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0.0.1 Transfer Matrix method

Given the Hamiltonian above we can write the corresponding partition function in the following symmetric form:

$$Z_N(k,h) = \sum_{S_1=\pm 1}\sum_{S_2=\pm 1}\cdots\sum_{S_N=\pm 1}\left[e^{kS_1S_2+\frac{h}{2}(S_1+S_2)}\right]\left[e^{kS_2S_3+\frac{h}{2}(S_2+S_3)}\right]\dots\left[e^{kS_NS_1+\frac{h}{2}(S_N+S_1)}\right] \tag{1}$$

Suppose you have a sort of $\sum_j M_{ij}P_{jk}$, what we have done is doing something like that. In the previous form Z_N can be written as a product of matrices

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

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

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

Note that the labels of the matrix corresponds to the values of S_i. Hence its dimension depdens 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 $S_i=\pm 1$ and neirest neighbour interaction implies that we have 2 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 now introduce some useful notations and relations using the bra-ket formalism: subequations

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

$$\left\langle S_i^{(+)}\right| = (1^*,0)_i \quad \left\langle S_i^{(-)}\right| = (0,1^*)_i \tag{7}$$

The identity relation is:

$$\sum_{S_i=\pm 1}|S_i\rangle\langle S_i| = \left|S_i^{(+)}\right\rangle\left\langle S_i^{(+)}\right| + \left|S_i^{(-)}\right\rangle\left\langle S_i^{(-)}\right| = \mathbb{1} = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \tag{8}$$

By using the last property we can write

$$\begin{aligned} Z_N(K,h) &= \sum_{S_1=\pm 1}\cdots\sum_{S_N=\pm 1}\langle S_1|\,\mathbb{T}\,|S_2\rangle\langle S_2|\,\mathbb{T}\,|S_3\rangle\dots|S_i\rangle\langle S_i|\,\mathbb{T}\,|S_{i+1}\rangle\dots \\ &= \sum_{S_1=\pm 1}\langle S_1|\,\mathbb{T}^N\,|S_1\rangle = \mathrm{Tr}\left[\mathbb{T}^N\right] \end{aligned} \tag{9}$$

this is exactly the trace of the matrix. Being $\mathbb{T}$ symmetric, we can diagonalize it by an unitary transformation

$$\mathbb{T}_D = \mathbb{P}^{-1}\mathbb{T}\mathbb{P} \tag{10}$$

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

$$\begin{aligned}
\mathrm{Tr}\left[\mathbb{T}^N\right] &= \mathrm{Tr}\left[\underbrace{\mathbb{T}\mathbb{T}\mathbb{T}\ldots\mathbb{T}}_{N}\right] = \mathrm{Tr}\left[\mathbb{P}\mathbb{P}^{-1}\mathbb{T}\mathbb{P}\mathbb{P}^{-1}\mathbb{T}\mathbb{P}\ldots\mathbb{P}^{-1}\mathbb{T}\mathbb{P}\mathbb{P}^{-1}\right] \\
&= \mathrm{Tr}\left[\mathbb{P}\mathbb{T}_D^N\mathbb{P}^{-1}\right] \underset{\substack{\text{ciclyc property}\\ \text{of the trace}}}{=} \mathrm{Tr}\left[\mathbb{T}_D^N\mathbb{P}^{-1}\mathbb{P}\right] \\
&= \mathrm{Tr}\left[\mathbb{T}_D^N\right]
\end{aligned} \tag{11}$$

where

$$\mathbb{T}_D = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix} \quad \mathbb{T}_D^N = \begin{pmatrix} \lambda_+^N & 0 \\ 0 & \lambda_-^N \end{pmatrix} \tag{12}$$

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:

$$Z_N(K,h) = \mathrm{Tr}\left[\mathbb{T}_{\mathbb{D}}^{\mathbb{N}}\right] = \lambda_+^N + \lambda_-^N \tag{13}$$

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 neirest neighbour and next neirest neighbour interactions. The hamiltonian is:

$$\mathcal{H} = k_1 \sum_i S_i S_{i+1} + k_2 \sum_i S_i S_{i+1} S_{i+2} S_{i+3} \tag{14}$$

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

$$\langle S_i S_{i+1} | \, \mathbb{T} \, | S_{i+2} S_{i+3} \rangle \tag{15}$$

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

General transfer matrix method

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

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

$$\left\langle S_i^{(3)} \right| = (0, 0, 1^*, 0, \ldots, 0) \qquad \left| S_i^{(3)} \right\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} \tag{16}$$

Similarly to the 2×2 (Ising) case it is easy to show that

$$\sum_{S_i} |S_i\rangle \langle S_i| = \mathbb{1}, \quad \mathbb{1} \in (n+2) \times (n+2) \tag{17}$$

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

Let us now 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)

$$\mathbb{S}_i \equiv \sum_{S_i} |S_i\rangle\, S_i \,\langle S_i| \tag{18}$$

Example 3. Ising model $n+2=2$

$$\begin{pmatrix}1\\0\end{pmatrix} S^{(1)}(1^*,0) + \begin{pmatrix}0\\1\end{pmatrix} S^{(2)}(0,1^*) = \begin{pmatrix}S^{(1)} & 0\\ 0 & 0\end{pmatrix} + \begin{pmatrix}0 & 0\\ 0 & S^{(2)}\end{pmatrix} = \begin{pmatrix}S^{(1)} & 0\\ 0 & S^{(2)}\end{pmatrix} \tag{19}$$

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

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

$$\mathbb{T} = \mathbb{P}\mathbb{T}_D\mathbb{P}^{-1} = \sum_i |t_i\rangle\, \lambda_i \,\langle t_i| \tag{20}$$

Indeed

$$\mathbb{T}\,|t_j\rangle = \sum_i |t_i\rangle\, \lambda_i \,\langle t_i|t_j\rangle = \sum_i |t_i\rangle\, \lambda_i \delta_{ij} = \lambda_j\,|t_j\rangle \tag{21}$$

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

$$Z_N(\{k\},h) = \lambda_+^N + \lambda_-^N + \sum_{i=1}^{n} \lambda_i^N \tag{22}$$

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

$$F_N() = -k_B T \log Z_N() \tag{23}$$

In general, looking at the thermodynamic limit, by factorizing λ_+

$$f_b(\{k\},h) = \lim_{N\to\infty} \frac{1}{N} F_N = \lim_{N\to\infty} \frac{1}{N}(-k_B T) \log \left[\lambda_+^N + \lambda_-^N + \sum_{i=1}^{n} \lambda_i^N\right] \tag{24}$$

by rearringing

$$f_b = \lim_{N\to\infty} \frac{-k_B T}{N} \log \left[\lambda_+^N \left(1 + \frac{\lambda_-^N}{\lambda_+^N} + \sum_{i=1}^{n} \left(\frac{\lambda_i}{\lambda_+}\right)^N\right)\right] \tag{25}$$

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

$$\left(\frac{\lambda_-}{\lambda_+}\right)^N \stackrel{N\to\infty}{\longrightarrow} 0, \quad \left(\frac{\lambda_i}{\lambda_+}\right)^N \stackrel{N\to\infty}{\longrightarrow} 0 \quad \forall i \tag{26}$$

we obtain

$$f_b = -k_B T \log \lambda_+ \tag{27}$$

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

Theorem 0.0.1 (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* $\{\lambda_i\}_{i=1,\dots,n-1}$. *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 trye for $T > 0$ since for $T = 0$ some T_{ij} can be either 0 or ∞ violating the hypothesis of the theorem.

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.

Two point correlation function

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

$$\Gamma_R \equiv \langle S_1 S_R \rangle - \langle S_1 \rangle \langle S_R \rangle \tag{28}$$

Since

$$\Gamma_R \underset{R\to\infty}{\sim} \exp[-R/\xi] \tag{29}$$

we can define the correlation length ξ as

$$\xi^{-1} \equiv \lim_{R\to\infty} \left[-\frac{1}{R} \log |\langle S_1 S_R \rangle - \langle S_1 \rangle \langle S_R \rangle| \right] \tag{30}$$

We have to compute the terms $\langle S_1 S_R \rangle_N$ and $\langle S_1 \rangle_N \langle S_R \rangle_N$. From the definition

$$\langle S_1 S_R \rangle_N = \frac{1}{Z_N} \sum_{\{S\}} S_1 S_R \exp[-\beta \mathcal{H}] \tag{31}$$

Let us now write this expression by using the transfer matrix formalism.

$$\langle S_1 S_R \rangle_N = \frac{1}{Z_N} \sum_{\{S\}} S_1 \langle S_1 | \mathbb{T} | S_2 \rangle \dots \langle S_{R-1} | \mathbb{T} | S_R \rangle S_R \langle S_R | \mathbb{T} | S_{R+1} \rangle \dots \langle S_N | \mathbb{T} | S_1 \rangle \tag{32}$$

Summing over the free spins

$$\langle S_1 S_R \rangle_N = \frac{1}{Z_N} \sum_{S_1, S_R} S_1 \langle S_1 | \mathbb{T}^{R-1} | S_R \rangle S_R \langle S_R | \mathbb{T}^{N-R+1} | S_1 \rangle \tag{33}$$

On the other hand since

$$\mathbb{T} = \sum_{i=1}^{n+2} |t_i\rangle\, \lambda_i \,\langle t_i| \tag{34}$$

we have

$$\mathbb{T}^{R-1} = \sum_{i=1}^{n+2} |t_i\rangle\, \lambda_i^{R-1} \,\langle t_i| \tag{35a}$$

$$\mathbb{T}^{N-R+1} = \sum_{i=1}^{n+2} |t_i\rangle\, \lambda_i^{N-R+1} \,\langle t_i| \tag{35b}$$

Hence

$$\langle S_1|\, \mathbb{T}^{R-1} \,|S_R\rangle = \sum_{i=1}^{n+2} \langle S_1|t_i\rangle\, \lambda_i^{R-1} \,\langle t_i|S_R\rangle \tag{36}$$

and plugging this expression in (33) one gets

$$\sum_{\{S\}} S_1 S_R e^{-\beta\mathcal{H}} = \sum_{S_1 S_R} S_1 \sum_{i=1}^{n+2} \langle S_1|t_i\rangle\, \lambda_i^{R-1} \,\langle t_i|S_R\rangle\, S_R \sum_{j=1}^{n+2} \langle S_R|t_j\rangle\, \lambda_j^{N-R+1} \,\langle t_j|S_1\rangle \tag{37}$$

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

$$\mathbb{S}_1 = \sum_{S_1} |S_1\rangle\, S_1 \,\langle S_1| \tag{38a}$$

$$\mathbb{S}_R = \sum_{S_R} |S_R\rangle\, S_R \,\langle S_R| \tag{38b}$$

one gets

$$\sum_{\{S\}} S_1 S_R e^{-\beta\mathcal{H}} = \sum_{ij} \langle t_j|\, \mathbb{S}_1 \,|t_i\rangle\, \lambda_i^{R-1} \,\langle t_i|\, \mathbb{S}_R \,|t_j\rangle\, \lambda_j^{N-R+1} \tag{39}$$