Computational Physics - PHYS 410/510
Spring 2025

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Homework

HW 6

due *2025-04-24*

Info	final project presentation: **Thursday, April 24, 2025**, *9:30* Program codes should be mailed to: aglatz@niu.edu (see also website). Other problem solutions can be handed in or mailed as well. Problems with points marked by * are for extra credit.

I. ISING MODEL *[30(+5*)+30+10* PTS]*

Here we consider the Ising model on a two-dimensional periodic grid defined by the Hamiltonian:

$$H = -J \sum_{\langle(i,j),(k,l)\rangle} \sigma_{i,j}\sigma_{k,l} - h \sum_{(i,j)} \sigma_{i,j} \,,$$

where $(i,j) \in [0,\ldots,N_x-1] \times [0,\ldots,N_y-1]$ index the x,y coordinates of the grid points and $\langle(i,j),(k,l)\rangle$ denotes the sum over all grid points and for each grid point over its 4 nearest neighbors (NN), i.e., $\sum_{\langle(i,j),(k,l)\rangle} = \sum_{(i,j)} \sum_{(k,l)\in \mathrm{NN}(i,j)}$. The spins can have values $\sigma_{i,j} = \pm 1$, J is the coupling constant, and h the external magnetic field. Boundary conditions are periodic. The system energy, E, for a given configuration $c = \{\sigma_{i,j}\}$ is simply given by the Hamiltonian and the magnetization, m, of the system for a given spin configuration by

$$m = \frac{M}{N_x N_y} = \langle \sigma_{i,j} \rangle \equiv \frac{1}{N_x N_y} \sum_{(i,j)} \sigma_{i,j} \,.$$

If a single spin $\sigma_{i,j}$ flips: $\sigma_{i,j} \to -\sigma_{i,j}$, the total system energy changes by

$$\Delta E = 2J\sigma_{i,j}(\sigma_{i+1,j} + \sigma_{i-1,j} + \sigma_{i,j+1} + \sigma_{i,j-1}) + 2h\sigma_{i,j}$$

and magnetization by $\Delta M = -2\sigma_{i,j} = N_x N_y \Delta m$.
Here we fix $J = 0.5$ and mostly $h = 0$.
For the initial condition you can either use random spins or aligned spins (ferromagnetic configuration). Calculate E and m for the initial condition and update both using ΔE and Δm above whenever a new configuration is accepted.
After a steady state is reached you should calculate the observables: $\langle E \rangle_c$, $\langle E^2 \rangle_c$, $|\langle m \rangle_c|$, and $\langle m^2 \rangle_c$, where $\langle . \rangle_c$ is the average over accepted configurations.
From these you get the susceptibility

$$\chi = (\langle m^2 \rangle_c - \langle m \rangle_c^2)/(k_B T)$$

and heat capacity

$$c_h/k_B = (\langle E^2 \rangle_c - \langle E \rangle_c^2)/(k_B T)^2 \,.$$

a) Implement the Metropolis algorithm for the Ising model using the above information and protocol given in the lecture. It might be useful to use a linear array instead of a two dimensional array with index $k = i + jN_x$ ($i = k \mod N_x$, $j = k \div N_x$, where $\div$ is the integer division). For the 'sweeps' (i.e., $N_x N_y$ trial configurations) go through all sites systematically, use randomly selected sites, or all systematically with permutation array which is shuffled occasionally (*: 5 extra points for the last option).

b) Run your code $N_x = N_y = 5, 20, 50, 100$ and reproduce the results for $\langle E \rangle_c (T)$ (with error), $| \langle m \rangle_c (T)|$, $c_h(T)$, and $\chi(T)$. Choose your initial and intermediate equilibration sweep numbers – the latter after temperature change – such that steady states are reached. Only then do the configuration averages for at least 10^5 accepted configurations. Choose about 100 equidistant temperature changes (between $k_B T = 0.03$ and $k_B T = 3$). Compare to the Onsager solution.

c) Rerun the above for $N_x = N_y = 50$ only with $h = 0.1$.