BB 626: Modeling biological systems and processes

Date : 24 Jan 2025 Max. Marks : 5

1. Consider a set of N=100 proteins arranged on a circle. Let S_i be the state of i^{th} protein. Each protein can be in two states $S_i = +1$ or $S_i = -1$. The total energy of the system is given

$$E = -J \sum_{i=1}^{N} S_i S_{i+1} + h \sum_{i=1}^{N} S_i$$

where the interaction is only between the nearest neighbors. Simulate this system using Monte Carlo simulation and calculate the following quantities. Unless specified otherwise do all the simulations for the following sets of parameters: (J,h)=(1,1), (1, 0.1), (10, 1), (1,-1).

(a) Calculate the total energy of the system as a function of Monte Carlo steps (2 Marks).

(b) Calculate the average magnetization of the system after the system has reached a steady state. $M = \sum_{i=1}^{N} S_i$, and compute magnetization per protein as m=M/N

Plot m versus h for a few different values of h values ($-5 < h < 5$). Take sufficient values of h to make the curve smooth. Here take $J = 1$ first; then repeat for $J = 10$

Try to fit the resulting curve with the known analytical solution

$$m(J,h) = \frac{\sinh(h)}{\sqrt{\cosh^2(h) - 2\exp(-2J)\sinh(2J)}}.$$

(3 Marks)

Optional question:

(c) Calculate the specific heat of the system $C = \langle E^2 \rangle - \langle E \rangle^2$, for the following sets of parameters: (J,h)=(1,1), (1, 0.1), (10, 1), (1,-1).