Lecture 7.
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0.0.1 Transfer Matrix method

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

$$Z_N(k,h) = \sum_{S_1=\pm1}\sum_{S_2=\pm1}\cdots\sum_{S_N=\pm1}\left[e^{KS_1S_2+\frac{h}{2}(S_1+S_2)}\right]\left[e^{KS_2S_3+\frac{h}{2}(S_2+S_3)}\right]\cdots\left[e^{KS_NS_1+\frac{h}{2}(S_N+S_1)}\right] \tag{1}$$

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

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

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

$$\langle S|\,\mathbb{T}\,|S'\rangle = \exp\left[KSS'+\frac{h}{2}(S+S')\right] \tag{3}$$

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 ($k_{LL}\sum S_iS_{i+1}S_{i+2}S_{i+3}$).

For Ising $S_i = \pm1$ and neirest neighbour interaction implies that we have two values and that $\mathbb{T}$ is a 2×2 matrix whose components are

$$\langle+1|\,\mathbb{T}\,|+1\rangle = \exp[K+h] \tag{4a}$$
$$\langle+1|\,\mathbb{T}\,|-1\rangle = \langle-1|\,\mathbb{T}\,|+1\rangle = \exp[K-h] \tag{4b}$$
$$\langle-1|\,\mathbb{T}\,|-1\rangle = \exp[-K] \tag{4c}$$

The explicit representation is

$$\mathbb{T} = \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix} \tag{5}$$

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

$$\left|S_i^{(+)}\right\rangle = \begin{pmatrix}1\\0\end{pmatrix}_i \quad \left|S_i^{(-)}\right\rangle = \begin{pmatrix}0\\1\end{pmatrix}_i \tag{6a}$$
$$\left\langle S_i^{(+)}\right| = (1^*,0)_i \quad \left\langle S_i^{(-)}\right| = (0,1^*)_i \tag{6b}$$

The identity relation is:

$$\sum_{S_i=\pm1}|S_i\rangle\langle S_i| = \left|S_i^{(+)}\right\rangle\left\langle S_i^{(+)}\right| + \left|S_i^{(-)}\right\rangle\left\langle S_i^{(-)}\right| = \mathbb{1} = \begin{pmatrix}1&0\\0&1\end{pmatrix} \tag{7}$$

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

By using the identity property we can write

$$\begin{aligned} Z_N(K,h) &= \sum_{S_1=\pm1} \cdots \sum_{S_N=\pm1} \langle S_1| \mathbb{T} |S_2\rangle \langle S_2| \mathbb{T} |S_3\rangle \dots |S_i\rangle \langle S_i| \mathbb{T} |S_{i+1}\rangle \dots \\ &= \sum_{S_1=\pm1} \langle S_1| \mathbb{T}^N |S_1\rangle = \mathrm{Tr}\big[\mathbb{T}^N\big] \end{aligned} \tag{8}$$

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

$$\mathbb{T}_D = \mathbb{P}^{-1}\mathbb{T}\mathbb{P} \tag{9}$$

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

$$\begin{aligned} \mathrm{Tr}\big[\mathbb{T}^N\big] &= \mathrm{Tr}\left[\underbrace{\mathbb{T}\mathbb{T}\mathbb{T}\dots\mathbb{T}}_{N}\right] = \mathrm{Tr}\big[\mathbb{P}\mathbb{P}^{-1}\mathbb{T}\mathbb{P}\mathbb{P}^{-1}\mathbb{T}\mathbb{P}\dots\mathbb{P}^{-1}\mathbb{T}\mathbb{P}\mathbb{P}^{-1}\big] \\ &= \mathrm{Tr}\big[\mathbb{P}\mathbb{T}_D^N\mathbb{P}^{-1}\big] \underset{\substack{\text{ciclyc property}\\ \text{of the trace}}}{=} \mathrm{Tr}\big[\mathbb{T}_D^N\mathbb{P}^{-1}\mathbb{P}\big] \\ &= \mathrm{Tr}\big[\mathbb{T}_D^N\big] \end{aligned} \tag{10}$$

where

$$\mathbb{T}_D = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix} \quad \Rightarrow \quad \mathbb{T}_D^N = \begin{pmatrix} \lambda_+^N & 0 \\ 0 & \lambda_-^N \end{pmatrix} \tag{11}$$

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

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

We finally have:

$$Z_N(K,h) = \mathrm{Tr}\big[\mathbb{T}_{\mathbb{D}}^{\mathbb{N}}\big] = \lambda_+^N + \lambda_-^N \tag{12}$$

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 ($S_i = \pm1$) with neirest neighbour and next neirest neighbour interactions. The hamiltonian is:

$$\mathcal{H} = k_1 \sum_i S_i S_{i+1} + k_2 \sum_i S_i S_{i+1} S_{i+2} S_{i+3} \tag{13}$$

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.

Let us now consider the transfer matrix formalism in a more general setting.

0.1 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 mary 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

$$\sum_{S_i} |S_i\rangle\langle S_i| = \mathbb{1}, \quad \mathbb{1}\in(n+2)\times(n+2) \tag{14}$$

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)

$$\mathbb{S}_i \equiv \sum_{S_i} |S_i\rangle\, S_i\, \langle S_i| \tag{15}$$

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.

Remark. By constrution $\langle S_i|$ 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

$$\mathbb{T} = \mathbb{P}\mathbb{T}_D\mathbb{P}^{-1} = \sum_i |t_i\rangle\,\lambda_i\,\langle t_i| \tag{16}$$

Indeed,

$$\mathbb{T}\,|t_j\rangle = \sum_i |t_i\rangle\,\lambda_i\,\langle t_i|t_j\rangle = \sum_i |t_i\rangle\,\lambda_i\delta_{ij} = \lambda_j\,|t_j\rangle \tag{17}$$

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

$$Z_N(\{K\},h) = \lambda_+^N + \lambda_-^N + \sum_{i=1}^{n}\lambda_i^N \tag{18}$$

0.1.1 The free energy

Now, we are interested in the limit of the bulk free energy

$$F_N() = -k_B T \log Z_N() \tag{19}$$

In general, looking at the thermodynamic limit $N \to \infty$, by factorizing λ_+

$$f_b(\{k\}, h) = \lim_{N\to\infty} \frac{1}{N} F_N = \lim_{N\to\infty} \frac{1}{N}(-k_B T) \log \left[\lambda_+^N + \lambda_-^N + \sum_{i=1}^{n} \lambda_i^N \right] \tag{20}$$

by rearringing,

$$f_b = \lim_{N\to\infty} \frac{-k_B T}{N} \log \left[\lambda_+^N \left(1 + \frac{\lambda_-^N}{\lambda_+^N} + \sum_{i=1}^{n} \left(\frac{\lambda_i}{\lambda_+} \right)^N \right) \right] \tag{21}$$

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

$$\left(\frac{\lambda_-}{\lambda_+} \right)^N \overset{N\to\infty}{\longrightarrow} 0, \quad \left(\frac{\lambda_i}{\lambda_+} \right)^N \overset{N\to\infty}{\longrightarrow} 0 \quad \forall i \tag{22}$$

we obtain:

$$f_b = -k_B T \log \lambda_+ \tag{23}$$

The limiting 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 0.1.1 (Perron-Frobenius). *Let $\mathbb{A}$ be a $n \times n$ matrix. If $\mathbb{A}$ is finite ($n < \infty$) and $\mathbb{A}_{ij} > 0, \forall i, j$, ($\mathbb{A}_{ij} = \mathbb{A}_{ij}(\vec{\mathbf{x}})$), 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!

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 any more and f_b can be non-analytic.

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

0.1.2 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 respect to the average is:

$$\Gamma_R \equiv \langle S_1 S_R \rangle - \langle S_1 \rangle \langle S_R \rangle \tag{24}$$

Since

$$\Gamma_R \underset{R\to\infty}{\sim} \exp[-R/\xi] \tag{25}$$

we can define the correlation length ξ as

$$\xi^{-1} \equiv \lim_{R\to\infty} \left[-\frac{1}{R} \log |\langle S_1 S_R \rangle - \langle S_1 \rangle \langle S_R \rangle| \right] \tag{26}$$

Now, let us compute the terms $\langle S_1 S_R \rangle_N$ and $\langle S_1 \rangle_N \langle S_R \rangle_N$. From the definition of average we obtain

$$\langle S_1 S_R \rangle_N = \frac{1}{Z_N} \sum_{\{S\}} S_1 S_R \exp[-\beta \mathcal{H}_N] \tag{27}$$

Remark. The subscript N denotes that we are again considering a ring of N spins. Z_N is known from equation (18).

Writing this expression by using the transfer matrix formalism one obtains

$$\langle S_1 S_R \rangle_N = \frac{1}{Z_N} \sum_{\{S\}} S_1 \langle S_1 | \mathbb{T} | S_2 \rangle \dots \langle S_{R-1} | \mathbb{T} | S_R \rangle S_R \langle S_R | \mathbb{T} | S_{R+1} \rangle \dots \langle S_N | \mathbb{T} | S_1 \rangle \tag{28}$$

Summing over the free spins,

$$\langle S_1 S_R \rangle_N = \frac{1}{Z_N} \sum_{S_1, S_R} S_1 \langle S_1 | \mathbb{T}^{R-1} | S_R \rangle S_R \langle S_R | \mathbb{T}^{N-R+1} | S_1 \rangle \tag{29}$$

On the other hand, since

$$\mathbb{T} = \sum_{i=1}^{n+2} |t_i\rangle \lambda_i \langle t_i| \tag{30}$$

we have

$$\mathbb{T}^{R-1} = \sum_{i=1}^{n+2} |t_i\rangle \lambda_i^{R-1} \langle t_i| \tag{31a}$$

$$\mathbb{T}^{N-R+1} = \sum_{i=1}^{n+2} |t_i\rangle \lambda_i^{N-R+1} \langle t_i| \tag{31b}$$

Hence,

$$\langle S_1 | \mathbb{T}^{R-1} | S_R \rangle = \sum_{i=1}^{n+2} \langle S_1 | t_i \rangle \lambda_i^{R-1} \langle t_i | S_R \rangle \tag{32}$$

and plugging this expression in (29) one gets

$$\sum_{\{S\}} S_1 S_R e^{-\beta \mathcal{H}_N} = \sum_{S_1 S_R} S_1 \sum_{i=1}^{n+2} \langle S_1 | t_i \rangle \lambda_i^{R-1} \langle t_i | S_R \rangle S_R \sum_{j=1}^{n+2} \langle S_R | t_j \rangle \lambda_j^{N-R+1} \langle t_j | S_1 \rangle \tag{33}$$

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

$$\mathbb{S}_1 = \sum_{S_1} |S_1\rangle S_1 \langle S_1| \tag{34a}$$

$$\mathbb{S}_R = \sum_{S_R} |S_R\rangle S_R \langle S_R| \tag{34b}$$

one gets

$$\sum_{\{S\}} S_1 S_R e^{-\beta \mathcal{H}_N} = \sum_{ij} \langle t_j | \, \mathbb{S}_1 \, | t_i \rangle \, \lambda_i^{R-1} \, \langle t_i | \, \mathbb{S}_R \, | t_j \rangle \, \lambda_j^{N-R+1} \tag{35}$$