Ising models

- originally it was suggested as a crude model of magnetic materials, but it can be used with a different interpretation also e.g. to model binary alloys or other systems.

- it was the first microscopic model with phase transition which can be solved in a closed form (at least in one and two dimensions)

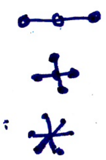
- the degrees of freedom (usually to be spins) are positioned on a lattice and interact only with the nearest neighbors

- Monte Carlo method can be used to calculate its thermodynamic properties by averaging over states of the system, thus it is also a useful toy model to show how MC works

• Hamiltonian – let σ_α denote a spin at the point α of the lattice (it can be 1D, 2D or 3D) which can be of value ± 1
(we will consider them as classical degrees of freedom, for the quantum case, look for the Heisenberg model)

- each spin is interacting with the external magnetic field B and its nearest neighbors:

1D: 2D: 3D:



$$H = -\mu B \sum_\alpha \sigma_\alpha - J \sum_{\langle\alpha\beta\rangle} \sigma_\alpha \sigma_\beta$$

μ: magnetic moment usually taken as 1

J: coupling constant

$\langle\alpha\beta\rangle$: sum is over nearest neighbor pairs only

(for $J>0$ we talk about „ferromagnetic" case
for $J<0$ about „antiferromagnetic" case)

and we will assume periodic boundary conditions

(in 1D σ_1 integracts with σ_N and σ_2

in 2D e.g. σ_{11} interacts with σ_{12}, σ_{21}, σ_{1N} and σ_{N1})

- the first term tends to align the spins along the field B

  the second term has a minimum for

  all spin aligned if $J>0$ $\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\ldots$

  or all spin alternating if $J<0$ $\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\ldots$

• <u>thermodynamics</u>

- if there are N spins in the model, there is

  2^N configurations of spins $\sigma = \{\sigma_\alpha\}_\alpha$

  runs over all lattice points

- in this canonical ensemble each state appear with probability

$$\rho(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z} \quad , \beta = \frac{1}{k_B T}$$

where

$$Z(B,T) = \sum_\sigma e^{-\beta H(\sigma)}$$

is the partition sum

- using Z we can calculate various quantities of interest like the free energy per site

$$f(B,T) = -\frac{1}{\beta N} \ln Z(B,T)$$

magnetization (averaged over ensemble) per site

$$M(B,T) = -\frac{\partial}{\partial B} f(B,T) = \frac{1}{\beta N} \frac{\frac{\partial Z}{\partial B}}{Z} =$$

$$= \frac{1}{\beta N} \sum_\sigma \left(\frac{e^{-\beta H}}{Z} \mu\beta \sum_\alpha \sigma_\alpha \right) = \frac{\mu}{N} \sum_\sigma \rho(\sigma) \left(\sum_\alpha \sigma_\alpha \right)$$

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

susceptibility per site

$$\chi = \frac{\partial M}{\partial B} = \frac{\mu}{N} \frac{\partial}{\partial B} \sum_\sigma \frac{e^{-\beta H}}{Z(B,T)} \left(\sum_\alpha \sigma_\alpha \right) =$$

$m = \mu \sum_\alpha \sigma_\alpha$

$$= \frac{\mu}{N} \sum_\sigma \Bigg[\underbrace{\frac{\mu\beta \left(\sum_\alpha \sigma_\alpha\right)^2 e^{-\beta H}}{Z}}_{\langle m^2 \rangle} - \frac{e^{-\beta H}}{Z^2} \left(\sum_\alpha \sigma_\alpha \right) \underbrace{\sum_\sigma \mu\beta \left(\sum_\alpha \sigma_\alpha \right) e^{-\beta H}}_{\beta \langle m \rangle} \Bigg] = \frac{\beta}{N} \left(\langle m^2 \rangle - \langle m \rangle^2 \right)$$

internal energy per site

$$U(B,T) = -T^2 \frac{\partial}{\partial T}\left(\frac{f(B,T)}{T}\right) = \frac{kT^2}{N}\frac{\partial \ln Z}{\partial T} = \frac{kT^2}{N}\frac{\sum_\sigma e^{-\frac{H}{kT}}\left(\frac{H}{kT^2}\right)}{Z}$$

$$= \frac{1}{N}\sum_\sigma \varrho(\sigma) H(\sigma)$$ as one could expect

and specific heat per site

$$c(B,T) = \frac{\partial u(B,T)}{\partial T} = \frac{1}{N}\sum_\sigma H(\sigma)\frac{\partial}{\partial T}\frac{e^{-\frac{H}{kT}}}{Z(B,T)} =$$

$$= \frac{1}{N}\sum_\sigma H(\sigma)\left[\frac{e^{-\frac{H}{kT}}}{Z}\frac{H(\sigma)}{kT^2} - \frac{e^{-\frac{H}{kT}}}{Z^2}\sum_\sigma e^{-\frac{H}{kT}}\frac{H}{kT^2}\right] =$$

$$= \frac{1}{NkT^2}\left[\sum_\sigma \varrho(\sigma) H(\sigma)^2 - \left(\sum_\sigma \varrho(\sigma) H(\sigma)\right)^2\right]$$

$$= \frac{1}{NkT^2}\left(\langle H(\sigma)^2\rangle - \langle H(\sigma)\rangle^2\right)$$

- implementation notes
  - to determine whether a new configuration is accepted in the Metropolis-Hastings algorithm we need to calculate the ratio

$$\frac{\varrho(\sigma_{try})}{\varrho(\sigma_{now})} = e^{-\beta[H(\sigma_{try}) - H(\sigma_{now})]} = e^{-\beta \Delta E}$$

where ΔE is a change in energy of the whole system when we change the configuration of spins σ_{now} to a new configuration σ_{try}

  - because we usually change only one spin at a random position σ_{ij} it is not necessary to calculate $H(\sigma)$ but only ΔE given by (in 2D)

$$\Delta E = 2\mu B \sigma_{ij} + 2J\sigma_{ij}\left(\sigma_{i^+j} + \sigma_{i^-j} + \sigma_{ij^+} + \sigma_{ij^-}\right)$$

where i^+ is $i+1$ for $i<N$ and 1 for $i=N$ (periodic boundary conditions)

and similarly for i^-, j^+ and j^-