Monte Carlo – Metropolis Application

Ising Model

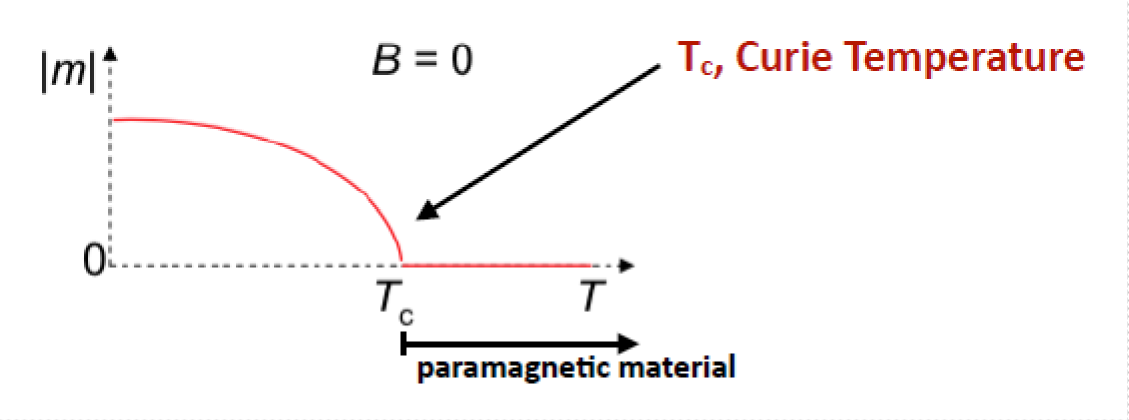
Model of a magnetic material

- The spins S_i can take two possible values +1 or -1
- Interaction only between pairs of nearest-neighbours <ij>
- $J > 0$ is the strength of exchange interaction (units of energy)

$$E = -J \sum_{<ij>} S_i S_j$$

The goal is to study the existence of a phase transition between an ordered (magnetized) phase with $m \neq 0$ and a disordered (non magnetic) phase $m=0$ depending on the temperature T (determine Tc, m=m(T), internal energy, specific heat…)

$$m = \frac{\langle S \rangle}{N},$$



Monte Carlo – Metropolis Example

"Direct" Monte Carlo (as in the calculation of Pi example)?

2^{NxN} states

=> for N=16 we have $\approx 10^{77}$ states
=> for N=64 we have $\approx 10^{8000}$ states

Impossible !!

- **But not all states are equally probable!!**
- Instead, we can consider a exploration of states following its probability in thermal equilibrium

$$p(E) \propto \exp(-E/k_{\mathrm{B}}T)$$

W. Krauth, "Statistical Mechanics: Algorithms and Computations".

Monte Carlo – Metropolis Example

Algorithm implemented

Monte Carlo – Metropolis Algorithm implemented in the code

- Generate initial state (*o*)

- Try a new state flipping a randomly selected spin (*n*)

- Decide to accept or reject the move from *o* to *n*

  If $U(n)-U(o) < 0$ => accept the move from *o* to *n*
  If $U(n)-U(o) > 0$ => accept the move from *o* to *n* with a probability given by the Boltzmann factor:

$$p(o \to n) = \exp\left[-\frac{U(n) - U(o)}{k_B T}\right]$$

- Repeat over and over again until some convergence criterion is achieved