(a)}{=} \sum_{\sigma_1=\pm 1} (\underbrace{\mathbf{T} \cdots \mathbf{T}}_{L \text{ times}})_{\sigma_1 \sigma_1} = \sum_{\sigma_1=\pm 1} (\mathbf{T}^L)_{\sigma_1 \sigma_1} = \text{Tr } \mathbf{T}^L \end{aligned}$$

In (a), note that all the sums except the first one lead to a *chain* of matrix multiplications:

$$\sum_a A_{ia} B_{aj} = C_{ij}$$

So, at the end, Z is the sum of the diagonal elements of \mathbf{T}^L , i.e. its **trace**.

\mathbf{T} is symmetric, and so it is diagonalizable, and its eigenvalues are **real** numbers. Moreover, the trace is basis independent, and so we may compute it in the basis where \mathbf{T} is diagonal. Let \mathbf{P} be the invertible matrix needed for diagonalizing \mathbf{T} , then $\mathbf{P} \mathbf{T} \mathbf{P}^{-1} = \text{diag}(\lambda_1, \lambda_2)$, where λ_1 and λ_2 are the *eigenvalues* of \mathbf{T} . Raising both sides to the L -th power, we get:

$$(\mathbf{P} \mathbf{T} \mathbf{P}^{-1})^L = \mathbf{P} \mathbf{T} \mathbf{P}^{-1} \mathbf{P} \mathbf{T} \mathbf{P}^{-1} \mathbf{P} \mathbf{T} \mathbf{P}^{-1} \cdots \mathbf{P} \mathbf{T} \mathbf{P}^{-1} = \mathbf{P} \mathbf{T}^L \mathbf{P}^{-1} = \begin{pmatrix} \lambda_1^L & 0 \\ 0 & \lambda_2^L \end{pmatrix}$$

Then:

$$\text{Tr}(\mathbf{P} \mathbf{T}^L \mathbf{P}^{-1}) = \text{Tr}(\mathbf{P}^{-1} \mathbf{P} \mathbf{T}^L) = \text{Tr}(\mathbf{T}^L) = \text{Tr} \begin{pmatrix} \lambda_1^L & 0 \\ 0 & \lambda_2^L \end{pmatrix} = \lambda_1^L + \lambda_2^L$$

And so:

$$Z = \text{Tr } \mathbf{T}^L = \lambda_1^L + \lambda_2^L \stackrel{(\text{??})}{=} e^{-\beta L f(K, h)}$$

Taking the logarithm of both sides:

$$\ln Z = -\beta L f(K, h) = \ln(\lambda_1^L + \lambda_2^L)$$

and dividing by L :

$$\frac{\ln Z}{L} = -\beta f(K, h) = \frac{1}{L} \ln(\lambda_1^L + \lambda_2^L)$$

Suppose (without loss of generality) that $\lambda_1 < \lambda_2$. Then:

$$-\beta f(K, h) = \frac{1}{L} \ln \left(\lambda_2^L \left[1 + \left(\frac{\lambda_1}{\lambda_2} \right)^L \right] \right) = \frac{1}{L} \ln \lambda_2 + \frac{1}{L} \ln \left[1 + \left(\frac{\lambda_1}{\lambda_2} \right)^L \right]$$

In the thermodynamic limit $L \rightarrow \infty$, the larger eigenvalue λ_2 *dominates*, and $(\lambda_1/\lambda_2)^L \rightarrow 0$, so that:

$$-\beta f(K, h) = \ln \lambda_2 + \frac{1}{L} \ln \left[1 + \left(\frac{\lambda_1}{\lambda_2} \right)^L \right] \xrightarrow{L \rightarrow +\infty} \ln \lambda_2 \quad (7)$$

The eigenvalues can be computed (as usual) as the roots of the *secular* (or *characteristic*) equation:

$$0 = \det(\mathbf{T} - \lambda \mathbf{I}) = \det \begin{vmatrix} e^{K+h} - \lambda & e^{-K} \\ e^{-K} & e^{K-h} - \lambda \end{vmatrix} = (e^{K+h} - \lambda)(e^{K-h} - \lambda) - e^{-2K} =$$

$$= \lambda^2 - \lambda e^K \frac{e^h + e^{-h}}{2} + \frac{e^{2K} - e^{-2K}}{2} = \lambda^2 - \lambda e^K \cosh h + 2 \sinh 2K$$

which are:

$$\lambda_{1,2} = e^K \cosh h \mp \sqrt{e^{2K} \cosh^2 h - 2 \sinh 2K} =$$

$$= e^K \cosh h \mp \sqrt{e^{2K} \sinh^2 h + e^{-2K}}$$

The **magnetization** is given by:

$$m \stackrel{(\text{??})}{=} -\frac{\partial}{\partial h}(\beta f) \stackrel{L \rightarrow \infty}{\stackrel{(\text{??})}{=}} \frac{\partial}{\partial h} \ln \lambda_2 = \frac{\partial}{\partial h} \ln \left(e^K \cosh h + \sqrt{e^{2K} \sinh^2 h + e^{-2K}} \right) =$$

$$= \frac{1}{e^K \cosh h + \sqrt{e^{2K} \sinh^2 h + e^{-2K}}} \left(e^K \sinh h + \frac{2e^{2K} \sinh h \cosh h}{2\sqrt{e^{2K} \sinh^2 h + e^{-2K}}} \right) =$$

$$= \frac{1}{e^K \cosh h + \sqrt{e^{2K} \sinh^2 h + e^{-2K}}} \frac{e^K \sqrt{e^{2K} \sinh^2 h + e^{-2K}} + e^{2K} \cosh h}{\sqrt{e^{2K} \sinh^2 h + e^{-2K}}} =$$

$$\stackrel{(a)}{=} \frac{1}{e^K \cosh h + \sqrt{e^{2K} \sinh^2 h + e^{-2K}}} \frac{e^K \cosh h + \sqrt{e^{2K} \sinh^2 h + e^{-2K}}}{\sqrt{\sinh^2 h + e^{-4K}}} =$$

$$= \frac{\sinh h}{\sqrt{\sinh^2 h + e^{-4K}}} \stackrel{(b)}{=} \frac{\tanh h}{\sqrt{1 - \frac{1-e^{-4K}}{\cosh^2 h}}} \quad (8)$$

where in (a) we divided numerator and denominator by e^K , and in (b) by $\cosh h$ and applied the identity $\cosh^2 h - \sinh^2 h = 1 \Rightarrow \sinh^2 h = \cosh^2 h - 1$.

Note that if $K = 0$, and so $J = 0$ (non-interacting case), (??) leads back to $m = \tanh h$, the result we already found in (??). Moreover, if $K > 0$ (ferromagnetic interaction), $m(K, h) > m(0, h)$ - meaning that spins align more easily to the external field if they can interact with their neighbours.

Again, if $h = 0$, $m(K, h = 0) = 0$, and so the system is unable to magnetize in absence of an external field.

In fact, consider any average spin, e.g. $\langle \sigma_0 \rangle$:

$$\langle \sigma_0 \rangle = \sum_{\{\sigma\}} \exp \left(K \sum_{\langle x, y \rangle} \sigma_x \sigma_y \right)$$

For any *finite* system ($L < +\infty$) the sum over all states is a *finite* sum, meaning that it evaluates to some finite number. Moreover, it is **odd** under the change of variables $\sigma_x \leftrightarrow \sigma'_x = -\sigma_x$:

$$\langle \sigma_0 \rangle = \sum_{\{\sigma\}} \exp \left(K \sum_{\langle x, y \rangle} \sigma_x \sigma_y \right) \sigma_0 = - \sum_{\{\sigma\}} \exp \left(K \sum_{\langle x, y \rangle} \sigma_x \sigma_y \right) \sigma_0 = -\langle \sigma_0 \rangle \quad (9)$$

and so $\langle \sigma_0 \rangle = 0$. Clearly, this arguments holds for any spin (by translation invariance), and so in general $\langle \sigma_k \rangle = 0 \forall k$.

0.1 Spontaneous magnetization

To observe the rise of a **spontaneous magnetization** (which is the experimental result we wish to model), i.e. a non zero m with no external field ($h = 0$), we need to be careful in the *order* of limits. In (??) taking $h = 0$ first leads to $m = 0$ for any finite V - and so also in the thermodynamic limit. The idea is then to *exchange* the two limits:

$$m(T) = \lim_{h \rightarrow 0^+} \lim_{V \rightarrow +\infty} \langle \sigma \rangle_{V,h} \quad (10)$$

So, first compute the magnetization $\langle \sigma \rangle$ for a finite volume V and in presence of an external field $h \neq 0$. Then perform the thermodynamic limit $V \rightarrow \infty$, and only then let go the field $h \rightarrow 0^+$. The $m(T)$ so defined is the **spontaneous magnetization** of the system, and it can be non-zero.

The idea is that the *presence* of $h \neq 0$ *breaks* the symmetry ($\sigma \leftrightarrow -\sigma$) of the system, invalidating argument (??) and thus allowing a spontaneous magnetization.

Equivalently, one can break the symmetry without using $h \neq 0$, but by imposing some *fixed* boundary conditions, for example by setting all spins at the boundaries set to $+1$. In this case, the magnetization for a finite volume V is denoted with $\langle \sigma \rangle_V^+$ (**plus** boundary condition). We can then take the thermodynamic limit:

$$m(T) = \lim_{V \rightarrow +\infty} \langle \sigma \rangle_V^+ \quad (11)$$

The boundary effect will vanish when $V \rightarrow \infty$, but it will always break the symmetry of the Hamiltonian ($\sigma \leftrightarrow -\sigma$).

Intuitively, (??) and (??) *break* the symmetry in the “same direction” (the first with $h > 0$, and the latter with $\sigma_i = +1$ at the boundaries), and so we expect them to lead to the same result at the end. For now, no instances in which (??) and (??) lead to different results are known.

Clearly, we can also consider the limits *from the other direction*, i.e. from $h < 0$, or with **down** boundary conditions ($\sigma_i = -1$ at the boundaries). The resulting magnetization will be the opposite:

$$\lim_{h \downarrow 0^+} m(K, h) = - \lim_{h \uparrow 0^-} m(K, h)$$

For the Ising Model in $d = 1$, $m(T) = 0$. In fact, in computing m in (??) we first considered the thermodynamic limit $L \rightarrow \infty$ for the free energy (??) with $h \neq 0$. Then, taking $h \rightarrow 0$ (as already observed), leads to $m = 0$. So, unfortunately, the $d = 1$ Ising Model does not suffice to capture the effect of spontaneous magnetization, even when spin-spin interactions are considered.

To observe a phase-transition, we need to find where the free energy $f(K, h)$ is non-analytic. In general, it can be shown that $\forall d > 1$, and $\forall h \neq 0$, $f(K, h)$ is analytic everywhere. The only singular points happen at $h = 0$ for $T < T_c$, where T_c is called the **critical temperature**.

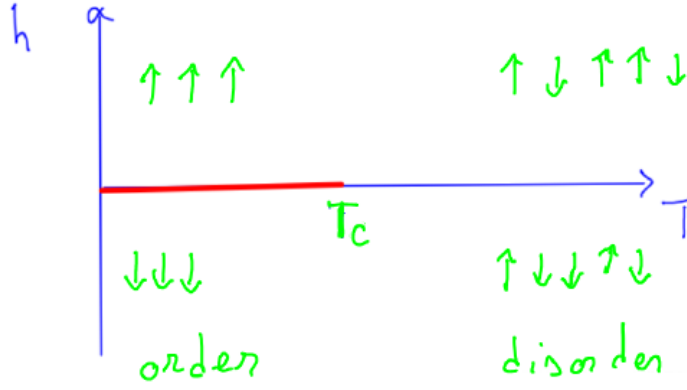


Figure (3) – Phase-diagram showing all parameters (h, T) for which the Ising Model’s free energy $f(K, h)$ is non-analytic, which lie on the red segment with $h = 0$ and $T = (0, T_c]$. Taking the limit $h \rightarrow 0^\pm$ when $T < T_c$ will lead to a non-zero magnetization m (positive if $h \downarrow 0^+$, negative if $h \uparrow 0^-$) - in other words the system “spontaneously organizes” in absence of an external field (**ordered phase**). The same limit when $T > T_c$ leads to $m = 0$ - here thermal fluctuations are too high, and the system remains in a random state (**disordered phase**).

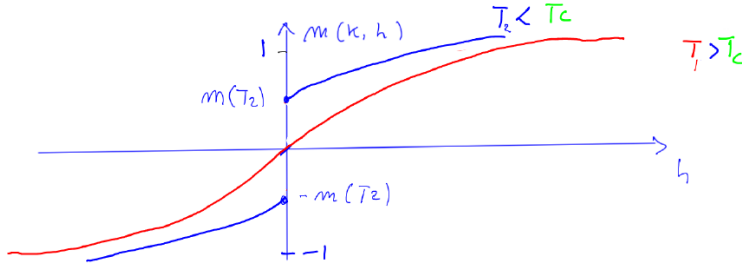


Figure (4) – Magnetization at constant temperature T as function of the field strength h (i.e. along a *vertical* line in fig. ??). If $T > T_c$, as for the red line, the result is the same we obtained in the non-interacting case (fig. ??), or the $d = 1$ model. On the other hand, for $T < T_c$ (blue line), a singularity appears at $h = 0$, with two possible limits for the magnetization.

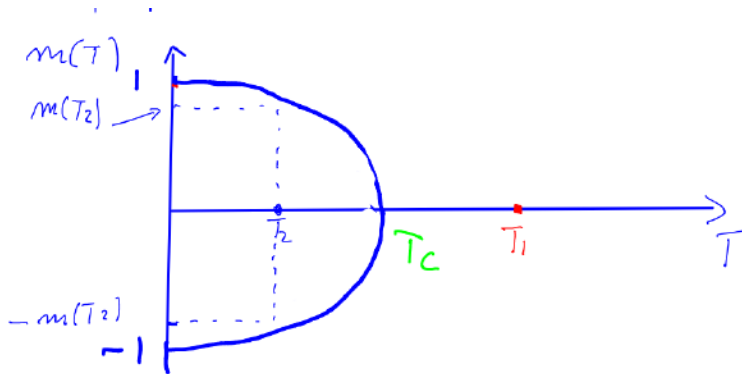


Figure (5) – Bifurcation plot for the **spontaneous magnetization** $m(T)$, i.e. the intercept at $h = 0$ of the curves in fig. ?? at various temperatures. For $T > T_c$, all curves $m(h)$ cross the origin, and so lead to no spontaneous magnetization $m(T) = 0$. Conversely, for $T < T_c$, two opposite values of $m(T)$ are possible, depending on the taken limit $h \rightarrow 0^\pm$. Note that the region “inside the arc” is not reachable (**unphysical region**): for example at $T = T_2$ it is impossible to obtain a magnetization $|m| < |m(T_2)|$.

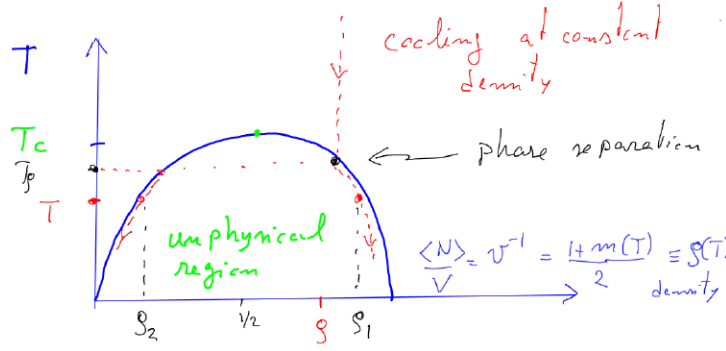


Figure (6) – The analogue of the magnetization m in the lattice gas is the **density** $\rho = v^{-1} = \langle N \rangle / V = (1 + m(T)) / 2$.

Consider the lattice gas model, with a fraction ρ of occupied cells. Suppose we want to keep $\langle N \rangle$ fixed. This can be done by changing the chemical potential, which is the conjugate variable to N , and in the lattice gas model takes the role the external magnetic field had in the ferromagnetic Ising Model (in fact the magnetic field b is a function of $\ln z$, which contains μ).

Lowering the temperature (moving along the red dashed line), to keep ρ fixed, μ has to change. When it reaches the blue curve, a *phase separation* is observed, and the gas divides in two parts: one of low density ρ_2 , and one with higher density ρ_1 . Graphically, until the blue curve is reached, the gas is “well mixed”: every region has almost the same density. After, it is divided in mostly empty regions and very dense regions (fig. ??).

⚠ This part is still under revision!

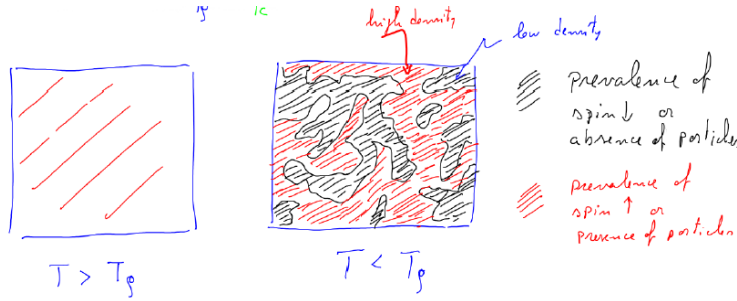


Figure (7) – The lattice gas is well-mixed for $T > T_p$ (left figure), but separates in two phases with different densities for $T < T_p$.

Let f_i be the fraction of volume occupied by the fluid with density ρ_i satisfies:

$$f_1 \rho_1 + f_2 \rho_2 = \rho$$

and ρ is fixed and remains constant. Also $f_1 + f_2 = 1$. Then:

$$\rho_1 = \frac{1 + m(T)}{2}; \quad \rho_2 = \frac{1 - m(T)}{2}$$

leading to:

$$f_1(T) = 1 - f_2(T) = \frac{1}{2} \left(1 + \frac{2\rho - 1}{m(T)} \right)$$

$$\rho = \begin{cases} \frac{1+m(T_\rho)}{2} & \rho > \frac{1}{2} \\ \frac{1-m(T_\rho)}{2} & \rho < \frac{1}{2} \end{cases}$$

T_ρ is defined as the temperature at which the red dashed line intercepts the blue curve, i.e. at which phase separation occurs.

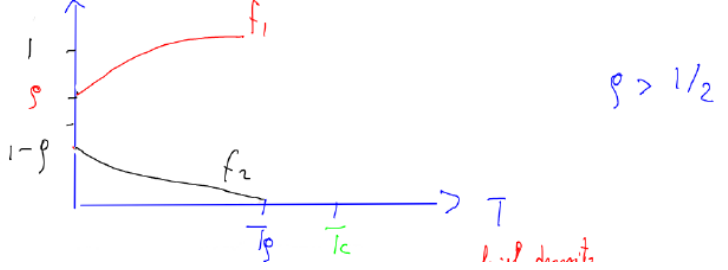


Figure (8)

Spinoidal decomposition: try to enter in the unphysical region by rapidly cooling the gas.

So we have found that the both the non-interacting case and the $d = 1$ Ising Model do not present any kind of phase transition. To proceed, we need to considerate a higher dimensional case. One possible way is through numerical simulations, or by considering the exact solution of the $d = 2$ case, for which the critical temperature turns out to be:

$$T_c = \frac{2\epsilon_0/k_B}{\ln(1 + \sqrt{2})}$$

Often one considers the *adimensional* critical parameter k_c , defined as:

$$k_c \equiv \frac{\epsilon_0}{k_B T_c} = \frac{1}{2} \ln(1 + \sqrt{2}) = 0.44 \dots$$

which is such that $\sinh(2k_c) = 1$. For details see [huang].

The specific heat at $b = 0$ is:

$$c_v(b = 0, T) \underset{T \sim T_c}{\propto} -\ln \left| 1 - \frac{T}{T_c} \right|$$

The magnetization is 0 above T_c , and for $T < T_c$ is given by:

$$m(T) = \left[1 - \frac{1}{\sinh^4(2K)} \right]^{1/8} \quad \theta(T_c - T) \propto \theta(T_c - T)(T_c - T)^{1/8}$$

The exponent $1/8$ is also called the β exponent (not to be confused with $1/k_B T$). We will study this kind of *power laws* for criticality in a later chapter. They are of particular importance because of their **universality** - i.e. very different systems sharing certain fundamental symmetries have the same behaviour when approaching T_c . (As anticipated, criticality is important to model complex systems).

No rigorous *exact* result is known for the case $h \neq 0$.

Another possibility to go on is to study low/high temperatures expansion of the Ising Model.

0.1.1 Low temperature expansion

Consider the partition function for the Ising Model in d dimensions:

$$Z = \sum_{\{\sigma\}} \exp \left(K \sum_{\langle x,y \rangle} \sigma_x \sigma_y + h \sum_x \sigma_x \right) = e^{-\beta V f(K,h)} \quad \begin{matrix} h=\beta b \\ K=\beta J \end{matrix} \quad (12)$$

The idea is to *approximate* Z with a truncated sum, considering only the most *relevant* states. Suppose $h \neq 0$ - for instance $h > 0$. Then, at very low temperature, we expect almost all spins to be aligned towards h . In this situation, the *most probable* configurations σ comprehend the one where all spins are aligned ($\sigma_i \equiv +1$), followed by the ones where only a few spins are *flipped*. Each of them *refines* the value of Z - and if a sufficient number of terms is considered, we can understand the low-temperature behaviour of the system.

In general, however, it is not clear how to find the **radius of convergence** of such a series. In practice, the low-temperature approximation works well for $T \sim 0$, and breaks down when approaching T_c , where Z is non-analytic.

So, let's start computing some terms. In the following we will assume for simplicity **periodic** boundary conditions, meaning that every cell has exactly $2d$ neighbours.

When no spins are flipped $\sigma_i \equiv +1$, the exponential becomes:

$$\mathcal{N}_0 = \exp \left(K \underbrace{\sum_{\langle x,y \rangle} 1}_A + h \underbrace{\sum_x 1}_B \right) \stackrel{(\text{??})}{=} \exp(KVd + hV) \quad (13)$$

Let's fix $d = 2$ to allow some visualization. Then:

$$\mathcal{N}_0 = \exp[V(2K + h)] \quad (14)$$

Suppose now we flip one spin $\sigma_i = -1$ (it does not matter which, as the system is transitionally invariant), and consider how much each of the two sums A and B in (??) changes (fig. ??).

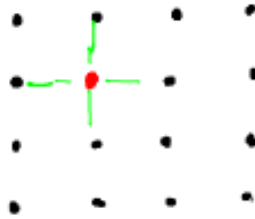


Figure (9) – Square lattice with one flipped spin (in red). The affected interactions are represented by the green edges.

B is just the sum over spins. As σ_i was $+1$ and now it is -1 , the change ΔB is $-1 - (+1) = -2$, so $B = N \rightarrow N - 2$.

On the other hand, changing one spin in A affects all the pairs (σ_j, σ_i) involving it, which are $2d = 4$ in our case (the green edges in fig. ??). The total change will then be $\Delta A = 4(-1 - (+1)) = 4 \cdot (-2) = -8$, and so $A = 2V \rightarrow 2V - 8$.

So, the exponential after one flipped spin will be:

$$\mathcal{N}_1 = \exp((2V - 8)K + (V - 2)h) \quad (15)$$

We can then begin to write Z (??) by summing all these terms. Note that while there is only one possible configuration σ resulting in the term \mathcal{N}_0 , there are V possibilities for \mathcal{N}_1 - because we can flip *any* of the V spins in the system:

$$Z = \mathcal{N}_0 + V\mathcal{N}_1 + \dots$$

Things start to become more difficult when considering *two* flipped spins σ_i and σ_j at once. Now their distance *matters* - and in particular if they are neighbouring or not.

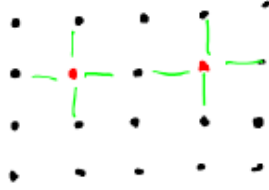


Figure (10) – Square lattice with two flipped non-neighbouring spins (in red).

Suppose σ_i and σ_j are **not neighbours** - meaning that they are independent (??). Then the change in the sums A and B will just be *twice* that produced by flipping only one spin, and the exponential will be:

$$\mathcal{N}_{2,\text{far}} = \exp[(2V - 16)K + (V - 4)h] \quad (16)$$

How many configurations $\{\sigma\}$ generate such term? The first spin to flip σ_i may be anyone of the V spins in the system, but the second σ_j cannot be in the same position, not in one of the 4 neighbouring cells, leaving available only $V - 5$ places. Thus, so far we have $V(V - 5)$ configurations. Exchanging σ_i and σ_j will not alter anything - as they are both -1 - and so we need to divide by 2 the previous total, leading to $V(V - 5)/2$:

$$Z = \mathcal{N}_0 + V\mathcal{N}_1 + \frac{V(V - 5)}{2}\mathcal{N}_{2,\text{far}} + \dots$$

If the two flipped spins are instead **neighbours**, then B will change the same (by -4), but for A we need to account only 6 changed interactions, and not 8: one *edge* is in common between the two spins, contributing with a $\sigma_i\sigma_j = (-1)(-1) = +1$, as if it was never changed, leaving 3 affected edges for each spin (fig. ??).

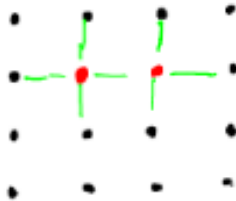


Figure (11) – Square lattice with two flipped neighbouring spins (in red).

So the new exponential term will be:

$$\mathcal{N}_{2,\text{close}} = \exp[(2V - 12)K + (V - 4)h]$$

The first spin can go in V places, but the second one must be its neighbour, leaving only 4 possibilities. Dividing by 2 to account for their permutation leaves us with $2V$ configurations forming $\mathcal{N}_{2,\text{close}}$:

$$\begin{aligned} Z &= \mathcal{N}_0 + V\mathcal{N}_1 + \frac{V(V-5)}{2}\mathcal{N}_{2,\text{far}} + 2V\mathcal{N}_{2,\text{close}} + \dots = \\ &= e^{2VK+hV} + Ve^{(2V-8)K+(V-2)h} + \frac{V(V-5)}{2}e^{(2V-16)K+(V-4)h} + 2Ve^{(2V-12)K+(V-4)h} + \dots \end{aligned}$$

Note that substituting $\sigma \leftrightarrow -\sigma$ is equivalent to changing the sign of h . In fact, any term of the sum in (??) changes by:

$$\exp\left(K \sum_{\langle x,y \rangle} \sigma_x \sigma_y + h \sum_x \sigma_x\right) \xrightarrow{\sigma \leftrightarrow -\sigma} \exp\left(K \sum_{\langle x,y \rangle} (\not\sigma_x)(\not\sigma_y) - h \sum_x \sigma_x\right)$$

So, by changing the sign of h in all the terms we already found, we can construct their *reflections* - i.e. the ones starting from all spins *down* and flipping *up* 1 or 2 of them. Adding them to Z we get:

$$\begin{aligned} Z &= e^{V(2K+h)} \left[1 + Ve^{-8K-2h} + \frac{V(V-5)}{2}e^{-16K-4h} + 2Ve^{-12K-4h} + O(e^{-16K-6h}) \right] + \\ &+ e^{V(2K-h)} \left[1 + Ve^{-8K+2h} + \frac{V(V-5)}{2}e^{-16K+4h} + 2Ve^{-12K+4h} + O(e^{-16K+6h}) \right] \end{aligned}$$

In fact, considering 3 spin-flips leads to new terms of order $O(e^{-16K-6h})$ (if they happen to be all neighbouring, as there are 8 affected interactions), or higher (if they are further apart, for up to 12 affected interactions).

Starting with $h > 0$ and taking first the thermodynamic limit $V \rightarrow \infty$ and then $h \downarrow 0^+$ we note that only the first series of terms *dominates*. In fact, for any $h > 0$:

$$\lim_{V \rightarrow \infty} \frac{e^{V(2K-h)}}{e^{V(2K+h)}} = \lim_{V \rightarrow \infty} e^{-2h} = 0 \quad \forall h > 0$$

So in the thermodynamic limit we can ignore the terms in the second row. Taking the logarithm and dividing by V we get the series expansion of the free energy:

$$\frac{\ln Z}{V} = -\beta f(K, h) = 2K + h + \frac{1}{V} \ln \left[1 + Ve^{-8K-2h} + \frac{V(V-5)}{2}e^{-16K-4h} + 2Ve^{-12K-4h} + \dots \right]$$

For $T \rightarrow 0$, $\beta \rightarrow \infty$, and so $K = \beta J \rightarrow \infty$, meaning that $e^{-K} \rightarrow 0$ and so we may expand in series the logarithm:

$$\ln(x) \approx x - \frac{x^2}{2} + O(x^3)$$

leading to:

$$\begin{aligned}
-\beta f(K, h) &= 2K + h + \underbrace{e^{-8K-2h} + \frac{V-5}{2}e^{-16K-4h} + 2e^{-12K-4h}}_{\text{First term}} \\
&\quad - \frac{1}{2V}(\cancel{Ve^{-8K-2h}})^2 + O(e^{-16K-6h}) = \\
&= 2K + h + e^{-8K-2h} + 2e^{-12K-4h} - \frac{5}{2}e^{-16K-4h} + O(e^{-16K-6h})
\end{aligned}$$

The spontaneous magnetization is then:

$$\begin{aligned}
m &\stackrel{(\text{??})}{=} \frac{1}{V} \frac{\partial \ln Z}{\partial h} \Big|_{h=0} = 1 - 2e^{-8K-2h} - 8e^{-12K-4h} + 10e^{-16K-4h} + \dots \Big|_{h=0} = \\
&\stackrel{(\text{??})}{=} 1 - 2e^{-8K} - 8e^{-12K} + 10e^{-16K} + \dots
\end{aligned} \tag{17}$$

and is plotted in fig. ??.

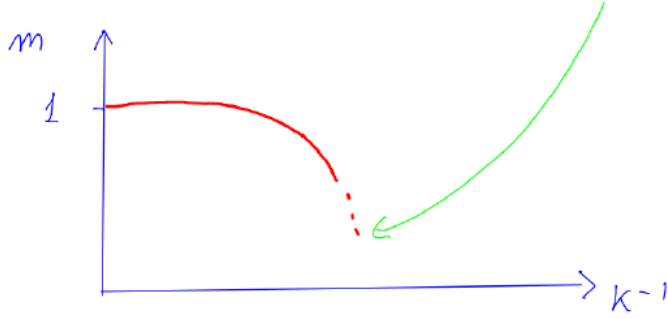


Figure (12) – Plot of the spontaneous magnetization as function of temperature $T \propto K^{-1} = 1/(\beta J)$. For $T \rightarrow 0$ ($K \rightarrow \infty$) m goes to 1. From Onsager's exact solution we know that m reaches 0 at T_c , but this cannot be observed in this expansion, as the radius of convergence never includes T_c .

More terms. For more terms of the expansion in (??) see [low-exp]. There also next nearest neighbours interactions are considered, with an interaction strength J_2 - so, to reconstruct our case, let $J_2 = 0$ and thus $y = e^{-4J_2\beta} = 1$. So, formula (3) in [low-exp] may be adapted as:

$$M(x) = 1 - 2x^2y^2 + \sum_{m,n} a(m,n)x^m y^n \Big|_{y=1} \quad x = e^{-4K}$$

Borrowing coefficients from table 1 in [low-exp] we get:

$$M(K) = 1 - 2e^{-8K} - 8e^{-12K} + (-8 + 18 - 24 - 20)e^{-16K} + \dots$$

So the first coefficients in (??) are correct, but the one for e^{-16K} not. In fact, to refine it, we should also consider the case of 3 and 4 neighbouring flips, which add terms of the same order e^{-16K} , but are much more difficult to compute.

Fortunately, there are more sophisticated methods for generating more terms, as can be seen in [ising-low]

0.1.2 Correlation functions

Until now we analysed the *magnetization*, i.e. the average local spin alignment:

$$m_x \equiv \langle \sigma_x \rangle$$

This can be interpreted as a **one-point** correlation function, measuring how much a spin σ_x is “correlated” with itself.

If we instead compare σ_x with a *different* spin σ_y , we get the **two-point** correlation function:

$$G_{x,y}^{(2)} = \text{Cov}[\sigma_x, \sigma_y] = \langle \sigma_x \sigma_y \rangle - \langle \sigma_x \rangle \langle \sigma_y \rangle \quad (18)$$

If σ_x and σ_y are independent, then immediately $\langle \sigma_x \sigma_y \rangle = \langle \sigma_x \rangle \langle \sigma_y \rangle$, and so $G_{x,y}^{(2)} = 0$. In general, however, the converse is not true: if the two-point correlation is 0, the two spin may still be interacting.

Consider each spin interacting with a local field h_x in the Ising Model. The partition function is then:

$$Z(\mathbf{h}) = \sum_{\{\boldsymbol{\sigma}\}} \exp \left(-\beta \mathcal{H}(\boldsymbol{\sigma}) + \sum_x h_x \sigma_x \right) \equiv e^{-\beta F(\mathbf{h})}$$

with F being the corresponding **free energy**. This is a generalization of the case (??), where $h_x \equiv h$ for all spins. Being able to *vary* the local field experienced by a single spin allows us to write correlation functions as derivatives of Z .

For the one-point correlation we get the same formula previously found in (??):

$$m_x = -\frac{\partial}{\partial h_x} (\beta F(\mathbf{h})) \quad (19)$$

On the other hand, for the two point correlation we get:

$$G_{xy}^{(2)} = -\frac{\partial^2}{\partial h_x \partial h_y} (\beta F(\mathbf{h})) = \langle (\sigma_x - \langle \sigma_x \rangle)(\sigma_y - \langle \sigma_y \rangle) \rangle \stackrel{(?)}{=} \frac{\partial m_y}{\partial h_x} \quad (20)$$

Similarly, for a 3-point correlation:

$$G_{xyz}^{(3)} = -\frac{\partial^3}{\partial h_x \partial h_y \partial h_z} (\beta F(\mathbf{h})) = \langle (\sigma_x - \langle \sigma_x \rangle)(\sigma_y - \langle \sigma_y \rangle)(\sigma_z - \langle \sigma_z \rangle) \rangle$$

and in general:

$$G_{x_1, \dots, x_n}^{(n)} = -\frac{\partial^n}{\partial h_{x_1} \dots \partial h_{x_n}} (\beta F)$$

We define the **susceptibility** as the derivative of the magnetization m with respect to the field h (when $h_x \equiv h \forall x$):

Susceptibility χ

$$\chi \equiv \frac{\partial m}{\partial h}$$

Inserting the definition of the magnetization (??) and computing the averages leads to:

$$\begin{aligned}
\chi &\equiv \frac{\partial m}{\partial h} = \frac{\partial}{\partial h} \left\langle \sum_x \sigma_x \right\rangle \frac{1}{V} = \frac{1}{V} \sum_x \frac{\partial}{\partial h} \langle \sigma_x \rangle = \frac{1}{V} \sum_x \frac{\partial}{\partial h} \frac{\overbrace{\sum_{\{\sigma\}} \sigma_x \exp \left(-\beta \mathcal{H}(\sigma) + \sum_y h \sigma_y \right)}^{\text{Num}}}{\underbrace{Z(\mathbf{h})}_{\text{Den}}} = \\
&= \frac{1}{V} \sum_x \frac{\overbrace{\sum_{\{\sigma\}} \exp \left(-\beta \mathcal{H}(\sigma) + \sum_y h \sigma_y \right) \sum_y \sigma_y}^{(\partial_h \text{Num})/\text{Den}}}{Z(\mathbf{h})} + \\
&\quad - \frac{1}{V} \sum_x \underbrace{\frac{\sum_{\{\sigma\}} \sigma_x \exp \left(-\beta \mathcal{H}(\sigma) + \sum_y h \sigma_y \right)}{Z(\mathbf{h})} \cdot \frac{\sum_{\{\sigma\}} \exp \left(-\beta \mathcal{H}(\sigma) + \sum_y h \sigma_y \right) \sum_y \sigma_y}{Z(\mathbf{h})}}_{-(\text{Num} \partial_h \text{Den})/\text{Den}^2} = \\
&= \frac{1}{V} \left[\left\langle \sum_{x,y} \sigma_x \sigma_y \right\rangle - \left\langle \sum_x \sigma_x \right\rangle \left\langle \sum_y \sigma_y \right\rangle \right]
\end{aligned}$$

So, rewriting the last step result in terms of (??) we get:

*Fluctuation
dissipation theorem*

$$\chi = \sum_x G_{x,y}$$

This is the **fluctuation dissipation theorem**. In other words, the “total” *correlation* between one spin σ_x and every other spin σ_y is equal to the “responsivity” of m_x to a change in h , i.e. how much the alignment of σ_x varies when the external field $b = h/\beta$ is adjusted.

\mathcal{H} is translational invariant if it does not change when *translating* spins:

$$\mathcal{H}(\sigma) = \mathcal{H}(\sigma')$$

with $\sigma'_x = \sigma_{x+x_0}$ for any x and x_0 fixed.

In this case, as we previously noted, the magnetization is constant: $m = \langle \sigma_x \rangle$, and the two-point correlation depends only on the distance between the two spins: $\langle \sigma_x \sigma_y \rangle = \langle \sigma_{x-y} \sigma_0 \rangle$.

Finally, we compute the Legendre transform $\Gamma(m)$ of βF with respect to h :

$$\Gamma(\mathbf{m}) = \beta F(\mathbf{j}) + \sum_x h_x m_x$$

where the $\{h_x\}$ have been calculated as a function of the local magnetizations $\{m_x\}$ by inverting (??). By property of the Legendre transform:

$$\frac{\partial \Gamma}{\partial m_x} = h_x$$

Differentiating both sides with respect to h_y leads to:

$$\delta_{xy} = \sum_z \frac{\partial^2 \Gamma}{\partial m_x \partial m_z} \frac{\partial m_z}{\partial h_y} \stackrel{(?)}{=} \sum_z \frac{\partial^2 \Gamma}{\partial m_x \partial m_z} G_{zy}$$

Thus $\frac{\partial^2 \Gamma}{\partial m_x \partial m_y}$ is the inverse of the two-point correlation function G_{xy} .

Exercise 0.1.1 (Ising Model):

Consider a 1-dimensional Ising Model with nearest-neighbour ferromagnetic interaction in an external uniform field with energy function given by:

$$\mathcal{H}(\boldsymbol{\sigma}) = -J \sum_{x=1}^N \sigma_x \sigma_{x+1} - B \sum_{x=1}^N \sigma_x \quad J > 0$$

where periodic boundary conditions are used, i.e. $\sigma_{N+1} \equiv \sigma_1$. Define $K = \beta J$ and $\beta B = h$.

Part A. Using the transfer matrix $T(\sigma, \sigma') = \exp(K\sigma\sigma' + h(\sigma + \sigma')/2)$ and its spectral decomposition, determine:

1. The **partition function** $Z(K, h)$
2. The **free energy** per node in the thermodynamic limit and its plot for $h = 0$ versus $1/K$
3. The **entropy** per node in the thermodynamic limit and its plot for $h = 0$ versus $1/K$
4. The **mean energy** per node in the thermodynamic limit and its plot for $h = 0$ versus $1/K$
5. The **specific heat** per node in the thermodynamic limit and its plot for $h = 0$ versus $1/K$
6. The **average magnetization** at x , $\langle \sigma_x \rangle$, in the thermodynamic limit and its plot for $h = 0, 0.1, 0.2, 0.5, 1$ versus $1/K$ and for $K = 1$ versus h in the range $(-5, 5)$
7. The **two-point correlation function** $\langle \sigma_x \sigma_{x+y} \rangle$ in the thermodynamic limit and its plot for $h = 0$ and $K = 1$ versus y .

Part B. Consider the same model with **open** boundary conditions (node 1 is linked only to node 2, and node N only to node $N - 1$):

$$\mathcal{H}(\boldsymbol{\sigma}) = -J \sum_{x=1}^{N-1} \sigma_x \sigma_{x+1} - B \sum_{x=1}^N \sigma_x$$

Show that the partition function for this case can be formally written as:

$$Z(K, h) = \mathbf{v}^T \mathbf{T}^N \mathbf{v} \equiv \sum_{\substack{\sigma_1 = \pm 1 \\ \sigma_N = \pm 1}} v(\sigma_1) \mathbf{T}^N(\sigma_1, \sigma_N) v(\sigma_N)$$

where $v(\sigma) = e^{h\sigma/2}$. Show that the free energy per node in the thermodynamic limit is the same as above.

Part C. Same as in part B with fixed boundary conditions $\sigma_1 = 1 = \sigma_2$, and $v(\sigma) = e^{h\sigma/2}$ for both $\sigma = \pm 1$.

Part D. How would you try to solve the Ising model in 1-dimension with nearest neighbour and next-to-nearest neighbour interaction and periodic boundary condition ($\sigma_{N+1} = \sigma_1$ and $\sigma_{N+2} = \sigma_2$):

$$\mathcal{H}(\boldsymbol{\sigma}) = - \sum_{x=1}^N (J_1 \sigma_x \sigma_{x+1} + J_2 \sigma_x \sigma_{x+2}) - B \sum_{x=1}^N \sigma_x$$

Solution. WIP