Problem 1: Ising model

Consider the Ising model in one dimension, whose Hamiltonian is given by

$$H = -J \sum_{i=1}^{L} \sigma_i \sigma_{i+1} + B \sum_{i=1}^{L} \sigma_i .$$

J represents the coupling between nearest neighbor spins, B denotes the magnetic field. We assume that $J > 0$, $B = 0$, and that $\sigma_{L+1} = \sigma_1$ (periodic boundary conditions). The spin variables can take the values $\sigma = \pm 1$.

- Determine one of the ground states under these conditions. Draw a picture of this state using upward arrows for spins $\sigma = 1$, and downward arrows for spins $\sigma = -1$.
- Give an example of a state A_1 with energy higher than the ground state, such that there are no states which lie between the ground state energy and the energy of the state A_1. In other words give an example of the first excited state. There are many such states.
- Give the entropy associated with the first excited state.
- **Extra credit:** Argue that at finite temperature in one dimension there is no long range order.

- ground state: $\uparrow\uparrow\uparrow\uparrow \ldots\ldots \uparrow$ $\quad E_0 = -JL$

  or $\downarrow\downarrow\downarrow\downarrow \ldots\ldots \downarrow$

- flip one continuous cluster of spins

  $\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow$ $\quad$ cluster can be of any size

  $-J\ -J\ +J\ -J\ -J\ -J\ +J\ -J\ -J$

  or $\uparrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow$ $\quad E = -JL + 4J$

- Entropy: two antiparallel bonds can be in $N \times (N-1)$ places

  $S = k \ln N(N-1) \longrightarrow 2k \ln N$

- $F = E - TS = -JL + 4J - 2kT \ln N \Rightarrow$ smaller than ground state energy for finite T and $N \to \infty$

Problem 2: Ising model (microcanonical ensemble)

Calculate the energy, entropy, temperature, and specific heat in the microcanonical ensemble for the model introduced in **Problem 1**. Based on investigating the specific heat, argue that there is no phase transition (a divergence in the specific heat indicates a phase transition).

there are L bonds, N_a anti-parallel, N_p parallel

$N_a + N_p = L$

$$E = -JN_p + JN_a = \cancel{-JN_p + J(L-N_a)} =$$
$$= -J(L-N_a) + JN_a = -JL + 2JN_a \Rightarrow N_a = \frac{E+JL}{2J} = \frac{E}{2J} + \frac{L}{2}$$

$$\Omega = \frac{L!}{N_a!\,(L-N_a)!} \rightarrow S = k \ln \Omega =$$
$$= k\left(L\ln L - N_a \ln N_a - (L-N_a)\ln(L-N_a)\right)$$

$$S = k\left(L\ln L - \left(\frac{L}{2}+\frac{E}{2J}\right)\ln\left(\frac{L}{2}+\frac{E}{2J}\right) - \left(\frac{L}{2}-\frac{E}{2J}\right)\ln\left(\frac{L}{2}-\frac{E}{2J}\right)\right)$$

$$\frac{1}{T} = \frac{\partial S}{\partial E} = k\left(-\frac{1}{2J}\ln\left(\frac{L}{2}+\frac{E}{2J}\right) \cancel{-\frac{1}{2J}} + \frac{1}{2J}\ln\left(\frac{L}{2}-\frac{E}{2J}\right) \cancel{+\frac{1}{2J}}\right)$$

$$\frac{2J}{kT} = \ln\left[\frac{\left(\frac{L}{2}-\frac{E}{2J}\right)}{\left(\frac{L}{2}+\frac{E}{2J}\right)}\right] \Rightarrow e^{\frac{2J}{kT}}\left(\frac{L}{2}+\frac{E}{2J}\right) = \left(\frac{L}{2}-\frac{E}{2J}\right)$$

$$e^{2J/kT}(JL+E) = (JL-E)$$

$$\Downarrow \qquad E(1+e^{2J/kT}) = JL(1-e^{2J/kT})$$

$$T = \frac{2J}{k \ln\frac{(JL-E)}{(JL+E)}} \qquad \Rightarrow E = -JL\tanh(J/kT)$$

$$C = \frac{\partial E}{\partial T} = -JL\left(1 - \tanh^2\left(\frac{J}{kT}\right)\right)\left(-\frac{J}{kT^2}\right)$$

$$C = \frac{J^2L}{kT^2}\left(1-\tanh^2\left(\frac{J}{kT}\right)\right) \rightarrow$$

continuous fn.
no phase transition

Problem 3 Ising model (canonical ensemble)

For the model introduced in **Problem 1**, calculate the canonical partition function, the average energy and the specific heat. Compare your results to those of **Problem 2**, when applicable. Assess whether a phase transition occurs, based on the behavior of the specific heat.

$$Q = \sum_{\sigma_1=\pm 1} \cdots \sum_{\sigma_L=\pm 1} \prod_{i=1}^{L} e^{+\beta J \sigma_i \sigma_{i+1}} = \operatorname{Tr} \bar{\bar{T}}^L$$

$$\bar{\bar{T}} = \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix} \Rightarrow \text{diagonalize}$$

$$\Rightarrow \left(e^{\beta J} - \lambda\right)^2 = e^{-2\beta J}$$

$$e^{\beta J} - \lambda = \pm e^{-\beta J}$$

$$\lambda = \underbrace{2\cosh \beta J}_{\text{larger}},\ 2 \sinh \beta J$$

$$Q = 2^L \left(\cosh^L \beta J + \sinh^L(\beta J)\right)$$

$$E = -\frac{\partial \ln Q}{\partial \beta} = -\frac{1}{Q}\frac{\partial Q}{\partial \beta} = -\frac{2^L L\left(\cosh^{L-1}\beta J \sinh \beta J + \sinh^{L-1}\beta J \cosh(\beta J)\right) J}{2^L\left(\cosh^L \beta J + \sinh^L(\beta J)\right)}$$

as $L \to \infty$ $\quad E = -JL\tanh(\beta J)$

$\Downarrow$

$$C = \frac{\partial E}{\partial T} = +\frac{J^2 L}{kT^2}\left(1 - \tanh^2(\beta J)\right)$$

no phase transition!