

The Ising Model

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History

- ▶ Proposed by Wilhelm Lenz to his student Ernst Ising
- ▶ 1924: Ernst Ising - *Beitrag zur Theorie des Ferromagnetismus*¹
"Es entsteht ... [durch] ... die Beschränkung der Wechselwirkung auf diejenige benachbarter Elemente [...] kein Ferromagnetismus."
- ▶ 1936: Rudolph Peierls - *On Ising's model of ferromagnetism*²
"[...] for sufficiently low temperatures the Ising model in two [or more] dimensions shows ferromagnetism [...]."

¹Zeitschrift für Physik Februar–April 1925, Volume 31, Issue 1, pp 253-258

²Cambridge Philosophical Society 1936, Volume 32, Issue 03, Oct.

Figure: Square Lattice in 1 dimension

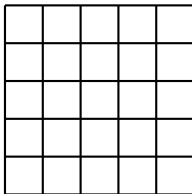


Figure: Square Lattice in 2 dimensions

Figure: Square Lattice in 1 dimension

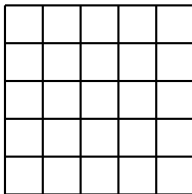


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Lattice



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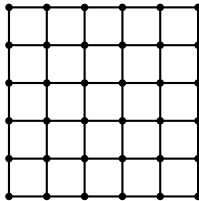


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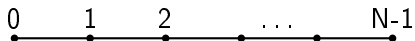


Figure: Square Lattice in 1 dimension

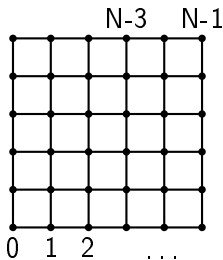


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Figure: Square Lattice in 1 dimension

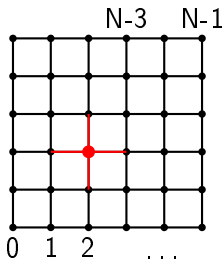


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Figure: Square Lattice in 1 dimension

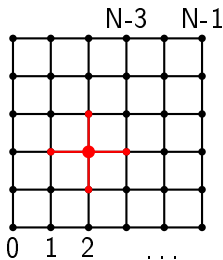


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Figure: Square Lattice in 1 dimension

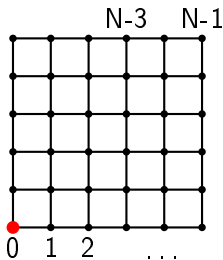


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Figure: Square Lattice in 1 dimension

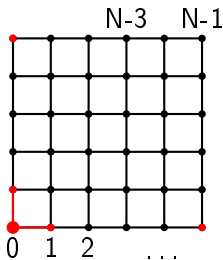


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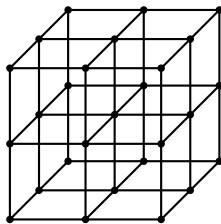
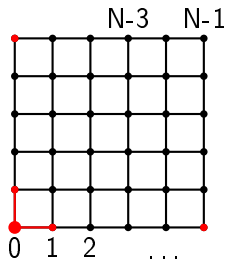


Figure: Square Lattice in 2 and 3 dimensions

Lattice



Figure: Square Lattice in 1 dimension

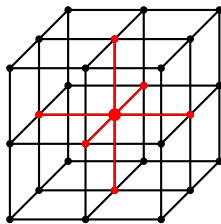
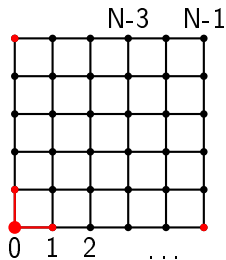


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Lattice Sites

- ▶ Each site has a state $s_i = -1 \vee 1$
- ▶ Assignment of states $S = (s_0, s_1, s_2, \dots, s_{N-1})$ to the lattice sites is called a configuration
- ▶ Therefore 2^N unique configurations for a lattice with N lattice sites.

Magnetization

- ▶ The magnetization of a configuration is calculated by

$$M_S = M(S) = \sum_i^N s_i \in [-N, N]$$

- ▶ The squared magnetization is an indicator for the degree of order

$$M_S^2 = \sum_i s_i^2 \in [0, N]$$

- ▶ Each configuration has a corresponding energy - the Hamiltonian.

$$E_S = E(S) = H(s_0, s_1, \dots, s_{N-1}) = -J \sum_{\langle i,j \rangle} s_i \cdot s_j - h \sum_i s_i$$

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$$H_S = -J \sum_{\langle i,j \rangle} s_i \cdot s_j \quad \in [-2NJ, 2NJ]$$

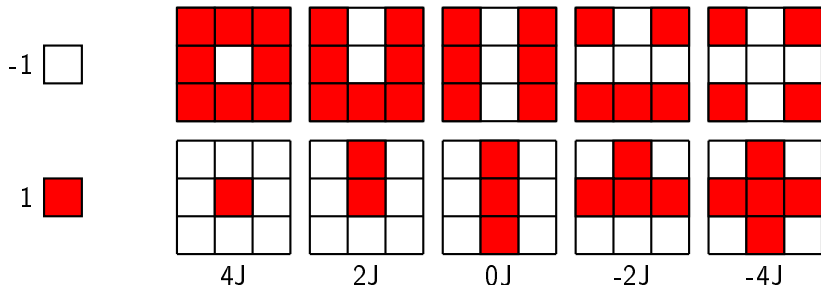


Figure: Energy contribution (nearest neighbor interaction) of the bonds connected to the central lattice site

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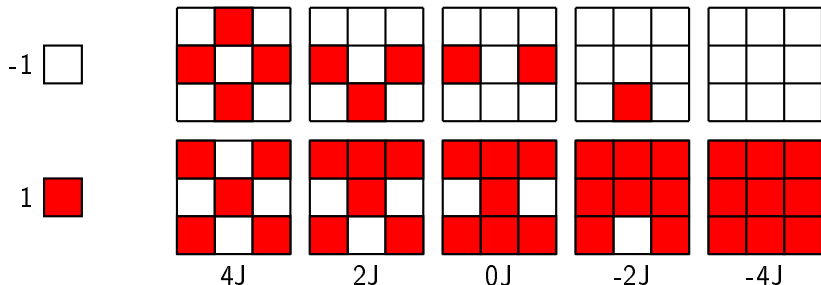


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Boltzmann distribution

Probability of system being in the state S is given by the Boltzmann distribution ($\beta = 1/kT$)

$$p_S = p(S) = \frac{e^{-\beta E_S}}{Z}$$

Z is the the partition function

$$Z = \sum_i^{2^N} e^{-\beta E_{S_i}}$$

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→ *importance sampling*

Markov Chain

- ▶ Chain of iteratively created configurations C_1, C_2, \dots, C_n
- ▶ Resulting configurations correspond to the desired probability distribution p and span the entire state space.
- ▶ Configuration C_t only depends on C_{t-1} (Markov property).

Transitions in the Markov Chain

Probability for being in state A:	p_A
Transition probability for transition $S_A \rightarrow S_B$:	p_{AB}

If it fulfills *detailed balance* (it must!)

$$p_A \cdot p_{AB} = p_B \cdot p_{BA}$$

the following relation for the transition probability follows:

$$\frac{p_{AB}}{p_{BA}} = \frac{p_B}{p_A} = \left(\frac{Z}{Z} \right) \frac{e^{-\beta E_B}}{e^{-\beta E_A}} = e^{-\beta(E_B - E_A)} = e^{-\beta \Delta E}$$

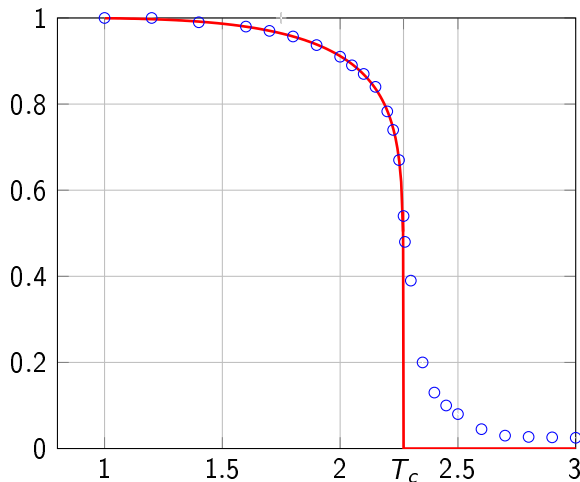
Metropolis- Hastings Algorithm

- ▶ Configuration after t steps is C_t
- ▶ Flip one lattice site $\rightarrow C'_t$
 - ▶ has to be chosen randomly - suitable RNG necessary
- ▶ Calculate energy difference $\Delta E = E'_t - E_t$
- ▶ Calculate acceptance probability P

$$P = \min \left(1, e^{-\beta \cdot \Delta E} \right), \quad \beta = 1/kT > 0$$

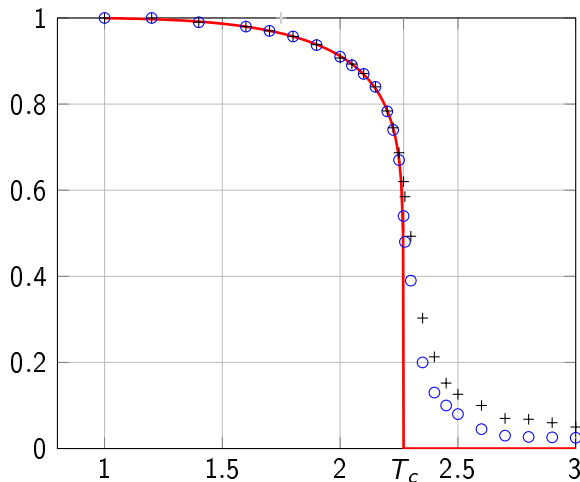
- ▶ Generate random number $r \in [0, 1[$
 - ▶ $r < P \rightarrow C_{t+1} = C'_t$
 - ▶ $r > P \rightarrow C_{t+1} = C_t$

Absolute magnetization per spin



?? MC 75×75
?? analytical solution

Absolute magnetization per spin



?? MC 50×50
?? MC 75×75
?? analytical solution

Properties of a configuration s

- ▶ Energy – Hamiltonian: $E(s) = H(s)$
- ▶ Internal energy (per spin): $e(s) = E/N \in [-2, 2]$
- ▶ Magnetization: $M(s) = \sum_i^N s_i$
- ▶ Magnetization (per spin): $m(s) = M/N \in [-1, 1]$

Temperature

Temperature in the Ising Model

$$P = \min \left(1, e^{-\beta \cdot \Delta H} \right), \quad \beta = 1/kT > 0$$

- ▶ $\Delta H < 0 \rightarrow P = 1$
- ▶ high temperature leads to higher acceptance probability \rightarrow unordered (low magnetization, Curie Temperature T_c)
- ▶ critical temperature T_c when $\langle \sum_i^N s_i \rangle / N \approx 0$

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 - ▶ $kT_c/J = 2.269$

Cluster Flip Algorithms

Summary - Ising Model

- ▶ molecules on a lattice - each with with one of two possible states
- ▶ (magnetic) moments prefer to align
- ▶ low temperatures: ordered
- ▶ high temperatures: disordered

Different Models

- ▶ Single value obtained from one configuration hasn't much significance
- ▶ Average from many (n) configurations instead:

$$\bar{E} = \frac{1}{n} \sum_i^n E_{S_i} \qquad \bar{M} = \frac{1}{n} \sum_i^n M_{S_i} \qquad \dots$$

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- ▶ Sampling from completely random configurations does not work well for ordered configurations seen in ferromagnets.