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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

For large N there are two limiting cases. If β is very large $\lambda_1/\lambda_3 \approx 1$ so $Z \approx 3\lambda_3^N$. If, on the other hand, β is small we get $Z \approx \lambda_3^N$, as the fraction goes to zero when N 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^N is irrelevant. An approximate expression for U is thus

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

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

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

and for $T \to \infty$ we get

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

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.