INTRODUCTION TO THE ISING MODEL

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1. The Ising Model

The Ising model is the simplest possible model of a magnetic system. It describes an assembly of magnetic dipoles which can interact with each other and also with an applied magnetic field. In this model, the individual magnetic dipole can only take up one of two possible polarizations. We describe such a dipole by a degree of freedom σ which can take one of two values, $\sigma = 1$ and $\sigma = -1$. We will typically denote the degree of freedom occupying the position x by σ_x. We will often refer to these degrees of freedom as "spins".

Typically, the positions x at which the spins are located are at the sites of a hypercubic lattice. We will consider such systems in any number of dimensions. In D dimensions, the positions would be located at the points

$$x = a\left[n_1\hat{1} + n_2\hat{2} + \ldots + n_D\hat{D}\right]$$

where a is the lattice constant. It is the distance between neighbouring lattice sites. $n_1, n_2, \ldots, n_D$ are integers and, for an infinite lattice they each run over all of the integers. Of the lattice is not infinite but has a boundary they run over a range that is enough to enumerate the lattice sites. The unit vectors $\hat{1}, \hat{2}, \ldots, \hat{D}$ are directed along the positive directions of the Cartesian coordinates in a Cartesian coordinate system in D-dimensional Euclidean space. We will sometimes label a generic one of these unit vectors or the set of all of these unit vectors by the symbol μ

The Ising model is further specified by its energy function which we will call its Hamiltonian. When each of the spins of the lattice have a given value (each being 1 or -1) we say that the energy of that configuration of the spins is

$$H \;=\; -J\sum_{x,\mu}\sigma_x\sigma_{x+\mu} - B\sum_x \sigma_x \tag{1}$$

The first term in the Hamiltonian is a quadratic in the spin variables. We will always assume that the constant J is positive. In this case, the first term in the energy is smallest if neighbouring spins are aligned since $-J\sigma_x\sigma_{x+\mu} = -J$ when both σ_x and $\sigma_{x+\mu}$ are equal to one or both are equal to -1 and this is the smallest value this term in the Hamiltonian can have. If σ_x and $\sigma_{x+\mu}$ differ in sign, $-J\sigma_x\sigma_{x+\mu} = J$ and the energy is higher. The last term in the Hamiltonian, $-B\sum_x \sigma_x$ is intended to emulate an external magnetic field whose role is played by B. Its role is to favour the alignment of spins with B.

The summation in the first term of the Hamiltonian covers all of the links of the lattice, where we call a segment that begins at a lattice site and ends at a neighbouring site a link.

In expanded form the sum is

$$\sum_{x,\mu} \sigma_x \sigma_{x+\mu} = \sum_x \left[\sigma_x \sigma_{x+\hat{1}} + \sigma_x \sigma_{x+\hat{2}} + \ldots + \sigma_x \sigma_{x+\hat{D}} \right]$$

and we can see that summing over x then gives one term for every link of the lattice.

We will analyze the thermodynamics of the Ising spin system by using the grand canonical ensemble. For this we need to compute the partition function

$$Z[T,B,N] = \sum_{\text{spins}} e^{-H/k_B T} \tag{2}$$

where N is the total number of sites, k_B is Boltzmann's constant and T is the temperature. We will only consider cases where N is a very large number, going to infinity. The summation $\sum_{\text{spins}}$ is over every possible configuration of the spins. The Helmholtz free energy is given by

$$F[T,B,N] = -k_B T \ln Z[T,B,N] \tag{3}$$

It is a function of the temperature, T, the magnetic field, B and the total number of spins. It has the differential

$$dF[T,B,N] = -SdT - MdB + \mu dN \tag{4}$$

implying that the partial derivatives of the free energy obtain

$$S[T,B,N] = -\left.\frac{\partial F}{\partial T}\right|_{B,N},\ M[T,B,N] = -\left.\frac{\partial F}{\partial M}\right|_{T,N},\ \mu[T,B,N] = \left.\frac{\partial \Phi}{\partial N}\right|_{T,B} \tag{5}$$

Here, the magnetization, M is given by the thermal expectation value of the total spin

$$M = \frac{\sum_{\text{spins}} \left[\sum_x \sigma_x\right] e^{-H/k_B T}}{\sum_{\text{spins}} e^{-H/k_B T}} \tag{6}$$

It is an extensive variable and often it is useful to consider the magnetization density, m which is defined by

$$m \equiv \frac{M}{N} \tag{7}$$

It is typically m that is finite in the limit as $N \to \infty$.

Sometimes a Legendre transformation of the Helmholtz Free energy with respect to the magnetization is of interest to us. For this, we form the quantity which is called the Landau potential,

$$\Phi[T,M,N] = F + MB \tag{8}$$

where $\Phi[T,M,N]$ is the grand canonical free energy. It has the differential

$$d\Phi[T,M,N] = -SdT + BdM + \mu dN \tag{9}$$

and its partial derivatives are

$$S[T,M,N] = -\frac{\partial \Phi}{\partial T}\bigg|_{M,N}, \; B[T,M,N] = \frac{\partial \Phi}{\partial M}\bigg|_{T,N}, \; \mu[T,M,N] = \frac{\partial \Phi}{\partial N}\bigg|_{T,M} \tag{10}$$

We will be interested in the behaviour of the Ising model as we vary the temperature T and the magnetic field B. We can plot the relevant regions in a phase diagram, the beginnings of which are depicted in figure 1.

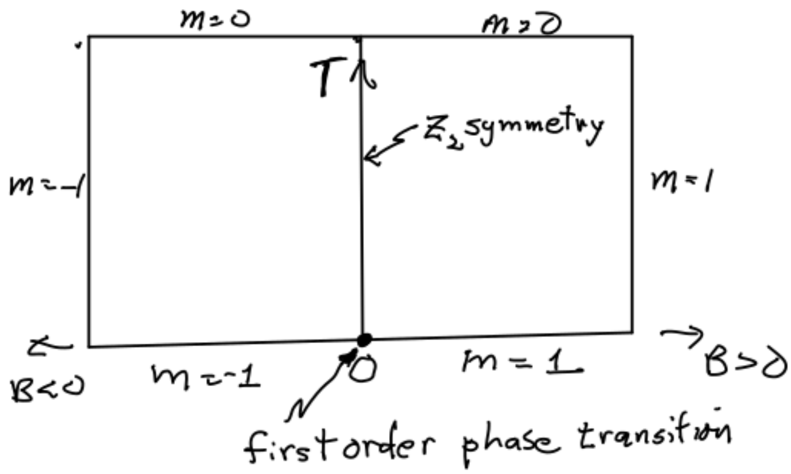

Figure 1. The space of possible physical values of the temperature are plotted on the vertical axis and magnetic field is plotted on the horizontal axis. The top of the diagram is intended to depict the region with very high temperature $k_BT/J, k_BT/|B| \to \infty$ where the sum over spins will average the magnetization density to zero. The extreme left and the extreme right of the figure are intended to depict regions with finite temperature but where the magnetic field has very large magnitude $\frac{|B|}{k_BT} \to \infty$. In these regions the magnetization density has its mazimum magnitude and the same sign as $m = \text{sign}(B)$. On the $T = 0$ axis the state of the system is the lowest energy state of the Hamiltonian which is a perfect ferromagnet with magnetization density $m = \text{sign}(B)$. This function is discontinuous on the $T = 0$ axis. As one follows the $T = 0$ axis from left to right, the magnetization density is a constant, equal to $m = -1$, then it jumps from -1 to $+1$ at $T = 0$. On the $T = 0$ axis, the magnetization is $M = \text{signB}N$ and the Helmholtz free energy is $F[T = 0.B, N] = -k_BTN|B|$. There is a first order phase transition that occurs at $T = 0$, as B passes through zero. The vertical, $B = 0$ line has enhanced symmetry – Z_2 – where the symmetry transformation is $\sigma_x \to -\sigma_x$, $\forall x$. This is a symmetry of the first term in the Hamiltonian (1) but not the second term. This symmetry is spontaneously broken at the point $(T, B) = (0, 0)$ as the value of m there is nonzero and it depends on history, whether we approached the point from the left or right – the system is a spontaneous ferromagnet at that point. There is the question as whether the spontaneous symmetry breaking persists along the line of enhanced symmetry where $T > 0$, $B = 0$.

In that diagram we can understand the phase of the system and compute the Helmholts free energy at the edges of the diagram. The remainder of our work on the Ising model will then be aimed at finding an understanding of what happens in the interior of the figure. In figure1.

The top of the phase diagram in figure 1 is the region with very high temperature $k_BT/J, k_BT/|B| \to \infty$ where the sum over spins average the magnetization density to zero. In that region the partition function is simply equal to the number of configuration of the spins $Z[T\to\infty, B, N] = 2^N$ and the Helmholtz free energy is

$$F[T\to\infty, B, N] = -k_BTN\ln 2$$

The extreme left and the extreme right of the figure depict regions with finite temperature but where the magnetic field has very large magnitude $\frac{|B|}{k_BT}\to\infty$. Alternatively we can think of this as a rebion where B is so large that we can neglect the first term in the Hamiltonian. Then, we can find the partition function and the Helmholtz free energy

$$Z[T, B\to\pm\infty, N] \approx \sum_{\text{spins}} e^{-\frac{B}{k_BT}\sum_x \sigma_x} = \prod_x \sum_{\sigma_x=1,-1} e^{-\frac{B}{k_BT}\sigma_x} = \left[2\cosh\frac{B}{k_BT}\right]^N$$

and

$$F[T, B\to\pm\infty, N] = -k_BTN\ln\left[2\cosh\frac{B}{k_BT}\right]$$

The magnetization density is equal to

$$m = \tanh\left(\frac{B}{k_BT}\right)$$

On the $T = 0$ axis the state of the system is the lowest energy state of the Hamiltonian which is a perfect ferromagnet with magnetization density

$$m = \text{sign}(B)$$

This function is discontinuous on the $T = 0$ axis. As one follows the $T = 0$ axis from left to right, the magnetization density is a constant, equal to $m = -1$, then it jumps from -1 to $+1$ at $T = 0$. On the $T = 0$ axis, the magnetization is $M = \text{signB}N$ and the Helmholtz free energy is

$$F[T = 0, B, N] = -k_BTN|B|$$

There is a phase transition that occurs at $T = 0$, as B passes through zero. This is a first order phase transition.

A phase transition occurs at a point where the free energy is not analytic. The order of a phase transition is the number of derivatives of the free energy by the parameter that drives the transition that exist at the point of the phase transition. Here, since $F[T, B\to\pm\infty, N] = -k_BTN|B|$ the phase transition is located at $(T, B) = (0, 0)$ and the number of derivatives of F by B which exist at $B = 0$ is one. Thus we say that this transition is of first order.

The vertical, $B = 0$ line has enhanced symmetry – Z_2 – where the symmetry transformation is $\sigma_x \to -\sigma_x$, $\forall x$. This is a symmetry of the first term in the Hamiltonian (1) but not the second term. This symmetry is spontaneously broken at the point $(T, B) = (0, 0)$ as the value of m there is nonzero and it depends on history, whether we approached the point from the left or right determines whether $m = -1$ or $m = 1$ – the system is a spontaneous ferromagnet at that point. There is the question as whether the spontaneous symmetry breaking persists along the line of enhanced symmetry where $T > 0$, $B = 0$. Indeed, for the Ising model in dimensions greater than one, it does and the final phase diagram is depicted in figure 2. There is a line of first order phase transitions along the $B = 0$ axis. The line ends at a critical point where the phase transition becomes a second order transition. We will see shortly that in one dimension, on the other hand, the only critical point is the one at $)T, B) = (0, 0)$.

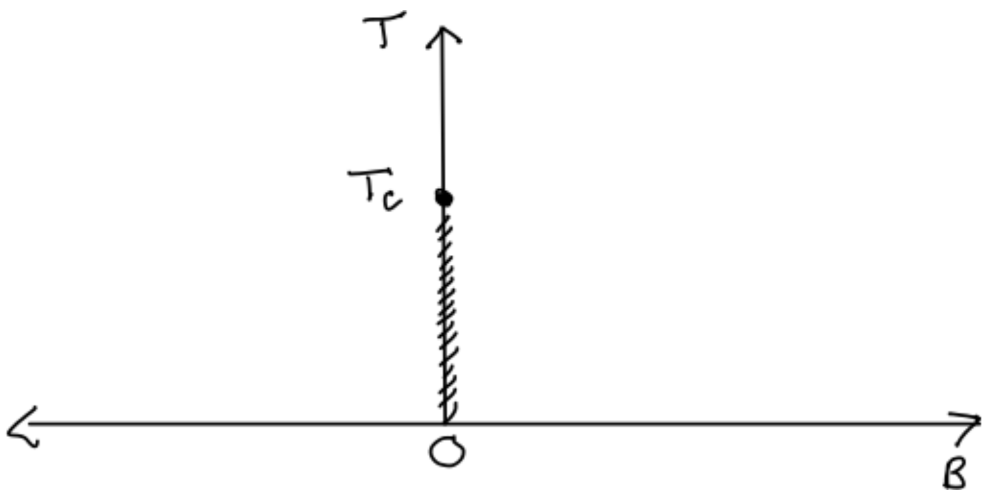

FIGURE 2. The phase diagram of the Ising model in $D > 1$ is depicted. There is a line of first order phase transitions located on the segment between zero and T_C of the $B = 0$ axis, denoted by the crosshatch, and ending at a second order phase transition at the critical point $(T, B) = (T_C, 0)$.

2. THE ISING MODEL IN $D = 1$

The Ising model is exactly solvable for the case of a one-dimensional chain of sites with nearest neighbour couplings. In this case, the lattice consists of a line of N equally spaced spins $\sigma_1, \sigma_2, .., \sigma_N$ and the Hamiltonian is written as

$$H- \; = \; -J \sum_{n=1}^{N-1} \sigma_n \sigma_{n+1} - B \sum_{n=1}^{N} \sigma_n \tag{11}$$

ake the thermodynamic limit, where the integer N is very large.

The partition function is given by the sum over all configurations of the spins, with each configuration weighted by the Boltzmann distribution.

$$Z[T,N,B] = \sum_{spins} e^{-H/k_BT}$$

or, more explicitly, using the Hamiltonian in equation (11),

(12)

$$Z[T,N,B] = \sum_{\sigma_1=1,-1}\sum_{\sigma_2=1,-1}\cdots\sum_{\sigma_N=1,-1}\exp\left(\frac{J}{K_BT}\sum_{n=1}^{N-1}\sigma_n\sigma_{n+1} + \frac{B}{k_BT}\sum_{n=1}^{N}\sigma_n\right)$$

$$= \sum_{\sigma_1=1,-1}\sum_{\sigma_2=1,-1}\cdots\sum_{\sigma_N=1,-1} e^{\frac{B}{k_BT}\frac{1}{2}\sigma_1}\left[e^{\frac{B}{k_BT}\frac{1}{2}\sigma_1+\frac{J}{k_BT}\sigma_1\sigma_2+\frac{B}{k_BT}\frac{1}{2}\sigma_2}\right]\cdot$$

$$\cdot\left[e^{\frac{B}{k_BT}\frac{1}{2}\sigma_2+\frac{J}{k_BT}\sigma_2\sigma_3+\frac{B}{k_BT}\frac{1}{2}\sigma_3}\right]\cdots\left[e^{\frac{B}{k_BT}\frac{1}{2}\sigma_{N-1}+\frac{J}{k_BT}\sigma_{N-1}\sigma_N+\frac{B}{k_BT}\frac{1}{2}\sigma_N}\right]e^{\frac{B}{k_BT}\frac{1}{2}\sigma_N} \tag{13}$$

We can easily evaluate this sum. For this purpose, we introduce the following matrix, sometimes called the "transfer matrix",

$$[T]_{ab} = \exp\left(\frac{B}{k_BT}\frac{1}{2}\sigma_a\right)\exp\left(\frac{J}{k_BT}\sigma_a\sigma_b\right)\exp\left(\frac{B}{k_BT}\frac{1}{2}\sigma_b\right) = \begin{bmatrix} e^{\frac{J+B}{k_BT}} & e^{-\frac{J}{k_BT}} \\ e^{-\frac{J}{k_BT}} & e^{\frac{J-B}{k_BT}} \end{bmatrix}$$

where the 11 component has $\sigma_a = \sigma_b = 1$, the 12-component has $\sigma_a = -\sigma_b = 1$, the 21-component has $-\sigma_a = \sigma_b = 1$ and the 22-component has $-\sigma_a = -\sigma_b = 1$.

Then we observe that the partition function can be written as a product over $N-1$ transfer matrices,

$$Z[T,N,B] = \sum_{\sigma_1=1,-1}\sum_{\sigma_N=1,-1} e^{\frac{B}{k_BT}\frac{1}{2}\sigma_1}[T^{N-1}]_{\sigma_1\sigma_N}e^{\frac{B}{k_BT}\frac{1}{2}\sigma_N} \tag{14}$$

Here we have taken the open boundary condition where we simply sum over the states of the first and last spin in the chain. Other alternatives, like fixing the values of the spins at one or the other or both ends of the chain or periodic boundary conditions where we put $\sigma_{i+N} = \sigma_i$ are also possible. One of our results will be that, when N is very large, the behaviour that we are looking for does not depend on which boundary condition we choose.

The transfer matrix is a real, symmetric matrix. Any real, symmetric matrix can be diagonalized by a similarity transform with orthogonal matrices. In this case of a 2×2 matrix, this statement takes the simple form

$$[T]_{ab} = R(\theta)\begin{bmatrix} t_+ & 0 \\ 0 & t_- \end{bmatrix}R^{-1}(\theta) \tag{15}$$

$$R(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \tag{16}$$

$$R^{-1}(\theta) = R(-\theta) \tag{17}$$

We can easily find the eigenvalues of a 2×2 matrix,

$$t_+ = \exp\left(\frac{J}{k_B T}\right)\cosh\frac{B}{k_B T} + \sqrt{\exp\left(\frac{2J}{k_B T}\right)\sinh^2\frac{B}{k_B T} + \exp\left(-2\frac{J}{k_B T}\right)} \tag{18}$$

$$t_- = \exp\left(\frac{J}{k_B T}\right)\cosh\frac{B}{k_B T} - \sqrt{\exp\left(\frac{2J}{k_B T}\right)\sinh^2\frac{B}{k_B T} + \exp\left(-2\frac{J}{k_B T}\right)} \tag{19}$$

where we confirm that both eigenvalues are positive real numbers and that $t_+ > t_-$. Moreover, it is easy to find the rotation angle which does the diagonalization,

$$\tan 2\theta = \frac{\exp\left(-\frac{2J}{k_B T}\right)}{\sinh\frac{B}{k_B T}} \tag{20}$$

Then

$$[T^{N-1}]_{ab} = \begin{bmatrix}\cos\theta & -\sin\theta \\ \sin\theta & \cos\theta\end{bmatrix}\begin{bmatrix}t_+^{N-1} & 0 \\ 0 & t_-^{N-1}\end{bmatrix}\begin{bmatrix}\cos\theta & \sin\theta \\ -\sin\theta & \cos\theta\end{bmatrix}$$

and equation (35) becomes

(21)

$$Z[T,N,B] = \sum_{\sigma_1=1,-1}\sum_{\sigma_N=1,-1} e^{\frac{B}{k_B T}\frac{1}{2}\sigma_1}\begin{bmatrix}\cos\theta & -\sin\theta \\ \sin\theta & \cos\theta\end{bmatrix}\begin{bmatrix}t_+^{N-1} & 0 \\ 0 & t_-^{N-1}\end{bmatrix}\begin{bmatrix}\cos\theta & \sin\theta \\ -\sin\theta & \cos\theta\end{bmatrix}_{\sigma_1\sigma_N} e^{\frac{B}{k_B T}\frac{1}{2}\sigma_N}$$

(22)

$$= \begin{bmatrix} e^{\frac{B}{2k_B T}}, e^{-\frac{B}{2k_B T}}\end{bmatrix}\begin{bmatrix}\cos\theta & -\sin\theta \\ \sin\theta & \cos\theta\end{bmatrix}\begin{bmatrix}t_+^{N-1} & 0 \\ 0 & t_-^{N-1}\end{bmatrix}\begin{bmatrix}\cos\theta & \sin\theta \\ -\sin\theta & \cos\theta\end{bmatrix}\begin{bmatrix} e^{\frac{B}{2k_B T}} \\ -\frac{B}{2k_B T}\end{bmatrix}$$

Since t_+ is the largest eigenvalue and $\sin\theta \neq 0$, the logarithm of the partition function will be dominated by the occurrence of t_+^{N-1} in the expression and, up to terms which grow slower with large N than N itself, the Helmholtz free energy is $F[T,N,B] = -Nk_B T \ln t_+$. This expression simplifies to

$$F[T,N,B] = -NJ - Nk_B T \ln\left(\cosh\frac{B}{k_B T} + \sqrt{\sinh^2\frac{B}{k_B T} + \exp\left(-4\frac{J}{k_B T}\right)}\right) \tag{23}$$

In particular, we use the second equation in (5) to find the magnetization density as

$$m \equiv \frac{M}{N} = \frac{\sinh\frac{B}{k_B T}}{\sqrt{\sinh^2\frac{B}{k_B T} + \exp\left(-4\frac{J}{k_B T}\right)}} \tag{24}$$

Then we note that for any $T > 0$, equation (24) indicates that

$$\lim_{B\to 0} m = 0 \ , \ T > 0 \tag{25}$$

It is only when we look at the zero temperature limit, where, from equation (24) we find that

$$\lim_{T\to 0} m = \text{sign}(B) \tag{26}$$

which exhibits a phase transition. It occurs at the point $(T, B) = (0, 0)$ in the phase diagram as B passes from negative to positive values. This was behaviour illustrated in figure 1. The point $(T, B) = (0, 0)$ is the only point where spontaneous symmetry breaking can occur, where the magnetization that is seen there depends on the direction from which the point is approached. If it is approached by increasing B along the $T = 0$ axis, $m = -1$. If it is approached by decreasing B along the $T = 0$ axis, $m = 1$. If it is approached from any other direction inside the diagram, $m = 0$.

We might wonder if the states with $m = -1, 1, 0$ are all degenerate $T \to 0, B \to 0$. Indeed,

$$\lim_{B\to 0} \lim_{T\to 0} F[T, B, N] = \lim_{B\to 0} (-N|B|) = -NJ \tag{27}$$

$$\lim_{F\to 0} \lim_{B\to 0} F[T, B, N] = \lim_{T\to 0} \left\{ -NJ - Nk_BT \ln \left(1 + \exp\left(-2\frac{J}{k_BT} \right) \right) \right\} = -NJ \tag{28}$$

one can see that the free energy goes the same constant, irregardless of the direction from which that point is approached. This indeed implies that the three states with $m = -1, 1, 0$ can occur, depending on the history of how the state is approached. This statement ignores "finite volume effects" which depend on the boundary conditions. Various boundary conditions could favour one of the three states.

To illustrate by example that the result for the free energy in equation (23) does not depend on the boundary conditions, we could also consider the spin chain with a periodic boundary condition. For this purpose, we set $\sigma_N - \sigma_1$. In order to ensure that each spin couples to the magnetic field B only once we need to drop one term from the second term in the Hamiltonian in equation (11) so that it now becomes

$$H \;=\; -J \sum_{n=1}^{N-1} \sigma_n \sigma_{n+1} - B \sum_{n=1}^{N-1} \sigma_n \tag{29}$$

and the partition function is now given by the simpler expression

$$Z[T, B, N] = \text{Tr} T^{N-1} \tag{30}$$

The trace of a real symmetric matrix is equal to the sum of its eigenvalues

$$Z[T, B, N] = t_+^{N-1} + t_-^{N-1} \tag{31}$$

and

$$F[T, B, N] = -k_B T N \ln t_+ + \dots \tag{32}$$

where the ellipses denote terms which, as N becomes very large, grow slower than N. The result agrees with our previous on in equation (23).

2.1. **Spin correlation functions.** The magnetization density that we have discussed above is the average expectation value of the orientation of a single spin,

$$m = \frac{1}{N}\sum_x < \sigma_x >$$

Sometimes it is of interest to know the single spin expectation value $< \sigma_x >$ itself. If we had a translation invariant boundary condition, like periodic boundary conditions, we expect that $< \sigma_x >$ is independent of x and it would therefore be equal to m. On the other hand, if we have the open boundary conditions that we have chosen (where we simply sum over both orientations of the spins at the ends of the chain) or if we fix one or both of the spins at the end of the chain to a given value, we expect that $< \sigma_x >$ will depend on x and perhaps be an approximate constant as x varies over values which are far from the boundaries.

In this simple one-dimensional spin chain, we can compute the expectation value $< \sigma_x >$ exilicitly

$$\langle \sigma_x \rangle = \frac{1}{Z}\sum_{\sigma_1=1,-1}\sum_{\sigma_N=1,-1} e^{\frac{B}{k_BT}\frac{1}{2}\sigma_1}\left\{T^{x-1}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}T^{N-x}\right\}_{\sigma_1\sigma_N} e^{\frac{B}{k_BT}\frac{1}{2}\sigma_N}$$

$$= \frac{\begin{bmatrix}e^{\frac{B}{2k_BT}}, e^{-\frac{B}{2k_BT}}\end{bmatrix}\begin{bmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{bmatrix}\begin{bmatrix}t_+^{x-1} & 0\\ 0 & t_-^{x-1}\end{bmatrix}\begin{bmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\begin{bmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{bmatrix}\begin{bmatrix}t_+^{N-x} & 0\\ 0 & t_-^{N-x}\end{bmatrix}\begin{bmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{bmatrix}\begin{bmatrix}e^{\frac{B}{2k_BT}}\\ e^{-\frac{B}{2k_BT}}\end{bmatrix}}{\begin{bmatrix}e^{\frac{B}{2k_BT}}, e^{-\frac{B}{2k_BT}}\end{bmatrix}\begin{bmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{bmatrix}\begin{bmatrix}t_+^{N-1} & 0\\ 0 & t_-^{N-1}\end{bmatrix}\begin{bmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{bmatrix}\begin{bmatrix}e^{\frac{B}{2k_BT}}\\ e^{-\frac{B}{2k_BT}}\end{bmatrix}}$$

$$= \frac{\begin{bmatrix}e^{\frac{B}{2k_BT}}\cos\theta + e^{-\frac{B}{2k_BT}}\sin\theta, -e^{\frac{B}{2k_BT}}\sin\theta + e^{-\frac{B}{2k_BT}}\cos\theta\end{bmatrix}\begin{bmatrix}t_+^{x-1} & 0\\ 0 & t_-^{x-1}\end{bmatrix}\begin{bmatrix}\cos 2\theta & -\sin 2\theta\\ -\sin 2\theta & -\cos 2\theta\end{bmatrix}\begin{bmatrix}t_+^{N-x} & 0\\ 0 & t_-^{N-x}\end{bmatrix}\begin{bmatrix}e^{\frac{B}{2k_BT}}\cos\theta + e^{-\frac{B}{2k_BT}}\sin\theta\\ -e^{\frac{B}{2k_BT}}\sin\theta + e^{-\frac{B}{2k_BT}}\cos\theta\end{bmatrix}}{\begin{bmatrix}e^{\frac{B}{2k_BT}}\cos\theta + e^{-\frac{B}{2k_BT}}\sin\theta, -e^{\frac{B}{2k_BT}}\sin\theta + e^{-\frac{B}{2k_BT}}\cos\theta\end{bmatrix}\begin{bmatrix}t_+^{N-1} & 0\\ 0 & t_-^{N-1}\end{bmatrix}\begin{bmatrix}e^{\frac{B}{2k_BT}}\cos\theta + e^{-\frac{B}{2k_BT}}\sin\theta\\ -e^{\frac{B}{2k_BT}}\sin\theta + e^{-\frac{B}{2k_BT}}\cos\theta\end{bmatrix}}$$

$$= \frac{\begin{bmatrix}t_+^{x-1}\left(e^{\frac{B}{2k_BT}}\cos\theta + e^{-\frac{B}{2k_BT}}\sin\theta\right), t_-^{x-1}\left(-e^{\frac{B}{2k_BT}}\sin\theta + e^{-\frac{B}{2k_BT}}\cos\theta\right)\end{bmatrix}\begin{bmatrix}\cos 2\theta & -\sin 2\theta\\ -\sin 2\theta & -\cos 2\theta\end{bmatrix}\begin{bmatrix}t_+^{N-x}\left(e^{\frac{B}{2k_BT}}\cos\theta + e^{-\frac{B}{2k_BT}}\sin\theta\right)\\ t_-^{N-x}\left(-e^{\frac{B}{2k_BT}}\sin\theta + e^{-\frac{B}{2k_BT}}\cos\theta\right)\end{bmatrix}}{\begin{bmatrix}t_+^{x-1}\left(e^{\frac{B}{2k_BT}}\cos\theta + e^{-\frac{B}{2k_BT}}\sin\theta\right), t_-^{x-1}\left(-e^{\frac{B}{2k_BT}}\sin\theta + e^{-\frac{B}{2k_BT}}\cos\theta\right)\end{bmatrix}\begin{bmatrix}t_+^{N-x}\left(e^{\frac{B}{2k_BT}}\cos\theta + e^{-\frac{B}{2k_BT}}\sin\theta\right)\\ t_-^{N-x}\left(-e^{\frac{B}{2k_BT}}\sin\theta + e^{-\frac{B}{2k_BT}}\cos\theta\right)\end{bmatrix}}$$

$$\begin{aligned}
&= \left\{\cos 2\theta\left(t_+^{N-1}\left(e^{\frac{B}{2k_BT}}\cos\theta + e^{-\frac{B}{2k_BT}}\sin\theta\right)^2 - t_-^{N-1}\left(-e^{\frac{B}{2k_BT}}\sin\theta + e^{-\frac{B}{2k_BT}}\cos\theta\right)^2\right)\right.\\
&\left. - \sin 2\theta(t_+^{x-1}t_-^{N-1} + t_+^{N-1}t_-^{x-1})\left(e^{\frac{B}{2k_BT}}\cos\theta + e^{-\frac{B}{2k_BT}}\sin\theta\right)\left(-e^{\frac{B}{2k_BT}}\sin\theta + e^{-\frac{B}{2k_BT}}\cos\theta\right)\right\}\cdot\\
&\cdot\left\{t_+^{N-1}\left(e^{\frac{B}{2k_BT}}\cos\theta + e^{-\frac{B}{2k_BT}}\sin\theta\right)^2 + t_-^{N-1}\left(-e^{\frac{B}{2k_BT}}\sin\theta + e^{-\frac{B}{2k_BT}}\cos\theta\right)^2\right\}^{-1}
\end{aligned} \tag{33}$$

The first line in the final equation above is independent of x. This is the part of the result which is independent of the boundary conditions. We are interested in the limit where $N >> x >> 1$. In that case, the first term in the denominator and the first term in the numerator dominate and we get

$$\lim_{N\to\infty} < \sigma_x >= \cos 2\theta = \frac{\sinh \frac{B}{k_BT}}{\sqrt{\sinh^2 \frac{B}{k_BT} + e^{-4\frac{J}{k_BT}}}} \tag{34}$$

where we have used equation (20) and some trigonometric identities to obtain the explicit form of $\cos\theta$. We also note that we could get exactly the same result by taking a derivative of the free energy. The magnetization is defined by

$$M = -\left.\frac{\partial F}{\partial B}\right|_{T,N}$$

and the magnetization density $m = M/N$. If we use the free energy that we computed above and which appears in equation (23) we get the same result – the expression for the magnetization that we have already quoted in equation (24).

Then, a correlation function of two spins is

$$\langle\sigma_x\sigma_y\rangle = \frac{1}{Z}\sum_{\sigma_1=1,-1}\sum_{\sigma_N=1,-1} e^{\frac{B}{k_BT}\frac{1}{2}\sigma_1}\left\{T^x\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}T^{y-x}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}T^{N-1-y}\right\}_{\sigma_1\sigma_N} e^{\frac{B}{k_BT}\frac{1}{2}\sigma_N} \tag{35}$$

where we will assume that both x and y are in the central part of the chain. The computation of this correlation function is straightforward if tedious. We will simplify our problem somewhat by changing to periodic boundary condition. This boundary condition identifies σ_1 and σ_N. What is more, we have to remove a term, $-B\sigma_N$ from the Hamilonian, otherwise the spin $\sigma_1 = \sigma_N$ would couple to B twice. Then, also, we will compute the connected correlation function. Using the transfer matrix, the correlation function is

$$\langle\sigma_x\sigma_y\rangle \; - \; \langle\sigma_x\rangle\langle\sigma_y\rangle = \tag{36}$$

$$\frac{\mathrm{Tr}\left\{T^{x-1}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}T^{y-x}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}T^{N-y}\right\}}{\mathrm{Tr}\left\{T^{N-1}\right\}} - \frac{\mathrm{Tr}\left\{T^{x-1}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}T^{N-x}\right\}}{\mathrm{Tr}\left\{T^{N-1}\right\}}\frac{\mathrm{Tr}\left\{T^{y-1}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}T^{N-y}\right\}}{\mathrm{Tr}\left\{T^{N-1}\right\}} \tag{37}$$

$$= \frac{\mathrm{Tr}\left\{\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}T^{y-x}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}T^{N-y+x}\right\}}{\mathrm{Tr}\left\{T^{N-1}\right\}} - \frac{\mathrm{Tr}\left\{\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}T^{N-1}\right\}}{\mathrm{Tr}\left\{T^{N-1}\right\}}\frac{\mathrm{Tr}\left\{c\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}T^{N-1}\right\}}{\mathrm{Tr}\left\{T^{N-1}\right\}} \tag{38}$$

where we have used the property of a trace over a product of matrices

$$\mathrm{Tr}(AB) \equiv \sum_a (AB)_{aa} = \sum_{ab} A_{ab}B_{ba} = \sum_{ab} B_{ba}A_{ab} = \sum_b (BA)_{bb} = \mathrm{Tr}(BA)$$

Some straightforward algebra leads to the result

$$\langle \sigma_x \sigma_y \rangle \ - \ \langle \sigma_x \rangle \langle \sigma_y \rangle = \frac{t_+^{y-x} t_-^{N-y+x} + t_-^{y-x} t_+^{N-y+x}}{t_+^N + t_-^N} \tag{39}$$

If we take the limit where N is large and, in particular, $N >> |y-x|$, we find the result

$$\langle \sigma_x \sigma_y \rangle \ - \ \langle \sigma_x \rangle \langle \sigma_y \rangle \ \approx \ \left(\frac{t_-}{t_+}\right)^{y-x} = e^{-|y-x|/\xi} \tag{40}$$

The correlation decays exponentially with distance. The distance scale ξ is called the correlation length. Here, it is given by

$$\xi = \frac{1}{\ln \frac{t_+}{t_-}} = \frac{1}{\ln \frac{1+\sqrt{\tanh^2 \frac{B}{k_B T} + \frac{\exp\left(-4\frac{J}{k_B T}\right)}{\cosh^2 \frac{B}{k_B T}}}}{1-\sqrt{\tanh^2 \frac{B}{k_B T} + \frac{\exp\left(-4\frac{J}{k_B T}\right)}{\cosh^2 \frac{B}{k_B T}}}}}$$

This correlation length is a positive real number in the entire (T, B) half-plane. When we switch off the magnetic field we get

$$\lim_{B\to 0} \xi = \frac{1}{\ln \frac{1+\exp\left(-2\frac{J}{k_B T}\right)}{1-\exp\left(-2\frac{J}{k_B T}\right)}}$$

and it diverges at the field and zero temperature limit where there can be a spontaneous magnetization,

$$\lim_{T\to 0} \lim_{B\to 0} \xi \ = \ \frac{1}{2} e^{2\frac{J}{k_B T}} \ \to \ \infty$$

3. Landau's Argument

The absence of spontaneous magnetization at any finite temperature can be understood from a physical argument which is originally attributed to L.D.Landau. Let us set $B = 0$. The lowest energy states of the Ising model are indeed spontaneously magnetized ferromagnets where all of the spins have value $+1$ or where all of the spins have value -1. Let us begin with the lowest energy state where all of the spins have value $+1$, that is, $\sigma_n = 1$ $\forall n$. At first sight, one might expect that this state with all spins aligned, having the lowest energy, therefore has the largest Boltzmann weight. Its Boltzmann weight is

$$e^{(N-1)\frac{J}{k_B T}}$$

However, as we shall now argue, it is not the case that other states necessarily make a smaller contribution.

A defect in the completely aligned state is a "domain wall" that separates a region where the spins are $\sigma = +1$ from a region where the spins are $\sigma = -1$. The energy of this domain wall is the energy of the lowest energy state plus the energy of a single misaligned pair of neighbouring spins, $-(N-1)J + 2J$. This domain wall which is a misaligned pair of neighbouring spins is also sometimes called a "misaligned bond". The total number of places where a domain wall can occur is $N-1$. The Boltzmann weight for such a state has the exponential of its energy divided by k_BT and this exponential should be multiplied by the degeneracy of the state, that is, the number of places where the domain wall could be located. A single domain wall can be located in $N-1$ different positions, so the net Boltzmann weight that we assign to it is

$$(N-1)e^{(N-1)\frac{J}{k_BT}-2\frac{J}{k_BT}} = e^{(N-1)\frac{J}{k_BT}}e^{\ln(N-1)-2\frac{J}{k_BT}}$$

we see that as well as the energy which gives a relative factor $e^{-2\frac{J}{k_BT}}$ which suppresses this state, there is a slight enhancement from the presence of the factor $N-1$ which is large, since N is large. The suppression of this one domain wall state compared to the state with no domain wall at all is

$$e^{\ln(N-1)-2\frac{J}{k_BT}}$$

which is greater than one when N is large enough. We can think of this as the entropy of domain walls as growing faster than their energy. It should lead to states where the density of domain walls is finite and where the magnetization is zero. This is basically Landau's argument as to why there is no ferromagnetism at any nonzero temperature in the one dimensional Ising model.

Now, to develop this idea a bit, let us consider a state of the system with two domain walls. The energy of that state is $-(N-1)J + 4J$ and the number of positions that the two domain walls can occupy is

$$\frac{(N-1)(N-2)}{2} = \frac{(N-1)!}{(N-3)!2!}$$

We get this factor by noting that there are $N-1$ positions where we can place the first domain wall and $N-2$ positions where we can place the second one, but this over-counts the number since the order in which we placed the domain walls is irrelevant, both orderings result in the same spin configuration. Therefore we must divide by the factor of 2. The net Boltzmann weight for the system with two domain walls is

$$\frac{(N-1)!}{(N-3)!2!}e^{(N-1)\frac{J}{k_BT}-4\frac{J}{k_BT}}$$

We can easily generalize this expression to consider spin configurations with q domain walls. The energy of the state with q domain walls is $-(N-1)J + 2qJ$ and the number of ways fo placing q domain walls on a chain with $N-1$ bonds is the combinatorial number $\frac{(N-1)!}{q!(N-1-q)!}$. The weight of a state with q domain walls is thus

$$\frac{(N-1)!}{q!(N-1-q)!}e^{(N-1)\frac{J}{k_BT}-2q\frac{J}{k_BT}}$$

To confirm that we are on the right track here, we can sum the Boltzmann weights for misaligned bonds to find the partition function

$$Z = \sum_{q=0}^{N-1} \frac{(N-1)!}{q!(N-1-q)!} e^{(N-1)\frac{J}{k_BT} - 2q\frac{J}{k_BT}} = e^{(N-1)\frac{J}{k_BT}} \left(1 + e^{-2\frac{J}{k_BT}}\right)^{N-1}$$

whose logarithm, at the large N limit (where $N-1$ is well approximated by N) indeed produces exactly the $B \to 0$ limit of the Helmholtz free energy that we found in equation (23),

$$F[T, N, B = 0] = -NJ - Nk_BT \ln\left(1 + \exp\left(-2\frac{J}{k_BT}\right)\right) \tag{41}$$

The most likely number of misaligned bonds is found by maximizing the Boltzmann weight, or its logarithm

$$\ln \frac{N!}{q!(N-q)!} \; - \; 2q\frac{J}{k_BT}$$

We assume q is large and use Stirling's formula,

$$-q \ln q/N - (N-q)\ln(N-q)/N - 2q\frac{J}{k_BT}$$

then we find that

$$\frac{\frac{q}{N}}{1 - \frac{q}{N}} = e^{-2\frac{J}{k_BT}}$$

which can be solved by

$$\frac{q}{N} = \frac{e^{-2\frac{J}{k_BT}}}{1 + e^{-2\frac{J}{k_BT}}} \tag{42}$$

This has two interesting features. First of all, as we have already noted should be the case, the density of domain walls, $\frac{q}{N}$ is nonzero at any finite temperature. Once there is a nonzero density of randomly placed domain walls, the average magnetization should be zero. This way we understand why there is no ferromagnetic phase of this system when $T > 0$.

Secondly, the expectation value of the number of domain walls in equation (42) is highly reminiscent of the expectation value of the number of particles in a Fermi-Dirac distribution where the particles are fermions which have a single energy level with energy $2J$.

In fact, the Helmholtz free energy in equation (41) is identical to the free energy of a quantum system of N non-interacting fermions where each of the fermions has only one energy level, with energy $2J$, and this fermion state can be either occupied or unoccupied. There is also a constant ground state energy NJ where the "ground state" is the state with no fermions at all. (This constant shift of the free energy is irrelevant to the thermodynamics of the system.)