FYS4130 - Oblig 2

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All code used in this oblig can be found on my Github: https://github.com/Vikenes/FYS4130

TASK 1 - TRANSFER MATRICES

a) Partition function and average internal energy

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

$$m \equiv \frac{1}{N} \sum_{j=0}^{N-1} m_j \tag{2}$$

$$\text{where} \quad m_j \equiv e^{i(2\pi/3)\sigma_j} \tag{3}$$

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

$$T_{\sigma_i, \sigma_{i+1}} = \begin{pmatrix} e^{\beta J} & 1 & 1 \\ 1 & e^{\beta J} & 1 \\ 1 & 1 & e^{\beta J} \end{pmatrix}$$

$$Z = \sum_{\{\sigma_j\}} \prod_{i=0}^{L-1} T_{\sigma_j, \sigma_{j+1}} = \sum_{\{\sigma_j\}} T_{\sigma_0, \sigma_1} T_{\sigma_1, \sigma_2} \cdots T_{\sigma_{L-1}, \sigma_0} = \mathrm{Tr}\big(T^L\big)$$

$$T = SDS^{-1}, \text{ where } D = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}$$

$$\begin{aligned} \lambda_1 &= e^{\beta J} - 1 \\ \lambda_2 &= e^{\beta J} - 1 \\ \lambda_3 &= e^{\beta J} + 2 \end{aligned}$$

$$\begin{aligned} Z &= \mathrm{Tr}\big(SDS^{-1} SDS^{-1} \cdots DS^{-1}\big) = Tr(D^L) = 2\lambda_1^L + \lambda_3^L \\ &= 2(e^{\beta J} - 1)^L + (e^{\beta J} + 2)^L \end{aligned}$$

$$U = \frac{\partial(\beta F)}{\partial\beta}$$

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

$$U = -L\frac{Je^{\beta J}}{e^{\beta J} - 1} - L\frac{Je^{\beta J}}{e^{\beta J} + 2}$$

For an approximate expression of U we can rewrite the partition function in a way that allows us to neglect a term.

$$Z = 2\lambda_1^L + \lambda_3^L = \lambda_3^L\left[2\left(\frac{\lambda_1}{\lambda_3}\right)^L + 1\right]$$

For large L there are two limiting cases. If β is very large $\lambda_1/\lambda_3 \approx 1$ so $Z \approx 3\lambda_3^L$. If, on the other hand, β is small we get $Z \approx \lambda_3^L$, as the fraction goes to zero when L becomes large. Since we have to differentiate the logarithm of Z with respect to β to obtain the approximate expression for U, the constant in front of λ_3^L is irrelevant. An approximate expression for U is thus

$$\begin{aligned} U &= -\frac{\partial}{\partial\beta}\ln Z \approx -\frac{\partial}{\partial\beta}L\ln\lambda_3 = -L\frac{\partial}{\partial\beta}\ln\left(e^{\beta J} + 2\right) \\ &= -\frac{LJ}{1 + 2e^{-\beta J}} \end{aligned}$$

For $T \to 0$ the approximate expression for U becomes

$$\lim_{\beta\to\infty} U = -LJ$$

and for $T \to \infty$ we get

$$\lim_{\beta\to 0} U = -\frac{LJ}{1+2} = -\frac{LJ}{3}$$

In the low temperature limit we get the minimum energy of our model, where all the spins are aligned. In the high temperature limit, we have disordered spin states. Since σ_j can take three possible values, the probability of neighbouring spins being aligned is 1/3, and we thus get one third of the total available energy.

b) - Average magnetization

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

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

$$m_j = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i(2\pi/3)} & 0 \\ 0 & 0 & e^{-i(2\pi/3)} \end{pmatrix}$$

$$
\begin{aligned}
\langle m_j \rangle &= \frac{1}{Z} \sum_{\{\sigma_j\}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i(2\pi/3)} & 0 \\ 0 & 0 & e^{-i(2\pi/3)} \end{pmatrix} T_{\sigma_0,\sigma_1} T_{\sigma_1,\sigma_2} \cdots T_{\sigma_{L-1},\sigma_0} \\
&= \frac{1}{Z} \operatorname{Tr} \left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i(2\pi/3)} & 0 \\ 0 & 0 & e^{-i(2\pi/3)} \end{pmatrix} \begin{pmatrix} e^{\beta J} & 1 & 1 \\ 1 & e^{\beta J} & 1 \\ 1 & 1 & e^{\beta J} \end{pmatrix}^L \right] \\
&= \frac{1}{Z} \operatorname{Tr} \left[\begin{pmatrix} \left(e^{\beta J}\right)^L & 0 & 0 \\ 0 & e^{i2\pi/3} \left(e^{\beta J}\right)^L & 0 \\ 0 & 0 & e^{-i2\pi/3} \left(e^{\beta J}\right)^L \end{pmatrix} \right] \\
&= \frac{1}{Z} e^{L\beta J} \left[1 + e^{i2\pi/3} + e^{-i2\pi/3} \right] = 0
\end{aligned}
$$

$$
\langle m_j \rangle = 0 \implies \langle m \rangle = 0
$$

c) - Correlation function

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

$$
\langle m_0^* m_r \rangle = \left\langle e^{i(2\pi/3)(\sigma_r - \sigma_0)} \right\rangle
$$

$$
m_0^* m_r = \begin{pmatrix} 1 & e^{i2\pi/3} & e^{-i2\pi/3} \\ e^{-i2\pi/3} & 1 & e^{i2\pi/3} \\ e^{i2\pi/3} & e^{-i2\pi/3} & 1 \end{pmatrix}
$$

$$
\begin{aligned}
\langle m_0^* m_r \rangle &= \frac{1}{Z} \sum_{\{\sigma_j\}} m_0^* m_r \, T^L = \frac{1}{Z} \operatorname{Tr} \left[\begin{pmatrix} \left(e^{\beta J}\right)^L & e^{i2\pi/3} & e^{-i2\pi/3} \\ e^{-i2\pi/3} & \left(e^{\beta J}\right)^L & e^{i2\pi/3} \\ e^{i2\pi/3} & e^{-i2\pi/3} & \left(e^{\beta J}\right)^L \end{pmatrix} \right] = \frac{1}{Z} 3 e^{L\beta J} \\
&= \frac{3 e^{L\beta J}}{2(e^{\beta J} - 1)^L + (e^{\beta J} + 2)^L}
\end{aligned}
$$