Monte Carlo Simulations in Statistical Physics

Classical interacting many-particle systems; examples

- atoms and molecules in simple liquids, gases, solids
- macromolecular systems; polymers, liquid crystals
- spin models of magnetism

Quantum fluctuations can often be neglected (not always)

Problem: Evaluate thermal expectation values

N particles with positions and momenta $\vec{x}_i,\ \vec{p}_i$

$$\langle A \rangle = \frac{1}{Z} \int \prod_{i=1}^{N} dx_i^d \int \prod_{i=1}^{N} dp_i^d A(\{x_i, p_i\}) \mathrm{e}^{-H(\{x_i,p_i\})/k_B T}$$

Partition function (state sum)

$$Z = \int \prod_{i=1}^{N} dx_i^d \int \prod_{i=1}^{N} dp_i^d \mathrm{e}^{-H(\{x_i,p_i\})/k_B T}$$

Hamiltonian (energy function) for identical particles in potential U and with pair-interaction V

$$H(\{\vec{x}_i, \vec{p}_i\}) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=1}^{N} U(\vec{x}_i) + \sum_{i \neq j} V(\vec{x}_i, \vec{x}_j)$$

If the observable A is velocity-independent (real-space correlation functions, response of local density to external perturbations, etc.), the momentum integrals cancel

$$\langle A \rangle = \frac{1}{Z} \int \prod_{i=1}^{N} dx_i^d A(\{x_i\}) \mathrm{e}^{-E(\{x_i\})/k_B T}$$

$$Z = \int \prod_{i=1}^{N} dx_i^d \mathrm{e}^{-E(\{x_i\})/k_B T}$$

Only the potential energy matters

$$E(\{x_i\}) = \sum_{i=1}^{N} U(\vec{x}_i) + \sum_{i \neq j} V(\vec{x}_i, \vec{x}_j)$$

For the kinetic energy the position integrals cancel

$$\left\langle \frac{p_i^2}{2m} \right\rangle = \frac{1}{Z_p} \int dp_i^d \frac{p_i^2}{2m} \mathrm{e}^{-p_i^2/2mk_BT}$$

$$Z_p = \int dp_i^d \mathrm{e}^{-p_i^2/2mk_BT}$$

This gives the equipartition theorem $\left\langle \frac{p_i^2}{2m} \right\rangle = \frac{d}{2} k_B T$

Most of statistical physics concerns velocity-independent quantities; the mathematical problem of interest is

$$\langle A \rangle = \frac{1}{Z} \int \prod_{i=1}^{N} dx_i^d A(\{x_i\}) \mathrm{e}^{-E(\{x_i\})/k_BT}$$

$$Z = \int \prod_{i=1}^{N} dx_i^d \mathrm{e}^{-E(\{x_i\})/k_BT}$$

With N approaching infinity (thermodynamic limit)

Few exact solutions; numerical simulations for finite N important

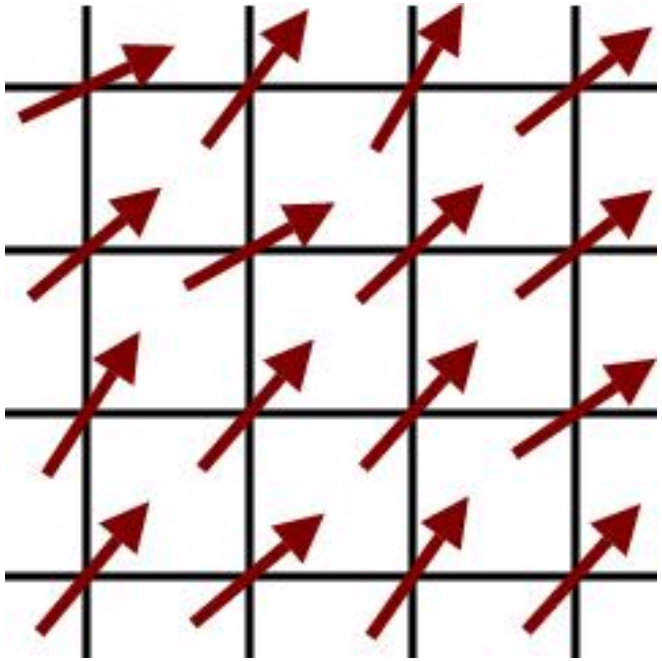
Lattice and spin models

Degrees of fredom "live" on vertices of a lattice

- Continuous or discrete variables on the vertices

Spin models, describing magnetism of solids with spinful atoms

- large spin S behaves as classical angular momentum
- quantum fluctuations important for small S (1/2,1,3/2)



Interactions: often of the Heisenberg form

$$E = \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

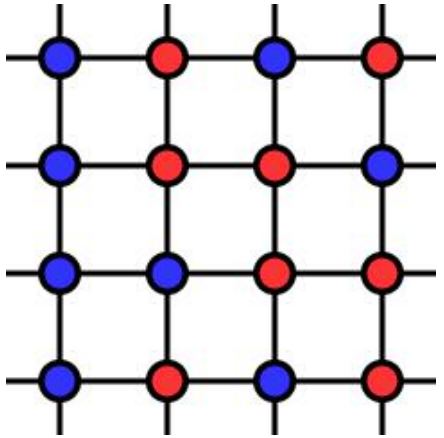
Ising models

Two states on each lattice site $\text{spin} \uparrow, \downarrow$

Can arise for quantum mechanical S=1/2: $S_i^z = \pm 1/2$

Strong anisotropies; z-interactions can dominate

$$E = \sum_{i,j} J_{ij} S_i^z S_j^z$$



This is the Ising model

- important in the theory of magnetism
- also effective model for other stat mech problems ("lattice gases", binary alloys, atom adsorption on surfaces,...)

With only nearest-neighbor interactions (J), the Ising model can be solved analytically in 1D and 2D

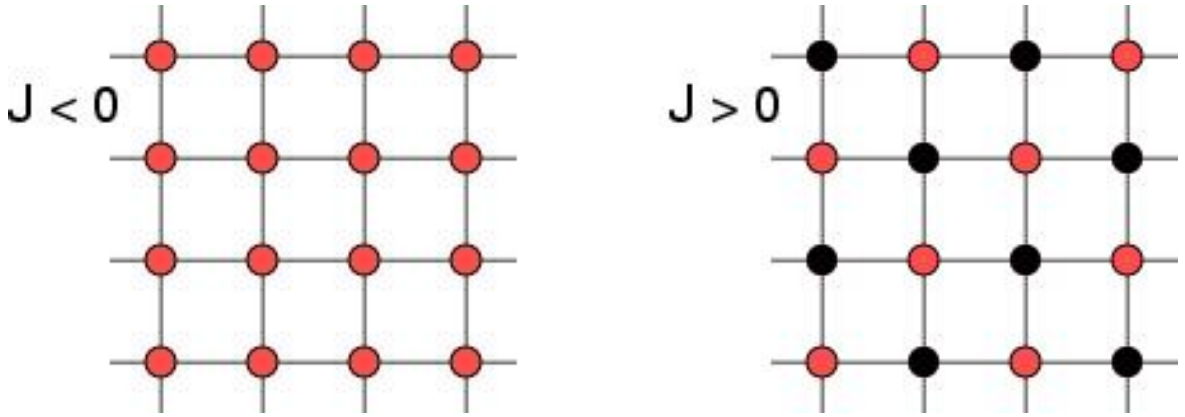
- Numerical simulations important in most other cases

Two-dimensional Ising model

$$E = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \quad \sigma_i = \pm 1$$

$\langle i, j \rangle$ denotes nearest neighbors

Ferromagnetic or antiferromagnetic ground state (T=0)



Related by transformation: $\sigma_i \longrightarrow -\sigma_i$ on one sublattice

Thermal expectation value of some quantity A

$$\langle A \rangle = \frac{1}{Z} \sum_S A(S) \mathrm{e}^{-E(S)/T}, \quad Z = \sum_S \mathrm{e}^{-E(S)/T}$$

Phase transition

Spontaneous ordering (symmetry breaking) at critical temperature

magnetization (ferromagnet)

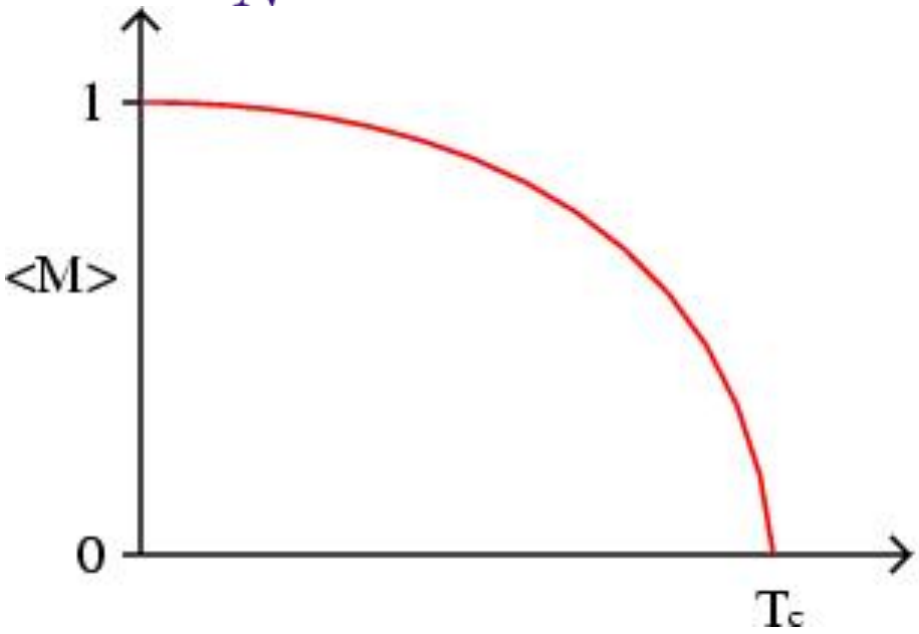
$$T_c/J = 2/\ln(1+\sqrt{2})$$

$$T_c/J \approx 2.269$$

$$M = \frac{1}{N}\sum_{i=1}^{N}\sigma_i$$

sublattice (staggered) magnetization (antiferromagnet)

$$M = \frac{1}{N}\sum_{}^{N}(-1)^{x_i+y_i}\sigma_i$$



Broken symmetry
only in infinite system

<M>=0 for finite N

<M^2> or <|M|> can be used