# Handin 3

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Date: February 8, 2024

## Problem 1

Consider the one-dimensional Ising-model.

### a)

In the thermodynamics limit and $H = 0$, write an expression of the free energy $\mathcal{F}$. Determine the low and high temperature limits of $\mathcal{F}$ and explain what they imply.

**Answer:** The partition function for the Ising model is given by:

$$Z = \sum_{\{S\}} \exp\left[h\sum_i S_i + K\sum_{\langle ij\rangle} S_iS_j\right],$$

and since $H = 0$, the first term is zero.

$$Z = \sum_{\{S\}} \exp\left[K\sum_{\langle ij\rangle} S_iS_j\right].$$

One rewrite the second sum in the following manner,

$$\begin{aligned}Z &= \sum_{\{S\}} \exp\left[K\sum_{i=1}^{N-1} S_iS_{i+1}\right]\\ &= 2\left(2\cosh(K)\right)^{N-1}.\end{aligned}$$

The free energy is then given by:

$$\begin{aligned}\mathcal{F} &= -k_bT\ln(Z)\\ &= -k_bT\ln\left(2\left(2\cosh(K)\right)^{N-1}\right)\\ &= -k_bT\left[\ln(2) + (N-1)\ln\left(2\cosh(K)\right)\right]\\ &= -k_bT\left[\ln(2) + (N-1)\ln\left(e^K + e^{-K}\right)\right]\\ &= -k_bT\left[\ln(2) + (N-1)\ln\left[e^K\left(1+e^{-2K}\right)\right]\right]\\ &= -k_bT\left[\ln(2) + (N-1)\left(K + \ln\left(1+e^{-2K}\right)\right)\right].\end{aligned}$$

The low and high temperature limits are given by:

$$\begin{aligned}
&\lim_{T\to 0}\lim_{N\to\infty}\left[-k_bT\left[\ln(2)+(N-1)\left(K+\ln\left(1+e^{-2K}\right)\right)\right]\right] \\
&=\lim_{T\to 0}\lim_{N\to\infty}\left[-k_bT\left[N\left(\frac{J}{k_bT}+\ln\left(1+e^{-\frac{2J}{k_bT}}\right)\right)\right]\right] \\
&=\lim_{T\to 0}\lim_{N\to\infty}\left[-k_bT\left[N\left(\frac{J}{k_bT}+\ln\left(1+e^{-\frac{2J}{k_bT}}\right)\right)\right]\right] \\
&=\lim_{N\to\infty}\left[-JN\right]=-\infty, \\
&\lim_{T\to \infty}\lim_{N\to\infty}\left(-k_bT\left[\ln(2)+(N-1)\left(K+\ln\left(1+e^{-2K}\right)\right)\right]\right)=-\infty,
\end{aligned}$$

In the thermodynamic limit, the free energy diverges.

## b)

Obtain expressions for the average energy $\langle E\rangle$ and the heat-capacity $C$ using the expression of $\mathcal{F}$.

**Answer:** The average energy is defined by:

$$\begin{aligned}
\langle E\rangle &= -\frac{1}{Z}\frac{\partial Z}{\partial\beta} \\
&= -\frac{1}{\left(2\cosh(J\beta)\right)^{N-1}}\frac{\partial}{\partial\beta}\left[\left(2\cosh(J\beta)\right)^{N-1}\right] \\
&= -\frac{2}{\left(2\cosh(J\beta)\right)^{N-1}}\left(N-1\right)J\sinh(J\beta)\left(2\cosh(J\beta)\right)^{N-2} \\
&= -J\left(N-1\right)\tanh(J\beta).
\end{aligned}$$

The heat capacity is defined by:

$$\begin{aligned}
C &= \frac{\partial\langle E\rangle}{\partial T} \\
&= \frac{\partial}{\partial\beta}\left(-J\left(N-1\right)\tanh\left(\frac{J}{k_bT}\right)\right) \\
&= \frac{J^2}{k_bT^2}\frac{(N-1)}{\cosh^2\left(\frac{J}{k_bT}\right)}.
\end{aligned}$$

## c)

Consider now the Ising model in a field and write an expression for $\mathcal{F}$ (again in the thermodynamic limit).

**Answer:** Now $H$ is non-zero, and thus the partition function is given by:

$$Z=\sum_{\{S\}}\exp\left[h\sum_i S_i+K\sum_{\langle ij\rangle}S_iS_j\right].$$

Furthermore, with introducing the transfer matrix, one obtains that the free energy can be written as:

$$\begin{aligned}\mathcal{F} &= -k_b T N \ln \left[ e^K \left( \cosh(h) + \sqrt{\sinh^2(h) + e^{-4K}} \right) \right] \\ &= -JN - k_b T N \ln \left[ \cosh(h) + \sqrt{\sinh^2(h) + e^{-4K}} \right].\end{aligned}$$

## d)

Compute the magnetization per spin $M$. What is $M$ in the limit $T \to 0$?

**Answer:** One computes the following expression for the magnetization per spin:

$$\begin{aligned}M &= \frac{1}{N} \frac{\partial \mathcal{F}}{\partial H} \\ &= \frac{1}{k_b T} \frac{\partial}{\partial h} \left( -J - k_b T \ln \left[ \cosh(h) + \sqrt{\sinh^2(h) + e^{-4K}} \right] \right) \\ &= \frac{\sinh^2(h)}{\cosh^2(h) + e^{-4K}}.\end{aligned}$$

# Problem 2

Consider the $d = 1$ Ising-model with periodic boundary conditions.

## a)

Construct the matrix $\mathbf{S}$ which diagonalises the transfer matrix $\mathbf{T}$. You will find it useful to write the matrix elements in terms of the variable $\theta$ given by:

$$\coth(2\theta) = e^{2K} \sinh(h).$$

**Answer:** Firstly, we define the transfer matrix $\mathbf{T}$ as:

$$\mathbf{T} = \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{-h+K} \end{pmatrix}.$$

A matrix $\mathbf{S}$ that diagonalises $\mathbf{T}$ is given by:

$$\mathbf{T}' = \mathbf{S}^{-1} \mathbf{T} \mathbf{S} \tag{1}$$

$$\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} = \mathbf{S}^{-1} \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{-h+K} \end{pmatrix} \mathbf{S}. \tag{2}$$

One needs to find the eigenvalues of $\mathbf{T}$, which is achieved by solving the characteristic equation:

$$\begin{aligned}\det(T - \lambda I) &= \begin{vmatrix} e^{K+h} - \lambda & e^{-K} \\ e^{-K} & e^{-h+K} - \lambda \end{vmatrix} \\ &= \left( e^{K+h} - \lambda \right) \cdot \left( e^{K-h} - \lambda \right) - e^{-2K} \\ &= \lambda^2 - \left( e^{K+h} + e^{K-h} \right) \lambda + e^{2K} - e^{-2K}\end{aligned}$$

The roots of this equation are given by:

$$\begin{aligned}\lambda_{1,2} &= \frac{e^{K+h}+e^{K-h}}{2} \pm \sqrt{\left(\frac{e^{K+h}+e^{K-h}}{2}\right)^2 - e^{2K} + e^{-2K}} \\ &= e^K\left[\cosh(h) \pm \sqrt{\sinh^2(h) + e^{-4K}}\right].\end{aligned}$$

Thus, $\lambda_1$ and $\lambda_2$ are the eigenvalues of $\mathbf{T}$, i.e. $\lambda_{1,2} = e^K\left[\cosh(h) \pm \sqrt{\sinh^2(h) + e^{-4K}}\right]$. Furthermore, we seek the eigenvectors corresponding to the eigenvalues of $\mathbf{T}$. The eigenvectors are given by:

$$\begin{aligned}(\lambda_1\mathbf{I} - \mathbf{T})\mathbf{v}_1 &= \mathbf{0}, \\ (\lambda_2\mathbf{I} - \mathbf{T})\mathbf{v}_2 &= \mathbf{0}.\end{aligned}$$

Looking at the first equation, one obtains:

$$\begin{gathered}\begin{pmatrix}\lambda_1 - e^{K+h} & -e^{-K} \\ -e^{-K} & \lambda_1 - e^{-h+K}\end{pmatrix}\begin{pmatrix}v_{11} \\ v_{12}\end{pmatrix} = \begin{pmatrix}0 \\ 0\end{pmatrix} \\ v_{11}\left(\lambda_1 - e^{K+h}\right) - v_{12}e^{-K} = 0 \\ v_{12}\left(\lambda_1 - e^{-h+K}\right) - v_{11}e^{-K} = 0\end{gathered}$$

This implies that one can write the eigenvector of $\lambda_1$ as:

$$\mathbf{v}_1 = \begin{pmatrix}v_{11} \\ v_{12}\end{pmatrix} = \begin{pmatrix}e^{-K} \\ -e^K\sinh(h) + \sqrt{e^{2K}\sinh^2(h) + e^{-2k}}\end{pmatrix},$$

and similarly, the eigenvector of $\lambda_2$ is given by:

$$\mathbf{v}_2 = \begin{pmatrix}v_{21} \\ v_{22}\end{pmatrix} = \begin{pmatrix}-e^K\sinh(h) + \sqrt{e^{2K}\sinh^2(h) + e^{-2k}} \\ -e^{-K}\end{pmatrix}.$$

Using $\cot(2\theta) = e^{2K}\sinh(h)$, on the term $-e^k\sinh(h) + \sqrt{e^{2K}\sinh^2(h) + e^{-2K}}$, one gets:

$$\begin{aligned}-e^k\sinh(h) + \sqrt{e^{2K}\sinh^2(h) + e^{-2K}} &= e^{-K}\left(-e^{2K}\sinh(h) + \sqrt{\cot^2(2\theta) + 1}\right) \\ &= e^{-K}\tan(\theta).\end{aligned}$$

Thus, the matrix $\mathbf{S}$ can be written as, after normalizing the eigenvectors, i.e $\mathbf{v_i}/\|\mathbf{v_i}\|$:

$$\mathbf{S} = \begin{pmatrix}\cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta)\end{pmatrix}.$$

## b)

Derive the relation:

$$\langle S_i\rangle = \frac{\mathrm{Tr}\left(\mathbf{S}^{-1}\sigma_z\mathbf{S}\mathbf{T}'^N\right)}{Z_N},$$

and use your answer from part a) to show that $\langle S_i \rangle = \cos(2\theta)$ as $N \to \infty$. Similarly compute $\langle S_i S_j \rangle$ and hence show that in the thermodynamics limit:

$$
\begin{aligned}
G(i, i+j) &= \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle \\
&= \sin^2(2\theta) \left( \frac{\lambda_2}{\lambda_1} \right)^j .
\end{aligned}
$$

**Answer:** We begin by stating that the average spin of a particle $i$ is given by:

$$
\begin{aligned}
\langle S_i \rangle &= \frac{1}{Z_n} \sum_{S_1} \ldots \sum_{S_N} T_{S_1,S_2} \ldots T_{S_{i-1},S_i} S_i \ldots T_{S_{N-1},S_N} \\
&= \frac{1}{Z_n} \sum_{S_1} \ldots \sum_{S_N} \ldots \mathbf{T} \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{=\sigma_z} \mathbf{T} \ldots \mathbf{T} \sigma_z \mathbf{T},
\end{aligned}
$$

This then yields that the average spin of particle $i$ can be written as:

$$
\langle S_i \rangle = \frac{\mathrm{Tr}\left(\sigma_z \mathbf{T}^N\right)}{Z_n}.
$$

From this, one then inverts eq (2), such that $\mathbf{T} = \mathbf{S}\mathbf{T}'\mathbf{S}^{-1}$, and thus:

$$
\langle S_i \rangle = \frac{\mathrm{Tr}\left(\sigma_z \left[\mathbf{S}\mathbf{T}'\mathbf{S}^{-1}\right]^N\right)}{Z_n}.
$$

From this, one expands the $(\mathbf{S}T'\mathbf{S}^{-1})^N$ term and utilizes that $\mathbf{S}^{-1} \cdot \mathbf{S} = \mathbf{I}$, such that one obtain:

$$
\begin{aligned}
\langle S_i \rangle &= \frac{\mathrm{Tr}\left(\sigma_z \mathbf{S}\mathbf{T}'\mathbf{S}^{-1}\mathbf{S}T' \ldots \mathbf{S}T'\mathbf{S}^{-1}\right)}{Z_N} \\
\langle S_i \rangle &= \frac{\mathrm{Tr}\left(\mathbf{S}^{-1}\sigma_z \mathbf{S}\mathbf{T}'^N\right)}{Z_N}.
\end{aligned}
$$

In order to evaluate $\langle S_i \rangle$ in the thermodynamic limit, one has to evaluate the expression $\mathbf{S}^{-1}\sigma_z\mathbf{S}$

$$
\begin{aligned}
\mathbf{S}^{-1}\sigma_z\mathbf{S} &= \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \\
&= \begin{pmatrix} \cos(2\theta) & -\sin(2\theta) \\ -\sin(2\theta) & -\cos(2\theta) \end{pmatrix}.
\end{aligned}
$$

Thus, $\langle S_i \rangle$ can be expressed as:

$$
\begin{aligned}
\langle S_i \rangle &= \frac{\mathrm{Tr}\left(\mathbf{S}^{-1}\sigma_z \mathbf{S}\mathbf{T}'^N\right)}{Z_N} \\
&= \frac{\mathrm{Tr}\left(\underbrace{\begin{pmatrix} \cos(2\theta) & -\sin(2\theta) \\ -\sin(2\theta) & -\cos(2\theta) \end{pmatrix}}_{=\delta} \cdot \begin{pmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{pmatrix}\right)}{\mathrm{Tr}\left(T^N\right)}
\end{aligned}
$$

In the thermodynamic limit, this then simplifies to:

$$
\langle S_i \rangle = \cos(2\theta).
$$

The correlation term $\langle S_i S_j \rangle$ is then given by:

$$\langle S_i S_j \rangle = \frac{1}{\mathrm{Tr}\left(T^N\right)} \left( \mathbf{T}'^i \cdot \delta \mathbf{T}'^j \delta \mathbf{T}'^{N-i-j} \right).$$

This, in the thermodynamic limit, can be written as:

$$\langle S_i S_j \rangle = \cos^2(2\theta) + \sin^2(2\theta) \left( \frac{\lambda_2}{\lambda_1} \right)^j.$$

Finally, the correlation function $G(i, i+j)$ is given by:

$$\begin{aligned} G(i, i+j) &= \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle \\ &= \cos^2(2\theta) + \sin^2(2\theta) \left( \frac{\lambda_2}{\lambda_1} \right)^j - \cos^2(2\theta) \\ &= \sin^2(2\theta) \left( \frac{\lambda_2}{\lambda_1} \right)^j. \end{aligned}$$

## c)

Calculate the isothermal suspectability $\chi_T$ from the formula given for $M(H)$ in the text. Verify explicitly that $\chi_T = \beta \sum_j G(i, i+j)$ (in the thermodynamic limit the sum runs from $-\infty \to \infty$).

**Answer:** The isothermal susceptibility is defined by:

$$\chi_T = \frac{\partial M}{\partial H}.$$

The magnetization per spin is given by:

$$M = \sum_{i=1}^{N} \langle S_i \rangle = N \cos(2\theta).$$

Thus, the isothermal susceptibility is given by:

$$\begin{aligned} \chi_T = \frac{\partial M}{\partial H} &= N \frac{\partial \cos(2\theta)}{\partial H} \\ &= N\beta \frac{\partial \cos(2\theta)}{\partial h} \\ &= -N\beta \sin(2\theta) \frac{\partial 2\theta}{\partial h}. \end{aligned}$$

We now need to find an explicit expression for $\theta$ which one does from $\cot(2\theta) = e^{2K} \sinh(h)$, such that:

$$\theta = \frac{1}{2} \cot^{-1} \left( e^{2K} \sinh(h) \right).$$

This then yields:

$$\begin{aligned} \chi_T &= -N\beta \sin(2\theta) \frac{\partial \theta}{\partial h} \\ &= -2N\beta \sin(2\theta) \frac{\partial}{\partial h} \left( \frac{1}{2} \cot^{-1} \left( e^{2K} \sinh(h) \right) \right) \\ &= N\beta \sin^3(2\theta) \, e^{2K} \cosh(h). \end{aligned}$$

To prove that the magnetic susceptibility is given by $\chi_T = \sum_j G(i, i+j)$, one needs to evaluate the sum:

$$
\begin{aligned}
\sum_j G(i, i+j) &= \sum_j \sin^2(2\theta) \left(\frac{\lambda_2}{\lambda_1}\right)^j \\
&= N \sin^2(2\theta) \left(\frac{\lambda_1 + \lambda_2}{\lambda_1 - \lambda_2}\right) \\
&= N \sin^2(2\theta) \left(\frac{e^{-K}\sqrt{\cot^2(2\theta) + 1}}{e^K \cosh(h)}\right)^{-1} \\
&= N \sin^2(2\theta) \left(\sin(2\theta) e^{2K} \cosh(h)\right) \\
&= N \sin^3(2\theta)\, e^{2K} \cosh(h).
\end{aligned}
$$

Since the $\beta G(i, i+j) = \chi_T$ one has proved that the identify holds.

## d)

We will now consider what happens at the boundaries. Consider the partition function:

$$
Z(h, K) = \sum_{S_1} \cdot ... \sum_{S_N} \exp\left[h\left(S_1 + ... + S_N\right) + K\left(S_1 S_2 + ... + S_{N-1} S_N\right)\right].
$$

In this case, the partition function is not simply $Z = \mathrm{Tr}\left(\mathbf{T}'\right)^N$. Work out what the correct expression is, you will have to introduce a new matrix in addition to $\mathbf{T}$, and show that the free energy is given by:

$$
\mathcal{F} = N f_b(h, K) + f_s(h, K) + F_{f_s}(N, h, K),
$$

where $f_b$ is the bulk free energy, $f_s$ is the surface free energy and $F_{f_s}$ is an intrinsic finite size contribution that depends on the system size as $e^{-C(h,K)N}$, where $C$ is function.

**Answer:**

## e)

Check that in the case $h = 0$ and $N \to \infty$, your result for the surface free energy agrees with that obtained from $\lim_{N\to\infty} \mathcal{F}_N^{free} - \mathcal{F}_N^{periodic}$.

**Answer:**