

Handin 3

Author : Andreas Evensen

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:

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

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

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

One rewrite the second sum in the following manner,

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

The free energy is then given by:

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

The low and high temperature limits are given by:

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

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:

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

The heat capacity is defined by:

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

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:

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

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 $T \rightarrow 0$?

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 θ 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:

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

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, λ_1 and λ_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:

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

This implies that one can write the eigenvector of λ_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 λ_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:

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

b)

Derive the relation:

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

and use your answer from part a) to show that $\langle S_i \rangle = \cos(2\theta)$ as $N \rightarrow \infty$. 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:

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

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

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

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

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

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

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

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:

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

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:

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

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 susceptibility χ_T from the formula given for $M(H)$ in the text. Verify explicitly that $\chi_T = \sum_j G(i, i+j)$ (in the thermodynamic limit the sum runs from $-\infty \rightarrow \infty$).

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:

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

We now need to find an explicit expression for θ 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:

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

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

$$\begin{aligned}\sum_j G(i, i+j) &= \sum_j \sin^2(2\theta) \left(\frac{\lambda_2}{\lambda_1}\right)^j \\ &= \sin^2(2\theta) \sum_j \left(\frac{\lambda_2}{\lambda_1}\right)^j \\ &= \sin^2(2\theta) \sum_j \left(\frac{e^K \left[\cosh(h) - \sqrt{\sinh^2(h) + e^{-4K}} \right]}{e^K \left[\cosh(h) + \sqrt{\sinh^2(h) + e^{-4K}} \right]} \right)^j\end{aligned}$$

d)

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

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

In this case, the partition function is not simply $Z = \text{Tr}(\mathbf{T}')^N$. 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 $N \rightarrow \infty$, your result for the surface free energy agrees with that obtained from $\lim_{N \rightarrow \infty} \mathcal{F}_N^{\text{free}} - \mathcal{F}_N^{\text{periodic}}$.

Answer: