INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI

PH 443: MONTE CARLO SIMULATION

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Assignment Report - 2

Name: Dewal Agarwal

Dept.: EEE

Objective:

Study of phase transitions in the spin-1/2 Ising model in two dimensions using Metropolis Algorithm for Monte Carlo Simulation.

Introduction:

Monte Carlo techniques will be used for the study of phase transitions in the spin-1/2 Ising model in two dimensions (2D). The spin-1/2 Ising model consists of spins which are confined to the sites of a lattice and which will have only the values +1 or −1. If there are N spins on the lattice, then the system can be in one of the 2^N states.

Summary of Metropolis Algorithm:

1) Initial conditions: Set the initial conditions of providing the values of the system size N (= 16), $J/k_B T$ and h = 0. Set time t = 0.

2) Choice of Initial State: Take a (N X N) square lattice. An arbitrary spin configuration is taken as initial state assigning s = +1 with probability p corresponding to up spin or assign s = -1 with probability (1-p) corresponding to down spin. Initialize the energy and magnetization.

3) Calculation of energy change: Choose a spin s_j at the site randomly (or sequentially) from initial configuration.

4) Accept or reject the spin flop: (a) If change in spin is negative the flip is allowed.

   (b) Else generate a random number, if it is less than the threshold. Flip allowed. Else reject.

5) Updates of physical quantities: Now one needs calculate or update various quantities of interest for which expectation values are required. Usually, expectation values of energy E Magnetization M and their second moments are calculated.

6) Repeat from step (3) until all the spins of the lattice are considered.

7) Monte Carlo cycle: Each time one sweeps through the lattice, i.e., summed over all spins, constitutes what is called a Monte Carlo cycle. Measure all the expectation values required. Increase the time unit by one, i.e., t → t+1. Go to step (3) and start new Monte Carlo cycle.

8) Calculation of expectation value.

Simulation:

The above mentioned algorithm is coded in python the useful plots for Magnetization, Susceptibility, Specific Heat and Energy with respect to temperature are displayed below.

Code: https://drive.google.com/open?id=1bYoEx2-MEyc07_lXs2gAuWCv1Bs_-M5Y

Number of Lattice Points N = 16 X 16

Number of temperature values n_t = 64 (Sampled from Gaussian distribution)

Critical Temp t_m = 2.269

PLOTS: