

# Computational Physics - PHYS 410/510

## Spring 2022

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www.aglatz.net/teaching/compphys\_S2022

### Homework

# 6

HW

due 2022-04-28

#### Info

final project presentation: **Thursday, May 5, 2022, 9:30**  
(will be assigned beginning of April.)

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  $(i, j) \in [0, \dots, N_x - 1] \times [0, \dots, N_y - 1]$  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.,  $\sum_{\langle(i,j),(k,l)\rangle} = \sum_{(i,j)} \sum_{(k,l) \in \text{NN}(i,j)}$ . 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

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

If a single spin  $\sigma_{i,j}$  flips:  $\sigma_{i,j} \rightarrow -\sigma_{i,j}$ , 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  $\Delta m = -2\sigma_{i,j}$ .

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  $\Delta E$  and  $\Delta m$  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  $\langle \cdot \rangle_c$  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  $k = i + jN_x$  ( $i = k \bmod N_x$ ,  $j = k \div N_x$ , 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  $h = 0.1$ .