Mandatory Assignment 2
Fys4130 - Statistical Mechanics

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Exercise 1

a)

For our system of L spins on a 1D chain with periodic boundary conditions we have the following Hamiltonian

$$H = -J \sum_{i=0}^{L-1} \delta_{\sigma_i, \sigma_{i+1}}$$

where each spin, σ, can take the values $\{0, 1, 2\}$.
As the Hamiltonian is known, the partiton function is given by

$$\begin{aligned} Z &= \sum_{\{\sigma\}} e^{-\beta H} \\ &= \sum_{\{\sigma\}} e^{\beta J \sum_{i=0}^{L-1} \delta_{\sigma_i, \sigma_{i+1}}} \\ Z &= \sum_{\{\sigma\}} \prod_{i=0}^{L-1} e^{\beta J \delta_{\sigma_i, \sigma_{i+1}}} \end{aligned}$$

where $\{\sigma\}$ denotes all possible spin configurations which can take place in the system. This is equivalent to stating

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

Note that for each i in the product there are nine different combinations of spins, three for each. These combinations can be written as a matrix, and in turn, the entire exponential factor can be written as a so-called *Transfer Matrix*.
We have

$$T = e^{\beta J \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}} = \begin{bmatrix} e^{\beta J} & 1 & 1 \\ 1 & e^{\beta J} & 1 \\ 1 & 1 & e^{\beta J} \end{bmatrix}$$

Let then $T(\sigma_i, \sigma_j)$ indicate element (σ_i, σ_j) of the matrix.
Example: $\sigma_i = 1$, $\sigma_j = 2$ gives $T(\sigma_i, \sigma_j) = T_{1,2} = 1$ where the indexing starts at zero.

Note that the transfer matrix is constant throughout the entire system as the Hamiltonian is constant. By diagonalizing the transfer matrix (wolfram alpha was used) the following decomposition is obtained

$$\begin{aligned} T &= VDV^{-1} \\ &= \begin{bmatrix} -1 & -1 & 1 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} e^{\beta J} - 1 & 0 & 0 \\ 0 & e^{\beta J} - 1 & 0 \\ 0 & 0 & e^{\beta J} + 2 \end{bmatrix} \begin{bmatrix} -1/3 & -1/3 & 2/3 \\ -1/3 & 2/3 & -1/3 \\ 1/3 & 1/3 & 1/3 \end{bmatrix} \\ &= \frac{1}{3} \begin{bmatrix} -1 & -1 & 1 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} e^{\beta J} - 1 & 0 & 0 \\ 0 & e^{\beta J} - 1 & 0 \\ 0 & 0 & e^{\beta J} + 2 \end{bmatrix} \begin{bmatrix} -1 & -1 & 2 \\ -1 & 2 & -1 \\ 1 & 1 & 1 \end{bmatrix} \end{aligned}$$

We may now rewrite the partition function as a series of sums over the product of transfer matrices.

$$\begin{aligned} Z &= \sum_{\{\sigma\}} \prod_{i=0}^{L-1} T(\sigma_i, \sigma_{i+1}) \\ &= \sum_{\sigma_0}\sum_{\sigma_1}\cdots\sum_{\sigma_{L-1}} T(\sigma_0, \sigma_1) T(\sigma_1, \sigma_2) \ldots T(\sigma_L - 1, \sigma_0) \end{aligned}$$

Where the last matrix element is a consequence of the periodic boundary conditions.

From linear algebra it is known that an element in a matric product can be written as

$$(AB)_{i,j} = \sum_k A_{i,k} B_{k,j}$$

Hence the partition function is given by

$$\begin{aligned}
Z &= \sum_{\sigma_0}\sum_{\sigma_1}\cdots\sum_{\sigma_{L-2}} T(\sigma_0,\sigma_1)T(\sigma_1,\sigma_2)\dots T(\sigma_{L-3},\sigma_{L-2}) \underbrace{\sum_{\sigma_{L-1}} T(\sigma_{L-2},\sigma_{L-1})T(\sigma_{L-1},\sigma_0)}_{T^2(\sigma_{L-2},\sigma_0)} \\
&= \sum_{\sigma_0}\sum_{\sigma_1}\cdots\sum_{\sigma_{L-3}} T(\sigma_0,\sigma_1)T(\sigma_1,\sigma_2)\dots T(\sigma_{L-4},\sigma_{L-3}) \underbrace{\sum_{\sigma_{L-2}} T(\sigma_{L-3},\sigma_{L-2})T^2(\sigma_{L-2},\sigma_0)}_{T^3(\sigma_{L-3},\sigma_0)} \\
&\vdots \\
Z &= \sum_{\sigma_0} T^L(\sigma_0,\sigma_0)
\end{aligned}$$

This final expression is the sum over the diagonal elements of the matrix T^L, also known as its trace. Thus we have

$$Z = \mathrm{Tr}\big(T^L\big)$$

Since T is a diagonalizable matrix, $T^L = VD^LV^{-1}$. Since the trace operation is invariant under cyclic permutation, we have that

$$\begin{aligned}
Z &= \mathrm{Tr}\big(T^L\big) = \mathrm{Tr}\big(VD^LV^{-1}\big) = \mathrm{Tr}\big(V^{-1}VD^L\big) = \mathrm{Tr}\big(D^L\big) \\
&= \mathrm{Tr}\left(\begin{bmatrix} \big(e^{\beta J}-1\big)^L & 0 & 0 \\ 0 & \big(e^{\beta J}-1\big)^L & 0 \\ 0 & 0 & \big(e^{\beta J}+2\big)^L \end{bmatrix}\right) \\
Z &= 2\big(e^{\beta J}-1\big)^L + \big(e^{\beta J}+2\big)^L
\end{aligned}$$

With an expression for the partition function we can calculate the internal energy of the system.

$$\begin{aligned}
U &= -\frac{\partial \ln Z}{\partial \beta} \\
&= -\frac{2LJe^{\beta J}\left(e^{\beta J}-1\right)^{L-1} + LJe^{\beta J}\left(e^{\beta J}+2\right)^{L-1}}{2(e^{\beta J}-1)^{L} + (e^{\beta J}+2)^{L}} \\
U &= -\frac{LJe^{\beta J}\left[2\left(e^{\beta J}-1\right)^{L-1} + \left(e^{\beta J}+2\right)^{L-1}\right]}{2(e^{\beta J}-1)^{L} + (e^{\beta J}+2)^{L}}
\end{aligned}$$

Using $\left(e^{\beta J}-1\right) = e^{\beta J}\left(1-e^{-\beta J}\right)$ and $\left(e^{\beta J}+2\right) = e^{\beta J}\left(1+2e^{-\beta J}\right)$ the above expression becomes

$$\begin{aligned}
U &= -\frac{LJe^{L\beta J}\left[2\left(1-e^{-\beta J}\right)^{L-1} + \left(1+2e^{-\beta J}\right)^{L-1}\right]}{e^{L\beta J}\left[2(1-e^{-\beta J})^{L} + (1+2e^{-\beta J})^{L}\right]} \\
U &= -LJ\frac{2\left(1-e^{-\beta J}\right)^{L-1} + \left(1+2e^{-\beta J}\right)^{L-1}}{2(1-e^{-\beta J})^{L} + (1+2e^{-\beta J})^{L}}
\end{aligned}$$

For high temperatures $\beta \to 0$, $\left(1-e^{-\beta J}\right) \Rightarrow 0$ and $(1+2e^{-\beta J}) \Rightarrow 3$. The energy then becomes

$$U_{High} = -LJ\frac{3^{L-1}}{3^{L}} = \frac{-LJ}{3}$$

For low temperatures $\beta \to \infty$, $\left(1-e^{-\beta J}\right) \Rightarrow 1$ and $\left(1+2e^{-\beta J}\right) \Rightarrow 1$. The energy then becomes

$$U_{Low} = -LJ\frac{2+1}{2+1} = -LJ$$

Explain these limiting behaviors

b)

Moving on to the mean magnetization, we have

$$
\begin{aligned}
\langle m \rangle &= \left\langle \frac{1}{N} \sum_{j=0}^{N-1} m_j \right\rangle \\
&= \frac{1}{N} \sum_{j=0}^{N-1} \langle m_j \rangle
\end{aligned}
$$

Since this sum is finite the above expression is valid.
The problem is now reduced to finding the expectation value for each of the local "magnetizations". Using the partition funciton as the probability distribution and the provided definiton of the local magnetization, we have

$$
\langle m_j \rangle = \frac{1}{Z} \sum_{\{\sigma\}} e^{i\frac{2\pi}{3}\sigma_j} \prod_{i=0}^{L-1} e^{\beta J \delta_{\sigma_i,\sigma_{i+1}}}
$$

Using a similar approach to finding the partition function, this can be expanded as a sum over the product of multiple transfer matrices.

$$
\begin{aligned}
\langle m_j \rangle &= \frac{1}{Z} \sum_{\sigma_0} \sum_{\sigma_1} \cdots \sum_{\sigma_{L-1}} e^{i\frac{2\pi}{3}\sigma_j} T(\sigma_0,\sigma_1)T(\sigma_1,\sigma_2)\ldots T(\sigma_{L-1},\sigma_0) \\
&= \frac{1}{Z} \sum_{\sigma_j} e^{i\frac{2\pi}{3}\sigma_j} \sum_{\sigma_0} \sum_{\sigma_1} \cdots \sum_{\sigma_{j-1}} \sum_{\sigma_{j+1}} \cdots \sum_{\sigma_{L-1}} T(\sigma_0,\sigma_1)T(\sigma_1,\sigma_2)\ldots T(\sigma_{L-1},\sigma_0) \\
&= \frac{1}{Z} \sum_{\sigma_j} e^{i\frac{2\pi}{3}\sigma_j} \sum_{\sigma_0} \sum_{\sigma_1} \cdots \sum_{\sigma_{j-1}} T(\sigma_0,\sigma_1)T(\sigma_1,\sigma_2)\ldots T(\sigma_{j-1},\sigma_j) \\
&\quad \sum_{\sigma_{j+1}} \cdots \sum_{\sigma_{L-1}} T(\sigma_j,\sigma_{j+1})T(\sigma_{j+1},\sigma_{j+2})\ldots T(\sigma_{L-1},\sigma_0) \\
&= \frac{1}{Z} \sum_{\sigma_j} e^{i\frac{2\pi}{3}\sigma_j} \sum_{\sigma_0} T^j(\sigma_0,\sigma_j) T^{L-j}(\sigma_j,\sigma_0)
\end{aligned}
$$

Where is has been used that $\sum_{\sigma_1} \cdots \sum_{\sigma_{j-1}} T(\sigma_0,\sigma_1)\ldots T(\sigma_{j-1},\sigma_j) = T^j(\sigma_0,\sigma_j)$ and $\sum_{\sigma_{j+1}} \cdots \sum_{\sigma_{L-1}} T(\sigma_j,\sigma_{j+1})\ldots T(\sigma_{L-1},\sigma_0) = T^{L-j}(\sigma_j,\sigma_0)$. Since $T^j(\sigma_0,\sigma_j)$ and $T^{L-j}(\sigma_j,\sigma_0)$ are elements of matrices, they are simply numbers, and thus commute. The order of multiplication can then be switched giving us

$$\langle m_j \rangle = \frac{1}{Z} \sum_{\sigma_j} e^{i\frac{2\pi}{3}\sigma_j} \sum_{\sigma_0} T^{L-j}(\sigma_j, \sigma_0) T^j(\sigma_0, \sigma_j)$$

$$\langle m_j \rangle = \frac{1}{Z} \sum_{\sigma_j} e^{i\frac{2\pi}{3}\sigma_j} T^L(\sigma_j, \sigma_j)$$

This final sum will only take the diagonal elements of the matrix T^L which can be calculated by $T^L = VD^LV^{-1}$ where V and D are the eigenvector and eigenvalue matrices from exercise a). Carrying out the full calculation;

$$\begin{aligned}
T^L &= VD^LV^{-1} \\
&= \frac{1}{3} \begin{bmatrix} -1 & -1 & 1 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} \left(e^{\beta J} - 1\right)^L & 0 & 0 \\ 0 & \left(e^{\beta J} - 1\right)^L & 0 \\ 0 & 0 & \left(e^{\beta J} + 2\right)^L \end{bmatrix} \begin{bmatrix} -1 & -1 & 2 \\ -1 & 2 & -1 \\ 1 & 1 & 1 \end{bmatrix} \\
&= \frac{1}{3} \begin{bmatrix} 2\left(e^{\beta J} - 1\right)^L + \left(e^{\beta J} + 2\right)^L & -\left(e^{\beta J} - 1\right)^L + \left(e^{\beta J} + 2\right)^L & -\left(e^{\beta J} - 1\right)^L + \left(e^{\beta J} + 2\right)^L \\ -\left(e^{\beta J} - 1\right)^L + \left(e^{\beta J} + 2\right)^L & 2\left(e^{\beta J} - 1\right)^L + \left(e^{\beta J} + 2\right)^L & -\left(e^{\beta J} - 1\right)^L + \left(e^{\beta J} + 2\right)^L \\ -\left(e^{\beta J} - 1\right)^L + \left(e^{\beta J} + 2\right)^L & -\left(e^{\beta J} - 1\right)^L + \left(e^{\beta J} + 2\right)^L & 2\left(e^{\beta J} - 1\right)^L + \left(e^{\beta J} + 2\right)^L \end{bmatrix}
\end{aligned}$$

Which gives

$$T^L(\sigma_j, \sigma_j) = \frac{2\left(e^{\beta J} - 1\right)^L + \left(e^{\beta J} + 2\right)^L}{3} \quad \forall \quad \sigma_j$$

Thus

$$\begin{aligned}
\langle m_j \rangle &= \frac{2\left(e^{\beta J} - 1\right)^L + \left(e^{\beta J} + 2\right)^L}{3Z} \sum_{\sigma_j} e^{i\frac{2\pi}{3}\sigma_j} \\
&= \frac{2\left(e^{\beta J} - 1\right)^L + \left(e^{\beta J} + 2\right)^L}{3Z} \underbrace{\left(1 + e^{i\frac{2\pi}{3}} + e^{i\frac{4\pi}{3}}\right)}_{=0} \\
\langle m_j \rangle &= 0
\end{aligned}$$

From this it follows that $\langle m \rangle = \frac{1}{N} \sum_j \langle m_j \rangle = 0$.

c)

Starting of by noting that the correlation function $C(r)$ is nothing else than the covariance between the complex conjugate magnetization at site zero and at a site distance r from site zero. Again using the partition function in constructing the probability distribution as well as the definition of the covariance, we have that

$$C(r) = \mathrm{Cov}(m_0^*, m_r) = \frac{1}{Z}\sum_{\{\sigma\}}\prod_i e^{\beta J\delta_{\sigma_i,\sigma_{i+1}}}(m_0^* - \langle m_0^*\rangle)(m_r - \langle m_r\rangle)$$

Knowing that the expectation value for magnetization is zero, we have

$$C(r) = \frac{1}{Z}\sum_{\{\sigma\}}\prod_i T(\sigma_i, \sigma_{i+1}) m_0^* m_r$$

The magnetization is only dependent on the spins at sites 0 and r, so these sums can be extracted. Using the provided definition, $m_j \equiv e^{i\frac{2\pi}{3}\sigma_j}$, we have

$$\begin{aligned}
C(r) = \frac{1}{Z}\sum_{\sigma_0} e^{-i\frac{2\pi}{3}\sigma_0}\sum_{\sigma_r} e^{i\frac{2\pi}{3}\sigma_r}\sum_{\sigma_1}\cdots\sum_{\sigma_{r-1}} T(\sigma_0,\sigma_1)\ldots T(\sigma_{r-1},\sigma_r)\\
\sum_{\sigma_{r+1}}\cdots\sum_{\sigma_{L-1}} T(\sigma_r,\sigma_{r+1})\ldots T(\sigma_{L-1},\sigma_0)\\
= \frac{1}{Z}\sum_{\sigma_0} e^{-i\frac{2\pi}{3}\sigma_0}\sum_{\sigma_r} e^{i\frac{2\pi}{3}\sigma_r} T^r(\sigma_0,\sigma_r)T^{L-r}(\sigma_r,\sigma_0)
\end{aligned}$$

The elements in the matrices T^r and T^{L-r} are known, and we can simply carry out the calculation

$$\begin{aligned}
C(r) &= \frac{1}{Z}\sum_{0} e^{-i\frac{2\pi}{3}\sigma_0}\Big(T^r(\sigma_0,0)T^{L-r}(0,\sigma_0) + e^{i\frac{2\pi}{3}}T^r(\sigma_0,1)T^{L-r}(1,\sigma_0) + e^{i\frac{4\pi}{3}}T^r(\sigma_0,2)T^{L-r}(2,\sigma_0)\Big)\\
&= \frac{1}{Z}[T^r(0,0)T^{L-r}(0,0) + e^{i\frac{2\pi}{3}}T^r(0,1)T^{L-r}(1,0) + e^{i\frac{4\pi}{3}}T^r(0,2)T^{L-r}(2,0)\\
&\quad e^{-i\frac{2\pi}{3}}T^r(1,0)T^{L-r}(0,1) + T^r(1,1)T^{L-r}(1,1) + e^{i\frac{2\pi}{3}}T^r(1,2)T^{L-r}(2,1)\\
&\quad e^{-i\frac{4\pi}{3}}T^r(2,0)T^{L-r}(0,2) + e^{-i\frac{2\pi}{3}}T^r(2,1)T^{L-r}(1,2) + T^r(2,2)T^{L-r}(2,2)]
\end{aligned}$$

Every diagonal element is the same, and every off-diagonal element is the same. Lets therefore introduce

$$
\begin{aligned}
\chi &= T^r(\sigma_i, \sigma_i) T^{L-r}(\sigma_i, \sigma_i) \\
&= \frac{1}{9}\Big(4\big(e^{\beta J} - 1\big)^L + \big(e^{\beta J} + 2\big)^L + 2\big(e^{\beta J} - 1\big)^r\big(e^{\beta J} + 2\big)^{L-r} + 2\big(e^{\beta J} - 1\big)^{L-r}\big(e^{\beta J} + 2\big)^r\Big)
\end{aligned}
$$

and

$$
\begin{aligned}
\xi &= T^r(\sigma_i, \sigma_j) T^{L-r}(\sigma_i, \sigma_j) \\
&= \frac{1}{9}\Big(\big(e^{\beta J} - 1\big)^L + \big(e^{\beta J} + 2\big)^L - \big(e^{\beta J} - 1\big)^r\big(e^{\beta J} + 2\big)^{L-r} - \big(e^{\beta J} - 1\big)^{L-r}\big(e^{\beta J} + 2\big)^r\Big)
\end{aligned}
$$

The correlationfunction is then

$$
\begin{aligned}
C(r) &= \frac{1}{Z}[3\chi + \xi \underbrace{\Big(2e^{i\frac{2\pi}{3}} + 2e^{-i\frac{2\pi}{3}} + e^{i\frac{4\pi}{3}} + e^{-i\frac{4\pi}{3}}\Big)}_{=-3}] \\
&= \frac{3}{Z}(\chi - \xi)
\end{aligned}
$$

From a) we have that $Z = 2\big(e^{\beta J} - 1\big)^L + \big(e^{\beta J} + 2\big)^L$, which in total gives us

$$
C(r) = \frac{\big(e^{\beta J} - 1\big)^L + \big(e^{\beta J} - 1\big)^r\big(e^{\beta J} + 2\big)^{L-r} + \big(e^{\beta J} - 1\big)^{L-r}\big(e^{\beta J} + 2\big)^r}{2(e^{\beta J} - 1)^L + (e^{\beta J} + 2)^L}
$$

"Is this correct?" - Daniel, 24 år
"Yes." - João, 21 anos