Computer modeling of physical phenomena: thermal Monte Carlo simulation

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19/04/2021, Pasteura 5, Warszawa

Plan

Plan

System in thermal equilibrium

- canonical ensamble: temperature T fixed by a big reservoir
- state occupation probability: Boltzman distribution

$$p_X = \frac{1}{Z} e^{-E(X)/k_B T},$$

where X denotes the state, $E(X)$ its energy.

- normalization constant

$$Z = \sum_X e^{-E(X)/k_B T},$$

is called the partition function (or statistical sum)

Observables

- expectation value of a physical quantity
- e.g. internal energy

$$U = \langle E \rangle = \frac{1}{Z} \sum_X E(X) e^{-\beta E(X)},$$

where $\beta = 1/k_B T$

Plan

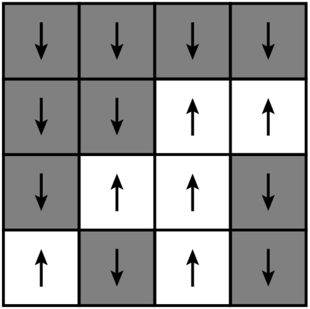
Ising model

Hamiltonian – or just energy function

$$H = -J \sum_{<ij>} s_i s_j - H \sum_i s_i$$

- spin (classical) $s_i = \pm 1$ on lattice sites i
- J – magnitude of nearest neighbour $< ij >$ interaction
- $X = \{s_i\}_{i=1\ldots N}$ – states of the system, total number 2^N
- external magnetic field H

Significance of the Ising model



- physically motivated model of magnetism
- playgroung for theoreticians to test methods, approaches, ideas

How to solve the Ising model

- exact solution of a phase transition (in 2D)
  given by Onsager in 1944
- important challenge: analytics for Ising model in 3D
- generate random, representative configurations:
  Monte Carlo simulations

Quantities to calculate

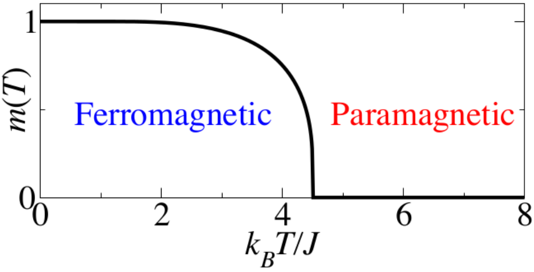
- mean magnetization per spin

$$\langle m \rangle = \frac{1}{N} \langle \sum_i s_i \rangle$$

- magnetic susceptibility
  (response to a small mag. field)

$$\chi = \frac{\partial \langle m \rangle}{\partial H} = \beta N (\langle m^2 \rangle - \langle m \rangle^2)$$

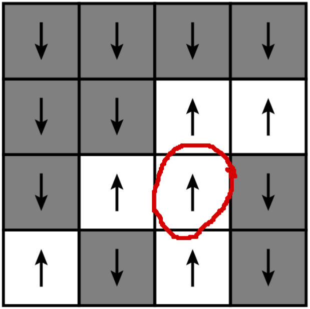
Qualitative behaviour



- low temperatures:
  spins organize themselfs to point in one direction
- high temperatures: spins fluctuate wildly,
  magnetization drops to zero

Heat-bath algorithm: idea

- thermalizes one spin at a time
- sets spin up/down with thermal distribution, given the neighbours are fixed



Heat-bath algorithm for the Ising model

1. Pick up a spin at random, lattice site i
2. Check how many neighbouring spins are "up"

$$m_i = \sum_{j:<ij>} s_j$$

3. Calculate the energy for spin i to be $+1$ or -1:

$$E_+ = -Jm_i - H; \quad E_- = +Jm_i + H$$

4. Set spin at $+1$ with probablity $p = \frac{e^{-\beta E_+}}{e^{-\beta E_+} + e^{-\beta E_-}}$ (at -1 with $1 - p$)
5. Repeat: 1MCS is performed
   after visiting every spin in the system on average

Draft of Python script

```
@jit(nopython=True)
def sweepHB(s,beta,L):
    # all variables we wish to change in the code should be listed
    # no need to return s -- it is just overwritten!

    for k in range(L*L):

        # pick a random site
        ix, iy = randint(L), randint(L)

        # calculate the sum over neighbouring spins
        sum_loc = ( s[(ix+1)%L,iy] + s[(ix-1)%L,iy]
                    + s[ix,(iy+1)%L] + s[ix,(iy-1)%L] )

        ## heat-bath
        prob_pls = 1./( 1. + np.exp(-2*beta*sum_loc) )
        if ( rand() < prob_pls ):
            s[ix,iy] =  1
        else:
            s[ix,iy] = -1
```