Chapter 1

Complex Systems Exercises

Exercise 1.0.1 (Ising Model)**:**

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

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

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

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

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

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

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

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

$$Z(K,h) = \boldsymbol{v}^T\mathrm{T}^N\boldsymbol{v} \equiv \sum_{\substack{\sigma_1=\pm1\\ \sigma_N=\pm1}} v(\sigma_1)\mathrm{T}^N(\sigma_1,\sigma_N)v(\sigma_N)$$

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

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

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

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

1.1 Solution

1.1.1 Part A

Consider a $d = 1$ system with N spins. The periodic boundary conditions are $\sigma_{N+1} = \sigma_1$.

1. The **partition function** is given by:

$$\begin{aligned} Z(K,h) &= \sum_{\{\boldsymbol{\sigma}\}} e^{-\beta\mathcal{H}(\boldsymbol{\sigma})} = \sum_{\{\boldsymbol{\sigma}\}} \exp\left(K\sum_{x=1}^{N} \sigma_x\sigma_{x+1} + h\sum_{x=1}^{N}\sigma_x \right) = \\ &= \sum_{\{\boldsymbol{\sigma}\}} \prod_{x=1}^{N} \underbrace{\exp\left(K\sigma_x\sigma_{x+1} + h\frac{\sigma_x + \sigma_{x+1}}{2} \right)}_{\mathrm{T}_{\sigma_x,\sigma_{x+1}}} = \\ &= \sum_{\sigma_1=\pm1} \cdots \sum_{\sigma_N=\pm1} \mathrm{T}_{\sigma_1\sigma_2}\mathrm{T}_{\sigma_2\sigma_3}\cdots\mathrm{T}_{\sigma_{N-1}\sigma_N}\mathrm{T}_{\sigma_N\sigma_1} = \\ &= \sum_{\sigma_1=\pm1} (\underbrace{\mathrm{T}\cdots\mathrm{T}}_{N \text{ times}})_{\sigma_1\sigma_1} = \sum_{\sigma_1=\pm1} (\mathrm{T}^N)_{\sigma_1\sigma_1} = \operatorname{Tr}\mathrm{T}^N \end{aligned}$$

where T is a 2×2 matrix given by:

$$\mathrm{T} = \begin{array}{cc} \sigma'=+1 & \sigma'=-1 \\ \left[\begin{array}{cc} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{array}\right. & \left.\begin{array}{c} \\ \\ \end{array}\right] \end{array} \begin{array}{c} \\ \sigma=+1 \\ \sigma=-1 \end{array} \tag{1.1}$$

As the trace is basis-independent, we can compute it in the basis that diagonalizes T. Let λ_1 and λ_2 be the eigenvalues of T, with $\lambda_1 < \lambda_2$. By solving:

$$\det(\mathrm{T} - \lambda\mathbb{I}) \overset{!}{=} 0$$

we find:

$$\lambda_{1,2} = e^K \cosh h \mp \sqrt{e^{2K}\sinh^2 h + e^{-2K}} \tag{1.2}$$

When diagonalized, $\mathrm{T} = \operatorname{diag}(\lambda_1, \lambda_2)$, and so:

$$Z(K,h) = \operatorname{Tr}\mathrm{T}^N = (\lambda_1^N + \lambda_2^N) \tag{1.3}$$

2. The **free energy** per node $f(K,h)$ is defined by the relation:

$$Z = e^{-\beta N f(K,h)} \underset{(1.3)}{=} (\lambda_1^N + \lambda_2^N)$$

Taking the ln of both sides and dividing by N leads to:

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

In the thermodynamic limit $N \to +\infty$ only the greatest eigenvalue (λ_1) will dominate:

$$= \frac{1}{N}\ln\left(\lambda_2^N\left[1 + \left(\frac{\lambda_1}{\lambda_2}\right)^N\right]\right) =$$

$$\xrightarrow[N\to+\infty]{} \frac{1}{\cancel{N}}\cancel{N}\ln\lambda_2 = \ln\lambda_2$$

Thus:

$$f(K,h) = -\frac{1}{\beta}\ln\lambda_2 = -\frac{1}{\beta}\ln[e^K\cosh h + \sqrt{e^{2K}\sinh^2 h + e^{-2K}}] \tag{1.4}$$

When $h = 0$:

$$\begin{aligned} f(K,h=0) &= -\frac{1}{\beta}\ln[e^K\cdot 1 + \sqrt{e^{2K}\cdot 0 + e^{-2K}}] = \\ &= -\frac{J}{\beta J}\ln 2\frac{[e^K + e^{-K}]}{2} = -\frac{J}{K}\ln(2\cosh K) \end{aligned} \tag{1.5}$$

where $K = \beta J = J/(k_B T)$, and so $1/K \propto T$.

As a function of T (or $1/K$), we have that:

$$f(K,0) \xrightarrow[T\to 0^+]{} -J$$

And for large T:

$$f(K,0) \underset{T\gg 1}{\sim} -JT\log 2$$

So, if $J = k_B = 1$, $f(K,0)$ stationarizes at -1 for $T \to 0^+$, and goes to $-\infty$ linearly (with a $\log 2$ factor) as $T \to +\infty$.

A plot of $f(1/K)$ is shown in fig. 1.1a.

3. The **entropy** per node is obtained by differentiating the free energy per node:

$$s \equiv -\frac{\partial f}{\partial T} = -\frac{\partial f}{\partial\beta}\frac{\partial\beta}{\partial T} = \frac{1}{k_B T^2}\frac{\partial f}{\partial\beta} \tag{1.6}$$

Using (1.4) we get:

$$\begin{aligned} \frac{\partial f}{\partial\beta} = +\frac{1}{\beta^2}\ln[e^K\cosh h + \sqrt{e^{2K}\sinh^2 h + e^{-2K}}]\cdot \\ \left(e^K J\cosh h + e^K B\sinh h + \frac{1}{2\sqrt{e^{2K}\sinh^2 h + e^{-2K}}}\cdot\right. \end{aligned}$$

$$\cdot \left[2e^{2K} J \sinh^2 h + 2e^{2K} B \cosh h \sinh h - 2Je^{-2K}\right]\Bigg)$$

Taking $h = 0$:

$$\left.\frac{\partial f}{\partial \beta}\right|_{h=0} = \frac{1}{\beta^2} \ln 2 \frac{[e^K + e^{-K}]}{2} - \frac{J\beta}{\beta \cdot \beta} \frac{e^K - e^{-K}}{e^K + e^{-K}} =$$
$$= \frac{1}{\beta^2} \ln[2\cosh(K)] - \frac{K}{\beta^2} \tanh(K)$$

The result is the same we would have obtained by directly differentiating (1.5), since:

$$\frac{\partial f}{\partial \beta}(K,h) = \frac{\partial f}{\partial K}\frac{\partial K}{\partial \beta} + \frac{\partial f}{\partial h}\underbrace{\frac{\partial h}{\partial \beta}}_{B}$$

and $h = 0 \Rightarrow B = 0$, meaning that the rightmost term vanishes (assuming that $\frac{\partial f}{\partial h}$ is well behaved).

Substituing back in (1.6) we get:

$$s = k_B \Big[\ln(2\cosh K) - K \tanh K\Big] \tag{1.7}$$

A plot of $s(1/K)$ is shown in fig. 1.1b.

4. The **mean energy** is given by:

$$\langle \epsilon \rangle = -\frac{\partial}{\partial \beta}\frac{\ln Z}{N} = -\frac{\partial}{\partial \beta}(\beta f(K,h)) =$$
$$= \frac{1}{e^K \cosh h + \sqrt{e^{2K}\sinh^2 h + e^{-2K}}} \Bigg(e^K J \cosh h + e^K B \sinh h +$$
$$+ \frac{1}{2\sqrt{e^{2K}\sinh^2 h + e^{-2K}}} \cdot \left[2e^{2K} J \sinh^2 h + 2e^{2K} B \sinh h \cosh h - 2Je^{-2K}\right]\Bigg)$$

When $h = 0$:

$$\epsilon(K, h = 0) = -J\frac{e^K - e^{-K}}{e^K + e^{-K}} = -J \tanh K \tag{1.8}$$

which is plotted in fig. 1.1c.

Note that, alternatively, we could have used the free energy definition to determine ϵ:

$$f = \epsilon - Ts$$

5. The **specific heat** *per node* is defined as:

$$c \equiv \frac{\partial \epsilon}{\partial T} = -\frac{\partial \epsilon}{\partial \beta}\frac{\partial \beta}{\partial T} = -k_B \beta^2 \frac{\partial \epsilon}{\partial \beta}$$

Since the expression is quite complicated, we use the argument we made when computing the entropy to take $h = 0$ *before* computing the derivative:

$$c(h = 0) = -k_B \beta^2 \frac{\partial}{\partial \beta}(-J \tanh K) = \frac{k_B K^2}{\cosh^2 K}$$

A plot of $c(1/K)$ is shown in fig. 1.1d.

6. The **magnetization** can be directly computed by differentiating the free energy:

$$
\begin{aligned}
\langle\sigma_x\rangle &= -\beta\frac{\partial}{\partial h}f(K,h) = \frac{\partial}{\partial h}(-\beta f(K,h)) = \\
&\underset{(1.4)}{=} \frac{\partial}{\partial h}\ln\Big(e^K\cosh h + \sqrt{e^{2K}\sinh^2 h + e^{-2K}}\Big) = \\
&= \frac{1}{e^K\cosh h + \sqrt{e^{2K}\sinh^2 h + e^{-2K}}}\left(e^K\sinh h + \frac{2e^{2K}\sinh h\cosh h}{2\sqrt{e^{2K}\sinh^2 h + e^{-2K}}}\right) = \\
&= e^K\sinh h\Big[1 + \frac{e^K\cosh h}{\sqrt{e^{2K}\sinh^2 h + e^{-2K}}}\Big]\frac{1}{e^K\cosh h + \sqrt{e^{2K}\sinh^2 h + e^{-2K}}} = \\
&= e^K\sinh h\frac{\sqrt{e^{2K}\sinh^2 h + e^{-2K}} + e^K\cosh h}{\sqrt{e^{2K}\sinh^2 h + e^{-2K}}}\frac{1}{e^K\cosh h + \sqrt{e^{2K}\sinh^2 h + e^{-2K}}} = \\
&= \frac{e^K\sinh h}{\sqrt{e^{2K}\sinh^2 h + e^{-2K}}} \qquad (1.9)
\end{aligned}
$$

For $h = 0$:

$$\langle\sigma_x\rangle \equiv 0$$

Plots of $\langle\sigma_x\rangle$ as function of h and K are shown in fig. 1.1e and 1.1f.

Alternatively, we can use the transfer matrix T. We start by writing explicitly the average:

$$\langle\sigma_x\rangle = \frac{1}{Z}\sum_{\{\boldsymbol{\sigma}\}}\sigma_x e^{-\beta\mathcal{H}(\boldsymbol{\sigma})} = \frac{1}{Z}\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_N=\pm1}\mathrm{T}_{\sigma_1\sigma_2}\cdots\mathrm{T}_{\sigma_{x-1}\sigma_x}\sigma_x\mathrm{T}_{\sigma_x\sigma_{x+1}}\cdots\mathrm{T}_{\sigma_N\sigma_1}$$

If we define:

$$\mathrm{T}'_{\sigma_i\sigma_j} \equiv \sigma_i\mathrm{T}_{\sigma_i\sigma_j} \qquad (1.10)$$

We can still write the sum over all spin configurations as the trace of a matrix product:

$$\langle\sigma_x\rangle = \frac{1}{Z}\,\mathrm{Tr}(\mathrm{T}^{x-1}\mathrm{T}'\mathrm{T}^{N-x})$$

Then, using the cyclic property of the trace:

$$\mathrm{Tr}(\mathrm{ABC}) = \mathrm{Tr}(\mathrm{CAB}) = \mathrm{Tr}(\mathrm{BCA})$$

we get:

$$\langle\sigma_x\rangle = \frac{1}{Z}\,\mathrm{Tr}(\mathrm{T}'\mathrm{T}^{N-x}\mathrm{T}^{x-1}) = \frac{1}{Z}\,\mathrm{Tr}(\mathrm{T}'\mathrm{T}^{N-1}) \qquad \forall x$$

As expected, $\langle\sigma_x\rangle$ does not depend on x, since the system is translational invariant.

Explicitly, T' is given by:

$$\mathrm{T}' = \begin{array}{cc} \scriptstyle\sigma'=+1 & \scriptstyle\sigma'=-1 & \\ \left[\begin{array}{c} e^{K+h} \\ -e^{-K} \end{array}\right. & \left.\begin{array}{c} e^{-K} \\ -e^{K-h} \end{array}\right] & \begin{array}{c} \scriptstyle\sigma=+1 \\ \scriptstyle\sigma=-1 \end{array} \end{array}$$

Note that it can be written as:

$$\mathrm{T}' = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mathrm{T} = \sigma_z \mathrm{T}$$

where σ_z is the third Pauli matrix (not to be confused with the z-th spin). Thus:

$$\langle \sigma_x \rangle = \frac{1}{Z} \operatorname{Tr}(\sigma_z \mathrm{T}^N)$$

As before, since the trace is basis independent, this computation is easier in the basis that diagonalizes T. Let $|v_{1,2}\rangle$ be the two eigenvectors of T, with eigenvalues $\lambda_{1,2}$. In the basis $\{|v_{1,2}\rangle\}$, $\mathrm{T}^N = \operatorname{diag}(\lambda_1^N, \lambda_2^N)$, while σ_z becomes:

$$\mathrm{V}^{-1} \sigma_z \mathrm{V} = \begin{pmatrix} \langle v_1 | \sigma_z | v_1 \rangle & \langle v_1 | \sigma_z | v_2 \rangle \\ \langle v_2 | \sigma_z | v_1 \rangle & \langle v_2 | \sigma_z | v_2 \rangle \end{pmatrix} \tag{1.11}$$

So, the argument of the trace in the $\{|v_\pm\rangle\}$ basis is:

$$\mathrm{V}^{-1} \sigma_z \mathrm{V} \operatorname{diag}(\lambda_1^N, \lambda_2^N) = \begin{pmatrix} \lambda_1^N \langle v_1 | \sigma_z | v_1 \rangle & \lambda_2^N \langle v_1 | \sigma_z | v_2 \rangle \\ \lambda_1^N \langle v_1 | \sigma_z | v_1 \rangle & \lambda_2^N \langle v_2 | \sigma_z | v_2 \rangle \end{pmatrix}$$

Thus:

$$\langle \sigma_z \rangle = \frac{1}{Z} \Big[\lambda_1^N \langle v_1 | \sigma_z | v_1 \rangle + \lambda_2^N \langle v_2 | \sigma_z | v_2 \rangle \Big] \tag{1.12}$$

$Z(K, h)$ is given by (1.3), which in the thermodynamic limit becomes:

$$Z(K, h) = (\lambda_1^N + \lambda_2^N) = \lambda_2^N \left(1 + \left(\frac{\lambda_1}{\lambda_2} \right)^N \right) \xrightarrow[N \to +\infty]{} \lambda_2^N \qquad \lambda_1 < \lambda_2$$

Substituting back in (1.12) we get:

$$\langle \sigma_z \rangle = \frac{1}{\lambda_2^N} \Big[\lambda_1^N \langle v_1 | \sigma_z | v_1 \rangle + \lambda_2^N \langle v_2 | \sigma_z | v_2 \rangle \Big] \xrightarrow[N \to +\infty]{} \langle v_2 | \sigma_z | v_2 \rangle \tag{1.13}$$

All that's left is to find the eigenvectors $\{|v_{1,2}\rangle\}$ and compute the required matrix element.

Since T is a 2×2 matrix, we can write it as a *linear combination* of the Pauli Matrices $\sigma_{x,y,z}$, which, together with the identity $\mathbb{1}$, form a basis of $\mathcal{M}_{2\times 2}(\mathbb{C})$. In other words, any 2×2 matrix M can be written as:

$$\mathrm{M} = a_0 \mathbb{1} + a_1 \sigma_x + a_2 \sigma_y + a_3 \sigma_z$$

with:

$$\sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

We can define a *vector of matrices* $\boldsymbol{\sigma} \equiv (\sigma_x, \sigma_y, \sigma_z)^T$, and write:

$$M = a_0 \mathbb{1} + \boldsymbol{a} \cdot \boldsymbol{\sigma} = a_0 \mathbb{1} + \underbrace{\|\boldsymbol{a}\|}_{a} (\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma})$$

where $\hat{\boldsymbol{n}} = (n_x, n_y, n_z)^T$ is a unitary vector ($\|\hat{\boldsymbol{n}}\| = 1$), and:

$$\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma} = \begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix}$$

This makes it simpler to find eigenvalues and eigenvectors of M. In fact, if $\boldsymbol{v}$ is an eigenvector of $\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}$ with eigenvalue λ:

$$(\boldsymbol{n} \cdot \boldsymbol{\sigma})\boldsymbol{v} = \lambda \boldsymbol{v}$$

then $\boldsymbol{v}$ is an eigenvector also of M, but with eigenvalue $a_0 + a\lambda$:

$$M\boldsymbol{v} = [a_0 \mathbb{1} + a(\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma})]\boldsymbol{v} = a_0 \boldsymbol{v} + a\lambda \boldsymbol{v} = (a_0 + a\lambda)\boldsymbol{v}$$

The eigenvalues of $\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}$ are ± 1:

$$\det(\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma} - \lambda \mathbb{1}) = \lambda^2 - \|\hat{\boldsymbol{n}}\|^2 \Rightarrow \lambda^2 = 1 \Rightarrow \lambda = \pm 1$$

If we parametrize the unit vector $\hat{\boldsymbol{n}}$ in spherical coordinates:

$$\begin{aligned} n_x &= \sin\theta \cos\varphi && (1.14) \\ n_y &= \sin\theta \sin\varphi && (1.15) \\ n_z &= \cos\theta \end{aligned}$$

Then a pair of *orthonormal* eigenvactors of $\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}$ is given by:

$$|v_1\rangle = \begin{pmatrix} -\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{pmatrix} \qquad |v_2\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}$$

$|v_1\rangle$ corresponds to $\lambda = -1$ and $|v_2\rangle$ to $\lambda_2 = +1$.

So, let's write T in the Pauli basis, using the Hilbert-Schmidt inner product ($\langle \mathrm{A}, \mathrm{B} \rangle = \mathrm{Tr}(\mathrm{AB}^*)$) to find the coefficients $a_{0,1,2,3}$:

$$\mathrm{T} = \underbrace{\frac{\mathrm{Tr}(\mathrm{T}\mathbb{1})}{2}}_{a_0} \mathbb{1} + \underbrace{\frac{\mathrm{Tr}(\mathrm{T}\sigma_x)}{2}}_{a_1} \sigma_x + \underbrace{\frac{\mathrm{Tr}(\mathrm{T}\sigma_y)}{2}}_{a_2} \sigma_y + \underbrace{\frac{\mathrm{Tr}(\mathrm{T}\sigma_z)}{2}}_{a_3} \sigma_z$$

In our case:

$$\begin{aligned} a_0 &= e^K \frac{e^h + e^{-h}}{2} = e^K \cosh h && (1.16) \\ a_1 &= \frac{2e^{-K}}{2} = e^{-K} \\ a_2 &= 0 \\ a_3 &= e^K \frac{e^h - e^{-h}}{2} = e^K \sinh h \end{aligned}$$

Thus:

$$a = \|\boldsymbol{a}\|^2 = \sqrt{a_1^2 + a_2^2 + a_3^2} = \sqrt{e^{-2K} + e^{2K} \sinh^2 h}$$

$$\hat{\boldsymbol{n}} = \frac{\boldsymbol{a}}{a}$$

Since the eigenvectors of T are the same of $\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}$ we can evaluate (1.13):

$$\langle v_2 | \sigma_z | v_2 \rangle = \cos^2 \frac{\theta}{2} - \sin^2 \frac{\theta}{2} = \cos\theta = n_z = \frac{a_3}{a} = \frac{e^K \sinh h}{\sqrt{e^{-2K} + e^{2K} \sinh^2 h}}$$

which coincides with the result we got in (1.9).

7. **Two-point correlation**

The same spectral method used to compute the magnetization can be used also for the two-point correlation $\langle \sigma_x \sigma_{x+y} \rangle$. As before, we start by explicitly writing the average:

$$\begin{aligned}
\langle \sigma_x \sigma_{x+y} \rangle &= \frac{1}{Z} \sum_{\{\boldsymbol{\sigma}\}} \sigma_x \sigma_{x+y} e^{-\beta \mathcal{H}(\boldsymbol{\sigma})} = \\
&= \frac{1}{Z} \sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_N = \pm 1} \mathrm{T}_{\sigma_1 \sigma_2} \cdots \mathrm{T}_{\sigma_{x-1} \sigma_x} \sigma_x \mathrm{T}_{\sigma_x \sigma_{x+1}} \cdots \\
&\qquad\qquad \cdots \mathrm{T}_{\sigma_{x+y-1} \sigma_{x+y}} \sigma_{x+y} \mathrm{T}_{\sigma_{x+y} \sigma_{x+y+1}} \cdots \mathrm{T}_{\sigma_N \sigma_1} = \\
&= \frac{1}{Z} \mathrm{Tr}(\mathrm{T}^{x-1} \sigma_x \mathrm{T}^y \sigma_{x+y} \mathrm{T}^{N-x-y+1}) = \\
&\underset{(a)}{=} \frac{1}{Z} \mathrm{Tr}(\sigma_z \mathrm{T}^y \sigma_z \mathrm{T}^{N-y})
\end{aligned}$$

where in (a) we used the cyclic property of the trace, and the fact that $\sigma_n \mathrm{T}_{\sigma_n \sigma_{n+1}}$ is equivalent to $\mathrm{T}' = \sigma_z \mathrm{T}$, where σ_z is the third Pauli matrix.

In the continuum limit $Z = \lambda_2^N$. If we compute the trace in the basis $|v_{1,2}\rangle$ that diagonalizes T, we get:

$$\langle \sigma_x \sigma_{x+y} \rangle = \frac{1}{\lambda_2^N} \Big[\langle v_1 | \sigma_z \mathrm{T}^y \sigma_z | v_1 \rangle \lambda_1^{N-y} + \langle v_2 | \sigma_z \mathrm{T}^y \sigma_z | v_2 \rangle \lambda_2^{N-y} \Big]$$

and since $\lambda_1 < \lambda_2$, when $N \to +\infty$ the first term vanishes, leaving:

$$\langle \sigma_x \sigma_{x+y} \rangle = \frac{\langle v_2 | \sigma_z \mathrm{T}^y \sigma_z | v_2 \rangle}{\lambda_2^y}$$

Be careful not to mix different bases! The matrix product can be done in the canonical basis - but it's difficult since here T has the form (1.1), thus making T^y quite hard to compute. A better choice is to compute everything in the $|v_{1,2}\rangle$ basis, where $\mathrm{T} = \mathrm{diag}(\lambda_1, \lambda_2)$, $|v_1\rangle = (1, 0)^T$, $|v_2\rangle = (0, 1)^T$ and σ_z is given by (1.11), i.e.:

$$\sigma_z = \begin{pmatrix} -\cos\theta & -\sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

An even better choice is to use completeness:

$$\langle v_2 | \sigma_z \mathrm{T}^y \sigma_z | v_2 \rangle = \sum_{i,j=1}^{2} \langle v_2 | \sigma_z | v_i \rangle \langle v_i | \mathrm{T}^y | v_j \rangle \langle v_j | \sigma_z | v_2 \rangle$$

Since $|v_{1,2}\rangle$ diagonalize T, we have:

$$\langle v_1 | \mathrm{T}^y | v_1 \rangle = \lambda_1^y \quad \langle v_2 | \mathrm{T}^y | v_2 \rangle = \lambda_2^y \quad \langle v_1 | \mathrm{T}^y | v_2 \rangle = \langle v_2 | \mathrm{T}^y | v_1 \rangle = 0$$

Thus:

$$\langle v_2| \sigma_z \mathrm{T}^y \sigma_z |v_2\rangle = \langle v_2| \sigma_z |v_1\rangle \lambda_1^y \langle v_1| \sigma_z |v_2\rangle + \langle v_2| \sigma_z |v_2\rangle \lambda_2^y \langle v_2| \sigma_z |v_2\rangle$$

Note that we already computed $\langle v_2| \sigma_z |v_2\rangle = \cos\theta$, and so we just need $\langle v_2| \sigma_z |v_1\rangle$, which is equal to $\langle v_1| \sigma_z |v_2\rangle$ since σ_z is symmetric in the canonical basis, and symmetry is preserved in an orthonormal change of basis. We then find $\langle v_1| \sigma_z |v_2\rangle = -\sin\theta$ and so:

$$\langle \sigma_x \sigma_{x+y}\rangle = \frac{\lambda_1^y \sin^2\theta + \lambda_2^y \cos^2\theta}{\lambda_2^y} = \cos^2\theta + \left(\frac{\lambda_1}{\lambda_2}\right)^y \sin^2\theta$$

$\lambda_{1,2}$ have been computed in (1.2), and from the parameterization of $\hat{\boldsymbol{n}}$ (1.14) we have $\cos^2\theta = n_3^2 = (a_3/a)^2$ and $\sin^2\theta = n_x^2 + n_y^2 = (a_1/a)^2$, with the values found in (1.16).

Since $\lambda_1 < \lambda_2$, when $y \to +\infty$ the second term vanishes, and:

$$\langle \sigma_x \sigma_{x+y}\rangle \xrightarrow[y\to\infty]{} \cos^2\theta = \cos\theta \cdot \cos\theta = \langle \sigma_x\rangle \langle \sigma_{x+y}\rangle$$

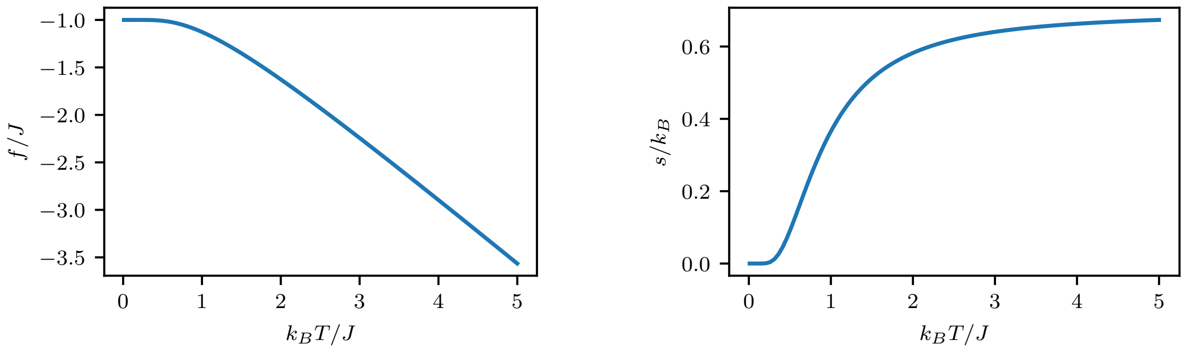
This means that two *spins* that are *infinitely* far apart are effectively *independent.*

When $h = 0$, the two-point correlation reduces to:

$$\langle \sigma_x \sigma_{x+y}\rangle = \left(\frac{e^K + e^{-K}}{e^K + e^{-K}}\right)^y = (\tanh K)^y$$

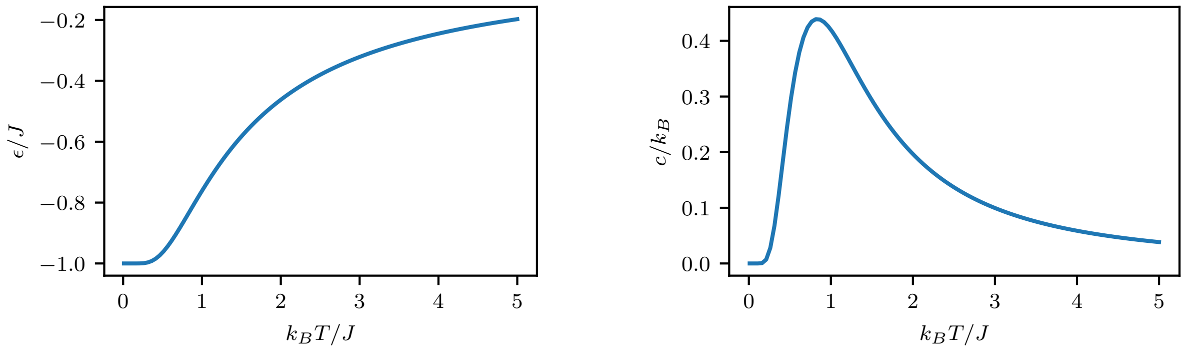
which coincides with the result already found in section 4.3.1 of the main notes, where we used *open* boundary conditions instead of periodic ones (in the thermodynamic limit they are effectively the same, as we will see in part B).

A plot of $\langle \sigma_x \sigma_{x+y}\rangle$ as a function of y is shown in fig. 1.1g.



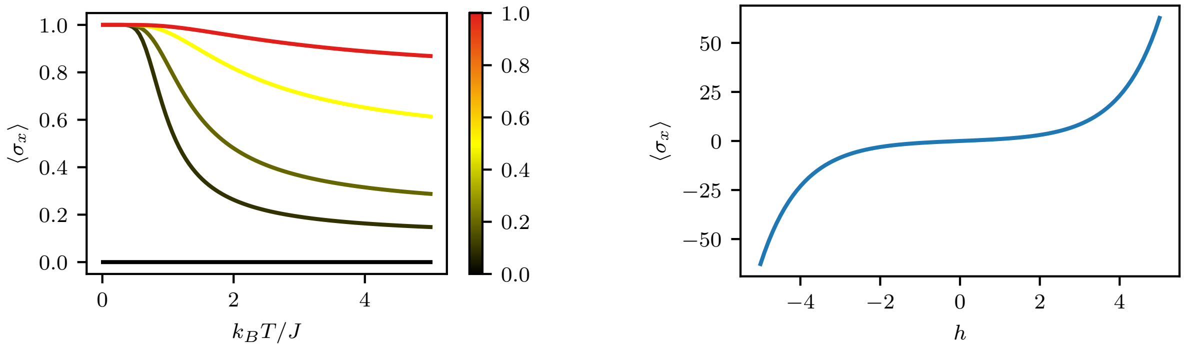
(a) Free energy f per node ($h = 0$).

(b) Entropy s per node ($h = 0$).



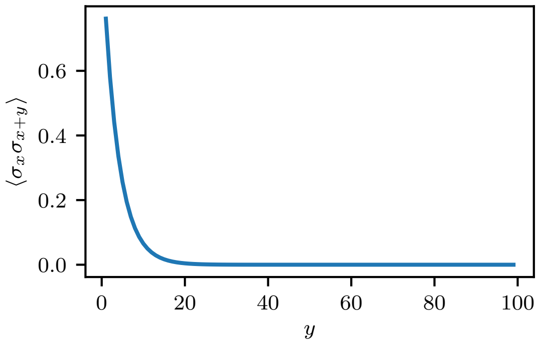
(c) Mean energy ϵ per node ($h = 0$).

(d) Specific heat c per node ($h = 0$).



(e) Average magnetization $\langle\sigma_x\rangle$ for $h = 0$, 0.1, 0.2, 0.5, 1.

(f) Average magnetization $\langle\sigma_x\rangle$ for $K = 1$.



(g) Two-point correlation function $\langle\sigma_x\sigma_{x+y}\rangle$ for $h = 0$ and $K = 1$.

Figure (1.1) – Plots of various quantities of interest. Note that $K_BT/J = 1/K$.

1.1.2 Part B

Let's consider the same model with **open boundary conditions**. The Hamiltonian is given by:

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

We begin by computing the partition function Z:

$$Z = \sum_{\{\boldsymbol{\sigma}\}} e^{-\beta\mathcal{H}(\boldsymbol{\sigma})} = \sum_{\{\boldsymbol{\sigma}\}} \exp\left(K\sum_{x=1}^{N-1}\sigma_x\sigma_{x+1} + h\sum_{x=1}^{N}\sigma_x\right)$$

We rewrite the sum $\sum_x \sigma_x$ in as follows:

$$\begin{aligned}\sum_{x=1}^{N}\sigma_x = \frac{1}{2}2\sum_{x=1}^{N}\sigma_x = \frac{1}{2}\Big[\quad & \sigma_1+\sigma_2+\cdots+\sigma_{N-1} + \sigma_N \\ & \sigma_1 + \sigma_2+\sigma_3+\cdots+\sigma_N\Big] = \\ = \frac{1}{2}&\left(\sum_{x=1}^{N-1}(\sigma_x+\sigma_{x+1}) + \sigma_1+\sigma_N\right)\end{aligned} \tag{1.17}$$

Substituting back:

$$Z = \sum_{\{\boldsymbol{\sigma}\}}\prod_{x=1}^{N-1} \underbrace{\exp\left(K\sigma_x\sigma_{x+1} + h\frac{\sigma_x+\sigma_{x+1}}{2}\right)}_{T_{\sigma_x\sigma_{x+1}}} \exp\left(h\frac{\sigma_1}{2}\right)\exp\left(h\frac{\sigma_N}{2}\right)$$

We define the 2×2 transfer matrix T as:

$$\mathrm{T}_{\sigma\sigma'} = \exp\left(K\sigma\sigma' + h\frac{\sigma_x+\sigma_{x+1}}{2}\right)$$

and the vector $\boldsymbol{v} = (v(+1), v(-1))$ as:

$$v(\sigma) = \exp\left(h\frac{\sigma}{2}\right)$$

Leading to:

$$\begin{aligned}Z &= \sum_{\{\sigma\}}\prod_{x=1}^{N-1} T_{\sigma_x\sigma_{x+1}} v(\sigma_1)v(\sigma_N) = \\ &= \sum_{\sigma_1=\pm1}\sum_{\sigma_2=\pm1}\cdots\sum_{\sigma_{N-1}=\pm1}\sum_{\sigma_N=\pm1} v(\sigma_1)T_{\sigma_1\sigma_2}\cdots T_{\sigma_{N-1}\sigma_N}v(\sigma_N) = \\ &= \sum_{\sigma_1=\pm1}\sum_{\sigma_N=\pm1} v(\sigma_1)(\mathrm{T}^{N-1})_{\sigma_1\sigma_N}v(\sigma_N) = \boldsymbol{v}^T\mathrm{T}^{N-1}\boldsymbol{v} = \langle v|\,\mathrm{T}^{n-1}\,|v\rangle\end{aligned}$$

The scalar product can be computed in the basis $|v_{1,2}\rangle$ where $\mathrm{T} = \mathrm{diag}(\lambda_1,\lambda_2)$. The change of basis can be done quickly by using completeness:

$$\langle v|\,\mathrm{T}^{n-1}\,|v\rangle = \sum_{i,j=1}^{2}\langle v|v_i\rangle\,\lambda_1^{N-1}\,\langle v_j|v\rangle = \langle v|v_1\rangle^2\,\lambda_1^{N-1} + \langle v|v_2\rangle^2\,\lambda_2^{N-1}$$

There is no necessity of computing $\langle v|v_1\rangle$ or $\langle v|v_2\rangle$, as they won't be significant in the thermodynamic limit.

In fact, let's consider the free energy per node f:

$$\begin{aligned}\frac{\ln Z}{N} \equiv -\beta f &= \frac{1}{N}\ln\left[\langle v|v_1\rangle^2 \lambda_1^{N-1} + \langle v|v_2\rangle^2 \lambda_2^{N-1}\right] = \\ &= \frac{1}{N}\ln\left[\lambda_2^{N-1}\Big(\langle v|v_1\rangle^2 \left(\frac{\lambda_1}{\lambda_2}\right)^{N-1} + \langle v|v_2\rangle^2\Big)\right]\end{aligned} \tag{1.18}$$

Since $\lambda_1 < \lambda_2$, when $N \gg 1$, the first term vanishes, leaving:

$$-\beta f = \frac{N-1}{N}\ln\lambda_2 + \frac{2}{N}\ln\langle v|v_2\rangle \xrightarrow[N\to+\infty]{} \ln\lambda_2$$

which is exactly the same result we found in (1.4). This also means that all the thermodynamic quantities we computed in part A have the same expression for the IM with o.b.c.

Intuitively, since in the thermodynamic limit the system is *infinite*, periodic and open boundary conditions are *effectively* the same.

1.1.3 Part C

We now consider the case with + boundary conditions: $\sigma_1 = \sigma_N = +1$. The partition function becomes:

$$Z = \sum_{\{\boldsymbol{\sigma}\}} e^{-\beta\mathcal{H}(\boldsymbol{\sigma})} = \sum_{\sigma_2=\pm1}\cdots\sum_{\sigma_{N-1}=\pm1}\exp\left(K\sum_{x=1}^{N-1}\sigma_x\sigma_{x+1} + h\sum_{x=1}^{N}\sigma_x\right) \qquad \sigma_1 = \sigma_N \equiv +1$$

We can repeat the argument we used in (1.17), leading to:

$$\begin{aligned}Z &= \sum_{\sigma_2=\pm1}\cdots\sum_{\sigma_{N-1}=\pm1}\exp\left(\frac{h}{2}\sigma_1\right)\mathrm{T}_{\sigma_1\sigma_2}\cdots\mathrm{T}_{\sigma_{N-1}\sigma_N}\exp\left(\frac{h}{2}\sigma_N\right) = \\ &= e^{h/2}(\mathrm{T}^{N-1})_{1,1}e^{h/2} = \\ &= e^{h/2}\begin{pmatrix}1 & 0\end{pmatrix}\mathrm{T}^{N-1}\begin{pmatrix}1\\0\end{pmatrix}e^{h/2} = \begin{pmatrix}e^{h/2} & 0\end{pmatrix}\mathrm{T}^{N-1}\begin{pmatrix}e^{h/2}\\0\end{pmatrix} = \\ &= \tilde{\boldsymbol{v}}^T\mathrm{T}^{N-1}\tilde{\boldsymbol{v}} = \langle\tilde{v}|\,\mathrm{T}^{N-1}\,|\tilde{v}\rangle\end{aligned}$$

where $\tilde{\boldsymbol{v}} = (e^{h/2}, 0)^T$. To compute the scalar product we use again *completeness*:

$$\langle\tilde{v}|\,\mathrm{T}^{N-1}\,|\tilde{v}\rangle = \langle\tilde{v}|v_1\rangle^2\lambda_1^{N-1} + \langle\tilde{v}|v_2\rangle^2\lambda_2^{N-1}$$

In the thermodynamic limit, the term λ_2 dominates, and everything else (including the prefactors) can be neglected. In fact, by repeating the same computation we did in (1.18), we obtain for the free energy:

$$-\beta f \xrightarrow[N\to+\infty]{} \ln\lambda_2$$

1.1.4 Part D

Consider the Ising Model with both nearest-neighbours and next-nearest-neighbours interactions in $d = 1$:

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

To compute the partition function Z, we can still use the same logic from before, i.e. construct a transfer matrix T. However, we first need to rewrite the Hamiltonian as the product of terms $\mathrm{T}_{\sigma,\sigma'}$, depending on only *two (consecutive) indices*. As of now, this is not possible - since we have 3 different indices: x, $x+1$ and $x+2$. There is no way to remove one of them if we want to account for both kind of interactions. So, the *trick* is to *add* a fourth index, and group them by 2, forming some kind of *multi-index* (or binary index).

We can do this by reasoning with **parity**. In fact, note that the nearest-neighbour interactions always involve spins with *different parity*, while the next-to-nearest-neighbour interactions only connect spins with the *same parity*. So, let's *group* the spins in two different *chains* depending on their parity. The first chain will contain all the *odd* spins $\sigma_i^{(1)} \equiv \sigma_{2i+1}$, and the second one all the *even* spins $\sigma_i^{(2)} \equiv \sigma_{2i}$. With this notation, the nearest neighbours interactions involve always spins of different chains (i.e. different parities), and the next-to-nearest-neighbours interaction always spins from the same chain.
We can then rewrite the Hamiltonian as follows (suppose, for simplicity, that N is even):

$$\mathcal{H}(\boldsymbol{\sigma}) = -J_1[\sum_{x=1}^{N/2}\sigma_x^{(1)}\sigma_x^{(2)} + \sigma_x^{(2)}\sigma_{x+1}^{(1)}] - J_2\sum_{x=1}^{N/2}[\sigma_x^{(1)}\sigma_{x+1}^{(1)} + \sigma_x^{(2)}\sigma_{x+1}^{(2)}] - B\sum_{x=1}^{N/2}[\sigma_x^{(1)} + \sigma_x^{(2)}] \tag{1.19}$$

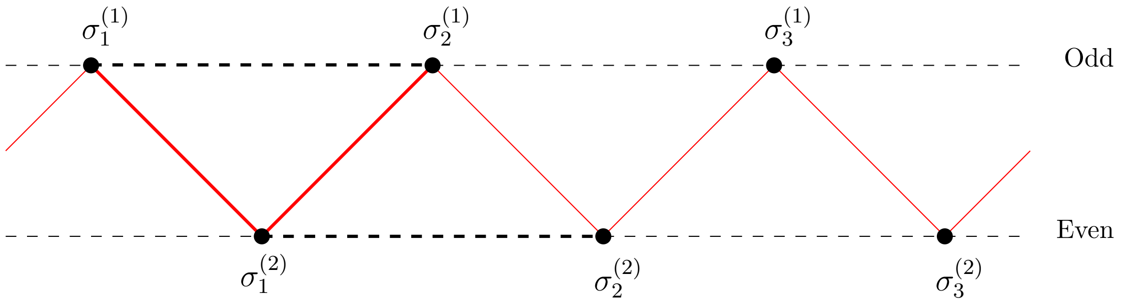


Figure (1.2) – Graphical representation of the IM model with both nearest-neighbour and next-to-nearest-neighbour interactions. Spins are represented as black dots, and ordered in two lines (chains) depending on their *parity*. The red continuous lines connect nearest-neighbours (J_1 terms), while the black dashed lines join next-to-nearest-neighbours (J_2 terms). The interactions described by the first term ($x = 1$) of (1.19) are highlighted in bold.

The two *multi*-indices of the transfer matrix will be $(\sigma_x^{(1)}, \sigma_x^{(2)})$ and $(\sigma_{x+1}^{(1)}, \sigma_{x+1}^{(2)})$, and so we need all terms to contain both of them:

$$\begin{aligned}\mathcal{H}(\boldsymbol{\sigma}) = -\Big[\frac{J_1}{2}\sum_{x=1}^{N/2}[\sigma_x^{(1)}\sigma_x^{(2)} + 2\sigma_x^{(2)}\sigma_{x+1}^{(1)} + \sigma_{x+1}^{(1)}\sigma_{x+1}^{(2)}] + J_2\sum_{x=1}^{N/2}[\sigma_x^{(1)}\sigma_{x+1}^{(1)} + \sigma_x^{(2)}\sigma_{x+1}^{(2)}] + \\ + \frac{B}{2}\sum_{x=1}^{N/2}[\sigma_x^{(1)} + \sigma_x^{(2)} + \sigma_{x+1}^{(1)} + \sigma_{x+1}^{(2)}]\Big]\end{aligned}$$

The partition function is given by:

$$Z = \sum_{\{\boldsymbol{\sigma}\}} e^{-\beta\mathcal{H}(\boldsymbol{\sigma})} = \sum_{\substack{\sigma_1^{(1)}=\pm 1\\ \sigma_1^{(2)}=\pm 1}} \cdots \sum_{\substack{\sigma_{N/2}^{(1)}=\pm 1\\ \sigma_{N/2}^{(2)}=\pm 1}} \prod_{i=1}^{N/2} \exp\left(\frac{K_1}{2}\left[\sigma_x^{(1)}\sigma_x^{(2)} + 2\sigma_x^{(2)}\sigma_{x+1}^{(1)} + \sigma_{x+1}^{(1)}\sigma_{x+1}^{(2)}\right]\right.$$

$$\left. K_2\left[\sigma_x^{(1)}\sigma_{x+1}^{(1)} + \sigma_x^{(2)}\sigma_{x+1}^{(2)}\right] + \frac{B}{2}\left[\sigma_x^{(1)} + \sigma_x^{(2)} + \sigma_{x+1}^{(1)} + \sigma_{x+1}^{(2)}\right]\right)$$

The exponential term is one entry of a 4 × 4 transfer matrix T:

$$\mathrm{T}_{(\sigma_x^{(1)},\sigma_x^{(2)}),(\sigma_{x+1}^{(1)},\sigma_{x+1}^{(2)})}$$

By mapping $\sigma_x = \pm 1 \to \{0, 1\}$, each "multi-index" is a binary number, defining a position in the matrix. For example, when $\sigma_x^{(1)} = \sigma_x^{(2)} = \sigma_{x+1}^{(1)} = \sigma_{x+1}^{(2)} = +1$, the matrix entry will be $\mathrm{T}_{(1,1),(1,1)} \equiv \mathrm{T}_{4,4}$. In this way, the sum of the product of exponentials can be interpreted as a *matrix product*, leading to:

$$Z = \mathrm{Tr}(\mathrm{T}^{N/2})$$