Chapter 1

Some exactly solvable models of phase transitions

1.1 *1-dim* Ising model

In this section, we arrive at the exact solution of the one dimensional Ising model. There are two techniques for solving the model:

1. the *recursive method*;

2. the *transfer matrix method*.

1.1.1 Recursive method

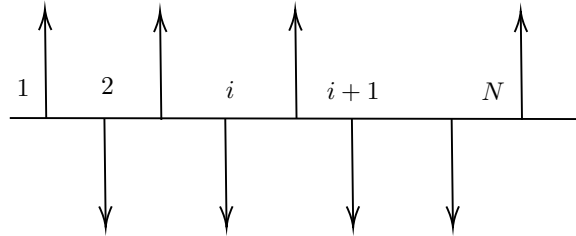**Case with $H = 0$ and free boundary conditions**

Figure 1.1: One dimensional Bravais Lattice.

Let us consider a Bravais lattice in the one dimensional case, that is just a one dimensional lattice, as in Figure 1.1.

The canonical partition function of such a system is:

$$Z_N(T) = \sum_{S_1=\pm 1} \sum_{S_2=\pm 1} \cdots \sum_{S_N=\pm 1} \exp\left[\overbrace{\beta J}^{K} \sum_{i=1}^{N-1} S_i S_{i+1} \right] \tag{1.1}$$

The two body interaction is the sum in all the neighbours that in that case are $(i-1)$ and $(i+1)$, but we have only to consider the one after, because the one behind is yet taken by the behind site.

We want to solve this partition function. If we consider *free boundary* condition, the N does not have a $N+1$, almost for the moment. Let us define

$$K \equiv \beta J, \quad h \equiv \beta H \tag{1.2}$$

Making explicit the sum in the exponential:

$$Z_N(K) = \sum_{S_1=\pm 1} \sum_{S_2=\pm 1} \cdots \sum_{S_N=\pm 1} e^{K(S_1 S_2 + S_2 S_3 + \cdots + S_{N-1} S_N)}$$

What does happen if we just add another spin at the end S_{N+1} ? Which is the partition function with that new spin? We obtain:

$$Z_{N+1}(K) = \sum_{S_{N+1}=\pm 1} \sum_{S_1=\pm 1} \sum_{S_2=\pm 1} \cdots \sum_{S_N=\pm 1} e^{K(S_1 S_2 + S_2 S_3 + \cdots + S_{N-1} S_N)} \, e^{K S_N S_{N+1}}$$

On the other hand, this sum is just involving this term:

$$\sum_{S_{N+1}=\pm 1} e^{K S_N S_{N+1}} = e^{K S_N} + e^{-K S_N} = 2\cosh(K S_N) = 2\cosh(K)$$

where the last equivalence derive from the fact that cosh is an even function and it does not depend on ± 1. Therefore,

$$Z_{N+1}(K) = (2\cosh(K))Z_N(K) \quad \text{and} \quad Z_N(K) = (2\cosh(K))Z_{N-1}(K)$$

By performing a backward iteration,

$$Z_N(K) = Z_1 (2\cosh(K))^{N-1}$$

Since $Z_1 = \sum_{S_1=\pm 1} 1 = 2$, we have

$$Z_N(T) = 2(2\cosh(K))^{N-1} \tag{1.3}$$

The free energy is

$$F_N(K) = -k_B T \ln Z_N(K) = -k_B T \ln 2 - k_B T(N-1)\ln(2\cosh(K)) \tag{1.4}$$

and taking the thermodynamic limit it becomes

$$f_b(T) \equiv \lim_{N \to \infty} \frac{1}{N} F_N(K) = -k_B T \ln\left(2\cosh\left(\frac{J}{k_B T}\right)\right) \tag{1.5}$$

As one can see (Figure 1.2) $f_b(T)$ is an analytic function of T, so we have no phase transition at $T \neq 0$.

Now, let us compute the magnetization (the average over the spin $\langle S_j \rangle$) for a generic site j (assume again that $S_i = \pm 1$). This can be done in many ways. Here, we choose one that consider another way to compute Z for the $1 - dim$ Ising model. This method can be useful for other calculations. It is based on the following identity:

$$\exp[K S_i S_{i+1}] \underset{(proof)}{=} \cosh(K) + S_i S_{i+1} \sinh(K) = \cosh(K)[1 + S_i S_{i+1} \tanh(K)] \tag{1.6}$$

Proof of identity (1.6)**.** Remind that

$$\cosh x = \frac{e^x + e^{-x}}{2}, \qquad \sinh x = \frac{e^x - e^{-x}}{2}$$

Hence,

$$e^x = \cosh x + \sinh x$$

In our case,

$$e^{k S_i S_{i+1}} = \cosh(K S_i S_{i+1}) + \sinh(K S_i S_{i+1}) = \cosh K + S_i S_{i+1} \sinh K$$

where the last step was obtained considering that cosh is an even function, while sinh is an odd one.   ■
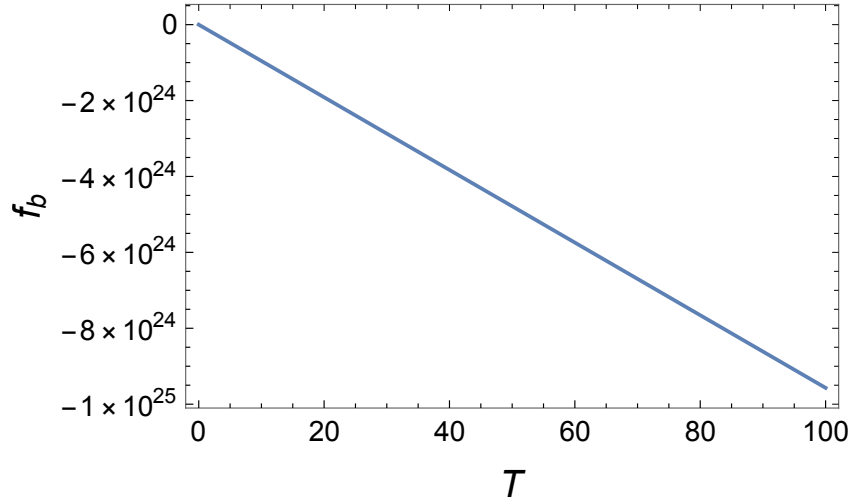
Figure 1.2: Free energy function in thermodynamic limit for the one dimensional Ising model, for $k_B = 1.38 \times 10^{23}, J = 1$.

Using identity (1.6), we obtain

$$Z_N(K) = \sum_{\{S\}} \exp\left[K \sum_{i=1}^{N-1} S_i S_{i+1} \right] = \sum_{\{S\}} \prod_{i=1}^{N-1} [\cosh(K)(1 + S_i S_{i+1} \tanh(K))]$$

by rearranging,

$$Z_N(K) = (\cosh K)^{N-1} \sum_{\{S\}} \prod_{i=1}^{N-1} (1 + S_i S_{i+1} \tanh K) \tag{1.7}$$

If we now expand the products, we get 2^{N-1} terms of the following form:

$$\sum_{\substack{S_{i_e}=\pm 1 \\ e=1,\dots,M}} (\tanh K)^M S_{i_1} S_{i_1+1} S_{i_2} S_{i_2+1} \dots S_{i_M} S_{i_M+1} = 0 \tag{1.8}$$

where $i_1 \dots i_M$ is a set of M sites of the lattice.

Remark. The terms above, when summed over $\{S\}$ are zero, except the term with $M = 0$ that is equal to 1 and, when summed over $\{S\}$, gives 2^N.

Therefore:

$$Z_N(K) = 2^N (\cosh K)^{N-1}$$

that coincides with the result obtained before.

If we now compute the average $\langle S_j \rangle$, the procedure is similar but now there will be terms as (1.8) with the addiction of an S_j:

$$(\tanh K)^M S_{i_1} S_{i_1+1} S_{i_2} S_{i_2+1} \dots S_{i_M} S_{i_M+1} \; S_j \tag{1.9}$$

that, when one sums over $\{S\}$ are all zero, included the term with $M = 0$ that now is equal to S_j and $\sum_{S_j=\pm 1} = 0$. Hence, we have the result

$$\langle S_j \rangle = 0 \quad \forall j \tag{1.10}$$

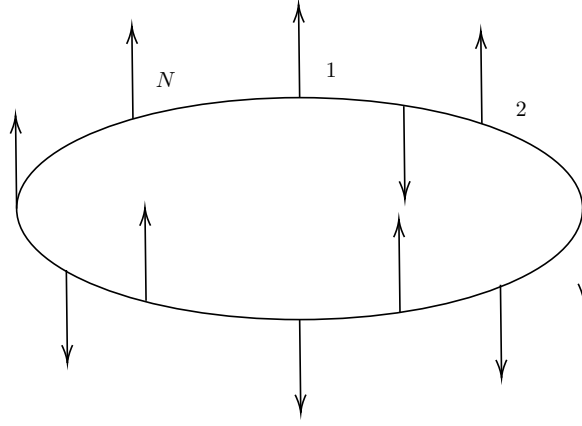The magnetization is always zero $\forall j \neq \infty$!

Figure 1.3: One dimensional lattice ring: Ising model with periodic boundary conditions.

Case with $H \neq 0$ and periodic boundary conditions

Consider the spins sitting on a 1D lattice ring as in Figure 1.3. The periodic boundary conditions are:

$$S_{N+1} = S_1$$

We have:

$$-\beta \mathcal{H}_\Omega(\{S\}) = K \sum_{i=1}^{N} S_i S_{i+1} + h \sum_{i=1}^{N} S_i \tag{1.11}$$

where

$$K \equiv \beta J, \quad h \equiv \beta H$$

The $1 - dim$ Ising model with this setup can be solved in several ways. Here we will use the method of the transfer matrix. This is a quite general technique that we will discuss within the Ising model.

1.1.2 Transfer Matrix method

Given the Hamiltonian (1.11)[1] we can write the corresponding partition function in the following symmetric form:

$$Z_N(k,h) = \sum_{S_1=\pm1} \sum_{S_2=\pm1} \cdots \sum_{S_N=\pm1} \left[e^{KS_1S_2+\frac{h}{2}(S_1+S_2)} \right] \left[e^{KS_2S_3+\frac{h}{2}(S_2+S_3)} \right] \cdots \left[e^{KS_NS_1+\frac{h}{2}(S_N+S_1)} \right]$$

We want to write the partition function in a form similarly to $\sum_j M_{ij} P_{jk}$. Note that, in the previous form Z_N can be written as a product of matrices

$$
\begin{aligned}
Z_N(h,k) &= \sum_{S_1=\pm1} \cdots \sum_{S_N=\pm1} \prod_{i=1}^{N} \exp\left[KS_iS_{i+1} + \frac{h}{2}(S_i + S_{i+1}) \right] \\
&= \sum_{S_1=\pm1} \cdots \sum_{S_N=\pm1} \langle S_1| \, \mathbb{T} \, |S_2\rangle \langle S_2| \, \mathbb{T} \, |S_3\rangle \ldots \langle S_N| \, \mathbb{T} \, |S_1\rangle
\end{aligned} \tag{1.12}
$$

where $\mathbb{T}$ is a 2×2 matrix defined as

$$\langle S| \, \mathbb{T} \, |S'\rangle = \exp\left[KSS' + \frac{h}{2}(S + S') \right] \tag{1.13}$$

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[1]The choice of boundary conditions becomes irrelevant in the thermodynamic limit, $N \to \infty$.

Remark. Note that the labels of the matrix corresponds to the values of S_i. Hence, its dimension depends on the number of possible values a spin S_i can assume. It can also depends on how many spins are involved in the interacting terms that are present in the Hamiltonian ($k_{LL} \sum S_i S_{i+1} S_{i+2} S_{i+3}$).

For the Ising model, we have $S_i = \pm 1$ and nearest neighbour interaction implies that we have two values and that $\mathbb{T}$ is a 2×2 matrix whose components are

$$\langle +1| \, \mathbb{T} \, |+1\rangle = \exp[K + h] \tag{1.14a}$$

$$\langle +1| \, \mathbb{T} \, |-1\rangle = \langle -1| \, \mathbb{T} \, |+1\rangle = \exp[-K] \tag{1.14b}$$

$$\langle -1| \, \mathbb{T} \, |-1\rangle = \exp[K - h] \tag{1.14c}$$

The explicit representation is

$$\mathbb{T} = \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix} \tag{1.15}$$

Let us introduce some useful notations and relations using the bra-ket formalism:

$$\left| S_i^{(+)} \right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_i, \quad \left| S_i^{(-)} \right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_i \tag{1.16a}$$

$$\left\langle S_i^{(+)} \right| = (1^*, 0)_i, \quad \left\langle S_i^{(-)} \right| = (0, 1^*)_i \tag{1.16b}$$

The identity relation is:

$$\sum_{S_i = \pm 1} |S_i\rangle \langle S_i| = \left| S_i^{(+)} \right\rangle \left\langle S_i^{(+)} \right| + \left| S_i^{(-)} \right\rangle \left\langle S_i^{(-)} \right| = \mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{1.17}$$

By using the identity property, we can rewrite the partition function as

$$\begin{aligned}
Z_N(K, h) &= \sum_{S_1 = \pm 1} \cdots \sum_{S_N = \pm 1} \langle S_1| \, \mathbb{T} \, |S_2\rangle \langle S_2| \, \mathbb{T} \, |S_3\rangle \ldots |S_i\rangle \langle S_i| \, \mathbb{T} \, |S_{i+1}\rangle \ldots \\
&= \sum_{S_1 = \pm 1} \langle S_1| \, \mathbb{T}^N \, |S_1\rangle = \text{Tr}\big[\mathbb{T}^N\big]
\end{aligned} \tag{1.18}$$

this is exactly the trace of the matrix, which is most usefully expressed in terms of the eigenvalues. Being $\mathbb{T}$ symmetric, we can diagonalize it by an unitary transformation as

$$\mathbb{T}_D = \mathbb{P}^{-1} \mathbb{T} \mathbb{P} \tag{1.19}$$

with $\mathbb{P}\mathbb{P}^{-1} = \mathbb{1}$. Hence,

$$\begin{aligned}
\text{Tr}\big[\mathbb{T}^N\big] &= \text{Tr}\Big[\underbrace{\mathbb{T}\mathbb{T}\mathbb{T}\ldots\mathbb{T}}_{N}\Big] = \text{Tr}\big[\mathbb{P}\mathbb{P}^{-1}\mathbb{T}\mathbb{P}\mathbb{P}^{-1}\mathbb{T}\mathbb{P}\ldots\mathbb{P}^{-1}\mathbb{T}\mathbb{P}\mathbb{P}^{-1}\big] \\
&= \text{Tr}\big[\mathbb{P}\mathbb{T}_D^N\mathbb{P}^{-1}\big] \underset{\substack{\text{ciclyc property} \\ \text{of the trace}}}{=} \text{Tr}\big[\mathbb{T}_D^N\mathbb{P}^{-1}\mathbb{P}\big] \\
&= \text{Tr}\big[\mathbb{T}_D^N\big]
\end{aligned}$$

where

$$\mathbb{T}_D = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix} \quad \Rightarrow \quad \mathbb{T}_D^N = \begin{pmatrix} \lambda_+^N & 0 \\ 0 & \lambda_-^N \end{pmatrix} \tag{1.20}$$

with $\lambda_\pm$ are the eigenvalues with $\lambda_+ > \lambda_-$.

Remark. $\mathbb{P}$ is the similitude matrix whose columns are given by the eigenvectors of $\lambda_\pm$.

We finally have:

$$Z_N(K, h) = \text{Tr}\left[\mathbb{T}_{\mathbb{D}}^{\mathbb{N}}\right] = \lambda_+^N + \lambda_-^N \tag{1.21}$$

Remark. As mentioned previously the dimension of the transfer matrix $\mathbb{T}$ and hence the number of eigenvalues $\{\lambda\}$ depend both on the possible values of S_i and on the number of sites involved in terms of the Hamiltonian (range of interaction).

Example 1

For example, consider the Ising ($S_i = \pm 1$) with n. n. and next n. n. interactions. The Hamiltonian is:

$$\mathcal{H} = k_1 \sum_i S_i S_{i+1} + k_2 \sum_i S_i S_{i+1} S_{i+2} S_{i+3}$$

Because of the second term, now there are $2^4 = 16$ possible configurations that can be described by using a 4×4 transfer matrix that we can write formally as

$$\langle S_i S_{i+1} | \, \mathbb{T} \, | S_{i+2} S_{i+3} \rangle$$

Example 2

For example, suppose $S_i = +1, 0, -1$, therefore the spin can assume three different values. This is a *deluted* Ising model.

Now, let us consider the transfer matrix formalism in a more general setting.

1.2   General transfer matrix method

The aim of this section is to describe how transfer matrices can be used to solve classical spin models. The idea is to write down the partition function in terms of a matrix, the transfer matrix. The thermodynamic properties of the model are then wholly described by the eigenspectrum of the matrix. In particular, the free energy per spin in the thermodynamic limit depends only on the largest eigenvalue and the correlation length only on the two largest eigenvalues through simple formulae.

Let $\mathbb{T}$ be a square matrix $(n+2) \times (n+2)$ that, for example, it is built if the spin variables may assume $(n+2)$ possible values. The k-esim value can be defined by the bra-ket notation where the two vectors are given by a sequence of "0" and a single "1" at the k-esim position.

Example 3

If $k = 3$ and there are $(n+2)$ possible values:

$$\left\langle S_i^{(3)} \right| = (0, 0, 1^*, 0, \ldots, 0) \qquad \left| S_i^{(3)} \right\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}$$

these are the bra-ket at the k-esim position.

Similarly to the 2×2 Ising case, it is easy to show the identity property

$$\sum_{S_i} |S_i\rangle \langle S_i| = \mathbb{1}, \quad \mathbb{1} \in (n+2) \times (n+2) \tag{1.22}$$

where now the sum is over $(n+2)$ values.

Let us consider the *diagonal matrix* $\mathbb{S}_i$, where the elements along the diagonal are all the $(n+2)$ possible values of the i-esim spin (or of some of their combination if longer interaction terms are considered)

$$\mathbb{S}_i \equiv \sum_{S_i} |S_i\rangle \, S_i \, \langle S_i| \tag{1.23}$$

Example 4: Ising model $n+2=2$

$$\begin{pmatrix}1\\0\end{pmatrix} S^{(1)}(1^*,0) + \begin{pmatrix}0\\1\end{pmatrix} S^{(2)}(0,1^*) = \begin{pmatrix}S^{(1)} & 0\\0 & 0\end{pmatrix} + \begin{pmatrix}0 & 0\\0 & S^{(2)}\end{pmatrix} = \begin{pmatrix}S^{(1)} & 0\\0 & S^{(2)}\end{pmatrix}$$

Ising: $S^{(1)} = +1, S^{(2)} = -1$.

Remark. Note that in this case the matrix $\mathbb{S}_i$ is equal to the Pauli matrix σ_z.

Example 5: Ising with Vacancies

We have $\sigma_i = +1, 0, -1$ so we have $n = 1$ and $n + 2 = 3$. We can write our vectors as:

$$+1 \to \left|S_i^{(+)}\right\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix} \quad \langle S_i^+| = (1^*, 0, 0)$$

$$0 \to \left|S_i^{(0)}\right\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix} \quad \langle S_i^0| = (0, 1^*, 0)$$

$$-1 \to \left|S_i^{(-)}\right\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix} \quad \langle S_i^-| = (0, 0, 1^*)$$

We then have

$$\mathbb{S}_i = \sum_{\sigma_i=\pm1,0} \left|S_i^{(\sigma_i)}\right\rangle \sigma_i \left\langle S_i^{(\sigma_i)}\right| = \begin{pmatrix}1 & 0 & 0\\0 & 0 & 0\\0 & 0 & -1\end{pmatrix}$$

Show at home that also in this case it is true that

$$\sum \left|S_i^{(\sigma_i)}\right\rangle \left\langle S_i^{(\sigma_i)}\right| = \mathbb{1}$$

Remark. By construction $\langle S_i|$ and $|S_i\rangle$ are the eigenvectors related to the eigenvalues $S_i = S^{(1)}, S^{(2)}, \ldots, S^{(n+2)}$.

Similarly. let $\langle t_i|$ and $|t_i\rangle$ be the eigenvectors related to the $(n+2)$ eigenvalues of the transfer matrix $\mathbb{T}$: $\{\lambda_+, \lambda_-, \lambda_1, \ldots, \lambda_n\}$, with $\lambda_+ > \lambda_- \geq \lambda_1 \geq \cdots \geq \lambda_n$.

Clearly,

$$\mathbb{T} = \mathbb{P}\mathbb{T}_D\mathbb{P}^{-1} = \sum_{i=1}^{n+2} |t_i\rangle \, \lambda_i \, \langle t_i| \tag{1.24}$$

Indeed

$$\mathbb{T}\,|t_j\rangle = \sum_{i=1}^{n+2} |t_i\rangle \, \lambda_i \, \langle t_i|t_j\rangle = \sum_{i=1}^{n+2} |t_i\rangle \, \lambda_i \delta_{ij} = \lambda_j \,|t_j\rangle \tag{1.25}$$

Given the set of λ described above, the N particle partition function is given by

$$Z_N = \lambda_+^N + \lambda_-^N + \sum_{i=1}^{n} \lambda_i^N \tag{1.26}$$

1.2.1 The free energy

Now, let us consider the free energy

$$F_N = -k_B T \log Z_N$$

In particular, we are interested in the limit of the bulk free energy. Looking at the thermodynamic limit $N \to \infty$ we have

$$f_b = \lim_{N \to \infty} \frac{1}{N} F_N = \lim_{N \to \infty} \frac{1}{N}(-k_B T) \log \left[\lambda_+^N + \lambda_-^N + \sum_{i=1}^n \lambda_i^N \right]$$

by factorizing λ_+, we obtain

$$f_b = \lim_{N \to \infty} \frac{-k_B T}{N} \log \left[\lambda_+^N \left(1 + \frac{\lambda_-^N}{\lambda_+^N} + \sum_{i=1}^n \left(\frac{\lambda_i}{\lambda_+} \right)^N \right) \right]$$

Since $\lambda_+ > \lambda_- > \lambda_1 > \ldots \lambda_n$,

$$\left(\frac{\lambda_-}{\lambda_+} \right)^N \xrightarrow{N \to \infty} 0, \quad \left(\frac{\lambda_i}{\lambda_+} \right)^N \xrightarrow{N \to \infty} 0 \quad \forall i$$

The result is

$$f_b = -k_B T \log \lambda_+ \tag{1.27}$$

The *limiting bulk free-energy depends only on the largest eigenvalue of the transfer matrix* $\mathbb{T}$! This is important since sometimes it is much simpler to compute only the largest eigenvalue than the whole spectrum of $\mathbb{T}$. Also an important theorem about λ_+ exists.

Theorem 1: Perron-Frobenius

Let $\mathbb{A}$ be a $n \times n$ matrix. If $\mathbb{A}$ is finite $(n < \infty)$ and $\mathbb{A}_{ij} > 0, \forall i, j, (\mathbb{A}_{ij} = \mathbb{A}_{ij}(\vec{x}))$, therefore its largest eigenvalue λ_+ has the following properties:

1. $\lambda_+ \in \mathbb{R}^+$

2. $\lambda_+ \neq$ from $\{\lambda_i\}_{i=1,\ldots,n-1}$. It means there is no degeneracy.

3. λ_+ is a analytic function of the parameters of $\mathbb{A}$.

Remark. Since in our case $\mathbb{A} \leftrightarrow \mathbb{T}$, λ_+ is related to f_b from the theorem. This means that f_b is an analytic function!

If the conditions of the Perron-Frobenius theorem are satisfied by $\mathbb{T}$, the model described by $\mathbb{T}$ cannot display a phase transition!

Remark. This is true for $T > 0$ since for $T = 0$ some $\mathbb{T}_{ij}$ can be either 0 or ∞ violating the hypothesis of the theorem.

Remark. If $\mathbb{T}$ has infinite dimension (see $d > 1$) the hypothesis of the theorem are not valid anymore and f_b can be non-analytic.

1.2.2 The correlation function

A second important quantity which is simply related to the eigenvalues of the transfer matrix is the correlation length. To calculate this, we need the spin-spin correlation function which serves as an example of how to obtain averages of products of spins using transfer matrices.

Let us consider the two point correlation between two spins at distance R to another. The fluctuation with respect to the average is:

$$\Gamma_R \equiv \langle S_1 S_R \rangle - \langle S_1 \rangle \langle S_R \rangle \tag{1.28}$$

Since

$$\Gamma_R \underset{R \to \infty}{\sim} \exp[-R/\xi]$$

we can define the correlation length ξ as

$$\xi^{-1} \equiv \lim_{R \to \infty} \left[-\frac{1}{R} \log |\langle S_1 S_R \rangle - \langle S_1 \rangle \langle S_R \rangle| \right] \tag{1.29}$$

Now, let us compute the terms $\langle S_1 S_R \rangle_N$ and $\langle S_1 \rangle_N \langle S_R \rangle_N$.

Term $\langle S_1 S_R \rangle_N$

From the definition of average we obtain

$$\langle S_1 S_R \rangle_N = \frac{1}{Z_N} \sum_{\{S\}} S_1 S_R \exp[-\beta \mathcal{H}_N] \tag{1.30}$$

Remark. The subscript N denotes that we are again considering a ring of N spins. Z_N is known from equation (1.26).

Writing this expression by using the transfer matrix formalism, one obtains

$$\langle S_1 S_R \rangle_N = \frac{1}{Z_N} \sum_{\{S\}} S_1 \langle S_1 | \mathbb{T} | S_2 \rangle \dots \langle S_{R-1} | \mathbb{T} | S_R \rangle S_R \langle S_R | \mathbb{T} | S_{R+1} \rangle \dots \langle S_N | \mathbb{T} | S_1 \rangle$$

Summing over the free spins,

$$\langle S_1 S_R \rangle_N = \frac{1}{Z_N} \sum_{S_1, S_R} S_1 \langle S_1 | \mathbb{T}^{R-1} | S_R \rangle S_R \langle S_R | \mathbb{T}^{N-R+1} | S_1 \rangle \tag{1.31}$$

On the other hand, since

$$\mathbb{T} = \sum_{i=1}^{n+2} |t_i\rangle \lambda_i \langle t_i|$$

we have

$$\mathbb{T}^{R-1} = \sum_{i=1}^{n+2} |t_i\rangle \lambda_i^{R-1} \langle t_i| \tag{1.32a}$$

$$\mathbb{T}^{N-R+1} = \sum_{i=1}^{n+2} |t_i\rangle \lambda_i^{N-R+1} \langle t_i| \tag{1.32b}$$

Hence,

$$\langle S_1 | \mathbb{T}^{R-1} | S_R \rangle = \sum_{i=1}^{n+2} \langle S_1 | t_i \rangle \lambda_i^{R-1} \langle t_i | S_R \rangle \tag{1.33a}$$

$$\langle S_R | \mathbb{T}^{N-R+1} | S_1 \rangle = \sum_{j=1}^{n+2} \langle S_R | t_j \rangle \lambda_j^{N-R+1} \langle t_j | S_1 \rangle \tag{1.33b}$$

and plugging these expressions in (1.31) one gets

$$\sum_{\{S\}} S_1 S_R e^{-\beta \mathcal{H}_N} = \sum_{S_1 S_R} S_1 \sum_{i=1}^{n+2} \langle S_1 | t_i \rangle \lambda_i^{R-1} \langle t_i | S_R \rangle S_R \sum_{j=1}^{n+2} \langle S_R | t_j \rangle \lambda_j^{N-R+1} \langle t_j | S_1 \rangle$$

Since the term $\langle t_j | S_1 \rangle$ is a scalar, it can be moved at the beginning of the product. Remembering the notations

$$\mathbb{S}_1 = \sum_{S_1} |S_1\rangle S_1 \langle S_1| \tag{1.34a}$$

$$\mathbb{S}_R = \sum_{S_R} |S_R\rangle S_R \langle S_R| \tag{1.34b}$$

one gets

$$\sum_{\{S\}} S_1 S_R e^{-\beta \mathcal{H}_N} = \sum_{ij} \langle t_j | \mathbb{S}_1 | t_i \rangle \lambda_i^{R-1} \langle t_i | \mathbb{S}_R | t_j \rangle \lambda_j^{N-R+1} \tag{1.35}$$

Since $\sum_k \lambda_k^N = Z_N$ for $k = +, -, 1, \ldots, n$, we have

$$\langle S_1 S_R \rangle_N = \frac{\sum_{ij} \langle t_j | \mathbb{S}_1 | t_i \rangle \lambda_i^{R-1} \langle t_i | \mathbb{S}_R | t_j \rangle \lambda_j^{N-R+1}}{\sum_{k=1}^n \lambda_k^N}$$

If we now multiply and divide by λ_+^N, we get

$$\langle S_1 S_R \rangle_N = \frac{\sum_{ij} \langle t_j | \mathbb{S}_1 | t_i \rangle (\lambda_i/\lambda_+)^{R-1} \langle t_i | \mathbb{S}_R | t_j \rangle (\lambda_j/\lambda_+)^{N-R+1}}{\sum_{k=1}^n (\lambda_k/\lambda_+)^N}$$

Remark. In the thermodynamic limit $N \to \infty$, only the terms with $j = +$ and $k = +$ will survive in the sum. Remind that R is fixed.

$$\langle S_1 S_R \rangle = \lim_{N \to \infty} \langle S_1 S_R \rangle_N = \sum_{i=\pm,1\ldots n} \left(\frac{\lambda_i}{\lambda_+} \right)^{R-1} \langle t_+ | \mathbb{S}_1 | t_i \rangle \langle t_i | \mathbb{S}_R | t_+ \rangle$$

Rembember that $\lambda_+ > \lambda_- \geq \lambda_1 \geq \cdots \geq \lambda_n$:

$$\langle S_1 S_R \rangle = \langle t_+ | \mathbb{S}_1 | t_+ \rangle \langle t_+ | \mathbb{S}_R | t_+ \rangle + \sum_{i \neq +}^n \left(\frac{\lambda_i}{\lambda_+} \right)^{R-1} \langle t_+ | \mathbb{S}_1 | t_i \rangle \langle t_i | \mathbb{S}_R | t_+ \rangle$$

Since one can prove

$$\lim_{N \to \infty} \langle S_R \rangle_1 = \langle t_+ | \mathbb{S}_1 | t_+ \rangle, \quad \lim_{N \to \infty} \langle S_R \rangle_N = \langle t_+ | \mathbb{S}_R | t_+ \rangle \tag{1.36}$$

we obtain

$$\langle S_1 S_R \rangle = \langle S_1 \rangle \langle S_R \rangle + \sum_{i \neq +} \left(\frac{\lambda_i}{\lambda_+} \right)^{R-1} \langle t_+ | \mathbb{S}_1 | t_i \rangle \langle t_i | \mathbb{S}_R | t_+ \rangle \tag{1.37}$$

Example 6: Show relation (1.36)

Let us prove (1.36) by a method analogous to that followed above.

$$\langle S_1 \rangle_N = \frac{1}{Z} \sum_{\{S\}} S_1 e^{-\beta \mathcal{H}_N} = \frac{1}{Z} \sum_{S_1} S_1 \langle S_1 | \mathbb{T}^N | S_1 \rangle = \frac{1}{Z} \sum_{S_1} S_1 \sum_i \langle S_1 | t_i \rangle \lambda_i^N \langle t_i | S_1 \rangle$$

$$= \frac{1}{Z} \sum_i \lambda_i^N \langle t_i | \mathbb{S}_1 | t_i \rangle = \frac{\sum_i (\lambda_i / \lambda_+)^N \langle t_i | \mathbb{S}_1 | t_i \rangle}{\sum_{k=1}^n (\lambda_k / \lambda_+)^N}$$

Taking the limit $N \to \infty$:

$$\langle S_1 \rangle = \lim_{N \to \infty} \langle S_1 \rangle_N = \langle t_+ | \mathbb{S}_1 | t_+ \rangle$$

The correlation function follows immediately from (1.37),

$$\Gamma_R = \langle S_1 S_R \rangle - \langle S_1 \rangle \langle S_R \rangle = \sum_{i \neq +}^n \left(\frac{\lambda_i}{\lambda_+} \right)^{R-1} \langle t_+ | \mathbb{S}_1 | t_i \rangle \langle t_i | \mathbb{S}_R | t_+ \rangle \tag{1.38}$$

Remark. Γ_R depends only on the eigenvalues and eigenvectors of the transfer matrix $\mathbb{T}$ and by the values of the spins S_1 and S_R.

A much simpler formula is obtained for the correlation length (1.29). Taking the limit $R \to \infty$ the ratio (λ_- / λ_+) dominates the sum and hence

$$\xi^{-1} = \lim_{R \to \infty} \left\{ -\frac{1}{R-1} \log |\langle S_1 S_R \rangle - \langle S_1 \rangle \langle S_R \rangle| \right\}$$

$$= \lim_{R \to \infty} \left\{ -\frac{1}{R-1} \log \left[\left(\frac{\lambda_-}{\lambda_+} \right)^{R-1} \langle t_+ | \mathbb{S}_1 | t_- \rangle \langle t_- | \mathbb{S}_R | t_+ \rangle \right] \right\}$$

$$= -\log \left[\left(\frac{\lambda_-}{\lambda_+} \right) \right] - \lim_{R \to \infty} \frac{1}{R-1} \log \langle t_+ | \mathbb{S}_1 | t_- \rangle \langle t_- | \mathbb{S}_R | t_+ \rangle$$

$$= -\log \left(\frac{\lambda_-}{\lambda_+} \right)$$

The important result is

$$\xi^{-1} = -\log \left(\frac{\lambda_-}{\lambda_+} \right) \tag{1.39}$$

It means that the *correlation length does depend only on the ratio between the two largest eigenvalues of the transfer matrix* $\mathbb{T}$.

1.2.3 Results for the *1-dim* Ising model

Let us now return to the example of the nearest neighbour Ising model in a magnetic field, to obtain explicit results for the bulk free energy f_b, the correlation function Γ and the correlation length ξ.

Recall that the transfer matrix of such a system is given by

$$\mathbb{T} = \begin{pmatrix} \exp(K+h) & \exp(-K) \\ \exp(-K) & \exp(K-h) \end{pmatrix}$$

Now, let us calculate the eigenvalues:

$$|\mathbb{T} - \lambda \mathbb{1}| = (e^{K+h} - \lambda)(e^{K-h} - \lambda) - e^{-2K} = 0$$

The two solutions are

$$\lambda_\pm = e^K \cosh(h) \pm \sqrt{e^{2K} \sinh^2(h) + e^{-2K}} \tag{1.40}$$

The free energy

The free energy is

$$f_b \equiv \lim_{N\to\infty} \frac{-k_B T}{N} \log Z_N(K, h)$$

$$= -k_B T \lim_{N\to\infty} \frac{1}{N} \log \left[\lambda_+^N \left(1 + \left(\frac{\lambda_-}{\lambda_+} \right)^N \right) \right]$$

$$= -k_B T \log \lambda_+$$

and inserting the explicit expression of λ_+ for the Ising model, we get

$$f_b = -k_B T \log \left(e^K \cosh h + \sqrt{e^{2K} \sinh^2(h) + e^{-2K}} \right)$$

$$= -K k_B T - k_B T \log \left(\cosh(h) + \sqrt{\sinh^2(h) + e^{-4K}} \right)$$

(1.41)

Remark. Remember that $K \equiv \beta J, h \equiv \beta H$.

Exercise 1

Check that if $h = 0$ we get back the expression found previously with the iterative method. What is the importance of boundary conditions?

Solution. If $h = 0$, we obtain

$$f_b = -K k_B T - k_B T \log \left(1 + \frac{1}{e^{2K}} \right) = -k_B T \left(\log e^K + \log(1 + e^{-2K}) \right)$$

$$= -k_B T \log \left(e^K + e^{-K} \right) = -k_B T \log \left(2 \frac{e^K + e^{-K}}{2} \right)$$

$$= -k_B T \log(2 \cosh K) = -k_B T \log \left(2 \cosh \left(\frac{J}{k_B T} \right) \right)$$

The choice of boundary conditions becomes irrelevant in the thermodynamic limit, $N \to \infty$.

Let us now consider the limits $T \to 0$ and $T \to \infty$ by keeping H fixed and J fixed.

- Case: $T \to 0 \Rightarrow K \to \infty, h \to \infty$.

$$e^{-4K} \overset{K\to\infty}{\longrightarrow} 0$$

$$\sqrt{\sinh^2 h} \overset{h\to\infty}{\sim} \sinh(h)$$

We have

$$\cosh h + \sinh h \sim \frac{2e^h}{2} \simeq e^h$$

and

$$f \overset{\substack{h\to\infty \\ K\to\infty}}{\sim} -K k_B T - k_B T \log e^h \sim -J - H \quad const$$

(1.43)

Therefore, as $T \to 0^+$, f goes to a constant that depends on J and H.

- Case: $T \to \infty \Rightarrow K \to 0, h \to 0$. In this case we suppose also that H and J (fixed) are also finite.

$$e^{-4K} \simeq 1$$

$$\sqrt{\sinh^2 h + e^{-4K}} \sim \sqrt{1}$$

Since $\cosh h \overset{h\to 0}{\sim} 1$:

$$f_B \sim -Kk_BT - k_BT\log(1+1) \sim -J - k_BT\ln 2 \tag{1.45}$$

Therefore, as $T \to \infty$, the free energy goes linearly to zero, as in Figure 1.4.
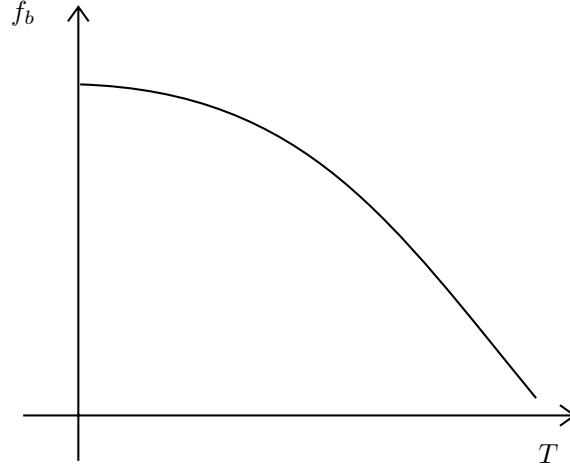
WHYYYYYYYYYY

Figure 1.4: Plot of the free energy f_b in function of the temperature T. For $T \to 0$, the free energy becomes constant, while for $T \to \infty$ it goes linearly to zero.

The magnetization

This can be obtained by differentiating the negative of the free energy with respect to the magnetic field H (or by using equation (1.36)):

$$m = -\frac{\partial f_b}{\partial H} = -\frac{1}{k_BT}\frac{\partial f_b}{\partial h} = \frac{\partial}{\partial h}\left[\log\left(\cosh(h) + \sqrt{\sinh^2(h) + e^{-4K}}\right)\right]$$

The result is

$$m = \frac{\sinh h + \frac{\sinh h \cosh h}{\sqrt{\sinh^2 h + e^{-4K}}}}{\cosh h + \sqrt{\sinh^2 h + e^{-4K}}} = \frac{\sinh h}{\sqrt{\sinh^2 h + e^{-4K}}} \tag{1.46}$$

- Case: $T > 0$ fixed, $H \to 0 \Rightarrow h \to 0$.

$$\sinh h \sim h \sim 0,$$
$$\cosh h \sim 1$$

In zero field $h \to 0$, we have $m \to 0$ for all $T > 0$. It means that there is no spontaneous magnetization!

The magnetic susceptibility

$$\chi_T \equiv \frac{\partial m}{\partial H} = \frac{1}{k_BT}\frac{\partial m}{\partial h} \tag{1.48}$$

If we consider the case $h \ll 1$, it is convenient first expand the (1.46) for $h \to 0$ and take the derivative to get χ_T.

Since $\sinh(h) \sim h + h^3$ and $\cosh(h) \sim 1 + h^2$, we have

$$m \stackrel{h \ll 1}{\sim} \frac{h(1 + e^{2K})}{1 + e^{-2K}}$$

If we now derive with respect to h

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

In the case of $h \ll 1$:

$$\chi_T = \frac{1}{k_B T}\frac{\partial m}{\partial h} \stackrel{h \ll 1}{\approx} \frac{1}{k_B T}\frac{(1 + e^{2K})}{(1 + e^{-2K})}$$

- Case: $T \to \infty \Rightarrow K \to 0$.

$$e^{2K} \simeq e^{-2K} \simeq 1$$

The *Curie's Law* for paramagnetic systems is:

$$\boxed{\chi_T \sim \frac{1}{k_B T}} \tag{1.49}$$

- Case: $T \to 0 \Rightarrow K \to \infty$.

$$e^{-2K} \simeq 0$$

$$\boxed{\chi_T \sim \frac{1}{k_B T}e^{2K} \sim \frac{1}{k_B T}e^{2J/k_B T}} \tag{1.50}$$

The correlation length

$$\xi^{-1} = -\log\left(\frac{\lambda_-}{\lambda_+}\right) = -\log\left[\frac{\cosh h - \sqrt{\sinh^2 h + e^{-4K}}}{\cosh h + \sqrt{\sinh^2 h + e^{-4K}}}\right] \tag{1.51}$$

For $h = 0$, we have $\cosh h \to 1, \sinh h \to 0$:

$$\xi^{-1} = -\log\left[\frac{1 - e^{-2K}}{1 + e^{-2K}}\right] = -\log\left[\frac{1}{\coth K}\right]$$

Therefore:

$$\xi = \frac{1}{\log(\coth K)}, = -\frac{1}{\log(\tanh K)}, \quad \text{for } h = 0 \tag{1.52}$$

- Case: $T \to 0 \Rightarrow K \to \infty$.

$$\coth K = \frac{e^K + e^{-K}}{e^K - e^{-K}} \stackrel{K \to \infty}{\simeq} 1 + 2e^{-2K} + \ldots \stackrel{K \to \infty}{\longrightarrow} 1$$

It implies

$$\xi \stackrel{K \gg 1}{\sim} \frac{1}{\ln(1 + 2e^{-2K})} \sim \frac{e^{2K}}{2}$$

Hence,

$$\xi \stackrel{T \to 0}{\sim} \frac{1}{2}e^{J/k_B T} \tag{1.53}$$

It diverges exponentially $\xi \to \infty$ as $T \to 0$.

- Case: $T \to \infty \Rightarrow K \to 0$.

$$\coth K = \frac{e^K + e^{-K}}{e^K - e^{-K}} \overset{K \to 0}{\simeq} \frac{1 + K + \frac{K^2}{2} + 1 - K + \frac{K^2}{2}}{1 + K + \frac{K^2}{2} - 1 + K - \frac{K^2}{2}} \sim \frac{2 + 2\frac{K^2}{2}}{2K} \sim \frac{1 + K^2}{K}$$

$$\xi^{-1} = \log\left(\coth K\right) \overset{K \to 0}{\sim} \ln \frac{1}{K} + \ln\left(1 + K^2\right) \sim +\infty$$

Therefore

$$\xi \overset{K \to 0}{\longrightarrow} 0$$

More precisely,

$$\xi \overset{K \to 0}{\sim} \frac{1}{\ln\left(1/K\right) + \ln\left(1 + K^2\right)} \overset{K \to 0}{\sim} -\frac{1}{\ln K} \tag{1.54}$$

1.3   Fluctuation-response for Ising-like models

We have an Hamiltonian like:

$$\mathcal{H}_N = -J \sum_{\langle ij \rangle} s_i s_j - \sum_i H_i s_i$$

And a partition function like this:

$$Z_N = \underset{\{s\}}{\mathrm{Tr}} \exp(-\beta \mathcal{H}_N)$$

If we compute the magnetisation we get:

$$M_i = \langle s_i \rangle_N = \frac{1}{\beta Z_N} \frac{\partial Z_N}{\partial H_i} = \frac{1}{\beta} \frac{\partial \ln Z_N}{\partial H_i}$$

So if we write the correlation function in this case is:

$$\langle s_i s_j \rangle_N = \frac{1}{\beta^2} \frac{1}{Z_N} \frac{\partial^2 Z_N}{\partial H_i \partial H_j}$$

The connected correlation function then is:

$$G_c(i,j) = \langle s_i s_j \rangle_c = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle = \frac{1}{\beta^2} \frac{\partial^2 \ln Z_N}{\partial H_i \partial H_j}$$

Remark. In general, differentiating Z_N to order k gives the k-point correlation function. So our partition function is the generating function of the correlations and the free-energy is the generating function of the connected correlations.

Setting $H_i = 0$ AFTER having taken the derivative gives:

$$G_c(i,j)\bigg|_{H_i=0} = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle = \frac{1}{\beta^2} \frac{\partial^2 \ln Z_n}{\partial H_i \partial H_j}\bigg|_{H_i=0}$$

That gives:

$$\frac{\partial M_i}{\partial H_j} = \frac{1}{\beta} \frac{\partial^2 \ln Z_N}{\partial H_i H_j} = \beta G_c(i,j)$$

This is the first form of the **Fluctuation-Response Relation**.

Spin Susceptibility

χ_N in a uniform magnetic field $H_i = H_i(H) = H$

$$\frac{\partial M_i}{\partial H} = \sum_j \frac{\partial M_i}{\partial H_j}\frac{\partial H_j}{\partial H} = \beta \sum_j G_c(i,j)$$

So

$$\chi = \frac{\partial M}{\partial H} = \beta \sum_j G_c(i,j) = \frac{\beta}{N}\sum_{i,j} G_c(i,j)$$

Remark. $M = \langle s_i \rangle$ is independent on i (it's translation invariant) so it is $\sum_j G_c(i,j)$ independent of i

1.4 Classical Heisenberg model for *d=1*

The Quantum Heisenberg Model is defined by the Hamiltonian Operator:

$$\mathcal{H} = -J\sum_{\langle ij \rangle} \vec{s}_i \cdot \vec{S}_j = -J\sum_{ij}(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z)$$

Since the different component S_x, S_y, S_z do not commute the full problem is not solvable analytically. On the other hand one can look at the associated model in which $|\vec{S}|$ goes to infinity and in the simples case of $d = 1$.

1.4.1 Classical Heisenberg Chain

Let us consider the Hamiltonian

$$\mathcal{H} = -J\sum_{i=1}^N \vec{S}_i \cdot \vec{S}_{i+1}$$

where the spins have infinite magnitude i.e. $|\vec{S}| \to \infty$. We introduce the unit vector operator:

$$s_i = \frac{\vec{S}_i}{|\vec{S}|}$$

It's commutation rules are:

$$[s_i^x, s_i^y] = i\frac{s_i^z}{S}$$
$$[s_i^y, s_i^z] = i\frac{s_i^x}{S}$$
$$[s_i^z, s_i^x] = i\frac{s_i^y}{S}$$

Where $S = |\vec{S}|$. In the limit $S \to \infty$ the components commute and the hamiltonian form can be written in classical form:

$$\mathcal{H} = -J\sum_i^N \vec{s}_i \cdot \vec{s}_{i+1}$$

Where $J = J_s S^2$. Note that now the spins are unit length vectors, so they are continuous values on the unit sphere. Let us consider periodic boundary conditions $s_{N+1} = s_1$ and $h = 0$. We can rewrite the Hamiltonian as:

$$-\beta\mathcal{H}(\{\vec{s}\}) = K\sum_{i=1}^N \vec{s}_i \cdot \vec{s}_{i+1}$$

The model satisfies $O(3)$ symmetry. We can then write the partition function:

$$Z_N = \sum_{\{\vec{s}\}} \exp[-\beta\mathcal{H}(\{\vec{s}\})] = \int \frac{d\Omega_1}{4\pi} \int \frac{d\Omega_2}{4\pi} \cdots \int \frac{d\Omega_N}{4\pi} \prod_{i=1}^{N} \exp(K\vec{s}_i \cdot \vec{s}_{i+1})$$

where the $d\Omega_i$ is the element of the solid angle for the unit vector $\vec{s}_i$. To compute Z_N one can either compute the integrals above (in spherical coordinates) or by using the Transfer Matrix Formalism

Transfer Matrix Formalism

In the transfer matrix formalism[2]:

$$Z_N(K) = \sum_{\{\vec{S}\}} e^{-\beta\mathcal{H}} = \sum_{\{\vec{S}\}} e^{K\sum_{i=1}^{N}\vec{S}_i\cdot\vec{S}_{i+1}} = \text{Tr}\left(\mathbb{T}^N\right) \tag{1.55}$$

where

$$\left\langle \vec{S}_i \middle| \mathbb{T} \middle| \vec{S}_{i+1} \right\rangle = e^{K\vec{S}_i\cdot\vec{S}_{i+1}}$$

Similarly to the Ising case,

$$\mathbb{T} = \sum_i |t_i\rangle \lambda_i \langle t_i|$$

and

$$\mathbb{T}_D = \mathbb{P}^{-1}\mathbb{T}\mathbb{P}$$

The problem is computing the eigenvalues λ_i of $\mathbb{T}$.

Formally, we should find

$$\exp\left[K\vec{S}_1 \cdot \vec{S}_2\right] = \left\langle \vec{S}_1 \middle| \mathbb{T} \middle| \vec{S}_2 \right\rangle = \sum_{i\in\text{eigenvalues}} \lambda_i \left\langle \vec{S}_1 \middle| t_i \right\rangle \left\langle t_i \middle| \vec{S}_2 \right\rangle = \sum_i \lambda_i f_i(\vec{S}_1)f^*(\vec{S}_2)$$

Remark. We start by noticing that the term $e^{K\vec{S}_1\cdot\vec{S}_2}$ is similar to the plane wave $e^{i\vec{q}\cdot\vec{r}}$, that in scattering problems is usually expanded in spherical coordinates. Plane wave can be expanded as a sum of spherical harmonics as

$$e^{i\vec{q}\cdot\vec{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (i)^l j_l(qr) Y_{lm}^*(\hat{\mathbf{q}}) Y_{lm}(\hat{\mathbf{r}})$$

where

$$j_l(qr) = -\frac{(i)^l}{2} \int_0^{\pi} \sin(\theta) e^{iqr\cos(\theta)} P_l(\cos(\theta))\,d\theta$$

are the *spherical Bessel functions*, while the $P_l(\cos(\theta))$ are the *Legendre polynomial* of order l.

From a formal comparison we have

$$\vec{S}_1 \leftrightarrow \hat{\mathbf{S}}_1, \qquad \begin{cases} i\vec{q} \cdot \vec{r} = iqr \\ K\vec{S}_1 \cdot \vec{S}_2 = K\left|\vec{S}_1\right|\left|\vec{S}_2\right| = K \end{cases} \tag{1.56}$$

multiplying by $(-i)$ we can write

$$qr = -iK\left|\vec{S}_1\right|\left|\vec{S}_2\right| = -iK \tag{1.57}$$

---

[2]Here we use $\vec{\mathbf{S}}$ but is the same as before

In our case, we have $\hat{\mathbf{q}} = \vec{\mathbf{S}}_1, \hat{\mathbf{r}} = \vec{\mathbf{S}}_2$. Hence,

$$e^{K\vec{\mathbf{S}}_1 \cdot \vec{\mathbf{S}}_2} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (i)^l j_l(-iK) Y_{lm}^*(\vec{\mathbf{S}}_1) Y_{lm}(\vec{\mathbf{S}}_2) = \sum_i \lambda_i f_i(\vec{\mathbf{S}}_1) f^*(\vec{\mathbf{S}}_2) \tag{1.58}$$

where

$$\lambda_i = \lambda_{lm}(K) = 4\pi(i)^l j_l(-iK) \tag{1.59}$$

Remark. Note that λ_i does not depend on m!

If $l = 0$, the largest eigenvalue is:

$$\lambda_+ = \lambda_0(K) = 4\pi j_0(-iK) = 4\pi \frac{\sinh K}{K}$$

and

$$\lambda_- = \lambda_1(K) = 4\pi i j_1(-iK) = 4\pi \left[\frac{\cosh K}{K} - \frac{\sinh K}{K^2} \right]$$

Exercise 2

Given the largest eigenvalue λ_+,

$$\lambda_+ = 4\pi \frac{\sinh K}{K}$$

find the bulk free energy density of the model and discuss its behaviour in the limits of low $(T \to 0)$ and high $(T \to \infty)$ temperatures.

Solution. The bulk free energy is

$$f_b = -k_B T \log \lambda_+ = -k_B T \log \left(4\pi \frac{\sinh K}{K} \right)$$

Remind that $K \equiv \beta J$ and consider the limits

- Case: $T \to 0 \Rightarrow K \to \infty$.

$$f_b = -\frac{J}{K} \log \left(4\pi \frac{\sinh K}{K} \right) \overset{K \to \infty}{\sim} \frac{J}{K} \log \left(\frac{K}{\sinh K} \right)$$

Hence,

$$f_b \overset{K \to \infty}{\sim} 0$$

- Case: $T \to \infty \Rightarrow K \to 0$.

$$\sinh K \overset{K \to 0}{\sim} K$$

$$\Rightarrow f_b = -k_B T \log \left(4\pi \frac{K}{K} \right) = -k_B T \log(4\pi)$$

In this case the free energy f_b goes linearly with respect to the temperature.

How can we violate the hypothesis of the Perron-Frobenius theorem hoping to find a phase transition also in a $d = 1$ model? One of the hypothesis of the Perron-Frobenius theorem is the one in which $A_{ij} > 0$ for all i, j. Hence, one possibility is to build a model in which its transfer matrix has same A_{ij} that are equal to zero also for $T \neq 0$.

1.5   Zipper model

The Zipper model is an unusually simple and interesting member of the class of one dimensional systems which exhibit a phase transition. It is a model introduced by Kittel [**?**] to describe

oligomers undergoing *denaturation transition*. Simplest model of DNA thermal denaturation transition (no bubbles). Better model for the denaturation of short oligomers.

The hypothesis are: the binding energy between two bases located at the end of the molecule is smaller than the one for pairs away from the ends. The unbinding starts and develops from the ends as a *zipper*.
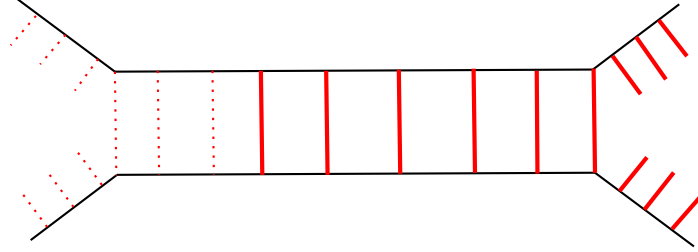

Figure 1.5: Sequential unzipping from the ends.
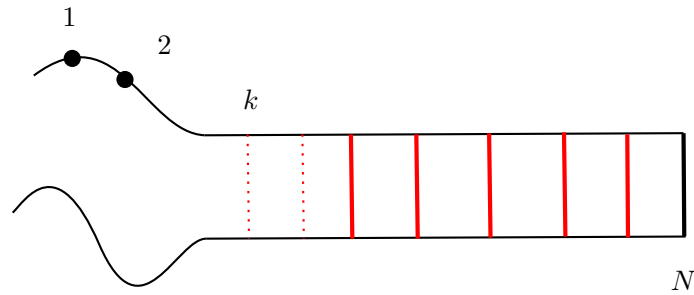

Figure 1.6: Open and closed links in a single-ended zipper.

In this denaturation transition we do not allow bubbles. Let us consider first the single-ended zipper, i.e. a molecular zipper of N parallel links that can be opened only from one end as in Figure 1.6. The single-ended zipper is simpler than any related problem which has been treated, and it offers a good way to introduce a biophysics example into a course of statistical mechanics.

If the first k bonds (or links) are open (unbounded pairs) the energy to open the $k+1$ is ε_0. Note that if at least one of the previous k bond is closed the energy needed to open the $k + 1$ band is infinite! We specify further that the last link, $k = N$, cannot be opened; this minor features serves only to distinguish one end from the other, and we shall say that the zipper is open when $N - 1$ links are open.

We suppose that there are G orientations which each open link can assume: that is, the open state of a link is G-fold degenerate, corresponding to the rotational freedom of a link. Hence, once a bond is open it can orient itself in G different ways. In other words, there is an entropy

$$S_0 = k_B \log G \tag{1.60}$$

associated to each open band. In the problem of DNA the empirical value of G may be of the order of 10^4.

Partition function

Let us suppose that the energy required to open the first k links is ε_0. If k links are open, the degeneracy is G^k, and the contribution of this configuration to the partition function is

$$G^k e^{-k\varepsilon_0/k_B T}$$

By summing over the possible values of k, the partition function is

$$Z_N(T, G, \varepsilon_0) = \sum_{k=0}^{N-1} G^k e^{-k\varepsilon_0/k_B T} = \sum_{k=0}^{N-1} e^{k(S_0 T - \varepsilon_0)/k_B T} \tag{1.61}$$

Let us call

$$\chi \equiv G e^{-\varepsilon_0/k_B T} \tag{1.62}$$

and simplify the previous expression

$$Z_N = \sum_{k=0}^{N-1} \chi^k = \frac{1 - \chi^N}{1 - \chi} \tag{1.63}$$

We see immediately there is a single pole singularity.

The free energy is

$$F_N = -k_B T \ln Z_N = -k_B T \ln \left[\frac{1 - \chi^N}{1 - \chi} \right] \tag{1.64}$$

We can now compute some observables of interest. The correct procedure is to evaluate thermodynamic quantities for finite N and then to examine the limit $N \to \infty$.

Calculate average number of open links

The thermodynamic average number of open links is

$$\langle k \rangle_N \equiv \frac{\sum_{k=0}^{N-1} k\chi^k}{\sum_{k=0}^{N-1} \chi^k} = \chi \frac{\mathrm{d}}{\mathrm{d}\chi} \ln Z_N = \frac{N\chi^N}{\chi^N - 1} - \frac{\chi}{\chi - 1} \tag{1.65}$$

The function is plotted in Figure 1.7. We examine the behaviour of $\langle k \rangle_N$ in the vicinity of the point $\chi_c = 1$ for which the denominators are equal to zero (pole).

Remark. In this model, we consider the average number of open links instead of the magnetization.
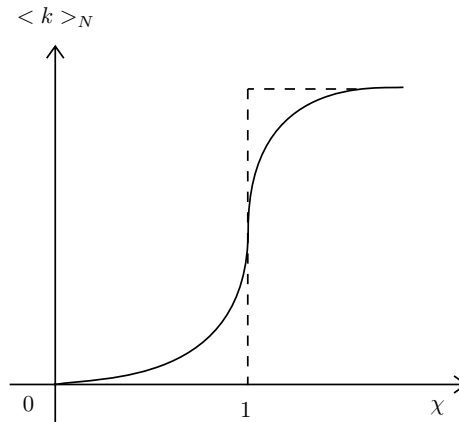

Figure 1.7: Thermodynamic average number of open links in a single-ended zipper of N links.

In order to analyze what happens near 1, we expand $\chi \equiv 1 + \varepsilon$:

$$\log Z_N(\chi) = \log \left[\frac{1 - (1+\varepsilon)^N}{1 - (1+\varepsilon)} \right]$$

$$= \log \left[\frac{1 - (1 + \varepsilon N + \frac{N(N-1)}{2!}\varepsilon^2 + \frac{N(N-1)(N-2)}{3!}\varepsilon^3 + O(\varepsilon^4))}{\varepsilon} \right]$$

$$= \log \left[N + \frac{N(N-1)}{2}\varepsilon + \frac{N(N-1)(N-2)}{6}\varepsilon^2 + \dots \right]$$

$$= \log N + \log \left[1 + \frac{N-1}{2}\varepsilon + \frac{(N-1)(N-2)}{6}\varepsilon^2 \right] \qquad (1.66)$$

$$= \log N + \log \left[1 + \frac{N\varepsilon}{2} + \frac{N^2\varepsilon^2}{6} + \dots \right]$$

$$= \log N + \left(\frac{N\varepsilon}{2} + \frac{N^2\varepsilon^2}{6} + \dots \right) + \frac{1}{2} \left(\frac{N\varepsilon}{2} + \frac{N^2\varepsilon^2}{6} + \dots \right)^2 + \dots$$

$$= \log N + \frac{N\varepsilon}{2} + \frac{N^2\varepsilon^2}{24} + \dots$$

By doing the same for $\langle k \rangle_N = \frac{N\chi^N}{\chi^N - 1} - \frac{\chi}{\chi - 1}$, one gets

$$\langle k \rangle_N = \frac{N}{2} \left(1 + \frac{N\varepsilon}{6} - \frac{N^3\varepsilon^3}{360} + \dots \right) \qquad (1.67)$$

this is true for $N \gg 1, \varepsilon \ll 1$.

At the transition point $\chi_c = 1$, where $\varepsilon = 0$:

$$\langle k \rangle_N \simeq \frac{N}{2}$$

We can define the variation (slope per site) as a response function (the derivative with respect to the parameter):

$$\frac{1}{N} \frac{\mathrm{d}\langle k \rangle}{\mathrm{d}\varepsilon} \simeq \frac{N}{12} - \frac{N^3\varepsilon^3}{240} + \dots \qquad (1.68)$$

is a maximum at $\varepsilon = 0$, and the slope at the transition point becomes infinite as $N \to \infty$ (linearly). The response function diverges linearly to N, this is a good signal that we have a transition.

Transition temperature

The temperature T_c corresponding to the pole $\chi_c = 1$ is given by

$$Ge^{-\varepsilon_0/k_B T_c} = 1$$

Hence,

$$T_c = \frac{\varepsilon_0}{k_B \log G} \qquad (1.69)$$

Note that as $G \to 1$, $T_c \to 0$. For $G = 1$ there is no solution at a finite temperature and hence the model does not display a phase transition for any finite T! This is telling you that if $G = 1$ what is important it is the energy, you have no entropy as disorder. At that point everything can happen.

There is a finite transition temperature if $G > 1$. One might perhaps argue that the model is now not strictly one-dimensional, for the degeneracy G arises from the rotational freedom of an open link.

Remark. Despite the model is 1-dim, for $G > 1$ there is a phase transition. This is due to two contributions:

1. Existence of forbidden configuration (infinite energy). It is a necessary condition, but not sufficient, for a phase transition in $d = 1$ with finite range interactions.

2. A further requirement may be that the degeneracy of the excited state (G) of a structural unit must be higher than the degeneracy of the ground state[3].

Unwinding from both ends

When the zipper is allowed to unwind from both ends, there are $k + 1$ ways in which a total of k links may be opened, so that the partition function for a double-ended zipper of N links is

$$Z_N(T, G, \varepsilon_0) = \sum_{k=0}^{N-1} (k+1) G^k e^{-k\varepsilon_0/k_B T} \tag{1.70}$$

and to this should be added a term for the state of N open links. This terminal term for a simple zipper is $G^N \exp(-N\varepsilon_0/k_B T)$.

1.5.1   Transfer matrix method for the Zipper model

The idea is: we want to map the Zipper model to an Ising model. The spin like model consists on associating to each bond a spin such that $S_i = 0$ if the i-esim bond is *closed* , while $S_i = 1, \ldots, G$ if the i-esim bond is *open* with G possible orientations. Therefore,

- Case: $S_i \neq 0$ open. We have two subcases:

  - S_{i-1} open: $S_{i-1} \neq 0 \Rightarrow E(S_i \neq 0 | S_{i-1} \neq 0) = \varepsilon_0$.
  - S_{i-1} closed: $S_{i-1} = 0 \Rightarrow E(S_i \neq 0 | S_{i-1} = 0) = \varepsilon_0 + V_0$

- Case: $S_i = 0$ closed. We have $E(S_i = 0) = 0$ irrespective of S_{i-1}.

Hence, considering all these cases, the energy results

$$E(S_i, S_{i-1}) = (\varepsilon_0 + V_0 \delta_{S_{i-1},0})(1 - \delta_{S_i,0}) \tag{1.71}$$

The boundary condition is $S_N = 0$ (always closed). The full Hamiltonian of the model can be written as (it could be also a function of delta, but it is not a problem):

$$\mathcal{H}_N = \varepsilon_0(1 - \delta_{S_1,0}) + \sum_{i=2}^{N-1} (\varepsilon_0 + V_0 \delta_{S_{i-1},0})(1 - \delta_{S_i,0}) \tag{1.72}$$

The Kittel's version is obtained by assuming $V_0 = \infty$.

The partition function is

$$Z_N = \sum_{\{S\}} \exp(-\beta \mathcal{H}_N)$$

In order to implement the transfer matrix formalism we rewrite Z_N as follows

$$Z_N = \sum_{\{S\}} e^{-\beta\varepsilon_0(1-\delta_{S_1,0})} \prod_{i=1}^{N-2} e^{-\beta\varepsilon_0(1-\delta_{S_{i+1},0})} \left[1 + (e^{-\beta V_0} - 1)\delta_{S_i,0}(1 - \delta_{S_{i+1},0})\right] \tag{1.73}$$

Let us consider the Kittel model, the condition $V_0 = \infty$ implies $\exp(-\beta V_0) = 0$. Hence, we can define the transfer matrix as

$$\mathbb{T} = \{\langle S| \mathbb{T} |S'\rangle \equiv t_{S,S'}\} \tag{1.74}$$

---

[3]In the mean-field approximation no transition can occur if the degeneracy of the ground state is higher than that of the excited state.

where

$$t_{S,S'} = e^{-\beta\varepsilon_0(1-\delta_{S',0})}[1 - \delta_{S,0}(1 - \delta_{S',0})] \tag{1.75}$$

or in matrix form

$$\mathbb{T} = \begin{bmatrix} 1 & 0 & \dots\dots 0 \\ 1 & a & \dots\dots a \\ \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots \\ 1 & a & \dots\dots a \end{bmatrix}, \qquad \text{with } a \equiv e^{-\beta\varepsilon_0}$$

The first think to notice is that the constraint that the bond S_{i+1} cannot be open if bond S_i is closed ($S_i = 0$) yields the null entries in the first row of $\mathbb{T}$. This violates the hypothesis of the Perron-Frobenius theorem!

The matrix $\mathbb{T}$ has three different eigenvalues

$$\lambda_1 = Ga, \quad \lambda_2 = 1, \quad \lambda_3 = 0 \tag{1.76}$$

The partition function can be written as

$$Z_N = (1, a, \dots, a)\mathbb{T}^{N-2} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \tag{1.77}$$

Moreover, we have

$$\lambda_1 \to \vec{\mathbf{v}}_1 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 1 \end{pmatrix}, \qquad \lambda_2 \to \vec{\mathbf{v}}_2 = \begin{pmatrix} 1 - Ga \\ 1 \\ \vdots \\ 1 \end{pmatrix}$$

and we can then write

$$\begin{pmatrix} 1 \\ a \\ \vdots \\ a \end{pmatrix} = \frac{a(1 - Ga) - 1}{1 - Ga}\vec{\mathbf{v}}_1 + \frac{1}{1 - Ga}\vec{\mathbf{v}}_2$$

$$\begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} = \frac{-Ga}{1 - Ga}\vec{\mathbf{v}}_1 + \frac{1}{1 - Ga}\vec{\mathbf{v}}_2$$

Therefore,

$$Z_N = \frac{1 - (Ga)^N}{1 - Ga} = \frac{1 - (Ge^{-\beta\varepsilon_0})^N}{1 - Ge^{-\beta\varepsilon_0}} = \frac{1}{1 - Ge^{-\beta\varepsilon_0}}(-\lambda_1^N + \lambda_2^N) \tag{1.79}$$

Since in the thermodynamic limit only the contribution of the largest eigenvalue matters for f_b we have

$$f_b = -k_B T \ln \max(\lambda_1, \lambda_2)$$

Remark. Given that the λ_1 and λ_2 are positive, analytic function of T ($\lambda_1 = Ga, \lambda_2 = 1$). In order to have a phase transition (i.e. non analiticity of f_b) the two eigenvalues must cross for a given value of T. It is true if and only if:

$$Ga_c = 1 \Leftrightarrow Ge^{-\beta_c\varepsilon_0} = 1 \Leftrightarrow T_c = \frac{\varepsilon_0}{k_B \ln G} \tag{1.80}$$

that agree with previous calculation (see Eq.(1.69)).

1.6   Transfer matrix for $2 - dim$ Ising

The two-dimensional Ising model for a system of interacting spins on a square lattice is one of the very few nontrivial many-body problems that is exactly soluble and shows a phase transition [?]. The exact solution in the absence of an external magnetic field ($H = 0$) was first given almost eighty years ago in a famous paper by Onsager [?], using the theory of Lie algebras. In particular, from Onsager's solution we can see that already in two dimensions an Ising model can exhibit phase transitions, showing a non null spontaneous magnetization for temperatures low enough.

Let us therefore consider a two-dimensional Ising model, defined on a lattice made of N rows and M columns, as in Figure 1.8. We apply periodic boundary conditions to the system in both directions (geometrically, this can be thought of as defining the model on a torus), and we consider only nearest neighbour interactions. The spin in a site is identified by $S_{\text{site}} = S_{m,n}$.
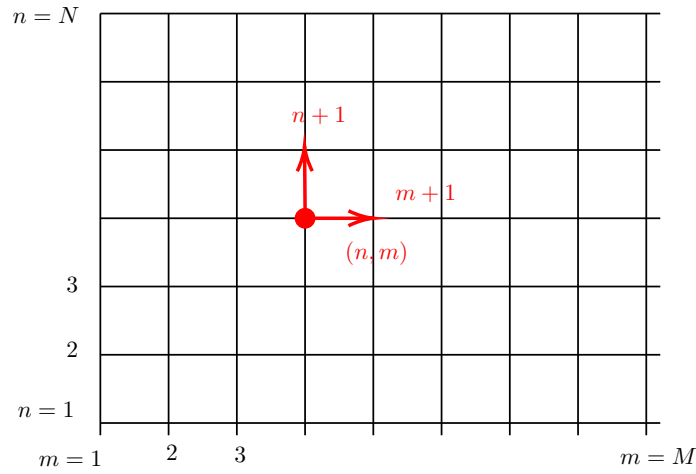

Figure 1.8: 2-dimensional Ising lattice of N rows and M columns.

We consider a set of spin arranged on a square lattice, interacting only with nearest neighbors and with a magnetic field $H \neq 0$. The reduced Hamiltonian of the system will be:

$$-\beta\mathcal{H}_\Omega(\{S\}) = K \sum_{\langle ij \rangle} S_i S_j + h \sum_i S_i$$

$$= K \sum_{n=1}^{N} \sum_{m=1}^{M} (S_{m,n}S_{m+1,n} + S_{m,n}S_{m,n+1}) + h \sum_{n=1}^{N} \sum_{m=1}^{M} S_{m,n}$$

This can be rewritten as follows:

$$-\beta\mathcal{H}_\Omega(\{S\}) = \sum_{m=1}^{M} [E_2(\mu_m, \mu_{m+1}) + E_1(\mu_m)] \tag{1.81}$$

where

$$E_1(\mu_m, h) = K \sum_{n=1}^{N} S_{m,n}S_{m,n+1} + h \sum_{n=1}^{N} S_{m,n} \tag{1.82a}$$

$$E_2(\mu_m, \mu_{m+1}, h) = K \sum_{n=1}^{N} S_{m,n}S_{m+1,n} \tag{1.82b}$$

the first equation is the one body interaction, while the second equation represents the interaction between nearest neighbours columns (two body interaction).

Moreover, μ is a N dimensional vector; in particular, each μ_m represents the set of N spins along column m:

$$\mu_m = \{S_{m,1}, S_{m,2}, \ldots, S_{m,N}\} \tag{1.83}$$

We can write a transfer matrix between columns, permitting to transfer along the m. As for the $d = 1$ case we can make the Hamiltonian symmetric:

$$-\beta \mathcal{H}_\Omega(\{S\}) = \sum_{m=1}^{M} \left[E_2(\mu_m, \mu_{m+1}) + \frac{1}{2}(E_1(\mu_m) + E_1(\mu_{m+1})) \right] \tag{1.84}$$

We have

$$
\begin{aligned}
Z_{N,M} &= \sum_{\mu_1} \cdots \sum_{\mu_M} \exp\left[\sum_{m=1}^{M} \left[E_2(\mu_m, \mu_{m+1}) + \frac{1}{2}(E_1(\mu_m) + E_1(\mu_{m+1})) \right] \right] \\
&= \sum_{\mu_1} \cdots \sum_{\mu_M} \left[\prod_{m=1}^{M} \exp\left[E_2(\mu_m, \mu_{m+1}) + \frac{1}{2}(E_1(\mu_m) + E_1(\mu_{m+1})) \right] \right] \\
&= \sum_{\mu_1} \cdots \sum_{\mu_M} \langle \mu_1 | \mathbb{T} | \mu_2 \rangle \langle \mu_2 | \mathbb{T} | \mu_3 \rangle \ldots \langle \mu_N | \mathbb{T} | \mu_1 \rangle
\end{aligned}
\tag{1.85}
$$

where

$$\langle \mu_m | \mathbb{T} | \mu_{m+1} \rangle = \exp\left[E_2(\mu_m, \mu_{m+1}) + \frac{1}{2}(E_1(\mu_m) + E_1(\mu_{m+1})) \right] \tag{1.86}$$

Remark. In the 2x2 transfer matrix in the 1-dim case we have two possible values. Now, we have to do the same in principle, but we have to do for all of the (1.83).

Remark. $\mathbb{T}$ is a matrix of dimension $2^N \times 2^N$, hence, in the thermodynamic limit is an infinite matrix (violation of Perron-Frobenius).

If we can find the set of eigenvalues $\lambda_+ > \lambda_- \geq \lambda_1 \geq \cdots \geq \lambda_{2^N - 2}$ of the $2^N \times 2^N$ matrix, we have

$$Z_{N,M} = \text{Tr}(\mathbb{T}^M) = \sum_{i=\pm,1}^{2^N - 2} \lambda_i^M(N) \tag{1.87}$$

Thermodynamic Limit

We can write our bulk free-energy as:

$$
\begin{aligned}
f_b &= -k_B T \lim_{N \to \infty} \lim_{M \to \infty} \frac{1}{MN} \ln(Z) \\
&= -k_B T \lim_{N \to \infty} \lim_{M \to \infty} \frac{1}{NM} \ln(\lambda_+^M + \lambda_-^M + \ldots) \\
&= -k_B T \lim_{N \to \infty} \frac{1}{N} \ln(\lambda_+) - k_B T \lim_{N \to \infty} \lim_{M \to \infty} \frac{1}{MN} \ln\left[1 + \sum_k \left(\frac{\lambda_k}{\lambda_+} \right)^M \right] \\
&= -k_B T \lim_{N \to \infty} \frac{1}{N} \ln(\lambda_+)(N) \quad (\star)
\end{aligned}
$$

Our ultimate goal is to find the largest eigenvalue of the $2^N \times 2^N$ matrix and take the limit $(\star)$. Not an easy task to achieve. The first solution was given by ONSAGER using Lie Algebra and group representation for $H = 0$ (1944). Subsequent alternative method include Pfaffian or other

combinatorial methods or mapping to a $1d$ quantum mechanics system. Let us jump directly to the final result:

$$\lambda_+(N) = \left[2\frac{\sinh}{2k}\right]^{\frac{N}{2}} \exp\left[\frac{1}{2}\sum_{i=1}^{2N-1}\psi_i\right]$$

where ψ_i are defined such that:

$$\cosh(\psi_i) = \coth(2k)\cosh(2k) - \cos\left(\frac{i\pi}{N}\right)$$

So we can write our bulk free-energy as:

$$f_b = -k_BT \lim_{N\to\infty}\ln(\lambda_+) = -\frac{k_BT}{2}\ln[2\sinh(2k)] - k_BT\lim_{N\to\infty}\frac{1}{2N}\sum_{i=1}^{N}\psi_{2i-1}$$

In the thermodynamic limit ($N\to\infty$):

$$\frac{1}{2N}\sum_{i=1}^{N}\psi_{2i-1} \sim \frac{1}{2\pi}\int_0^\pi \psi(\theta)\,d\theta = \frac{1}{2\pi}\int_0^\pi \text{arccosh}[\coth(2k)\cosh(2k) - \cos(\theta)]\,d\theta$$

using the identity

$$\text{arcosh}(x) = \frac{1}{\pi}\int_0^\pi \ln[2(x - \cos(\phi))]\,d\phi$$

we can write finally

$$f_b = -\frac{k_BT}{2}\ln[2\sinh(2k)] - \frac{k_BT}{2}\ln 2 - \frac{k_BT}{2\pi^2}\int_0^\pi\int_0^\pi \ln[\coth(2k)\cosh(2k) - \cos(\theta) - \cos(\phi)]\,d\phi\,d\theta$$

From the expression f_b one can deduce all the thermodynamic properties of the $2D$ Ising Model for $H = 0$. Where the expression from which derive T_c is:

$$2\tanh^2\left(\frac{2J}{k_BT_c}\right) = 1$$

which yields the numeric result:

$$\Rightarrow T_c \simeq 2,264J/k_B \neq 0$$

hence, we have a phase transition at a critical temperature T_c different from 0! Onsager also showed that the critical exponents of this model are:

$$\alpha = 0, \quad \beta = \frac{1}{8}, \quad \gamma = \frac{7}{4}$$

where $\alpha = 0$ because the specific heat diverges logarithmically for $T \sim T_c$:

$$c \propto A\left[-\ln\left(1 - \frac{T}{T_c}\right) + B\right]$$

It means that the specific heat displays at the transition a logarithmic divergence (no power law!).