PHYS 3142 Spring 2021
Computational Methods in Physics
Assignment 6
Due: 11:59 p.m. 21st Mar. 2021

Before you submit your assignment, do remember:

1. the due day
2. submit a report which contains your figures and results along with your code
3. make sure your code can run
4. do not forget to write comments in your codes.
5. label your figures and describle your results

The basic scoring rubric is :

1. **If you submit the assignment after the deadline or do not submit the report, you can only get up to 80% of grade**
2. **If there is any kind of plagiarism, all of the student involving will get zero mark! (except that the one can really prove the code is written by himself or herself and others copied it without telling him or her)**

1. Ising Model for ferromagnetic materials

Use MCMC (Markov chain Monte Carlo) method to simulate the Ising model in square lattice with 10*10 sites. The lattice is set as periodic. The Hamiltonian is

$$H = -J \sum_{<i,j>}^{N} S_i S_j$$

where J is set to be 2. Please calculate the Energy, Magnetization, Heat capacity and Susceptibility of the system, and plot the figure of these observables over Temperature from T=1 to T=20 with $\triangle T = 0.2$

Note 1: the Boltzmann constant k_B is set to be 1.

Note 2: The Heat capacity can be calculated by $C_v = \frac{[<E^2>-<E>^2]}{k_B T^2}$, where E is energy.

Note 3: The Susceptibility is $\chi = \frac{[<M^2>-<M>^2]}{T}$, where M is the magnetization.

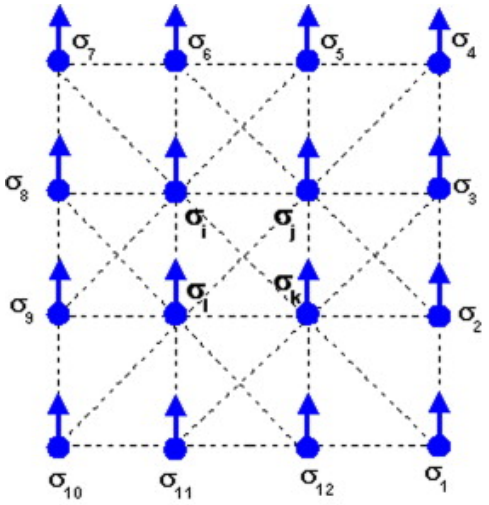
The following questions are optional, just for exercise and will not be marked.

2. Ising Model considering antiferromagnetic interactions

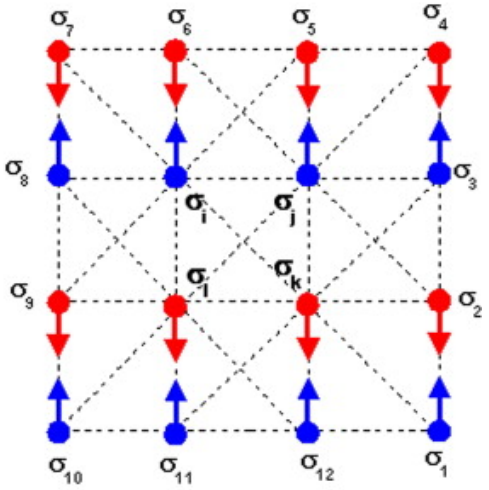
Use MCMC (Markov chain Monte Carlo) method to simulate the Ising model in square lattice with 10*10 sites. The lattice is set as periodic. The Hamiltonian is

$$H = -\sum_{<i,j>}^{N} J_{ij} S_i S_j$$

Now we assume that $J_x = 2$ while $J_y = -1$. (i.e. now the coefficient J is different along x and y direction. The lattice has ferromagnetic interaction along x direction and antiferromagnetic interaction along y direction.) What's the Energy, Magnetization, Heat capacity and Susceptibility of the system then? Please plot the figure of these observables over Temperature from T=1 to T=20 with $\triangle T = 0.2$



(a) ferromagnetic state



(b) superantiferromagnetic state