# FYS4130 - Oblig 2

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## Problem 1

The analytical calculations in problem 1 were done by hand on iPad. Unfortunately I don't have the time to write these into LaTeX, so I have instead included my iPad notes in the next pages.

# Problem 1

$$\begin{array}{cccccc} \uparrow & \times & \uparrow & \downarrow & \cdots & \times \\ 0 & 1 & 2 & 3 & & L-1 \end{array}$$

"x" = spin 0

a) $$Z = \sum_{\{\sigma\}} e^{-\beta H}$$

$$= \sum_{\{\sigma\}} e^{\sum_{i=0}^{L-1} \beta J \delta_{\sigma_i \sigma_{i+1}}}$$

$$= \sum_{\{\sigma\}} \prod_{i=0}^{L-1} e^{\beta J \delta_{\sigma_i \sigma_{i+1}}}$$

Let's define the transfer matrix

$$T_{\sigma_i \sigma_{i+1}} = e^{\beta J \delta_{\sigma_i \sigma_{i+1}}}$$

$$\underline{= \begin{pmatrix} e^{\beta J} & 1 & 1 \\ 1 & e^{\beta J} & 1 \\ 1 & 1 & e^{\beta J} \end{pmatrix}}$$

We then have

$$Z = \sum_{\{\sigma\}} \prod_{i=0}^{L-1} e^{\beta J \delta_{\sigma_i \sigma_{i+1}}}$$

$$= \sum_{\{\sigma\}} \prod_{i=0}^{L-1} T_{\sigma_i \sigma_{i+1}}$$

$$= \sum_{\{\sigma\}} T_{\sigma_0 \sigma_1} T_{\sigma_1 \sigma_2} \cdots T_{\sigma_{L-1} \sigma_0}$$

$$= \sum_{\{\sigma_0\}} (T^N)_{\sigma_0 \sigma_0} \qquad (N = L)$$

$$= \mathrm{Tr}\{T^N\}$$

$$= \mathrm{Tr}\left\{ \begin{pmatrix} e^{\beta J} & 1 & 1 \\ 1 & e^{\beta J} & 1 \\ 1 & 1 & e^{\beta J} \end{pmatrix}^N \right\}$$

We need to diagonalize T. We start by finding its eigenvalues:

$$0 = \det(T - \lambda \mathbb{1})$$

$$= \begin{vmatrix} e^{\beta J}-\lambda & 1 & 1 \\ 1 & e^{\beta J}-\lambda & 1 \\ 1 & 1 & e^{\beta J}-\lambda \end{vmatrix}$$

$$0 = (e^{\beta J}-\lambda)^3 + 2 - 3(e^{\beta J}-\lambda)$$

Get rid of exponents by guessing $\lambda = e^{\beta J} - \lambda_0$ for some $\lambda_0$. This gives

$$0 = \lambda_0^3 + 2 - 3\lambda_0$$

Can quickly see that $\lambda_0 = 1$ is a solution. Using polynomial division we find

$$(\lambda_0^3 - 3\lambda_0 + 2) : (\lambda_0 - 1) = \underline{\lambda_0^2 + \lambda_0 - 2}$$

$$\begin{array}{l} \underline{\lambda_0^3 - \lambda_0^2} \\ \lambda_0^2 - 3\lambda_0 + 2 \\ \underline{\lambda_0^2 - \lambda_0} \\ -2\lambda_0 + 2 \\ \underline{-2\lambda_0 + 2} \\ 0 \end{array}$$

$$\Rightarrow \quad \lambda_0 = \frac{-1 \pm \sqrt{1+8}}{2} = \frac{-1 \pm 3}{2}$$

$$\Rightarrow \quad \lambda_0 = 1 \quad \vee \quad \lambda_0 = -2$$

Thus we have

$\lambda = e^{\beta J} + 2$ with multiplicity 1

$\lambda = e^{\beta J} - 1$ with multiplicity 2

Diagonalizing gives

$$T = RDR^{-1}$$

with $D = \begin{pmatrix} e^{\beta J}+2 & 0 & 0 \\ 0 & e^{\beta J}-1 & 0 \\ 0 & 0 & e^{\beta J}-1 \end{pmatrix}$ and $R$ an invertible matrix with the eigenvectors of $T$ as columns.

Using this we have

$$Z = \mathrm{Tr}\{T^N\}$$

$$= \mathrm{Tr}\{\overbrace{\cancel{R^{-1}} D \cancel{R R^{-1}} D \cancel{R} \cdots \cancel{R^{-1}} D \cancel{R}}^{N \text{ times}}\}$$

↳ cyclic property

$$= \mathrm{Tr}\{D^N\}$$

$$Z = \left(e^{\beta J}+2\right)^N + 2\left(e^{\beta J}-1\right)^N$$

Average total internal energy:

$$U = \frac{1}{Z}\sum_{\{\sigma\}} H e^{-\beta H}$$

$$= -\frac{1}{Z}\frac{\partial Z}{\partial \beta}$$

$$= -\frac{1}{Z}\left[\frac{\partial}{\partial\beta}\left(e^{\beta J}+2\right)^N + 2\frac{\partial}{\partial\beta}\left(e^{\beta J}-1\right)^N\right]$$

$$= -\frac{1}{Z}\left[N\left(e^{\beta J}+2\right)^{N-1} e^{\beta J}\cdot J + 2N\left(e^{\beta J}-1\right)^{N-1} e^{\beta J}\cdot J\right]$$

$$= -NJe^{\beta J}\frac{\left(e^{\beta J}+2\right)^{N-1} + 2\left(e^{\beta J}-1\right)^{N-1}}{\left(e^{\beta J}+2\right)^{N} + 2\left(e^{\beta J}-1\right)^{N}}$$

At very high temperatures, $\beta \to 0$:

$$\lim_{\beta\to 0} U = -NJ\frac{(1+2)^{\cancel{N-1}} + \cancel{2\cdot(1-1)^{N-1}}}{\cancel{(1+2)^N} + \cancel{2\cdot(1-1)^N}}$$

$$= -\frac{1}{3}NJ \qquad \text{High } T$$

At very low temperatures, $\beta \to \infty$:

$$\lim_{\beta\to\infty} U = -NJ\lim_{\beta\to\infty} e^{\beta J}\frac{\left(e^{\beta J}\cancel{+2}\right)^{N-1} + 2\left(e^{\beta J}\cancel{-1}\right)^{N-1}}{\left(e^{\beta J}\cancel{+2}\right)^{N} + 2\left(e^{\beta J}\cancel{-1}\right)^{N}}$$ negligible as $\beta\to\infty$

$$= -NJ\lim_{\beta\to\infty}\frac{e^{N\beta J}+2e^{N\beta J}}{e^{N\beta J}+2e^{N\beta J}}$$

$= -NJ$ Low T

At low T all the spins have the same alignment. This can be seen since it is the only way to get $H = -J\sum_{i=0}^{L-1} \delta_{\sigma_i \sigma_{i+1}}$ to be $-JN$.

At high T the spin alignments are more random, with every spin taking on a random of the three possible values. On average, two neighbouring spins take the same value only one third of the time, resulting in $U = -\frac{1}{3}NJ$.

b) $\langle m\rangle = \frac{1}{Z}\sum_{\{\sigma\}}\frac{1}{N}\sum_{i=0}^{N-1} e^{i\frac{2\pi}{3}\sigma_i}\prod_{i=0}^{N-1} T_{\sigma_i\sigma_{i+1}}$

$$= \frac{1}{NZ}\sum_{i=0}^{N-1}\sum_{\{\sigma\}} e^{i\frac{2\pi}{3}\sigma_i} T_{\sigma_0\sigma_1}\cdots T_{\sigma_{N-1}\sigma_0}$$

$$= \frac{1}{NZ}\sum_{i=0}\sum_{\{\sigma\}} T_{\sigma_0\sigma_1}\cdots T_{\sigma_{i-1}\sigma_i} e^{i\frac{2\pi}{3}\sigma_i} T_{\sigma_i\sigma_{i+1}}\cdots T_{\sigma_{N-1}\sigma_0}$$

Let's define a matrix with the possible $m_i$-values along the diagonal:

$$M = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\frac{2\pi}{3}} & 0 \\ 0 & 0 & e^{i\frac{4\pi}{3}} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\frac{2\pi}{3}} & 0 \\ 0 & 0 & e^{-i\frac{2\pi}{3}} \end{pmatrix}$$

We then have

$$\langle m\rangle = \frac{1}{NZ}\sum_{i=0}^{N-1}\sum_{\{\sigma\}} T_{\sigma_0\sigma_1}\cdots T_{\sigma_{i-1}\sigma_i} M_{\sigma_i\sigma_i} T_{\sigma_i\sigma_{i+1}}\cdots T_{\sigma_{N-1}\sigma_0}$$

$$= \frac{1}{NZ}\sum_{i=0}^{N-1} \mathrm{Tr}\{T^i M T^{N-i}\}$$

$$= \frac{1}{NZ}\sum_{i=0}^{N-1} \mathrm{Tr}\{M T^N\}$$

$$= \frac{1}{NZ}\sum_{i=0}^{N-1} \mathrm{Tr}\{M R D^N R^{-1}\}$$

Need eigenvectors of $T$ to construct $R$. Let $\lambda_0 = e^{\beta J}+2$, $\lambda_1=\lambda_2=e^{\beta J}-1$. We find the eigenvectors by Gaussian elimination:

$$\lambda_0: \quad T-\lambda\mathbb{1} = \begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix} \overset{\text{Wolfram}}{\sim} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \end{pmatrix} \Rightarrow \vec{v}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$\lambda_{1,2}: \quad T-\lambda\mathbb{1} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \sim \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \Rightarrow \vec{v}_2 = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \ \vec{v}_3 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

$$\Rightarrow R = \begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & 0 \\ 1 & 0 & -1 \end{pmatrix}, \quad R^{-1} \overset{\text{Wolfram}}{=} \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix}$$

Using this we find

$$T^N = R D^N R^{-1}$$

$$= \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & 0 \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} \lambda_0^N & 0 & 0 \\ 0 & \lambda_1^N & 0 \\ 0 & 0 & \lambda_1^N \end{pmatrix}\begin{pmatrix} 1 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix}$$

$$= \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & 0 \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} \lambda_0^N & \lambda_0^N & \lambda_0^N \\ \lambda_1^N & -2\lambda_1^N & \lambda_1^N \\ \lambda_1^N & \lambda_1^N & -2\lambda_1^N \end{pmatrix}$$

$$= \frac{1}{3}\begin{pmatrix} \lambda_0^N + 2\lambda_1^N & \lambda_0^N - \lambda_1^N & \lambda_0^N - \lambda_1^N \\ \lambda_0^N - \lambda_1^N & \lambda_0^N + 2\lambda_1^N & \lambda_0^N - \lambda_1^N \\ \lambda_0^N - \lambda_1^N & \lambda_0^N - \lambda_1^N & \lambda_0^N + 2\lambda_1^N \end{pmatrix}$$

Furthermore, this gives

$$MT^N = \frac{1}{3}\begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\frac{2\pi}{3}} & 0 \\ 0 & 0 & e^{-i\frac{2\pi}{3}} \end{pmatrix}\begin{pmatrix} \lambda_0^N + 2\lambda_1^N & \lambda_0^N - \lambda_1^N & \lambda_0^N - \lambda_1^N \\ \lambda_0^N - \lambda_1^N & \lambda_0^N + 2\lambda_1^N & \lambda_0^N - \lambda_1^N \\ \lambda_0^N - \lambda_1^N & \lambda_0^N - \lambda_1^N & \lambda_0^N + 2\lambda_1^N \end{pmatrix}$$

$$\overset{\text{Wolfram}}{=} \frac{1}{3}\begin{pmatrix} \lambda_0^N + 2\lambda_1^N & \lambda_0^N - \lambda_1^N & \lambda_0^N - \lambda_1^N \\ e^{i\frac{2\pi}{3}}(\lambda_0^N - \lambda_1^N) & e^{i\frac{2\pi}{3}}(\lambda_0^N + 2\lambda_1^N) & e^{i\frac{2\pi}{3}}(\lambda_0^N - \lambda_1^N) \\ e^{-i\frac{2\pi}{3}}(\lambda_0^N - \lambda_1^N) & e^{-i\frac{2\pi}{3}}(\lambda_0^N - \lambda_1^N) & e^{-i\frac{2\pi}{3}}(\lambda_0^N + 2\lambda_1^N) \end{pmatrix}$$

Thus we find

$$\langle m \rangle = \frac{1}{NZ}\sum_{j=0}^{N-1} \mathrm{Tr}\{MT^N\}$$

$$= \frac{1}{NZ}\sum_{j=0}^{N} \frac{1}{3}\left(1 + \underbrace{e^{i\frac{2\pi}{3}} + e^{-i\frac{2\pi}{3}}}_{\substack{=2\cos(\frac{2\pi}{3}) \\ =-1}}\right)\left(\lambda_0^N + 2\lambda_1^N\right)$$

$$\boxed{\langle m \rangle = 0}$$

c) We have that

$$\langle m \rangle = \frac{1}{Z} \sum_{\{\sigma\}} \frac{1}{N} \sum_{i=0}^{N-1} m_i \, e^{-\beta H}$$

$$= \frac{1}{N} \sum_{i=0}^{N-1} \frac{1}{Z} \sum_{\{\sigma\}} m_i \, e^{-\beta H}$$

$$= \frac{1}{N} \sum_{i=0}^{N-1} \langle m_i \rangle$$

From the calculation in b) we know the content of this sum is zero, thus

$$\underline{\langle m_i \rangle = 0} \quad \forall i$$

We thus have

$$C(r) = \langle m_0^* m_r \rangle$$

$$= \frac{1}{Z} \sum_{\{\sigma\}} e^{-i\frac{2\pi}{3}\sigma_0} e^{i\frac{2\pi}{3}\sigma_r} \prod_{i=0}^{N-1} T_{\sigma_i \sigma_{i+1}}$$

$$= \frac{1}{Z} \sum_{\{\sigma\}} e^{-i\frac{2\pi}{3}\sigma_0} T_{\sigma_0\sigma_1} \cdots T_{\sigma_{r-1}\sigma_r} e^{i\frac{2\pi}{3}\sigma_r} T_{\sigma_r\sigma_{r+1}} \cdots T_{\sigma_{N-1}\sigma_0}$$

$$= \frac{1}{Z} \sum_{\{\sigma\}} M^\dagger_{\sigma_0\sigma_0} T_{\sigma_0\sigma_1} \cdots T_{\sigma_{r-1}\sigma_r} M_{\sigma_r\sigma_r} T_{\sigma_r\sigma_{r+1}} \cdots T_{\sigma_{N-1}\sigma_0}$$

$$= \frac{1}{Z} \operatorname{Tr}\{M^\dagger T^r M T^{N-r}\}$$

From b) we have

$$MT^{N-r} = \frac{1}{3} \begin{pmatrix} \lambda_0^{N-r} + 2\lambda_1^{N-r} & \lambda_0^{N-r} - \lambda_1^{N-r} & \lambda_0^{N-r} - \lambda_1^{N-r} \\ e^{i\frac{2\pi}{3}}(\lambda_0^{N-r} - \lambda_1^{N-r}) & e^{i\frac{2\pi}{3}}(\lambda_0^{N-r} + 2\lambda_1^{N-r}) & e^{i\frac{2\pi}{3}}(\lambda_0^{N-r} - \lambda_1^{N-r}) \\ e^{-i\frac{2\pi}{3}}(\lambda_0^{N-r} - \lambda_1^{N-r}) & e^{-i\frac{2\pi}{3}}(\lambda_0^{N-r} - \lambda_1^{N-r}) & e^{-i\frac{2\pi}{3}}(\lambda_0^{N-r} + 2\lambda_1^{N-r}) \end{pmatrix}$$

and similarly we find

$$M^\dagger T^r = \frac{1}{3}\begin{pmatrix} \lambda_0^r+2\lambda_1^r & \lambda_0^r-\lambda_1^r & \lambda_0^r-\lambda_1^r \\ e^{-i\frac{2\pi}{3}}(\lambda_0^r-\lambda_1^r) & e^{-i\frac{2\pi}{3}}(\lambda_0^r+2\lambda_1^r) & e^{-i\frac{2\pi}{3}}(\lambda_0^r-\lambda_1^r) \\ e^{i\frac{2\pi}{3}}(\lambda_0^r-\lambda_1^r) & e^{i\frac{2\pi}{3}}(\lambda_0^r-\lambda_1^r) & e^{i\frac{2\pi}{3}}(\lambda_0^r+2\lambda_1^r) \end{pmatrix}$$

Putting the two together gives

$$\mathrm{Tr}\left\{M^\dagger T^r M T^{N-r}\right\} = \frac{1}{9}\underset{\text{Trace, so we only need diagonal elements}}{\mathrm{Tr}}\left\{\begin{pmatrix} \lambda_0^r+2\lambda_1^r & \lambda_0^r-\lambda_1^r & \lambda_0^r-\lambda_1^r \\ e^{-i\frac{2\pi}{3}}(\lambda_0^r-\lambda_1^r) & e^{-i\frac{2\pi}{3}}(\lambda_0^r+2\lambda_1^r) & e^{-i\frac{2\pi}{3}}(\lambda_0^r-\lambda_1^r) \\ e^{i\frac{2\pi}{3}}(\lambda_0^r-\lambda_1^r) & e^{i\frac{2\pi}{3}}(\lambda_0^r-\lambda_1^r) & e^{i\frac{2\pi}{3}}(\lambda_0^r+2\lambda_1^r) \end{pmatrix} \cdot \begin{pmatrix} \lambda_0^{N-r}+2\lambda_1^{N-r} & \lambda_0^{N-r}-\lambda_1^{N-r} & \lambda_0^{N-r}-\lambda_1^{N-r} \\ e^{i\frac{2\pi}{3}}(\lambda_0^{N-r}-\lambda_1^{N-r}) & e^{i\frac{2\pi}{3}}(\lambda_0^{N-r}+2\lambda_1^{N-r}) & e^{i\frac{2\pi}{3}}(\lambda_0^{N-r}-\lambda_1^{N-r}) \\ e^{-i\frac{2\pi}{3}}(\lambda_0^{N-r}-\lambda_1^{N-r}) & e^{-i\frac{2\pi}{3}}(\lambda_0^{N-r}-\lambda_1^{N-r}) & e^{-i\frac{2\pi}{3}}(\lambda_0^{N-r}+2\lambda_1^{N-r}) \end{pmatrix}\right\}$$

$$\begin{aligned} &= \frac{1}{9}\Big[(\lambda_0^r+2\lambda_1^r)(\lambda_0^{N-r}+2\lambda_1^{N-r}) + \left(e^{i\frac{2\pi}{3}}+e^{-i\frac{2\pi}{3}}\right)(\lambda_0^r-\lambda_1^r)(\lambda_0^{N-r}-\lambda_1^{N-r}) \\ &\qquad + (\lambda_0^r+2\lambda_1^r)(\lambda_0^{N-r}+2\lambda_1^{N-r}) + \left(e^{-i\frac{2\pi}{3}}+e^{\overset{i\frac{2\pi}{3}}{\cancel{-i\frac{4\pi}{3}}}}\right)(\lambda_0^r-\lambda_1^r)(\lambda_0^{N-r}-\lambda_1^{N-r}) \\ &\qquad + (\lambda_0^r+2\lambda_1^r)(\lambda_0^{N-r}+2\lambda_1^{N-r}) + \left(e^{i\frac{2\pi}{3}}+e^{\overset{-i\frac{2\pi}{3}}{\cancel{i\frac{4\pi}{3}}}}\right)(\lambda_0^r-\lambda_1^r)(\lambda_0^{N-r}-\lambda_1^{N-r})\Big] \end{aligned}$$

$$= \frac{1}{3}\Big[(\lambda_0^r+2\lambda_1^r)(\lambda_0^{N-r}+2\lambda_1^{N-r}) + \underbrace{2\cos\left(\tfrac{2\pi}{3}\right)}_{=-1}(\lambda_0^r-\lambda_1^r)(\lambda_0^{N-r}-\lambda_1^{N-r})\Big]$$

$$= \frac{1}{3}\Big[(\lambda_0^r+2\lambda_1^r)(\lambda_0^{N-r}+2\lambda_1^{N-r}) - (\lambda_0^r-\lambda_1^r)(\lambda_0^{N-r}-\lambda_1^{N-r})\Big]$$

$$= \frac{1}{3}\Big[\cancel{\lambda_0^N} + \overset{3}{\cancel{2}}\lambda_0^r\lambda_1^{N-r} + \overset{3}{\cancel{2}}\lambda_0^{N-r}\lambda_1^r + \overset{3}{\cancel{4}}\lambda_1^N - \cancel{\lambda_0^N} + \cancel{\lambda_0^r\lambda_1^{N-r}} + \cancel{\lambda_0^{N-r}\lambda_1^r} - \cancel{\lambda_1^N}\Big]$$

$$= \underline{\lambda_1^N + \lambda_0^r\lambda_1^{N-r} + \lambda_0^{N-r}\lambda_1^r}$$

Thus we get

$$C(r) = \frac{\lambda_1^N + \lambda_0^r\lambda_1^{N-r} + \lambda_0^{N-r}\lambda_1^r}{Z}$$

$$\underline{\underline{C(r) = \frac{\lambda_1^N + \lambda_0^r\lambda_1^{N-r} + \lambda_0^{N-r}\lambda_1^r}{\lambda_0^N + 2\lambda_1^N}}} \qquad = \frac{\lambda_1^r}{\lambda_0^r}$$

The limit $L \to \infty$ is equivalent to $N \to \infty$. Using $\lambda_0 > \lambda_1$ we find in this limit:

$$\lim_{N\to\infty} C(r) = \frac{\lambda_1^N + \lambda_0^r \lambda_1^{N-r} + \lambda_0^{N-r}\lambda_1^r}{\lambda_0^N + 2\lambda_1^N} \quad \begin{array}{l} \cdot \frac{1}{\lambda_0} \\ \cdot \frac{1}{\lambda_0} \end{array}$$

$$= \lim_{N\to\infty} \frac{\left(\frac{\lambda_1}{\lambda_0}\right)^N + \left(\frac{\lambda_1}{\lambda_0}\right)^{N-r} + \left(\frac{\lambda_1}{\lambda_0}\right)^r}{1 + 2\left(\frac{\lambda_1}{\lambda_0}\right)^N}$$

$0 < \frac{\lambda_1}{\lambda_0} < 1$

$$= \left(\frac{\lambda_1}{\lambda_0}\right)^r$$

$$= \underline{\underline{\left(\frac{e^{\beta J} - 1}{e^{\beta J} + 2}\right)^r}} \qquad \text{for } L \to \infty$$

For $T=0$ we have $\beta \to \infty$, thus $\lambda_0 \approx \lambda_1 \approx e^{\beta J}$, so we get

$$\lim_{\beta\to\infty} C(r) = \lim_{\beta\to\infty} \frac{\lambda_1^N + \lambda_0^r \lambda_1^{N-r} + \lambda_0^{N-r}\lambda_1^r}{\lambda_0^N + 2\lambda_1^N}$$

$$= \lim_{\beta\to\infty} \frac{e^{\beta N J} + \cancel{e^{\beta r J}} e^{\beta(N-\cancel{r})J} + e^{\beta(N-\cancel{r})J}\cancel{e^{\beta r J}}}{e^{\beta N J} + 2e^{\beta N J}}$$

$$= \lim_{\beta\to\infty} \frac{3e^{\beta N J}}{3e^{\beta N J}}$$

$$= \underline{\underline{1}} \qquad \text{for } T=0$$

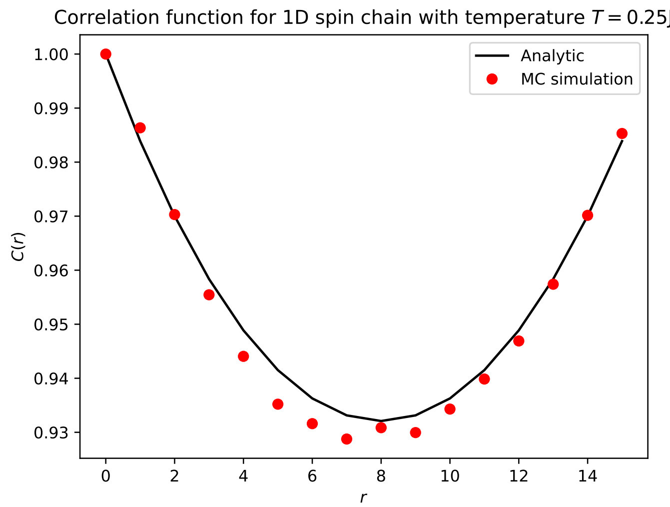


Figure 1: Correlation function $C(r)$ as a function of distance $r$ for temperature $T/J = 0.25$.

# Problem 2

## 2a)

The code I have used can be found at my Github page.[1]

## 2b)

The correlation function $C(r)$ from the Monte Carlo simulation for the one-dimensional spin chain is shown together with the analytical solution in Figures 1 and 2 for temperatures $T/J = 0.25$ and $T/J = 0.5$ respectively. The measurement points from the Monte Carlo simulation closely follows the analytical curve in both cases, although it is slightly off for some values in the $T/J = 0.25$ case. It is clear that the code works properly as the simulated results match the analytical results so well.

## 2c)

In Figure 3 I have plotted the real part of the average magnetization per site $\langle m \rangle$ as a function of temperature $T/J$ for the two-dimensional spin lattice. From the Figure it is clear that $\mathrm{Re}\{\langle m \rangle\} = 0$ at $T/J = 0$, meaning that the different spin sites take on varying values, representing a disordered system. This is counter-intuitive, as we would expect the spin states at low temperatures to be ordered,

[1] `https://github.com/Bragit123/FYS4130/tree/main/Oblig2`

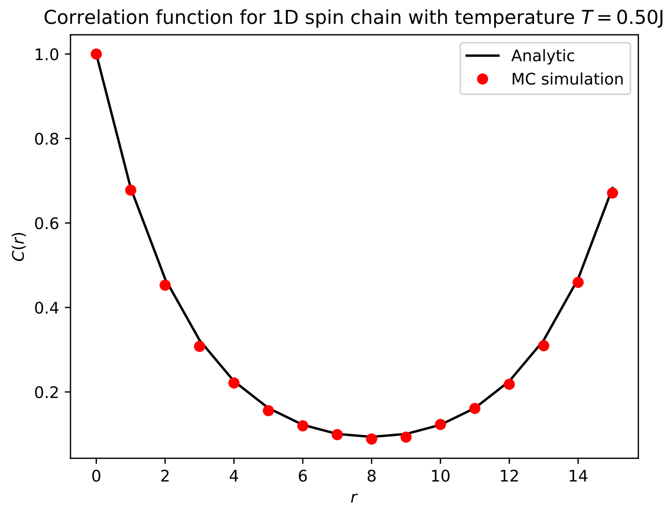


Figure 2: Correlation function $C(r)$ as a function of distance $r$ for temperature $T/J = 0.5$.

i.e. all spin states should point in the same direction. For $T \to \infty$ the average magnetization begins to oscillate slightly, but as it still remains close to zero this doesn't seem to signify any real physical change of the system, but rather some statistical errors in the simulation.

## 2d)

The average square magnetization per site $\langle |m|^2 \rangle$ is plotted against temperature $T/J$ in Figure 4, still for the two-dimensional lattice system. At $T = 0$ the average square magnetization goes to one, which seems to signify a disordered system consistent with the result in problem 2c). For $T \to \infty$, however, the average square magnetization approaches zero, implying an ordered state where all the spin states take on the same value, thus giving zero variance for the magnetization. This is again counter-intuitive as we would expect it to be the other way around (higher temperatures should lead to more disorder). In addition, this result seems to disaggree with the result in problem 2c), which implied that the system would still be disordered at high temperatures. This might, however, just be confusion on my part, as I am not entirely sure how to interpret the sudden oscillations in Figure 3, and the fact that we only include the real part instead of taking the absolute value might have something to do with this issue.

Despite the average magnetization and average square magnetization implying different results, the fact that we get a counter-intuitive image of how the system behaves, becoming increasingly ordered as the temperature rises, sug-

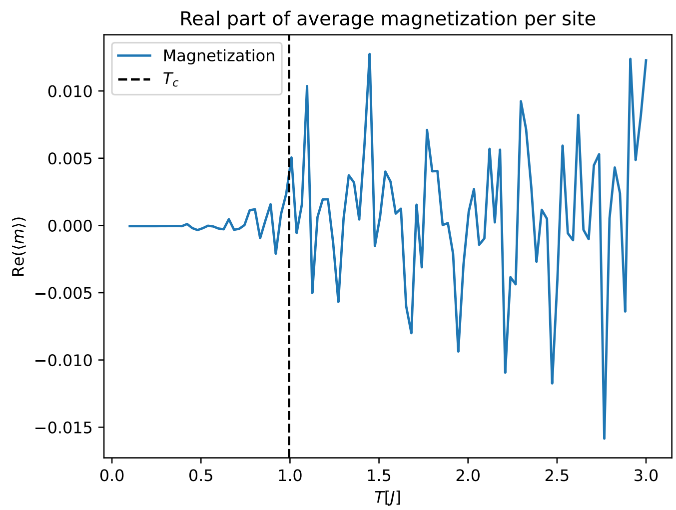


Figure 3: Real part of the average magnetization per site $\langle m \rangle$ as a function of temperature $T/J$.

gests that there is some error in the way the system is simulated, or the way the measurements have been done in the code. Unfortunately, I have spent a lot of time on figuring out what these issues can be, but I have not found any solution.

It should also be noted that the average square magnetization makes a sudden (near-discontinuous) jump from values close to one down to values close to zero. This sudden jump happens near the critical temperature $T_c/J = \frac{1}{\ln(1+\sqrt{3})} \approx 0.9950$, and might signify a phase transition of some sort. Since I believe that there is something wrong with the code I don't want to make too many conclusions based on the resulting plots, but it appears that the simulation is picking up on *something* at the critical temperature.

## 2e)

The critical temperature corresponds to $t = 0$, so we want to consider the behaviour of $\Gamma = \Gamma(0, L^{-1})$. If we can show that $\Gamma(0, L^{-1})$ is independent of $L$, i.e., that it is constant, this is sufficient to prove that the curves of $\Gamma$ will intersect at the critical temperature.

To do this, we consider finite-size scaling. Let $s$ represent the scale factor such that $t \to s^{y_t} t$ and $L^{-1} \to s^{y_L} L^{-1}$ for some exponents $y_t$ and $y_L$. Any order

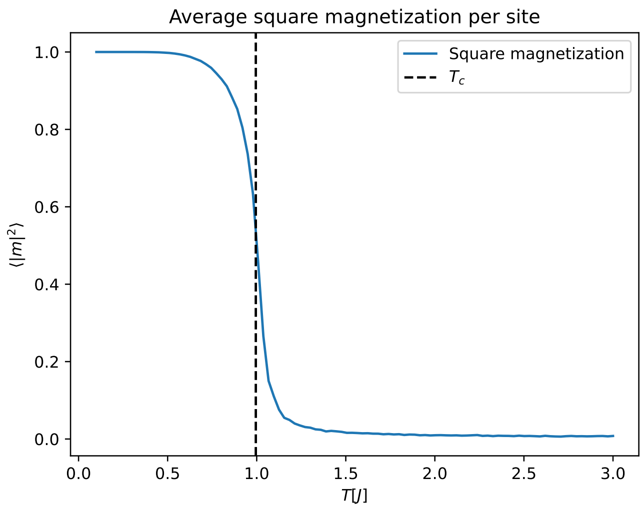


Figure 4: The average magnetization squared per site $\langle |m|^2 \rangle$ as a function of temperature $T/J$.

parameter $f(t, L)$ will then scale as

$$\begin{aligned} f(t, L^{-1}) \rightarrow f(s^{y_t}t, s^{y_L}L^{-1}) &= s^d f(t, L^{-1}) \\ f(t, L^{-1}) &= s^{-d} f(s^{y_t}t, s^{y_L}L^{-1}). \end{aligned}$$

In our case, $m$ is the order parameter, and from the definition of $\Gamma$ we have that

$$\begin{aligned} \Gamma(t, L^{-1}) &= \frac{\langle |m(t, L^{-1})|^4 \rangle}{\langle |m(t, L^{-1})|^2 \rangle^2} \\ &= \frac{\langle |s^{-d} m(s^{y_t}t, s^{y_L}L^{-1})|^4 \rangle}{\langle |s^{-d} m(s^{y_t}t, s^{y_L}L^{-1})|^2 \rangle^2} \\ &= \frac{\cancel{s^{-4d}} \langle |m(s^{y_t}t, s^{y_L}L^{-1})|^4 \rangle}{\cancel{s^{-4d}} \langle |m(s^{y_t}t, s^{y_L}L^{-1})|^2 \rangle^2} \\ &= \frac{\langle |m(s^{y_t}t, s^{y_L}L^{-1})|^4 \rangle}{\langle |m(s^{y_t}t, s^{y_L}L^{-1})|^2 \rangle^2} \\ \Gamma(t, L^{-1}) &= \Gamma(s^{y_t}t, s^{y_L}L^{-1}). \end{aligned}$$

This equality must hold for any scale factor $s$, so we can choose it freely. If we let $s = L^{1/y_L}$ we have that

$$\Gamma(t, L^{-1}) = \Gamma(L^{y_t/y_L}t, 1),$$

and inserting the critical temperature $t = 0$ gives

$$\Gamma(0, L^{-1}) = \Gamma(0, 1),$$

which is independent of the system size $L$. Since $\Gamma$ is independent of $L$ at the critical temperature, all curves of $\Gamma$ versus temperature for different $L$ must cross at the critical temperature, which is what we wanted to show.

## 2f)

In Figure 5 you can see a plot of $\Gamma = \frac{\langle |m|^4 \rangle}{\langle |m|^2 \rangle^2}$ as a function of the temperature $T/J$ for three different lattice sizes $L = 8, 16, 32$. The three curves corresponding to the different system sizes look pretty much identical. They all start at $\Gamma = 1$ at $T/J = 0$, remain close to constant at this value for low temperatures. At the critical temperature the three curves make a sudden jump to $\Gamma \approx 2$, although the jump is slightly slower for lower system sizes. After the critical temperature the curves oscillate frantically, but generally staying close to $\Gamma \approx 2$.

This is odd behaviour, and not what we would expect. We would expect the three curves to be more distinct, and then cross at some specific temperature that we would identify as the critical temperature $T_c/J$. Instead the three curves don't "cross" at any specific point, but stay pretty much equal to each other at all times. This observation combined with the strange behaviour in Figure 3 and 4 convinces me that there is some flaw in the simulation. This could be an error in the code, or the way I calculate the average and moments of the magnetization in the code is wrong. Sadly, I have not been able to identify the problem, but if the error is obvious I would appreciate any feedback.

I should note that the sudden jump in Figure 5 is close to the critical temperature, consistent with the result in problem 2d). Since we get strange behaviour at the critical temperature in both these plots it appears that we are capturing the phase transition of the system in some way. Therefore, I would guess the problem lies in the way the moments of the magnetization are "measured", not in the way the lattice is simulated, since an error in the simulation itself should not capture the phase transition at all, while signs of phase transitions might appear even if I "measure" the wrong thing.

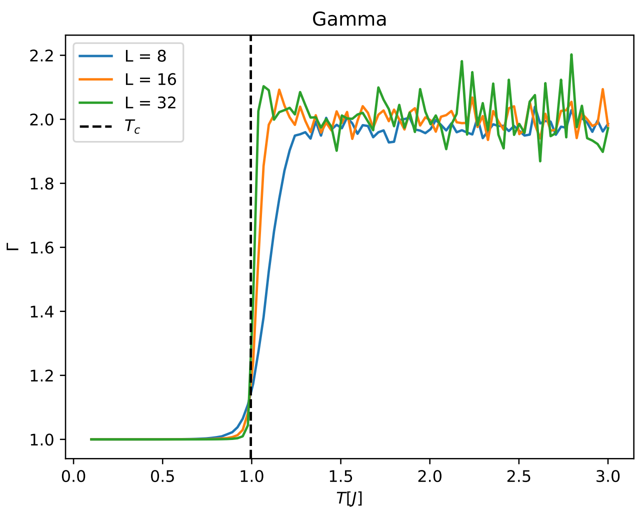


Figure 5: Magnetization moment ratio $\Gamma$ as a function of temperature $T/J$ for Lattice sizes $L = 8, 16, 32$.