The Ising Model and Markov Chain Monte Carlo

Vladimir Parfenyev

parfenius@gmail.com

Skolkovo Tech

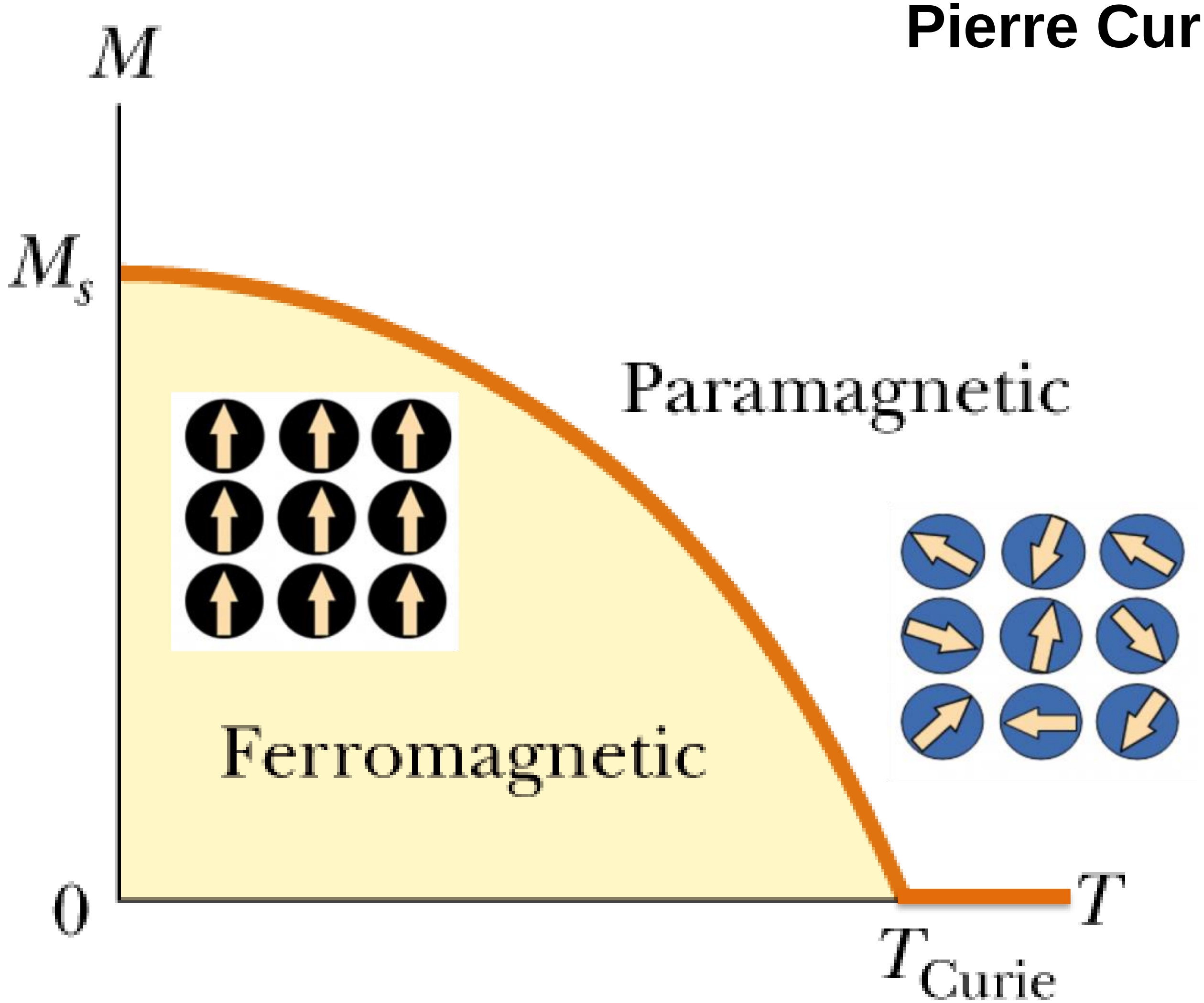
Skolkovo Institute of Science and Technology

17 April 2017

I. The Ising Model

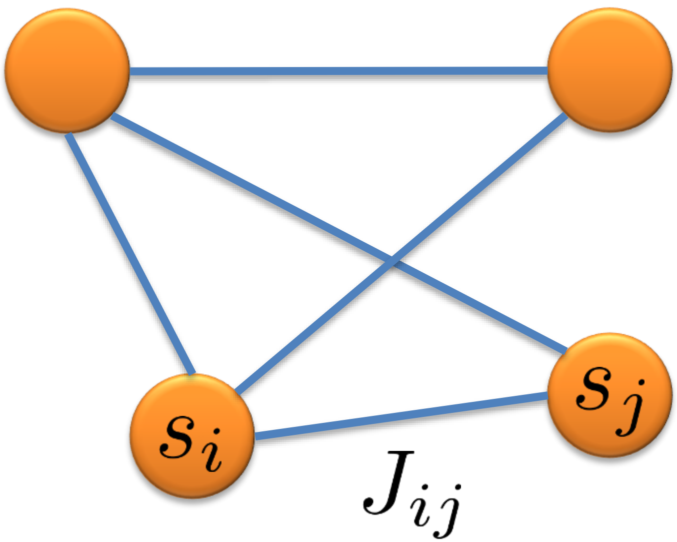
Block of Iron

Pierre Curie, 1895



The Ising Model

Each site *i* has a spin $s_i = \pm 1$ and each edge corresponds to interaction between spins:



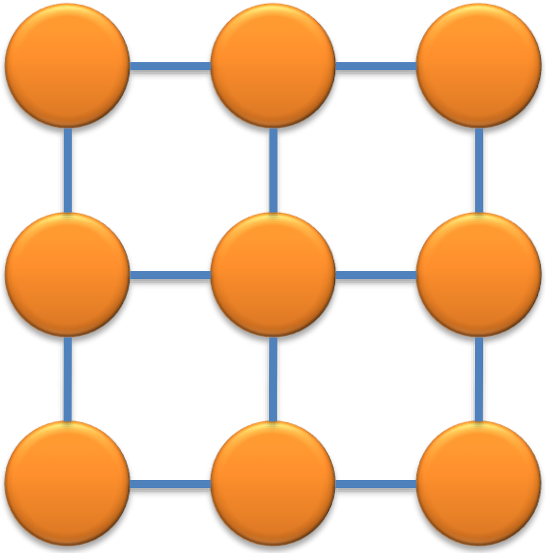
$$E = -\sum_{\langle ij \rangle} J_{ij} s_i s_j - \mu \sum_j s_j h_j$$

external magnetic field

Regular lattices are common for physical applications.

Physical Model

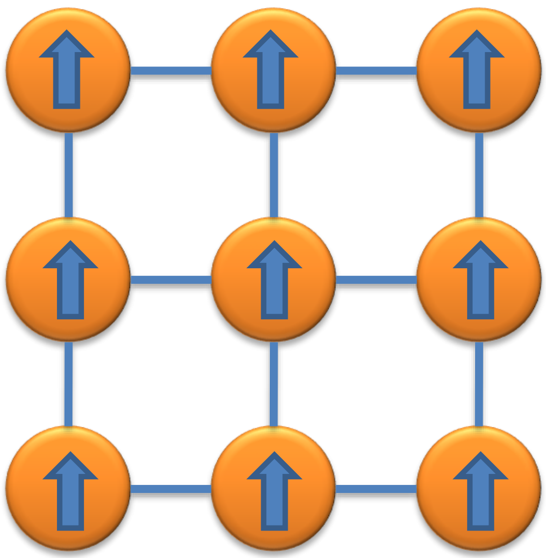
Square lattice with **periodic boundary conditions** and without external magnetic field:



$$E = -\sum_{\langle ij \rangle} s_i s_j$$

Physical Model

Square lattice with **periodic boundary conditions** and without external magnetic field:



$$E = -\sum_{\langle ij \rangle} s_i s_j$$

Lowest energy state – all spins point in the **same direction** – ferromagnetic order.

Boltzmann Distribution

System is not always in the lowest energy state – depending on temperature its energy is sometimes higher.

$$P_{eq}(s) = \frac{1}{Z} e^{-\beta E(s)}, \quad \beta = 1/T$$

$T \to 0, \ \beta \to \infty$ -- lowest energy state

$T \to \infty, \ \beta \to 0$ -- all states are equally likely

Free Energy *F = E - TS*

Macrostate – grouped states with the same energy *E*

The probability of being into macrostate:

$$\frac{W}{Z}e^{-\beta E} = \frac{1}{Z}e^{S-\beta E} = \frac{1}{Z}e^{-\beta(E-TS)}$$

The likeliest macrostate minimizes the **free energy**.

II. Direct Sampling

Problem Formulation

We want to generate a random state of the Ising model, according to the Boltzmann distribution:

$$P_{eq}(s) = \frac{1}{Z} e^{-\beta E(s)}, \quad \beta = 1/T.$$

By generating a large number of such states we can estimate **magnetization**:

$$X = \frac{1}{N} \sum_i s_i .$$

Brute-Force Sampling

1. Enumerate all states, calculate their energies, partition function and Boltzmann probabilities.

2. Split the interval [0,1) in sections and weight sections according to enumerated states.

3. Generate random variable uniformly distributed over [0,1) interval, and associate it with a state.

Brute-Force Sampling

1. Enumerate all states, calculate their energies, partition function and Boltzmann probabilities.

2. Split the interval [0,1) in sections and weight sections according to enumerated states.

3. Generate random variable uniformly distributed over [0,1) interval, and associate it with a state.

Exponential in the number of spins with respect both memory (save information about configurations) and time (calculate partition function).

Sampling by Rejection

1. Set each spin randomly with equal probability.

2. Calculate energy E of the state.

3. Accept it as a sample with probability

$$p = e^{-\beta(E - E_{min})} \leq 1.$$

Sampling by Rejection

1. Set each spin randomly with equal probability.

2. Calculate energy E of the state.

3. Accept it as a sample with probability

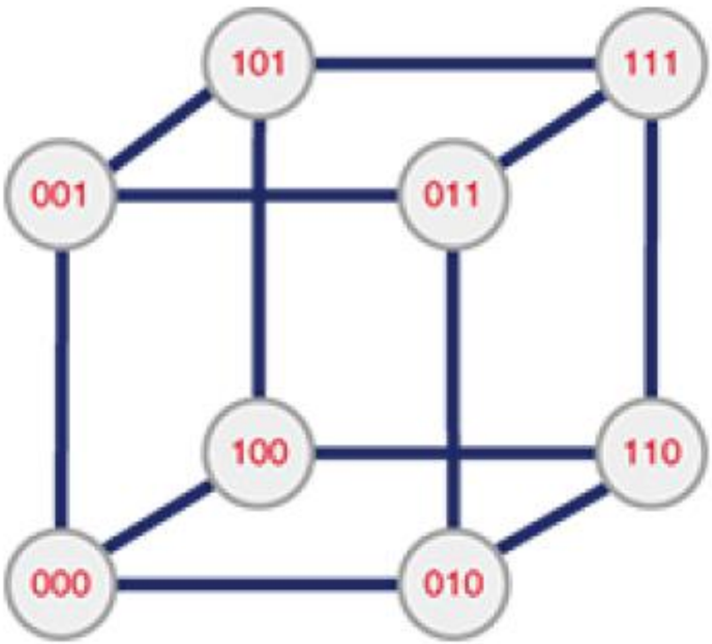
$$p = e^{-\beta(E - E_{min})} \leq 1.$$

For almost all states *p* is exponentially small, so we would have to generate an exponential number of trial states.

III. Markov Chain Monte Carlo

Markov Chain

The states of system are organized in hypercube graph:



2^n configurations

Metropolis-Hastings

1. Start from an arbitrary state.

repeat steps 2-4

2. Choose the random site *i* and calculate what change in the energy would result if we flipped it.

3. Flip the spin s_i with the following probability:

$$p = \begin{cases} 1, & \text{if } \Delta E < 0 \\ e^{-\beta \Delta E}, & \text{if } \Delta E \geq 0. \end{cases}$$

4. Accept the current state as new configuration.

Mixing Time

In practice the convergence can be verified **empirically** by checking if the expectation we compute saturated.

Mixing Time

In practice the convergence can be verified **empirically** by checking if the expectation we compute saturated.

At high temperature the evolution is like a random walk over hypercube. The mixing time can be estimated by **diffusion model**.

Mixing Time

In practice the convergence can be verified **empirically** by checking if the expectation we compute saturated.

At high temperature the evolution is like a random walk over hypercube. The mixing time can be estimated by **diffusion model**.

One can walk from one state to another in N steps – **diffusion** will take N^2 steps.

Gibbs Sampling

repeat steps 2-4

1. Start from an arbitrary state.

2. Choose the random site *i* and construct two possible configuration $s_i = +1$ and $s_i = -1$.

3. Calculate conditional probabilities

$$p_+ + p_- = 1, \quad p_+/p_- = e^{-\beta \Delta E}.$$

4. Accept $s_i = +1$ with probability p_+ and $s_i = -1$ with probability p_-.

Gibbs Sampling

repeat steps 2-4

1. Start from an arbitrary state.

2. Choose the random site *i* and construct two possible configuration $s_i = +1$ and $s_i = -1$.

3. Calculate conditional probabilities

$$p_+ + p_- = 1, \quad p_+/p_- = e^{-\beta\Delta E}.$$

4. Accept $s_i = +1$ with probability p_+ and $s_i = -1$ with probability p_-.

Both algorithms have comparable characteristics (e.g. mixing time).