Project I

Due Thursday, July 14, 2016

Develop a program using Monte Carlo method to simulate the Ising model on a square lattice (2-dimension: L×L) at the **no** external magnetic field case (H=0). Choose the lattice edge **L=20**. Use the periodic boundary condition.

Required format of the project:

1. Introduction
   - Briefly describe the phases (ferromagnetic and paramagnetic) and the phase transition; Microstates and its probability; Statistical average;
   - Ising model: spin and its possible values; the energy of the system; how many microstates for N spins (N= L×L).
   - Monte Carlo method on a Ising model; Important sampling; How to calculate E_{flip}.

2. Pseudocode of 'float chart' of your design of the Monte Carlo simulation.

3. Write **your own code** (in FORTRAN, C/C++ or python). Attach your code (better use 'script' on omega).

4. Calculate the magnetization M (=<s>) and the total energy <E> for 50 different temperature steps from T=0.0 to T=5.0 (or a range your can observe a phase transition). Plot them against T's. Discuss the physics from your results. Use the unit $J/k_B=1$ (so your T is in J/k_B and <E> is in J). Estimate the Curry temperature T_c.

The total point is 100, distributed as 20/20/30/30 points for Section 1/2/3/4.

Hint on the structure of the code

Use (declare) a two dimension array (L×L) (e.g. L=20)
isp(L,L), one dimension for columns and another for rows
Initialize the value to all "1", i.e. all up.

At a given T (temperature):
Do a few hundred steps sweeps for initial transient (bring the system in equilibrium with the heat bath);

Start the real N sweeps to collect the average $<M>=\Sigma M_\alpha/N$, $<E>=\Sigma E_\alpha/N$; where α is a microstate or a sweep.

Output T, M, E

Repeat for a new T. (outer loop)

One Monte Carlo sweep with the periodic boundary:

```
        loop i=1, L
            i1=i-1
            if(i.eq.1) i1=L
            i2=i+1
            if(i.eq.L) i2=1
            loop j=1, L
                j1=j-1
                if(j.eq.1) j1=L
                j2=j+1
                if(j.eq.L) j2=1
                isum=isp(i1,j)+isp(i2,j)+isp(i,j1)+isp(i,j2)
c eflip is the flip energy
                eflip=2*isp(i,j)*isum
                if(eflip.lt.0) then
                    isp(i,j)=-isp(i,j)
                elseif(rand().le.dexp(-eflip/T)) then
                    isp(i,j)= -isp(i,j)
                endif
            end loop j
        end loop i
```