The Ising Model

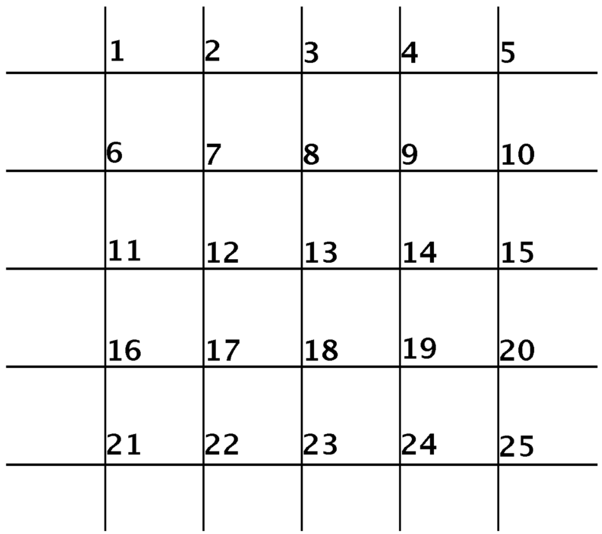
Monte Carlo Methods and Simulations

Ising Model

- A particular case of a lattice model
- It describes a very simple magnetic model (well... not really)
- It is solvable and exhibits a phase transition

Lattice

- Size $L{\times}L$, in the thermodynamic limit $L{\to}\infty$
- Each lattice point is labeled with one single index i
- $<i,j>$ denotes a pair
- We employ periodic boundary conditions



Hamiltonian

- On each node *i* we place a spin s_i
  - Two possible values $s_i = \pm 1$
  - The spins are the degrees of freedom
  - The Hamiltonian is:

$$H\{s_i\} = -J \sum_{<i,j>} s_i s_j - H \sum_i s_i$$

  - With J a coupling constant
  - And H the external magnetic field

Properties

- It only couples nearest neighbors spins, so
  - if $i=8 \Rightarrow j = 3, 7, 9, 13 \Rightarrow J \neq 0$ else $J=0$ end if
- Positive, $J>0$, favors nearest neighbors to be like i. This is called ferromagnetic
- Negative, $J<0$, favors nearest neighbors to NOT be like i. This is called antiferromagnetic
- Second term favors the spins to have a sign equal to that of magnetic field H

Partition function

$$Z = \sum_{\{s_i\}} \exp\left[\beta J \sum_{<i,j>} s_i s_j + \beta H \sum_i s_i\right]$$

- If *H=0* the model can be solved analitically

We can study

- Average value of the spins → magnetization
  - Let's start with all the spins in +
  - Flipping a spin with four equal nearest neighbors induces a penalty via Boltzmann factor $\exp[-8\beta J]$
  - For low temperature, as β is large, a particular spin flip is a very rare event

Raising T

- If we raise the temperature, the probability of having one or more spins turned over increases and therefore the magnetization decreases
- $T \rightarrow \infty \Rightarrow \beta = 0$
  - All configurations have a Boltzmann factor of 1 and the coupling of the spins is no longer noticeable
  - Each spin will assume values ± 1 with equal probability
  - Magnetization vanishes

Intermediate temperature

- To scenarios:
    - Magnetization decays asymptotically with increasing temperature
    - It will vanish at a certain temperature
        - Implies a non-analytical behavior in the magnetization curve

But...

- Hamiltonian depends analytically on all spins for finite systems
- All physical variables are analytic functions of the system parameters
- For $N \to \infty$, non-analytical behavior might show up
    - ... and actually happens!

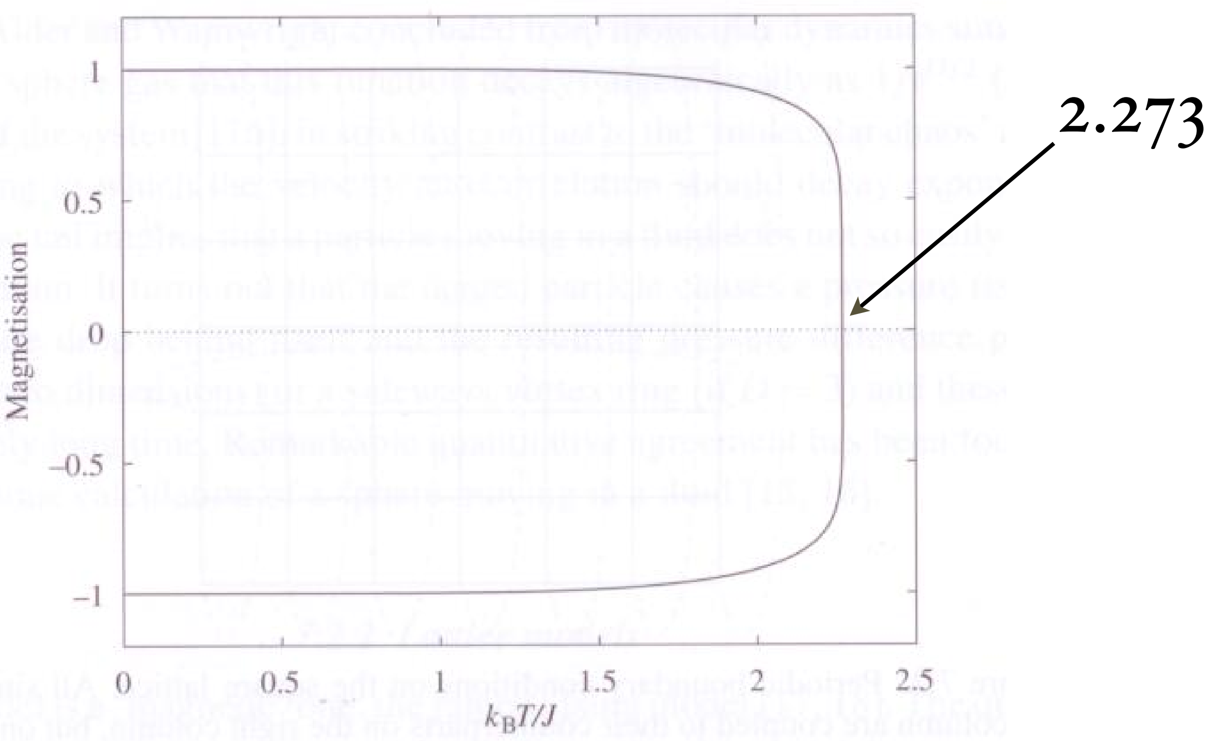
Phase transition

- For

$$\frac{J}{k_B T_c} \approx 0.44$$

Magnetization for the infinite system disappears

Magnetization curve



Final remarks

- The picture here is a dynamic one:
  We start with a particular state (all spins +1) and we increase temperature
  Average values of physical quantities are given by ensemble averages, so the average magnetization
- It is believed that in a realistic magnetic system spins flip one after another or in small groups
- Then turning over magnetization requires a large number of spin flips and the ocurrence of a domain wall between two regions

Metropolis & Ising Model

- 2D Ising model
- We must make a choice for the matrix $\omega_{XX'}$
  - For a 2D L×L lattice

$$\omega_{XX'} = 1/L^2 \quad \text{if X and X' differ by one spin}$$
$$\omega_{XX'} = 0 \quad \text{otherwise}$$

Algorithm

- Generate the initial configuration
- Choose one spin at random
- Flip spin, generating the trial configuration
- Calculate the energy difference

$$\Delta E\left(X \to X'\right) = E(X') - E(X)$$

- If the energy increases the trial state is accepted with probability $\exp\left[-\beta \Delta E\left(X \to X'\right)\right]$
- If energy decreases ⇒ always accept

Algorithm (II)

- The average number of steps between two updates in one particular spin is equal to L^2
- Therefore the time is usually expressed in MCS, Monte Carlo Steps per spin where
  1 MCS = L^2 trials