Boğaziçi University
Department of Physics

Phys 496/68N Fall 2011

Project 2

Due on December 30th, 2011

Monte Carlo Simulation of 1D Ising Model

1D Ising Model

The energy of the system is given by:

$$E(S) = -J \sum_{k=1}^{N} s_k \, s_{k+1} - B \sum_{k=1}^{N} s_k$$

Assume a periodic boundary condition; the last particle is next to the first particle: $s_{N+1} \equiv s_1$ Write a Monte Carlo code using Metropolis *et. al.* algorithm to simulate this system for a given N, J, B, and T. Note that the probability of being in a state $S = \{s_1, s_2, \dots, s_N\}$ is, according to statistical mechanics, related as:

$$P_S \sim e^{-\beta \cdot E(S)}$$

Then the acceptance comparison is done using

$$r = \exp(-\beta \cdot \Delta E)$$

where $\Delta E = E(S_{trial}) - E(S)$, and one can show that it is equal to

$$\Delta E = 2 s_i [J(s_{i-1} + s_{i+1}) + B]$$

for the case of flipping s_i to $s_i^{trial} = -s_i$. Note that, ΔE depends on only three particles, and there are limited number of different ΔE values, thus one can pre-calculate $r = \exp(-\beta \cdot \Delta E)$ for all possible cases and create a short table (possible 3D table) to speed up the simulation by not calculating the same exponential over and over again.

The magnetization per spin of the system is simply the average of the spins.

$$\frac{1}{N} M = \frac{1}{N} \sum_{k=1}^{N} s_k$$

In class, we derived the analytical solution for the average value of magnetization at the thermodynamic limit. The magnetization per particle for a 1D Ising system at given J, B, and T is calculated by:

$$\frac{1}{N} M = \frac{\sinh B/kT}{\sqrt{\sinh^2 B/kT + e^{-4J/kT}}}$$

Project:

- Take $N = 50$,
- Take $N_{sweep} = 50$ for a measurement
- Start with hot configuration (randomly distributed spins)
- Sweep $10 \times N_{sweep}$ for relaxation
- Make $N_{measure} = 20$ measurements with $N_{sweep} = 50$ sweeps separated with each measurements

- Make a series of measurements for $J = 1k$, $T = 1$ K for $B = \{-1, ..., 1\}k$ with $0.1k$ steps.
- Make a series of measurements for $J = 1k$, $T = 2$ K for $B = \{-1, ..., 1\}k$ with $0.1k$ steps.
- Make a plot showing your simulation results with their corresponding error bars for $N_{measure}$ measurements, and the expected curve calculated by the analytical solution in a single figure as shown below: