UNIVERSITY OF TEXAS ARLINGTON

PHYS 5319-001: Math Methods in Physics III

Monte Carlo Simulation on Ising Model

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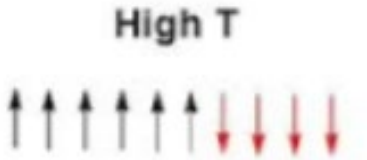
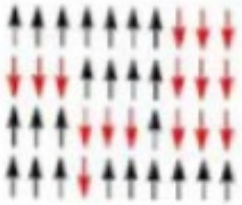
Ising Model

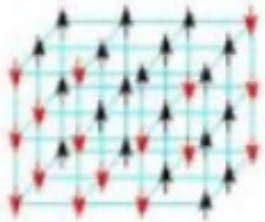


Solved

Ising – 1925



Onsager – 1944



Proven computationally intractable - 2000

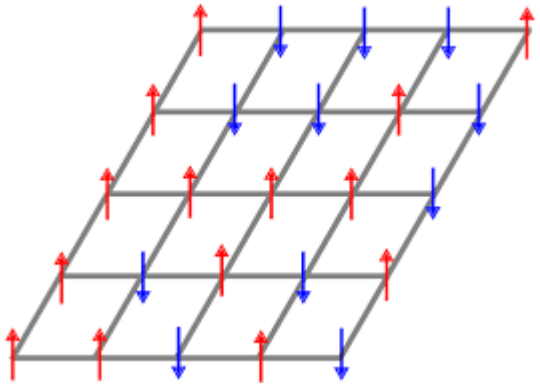
An array of *N* magnetic dipoles ("spins") on fixed points (lattice) in a uniform magnetic field *H*.

$$E_I\{s_i\} = -\sum_{<ij>} J_{ij} s_i s_j - H \sum_{i=1}^{N} s_i$$

S_i=1 or -1 (up or down); <ij> only consider the nearest neighbor; J_{ij} *(>0)* is the coupling constants.

For a system of *N* spins ($N \to \infty$), each spin configuration is a micro-state (α).

probability $P_\alpha \sim e^{-E_\alpha/kT}$

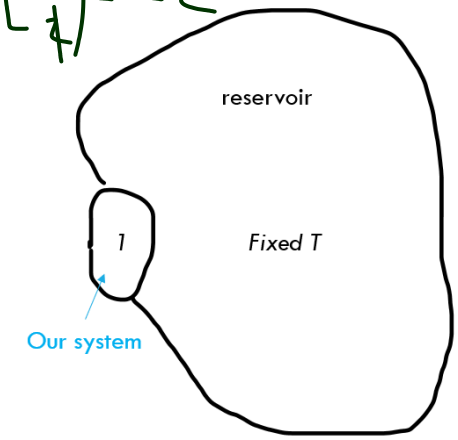


A macroscopic measurement $\langle A \rangle = \sum_\alpha A_\alpha P_\alpha$ e.g. $M = \sum_\alpha M_\alpha P_\alpha$

how many α? 2^N

Monte Carlo simulation of Ising model

- Here we use 2-d Ising model as an example;
- System in equilibrium with a heat reservoir;
- Canonical ensemble: $P_\alpha \sim e^{-E_\alpha/kT}$
- We *cannot* take all the micro states α (2^N);
- "random shooting" is just a uniform sampling;
- Important sampling: Metropolis algorithm:



-initialize the spin configuration (random or uniform)

-given a temperature (*T*) and field *H* (here =0)

-choose a spin (start from the 1st one) and flip it (a new configuration), calculate the energy change E_{flip};

*if $E_{flip}<0$, accept it. A new micro state α' is obtained (stored)

*if $E_{flip}>0$, $p = e^{-E_{flip}/kT}$; and generate a random number *r*.

if $p>r$, accept (the flip), a new state α' is obtained

if $p<r$, reject it (don't flip)

-move to the next spin.

a 5 × 5 model

Project I

Due Thursday, July 15, 2021

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. And only consider the nearest coupling/interaction.

Required parts 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 Matlab or python). Attach your code.

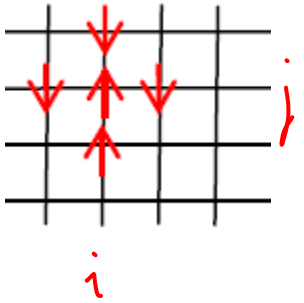
4. Calculate the magnetization M (=<s>) and the total energy <E> for 50 different temperature steps from T=0.0 to T=5.0 (or a range your can observe a phase transition). Plot them against T's. Discuss the physics from your results. **Use the unit $J/k_B=1$** (so your T is in J/k_B and <E> is in J). Estimate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

The core part

at a given temperature T, and the cell size L: S_{ij} initialized

One Monte Carlo sweep with the periodic boundary:

```
loop i=1, L                                   column index
      i1=i-1                                  left neighbor
      if(i=1) i1=L
      i2=i+1                                  right neighbor
      if(i=L) i2=1
      loop j=1, L                             row index
            j1=j-1                            up neighbor
            if(j=1) j1=L
            j2=j+1                            down neighbor
            if(j= 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< 0) then                 flip
                  isp(i,j)=-isp(i,j)
            elseif(rand()<exp(-eflip/T)) then flip
                  isp(i,j)= -isp(i,j)
            endif
      end loop j
end loop i
```



$$E_\alpha = \sum_{<n.n.>} J s_{ij} s_{i'j'}$$

$$\Delta E = E_1 - E_2 = 2J s_{ij} \sum_{<n.n.>} s_{i'j'}$$

function/subroutine. Let's call it **sweep**

More about the project-1

- For each call of function *sweep*, pass in: isp(L,L) array, *T*, and L
  pass out: isp(L,L) array ($\{S_{i,j}\}$)
- At a new *T*, since isp() is randomly initialized, you need at least run 500 sweeps to reach the equilibrium state.
- Then, start the simulation for that specific *T* for *N* sweeps
  at the end of each sweep (state α), calculate

$$\boldsymbol{M_\alpha = \sum_{ij} \langle S_{ij} \rangle}$$

$$E_\alpha = -J \sum_{<ij,i'j'>} S_{ij} S_{i'j'}$$

  at the end of this T, average *M* and *E* over *N* configurations (micro states).
- Repeat this for all T values
- Plot *M(T)* and *E(T)*

Have fun!