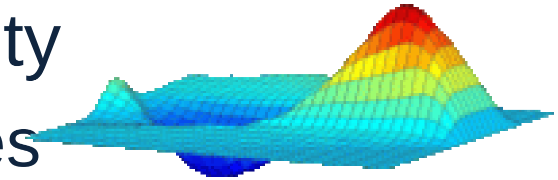
Far Eastern Federal University

The School of Natural Sciences



## High Performance Scientific Computing

**Modeling, Simulation and Optimization of Complex Processes**

# New Order Parameter for second-order Phase Transition


**P.D.Andrushchenko** PitAndMind@gmail.ru

Far Eastern Federal University, School of Natural Sciences,
Dept. of Computer Security, Vladivostok, ul. Sukhanova 8 , 690950

**K.V.Nefedev** knefedev@phys.dvgu.ru

The Far Eastern Federal University, School of Natural Sciences,
Department of Computer Systems, Vladivostok, ul. Sukhanova 8 , 690950

# Phase transition

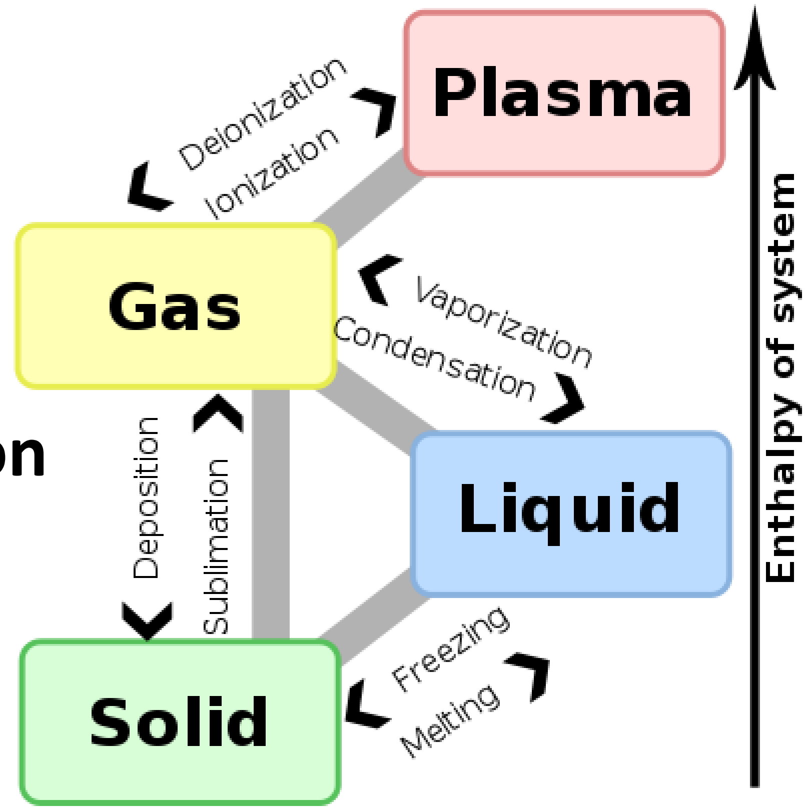
## 1.First-order phase transition

abrupt change of the most important, extensive primary parameters: the specific volume, the amount of stored internal energy, the concentration of components, etc.

## 2.Second-order phase transition

density and internal energy do not change

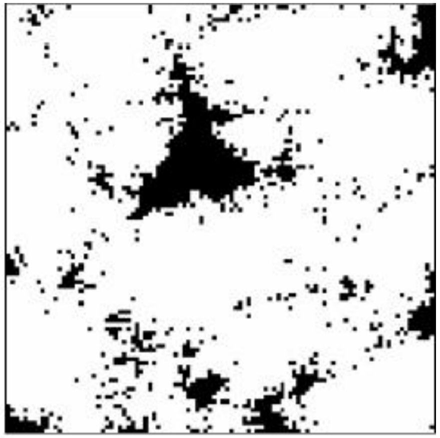
abrupt change of density and internal derivatives with respect to the temperature and pressure: heat capacity, thermal expansion coefficient, the different susceptibility, etc.

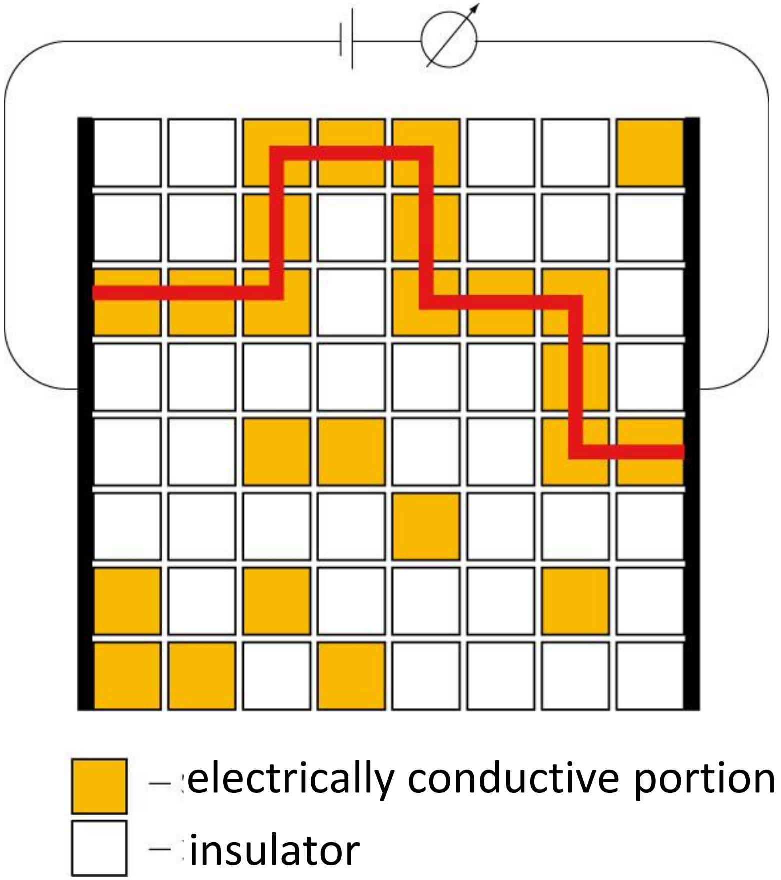


# Percolation theory

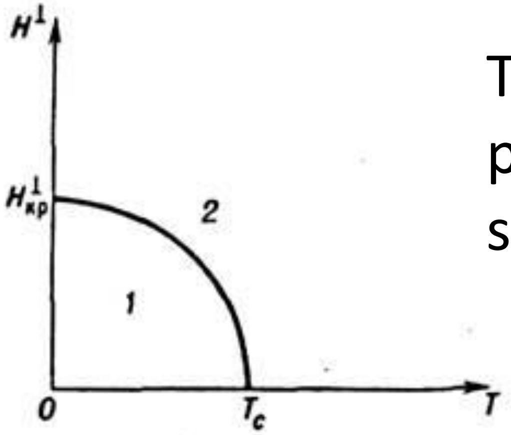
**Percolation theory**

The theory describes the appearance of infinite connected structures (clusters) consisting of individual elements



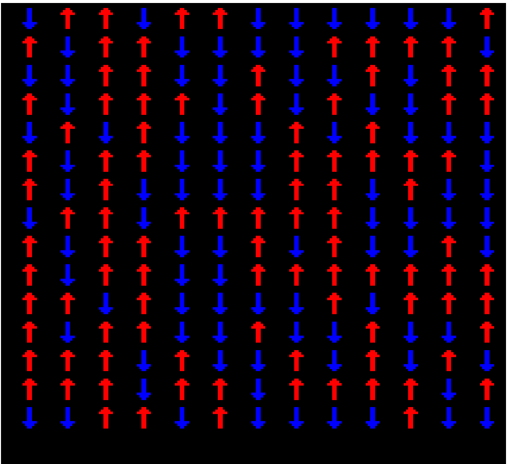


# Ferromagnetic



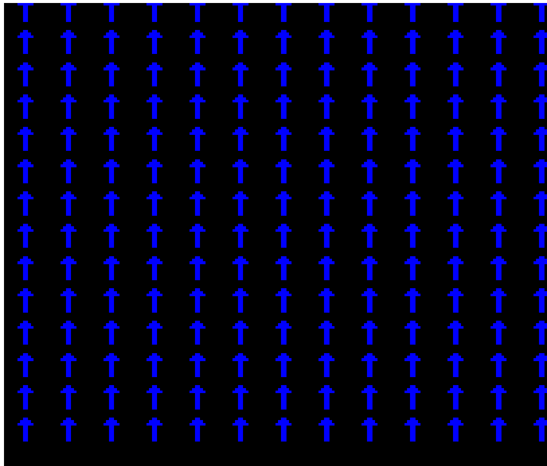

The magnetization is an order parameter for ferromagnetic systems

The order parameter of the ferromagnetic separates two phases of substance - the paramagnetic phase and ferromagnetic phase.

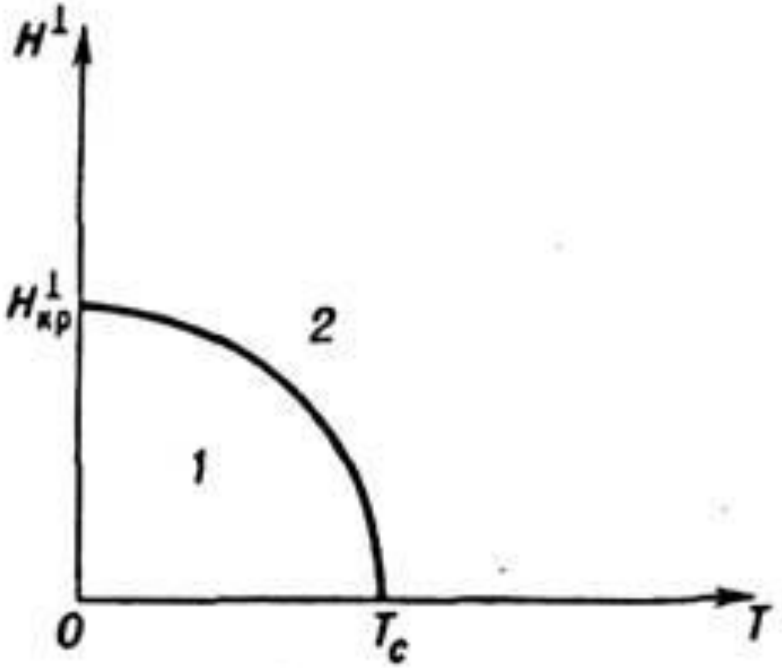


paramagnetic phase

ferromagnetic phase

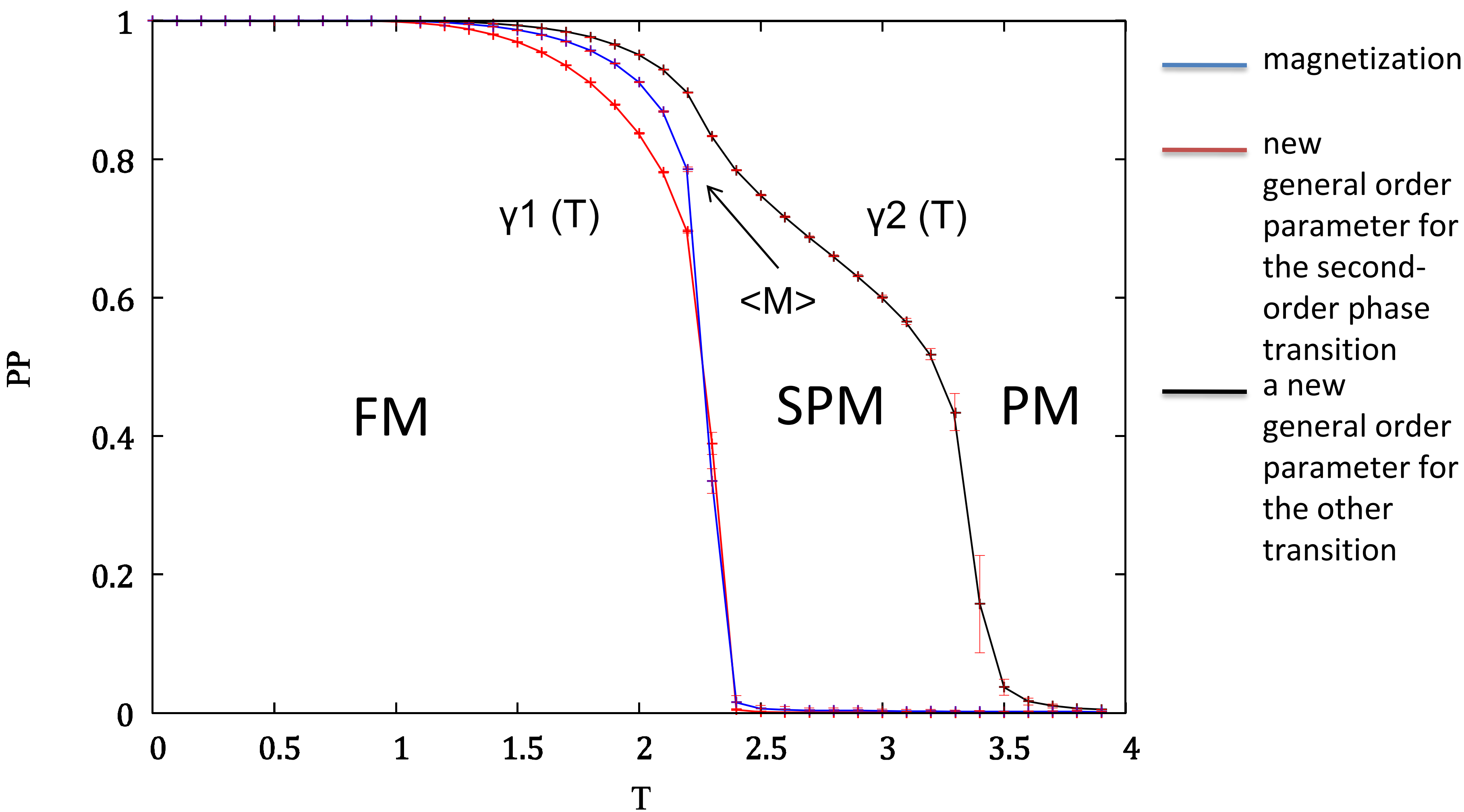


# Ferromagnetic

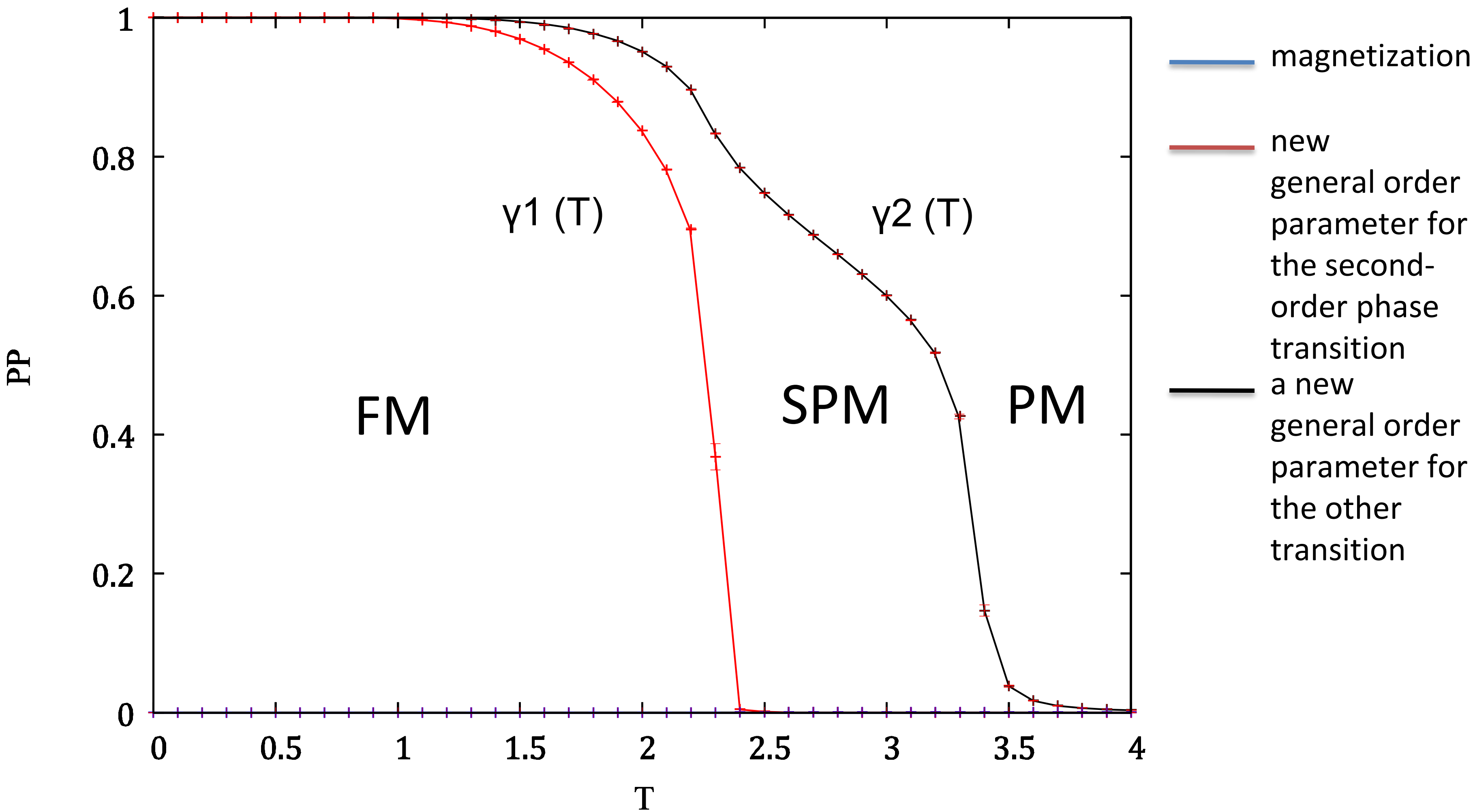



Tc – a critical temperature of the phase transition: a substance moves from one phase to another.

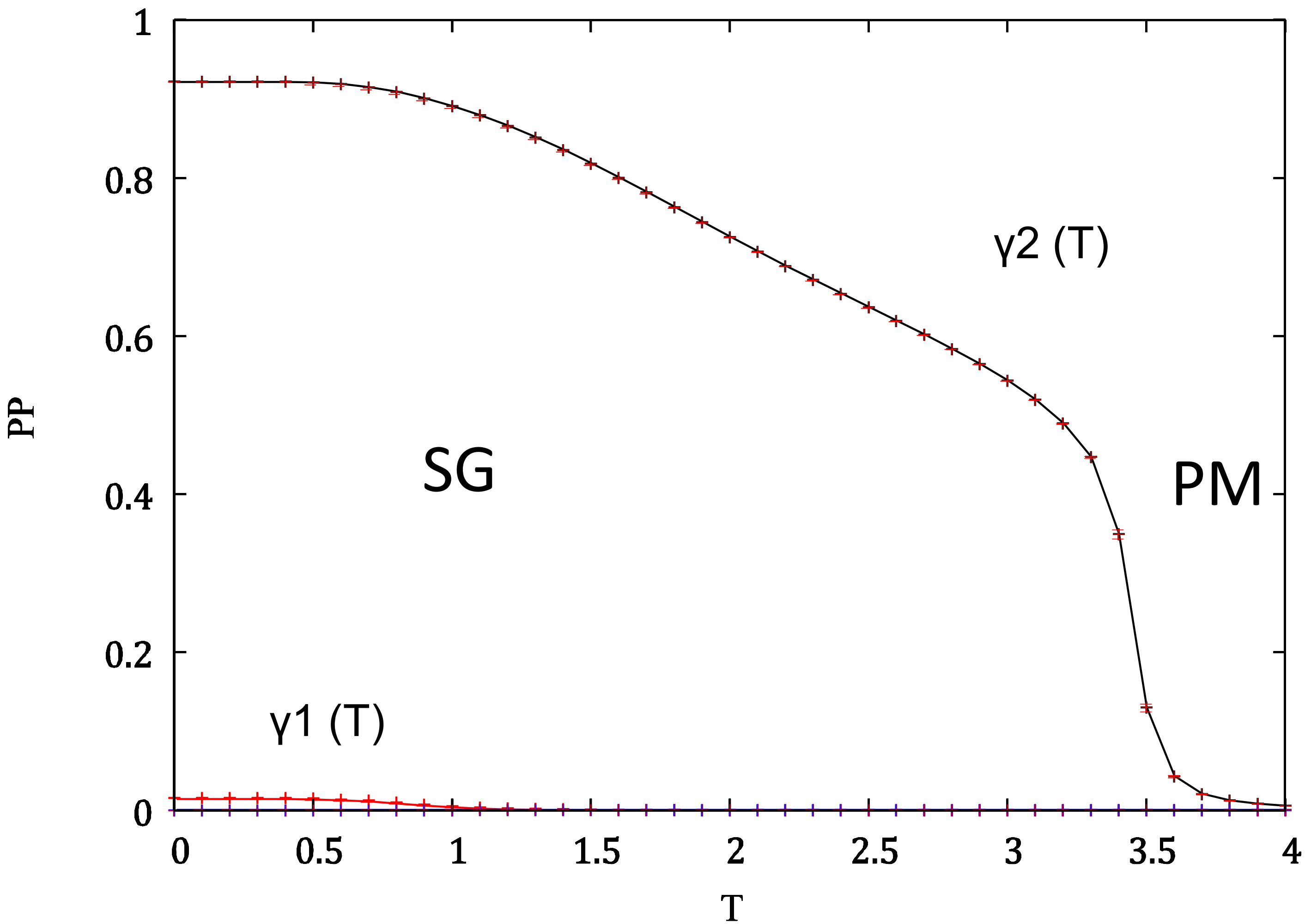
# Ferromagnetic



# Antiferromagnetic



# SpinGlass




new general order parameter for the second-order phase transition

a new general order parameter for the other transition

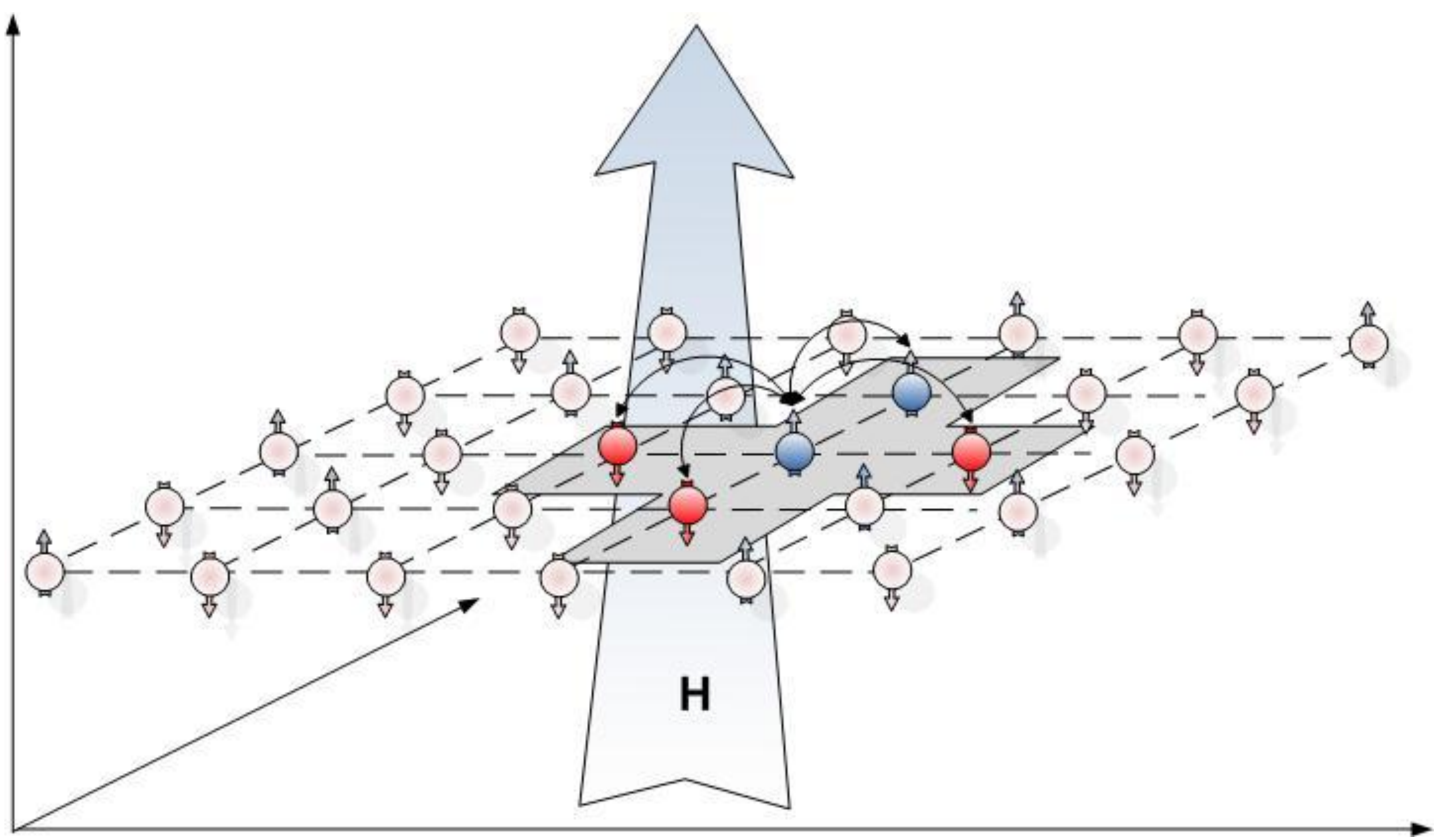
# Question

**1.What is the difference between these systems.**

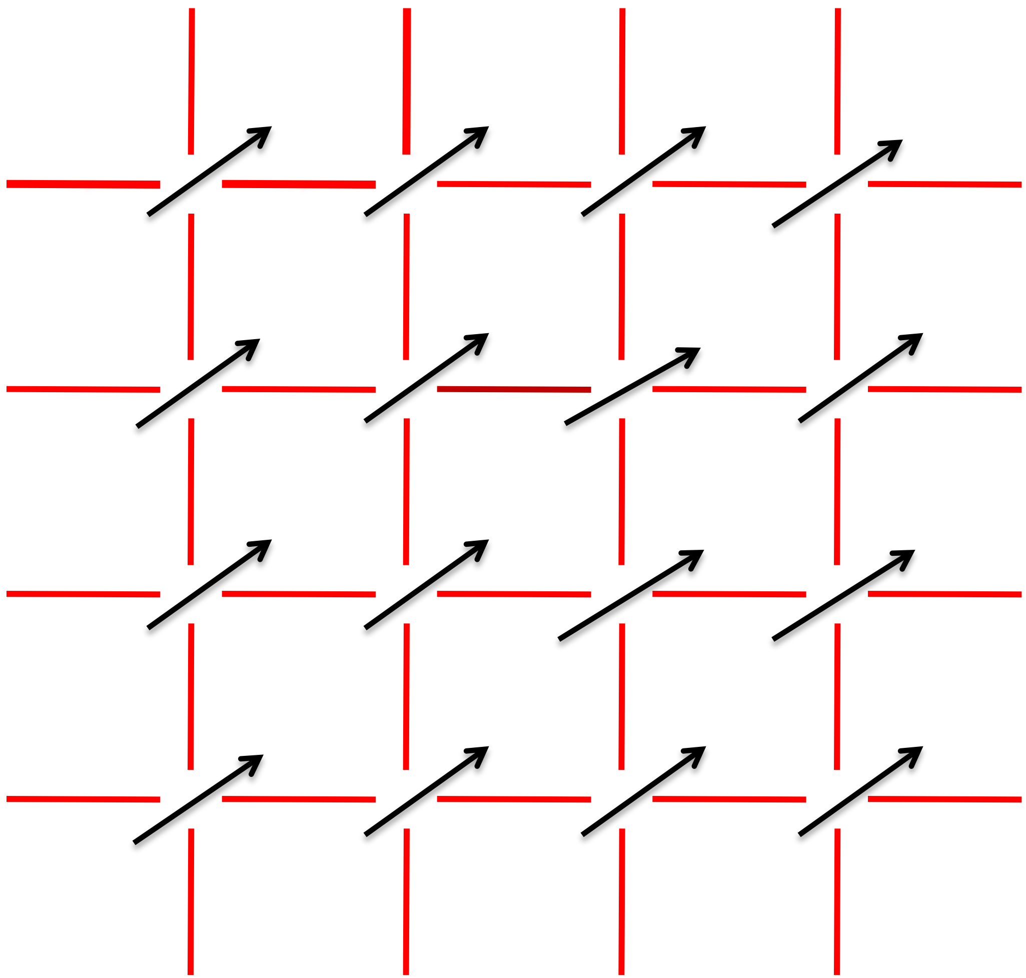
**2.Why is Onsager's magnetization order parameter does not work in non-ferromagnetic systems?**

**3.How to calculate order parameter?**

# 1.Ising's model



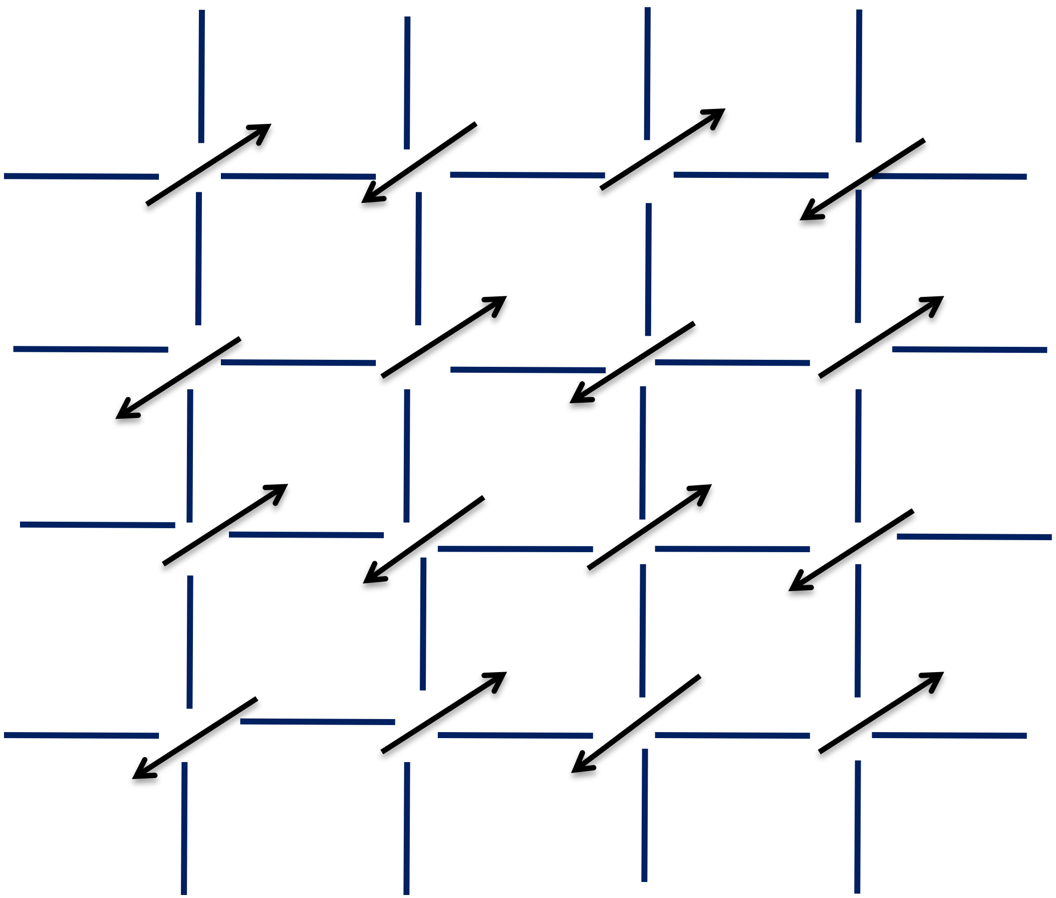
# Ferromagnet in Ising's model



***+J***

positive exchange integral

# Antiferromagnet in Ising's model



***-J***

**negative exchange integral**

# Calculation of energy

**This system is described by the energy functional, called Hamiltonian, which matchs each unique configuration of the system and the concrete value of energy**

$$H = -\sum_{i \neq j} J_{ij} S_i S_j - h \sum_i S_i \qquad [2]$$

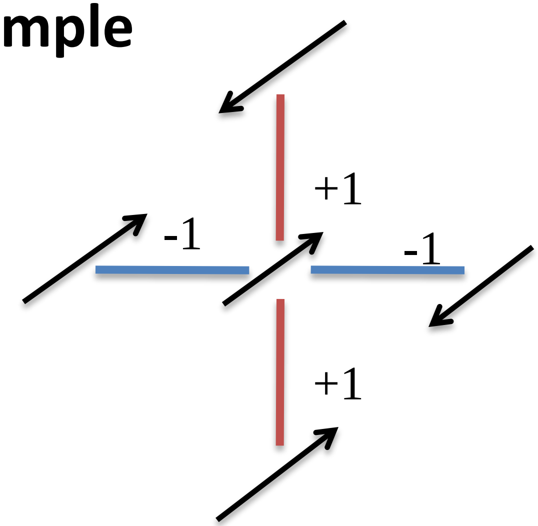
$J_{ij}$ - The exchange integral

h - external magnetic field

[2]Гинзбург С. Л., Необратимые явления в спиновых стеклах, М., 1989

# Calculation of energy

**Example**

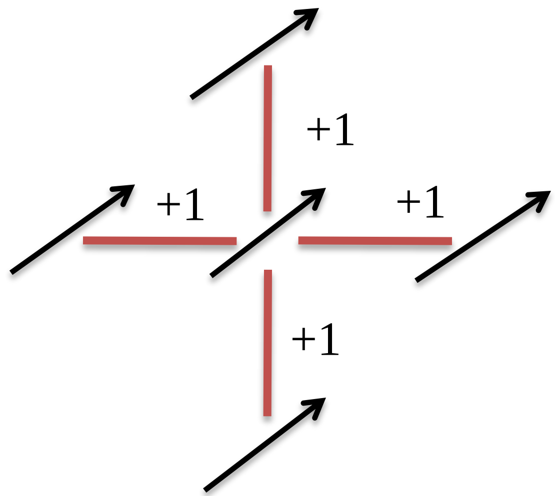



$$E = -[(+1)(+1)(-1)] - [(-1)(+1)(-1)] - [(+1)(+1)(+1)] - [(-1)(+1)(+1)] - 0$$

$$H = -\sum_{i \neq j} J_{ij} S_i S_j - h \sum_i S_i$$

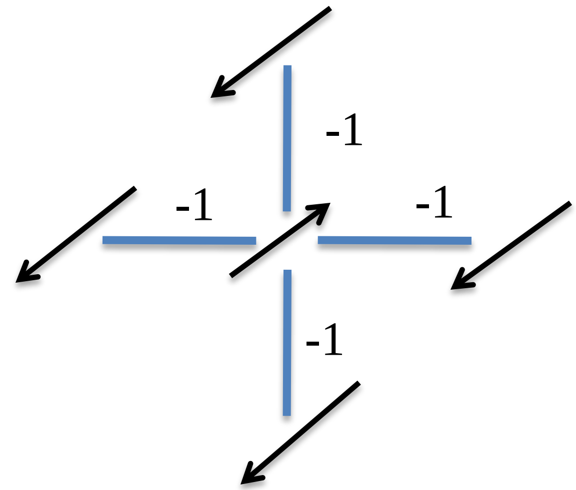
# Calculation of energy

**Ferromagnet**




$$E = -4$$

**AntiFerromagnet**

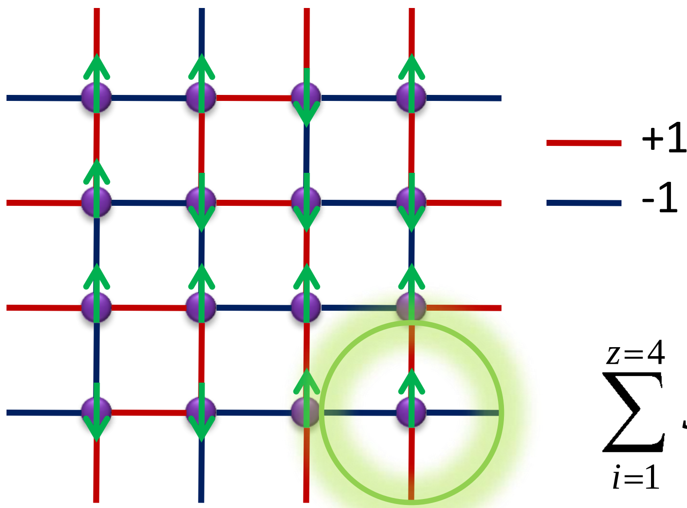



$$E = -4$$

$$H = -\sum_{i \neq j} J_{ij} S_i S_j - h \sum_i S_i$$

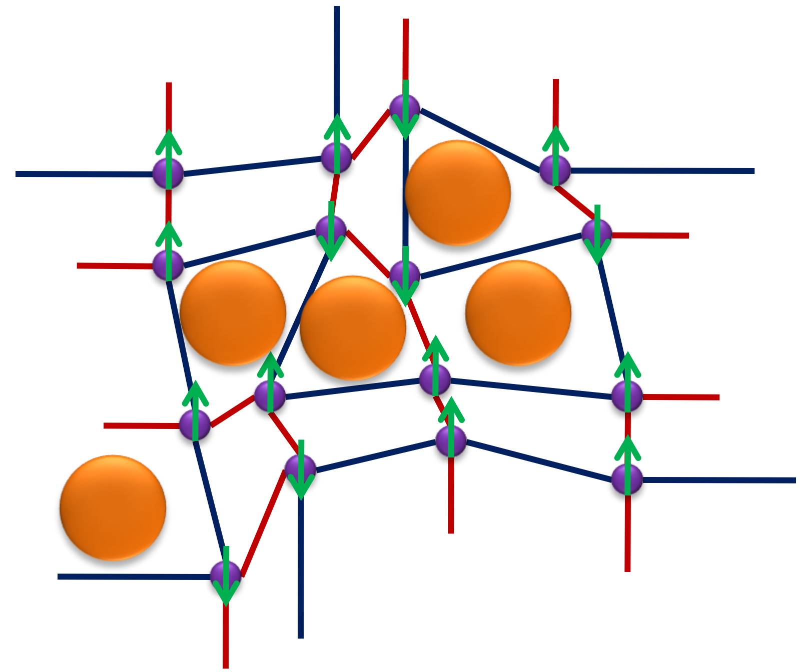
# Spin glass in the Ising model

**Scheme**




$$\sum_{i=1}^{z=4} J_i = 0$$

**Real lattice**



 The atoms of the host lattice

 Impurity atoms

Frustrated spin-glass model on a simple square lattice of Ising's model

# Spin glass in the Ising model

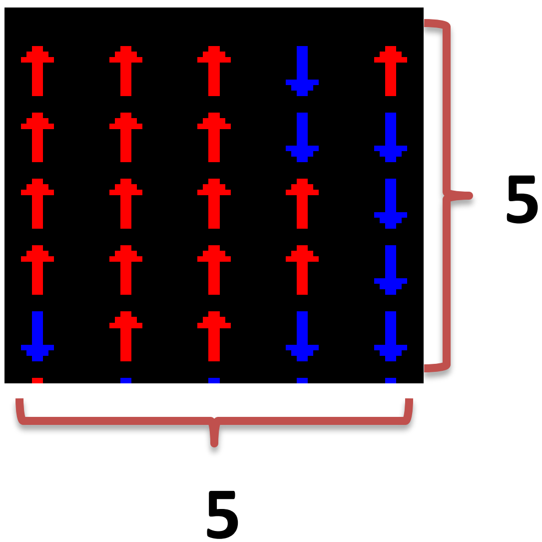
Herewith, the probability of any possible configuration is defined by **Gibbs distribution**.

$$P(X = x) = \frac{1}{Z(\beta)} \exp(-\beta E'(x))$$

In this model each spin interacts only with the nearest **z = 4** neighbours through the direct ferromagnetic or anti-ferromagnetic exchange interaction, randomly distributed in the lattice sites, on condition that

$$\sum_{i=1}^{z=4} J_i = 0$$

# How to calculate magnetization



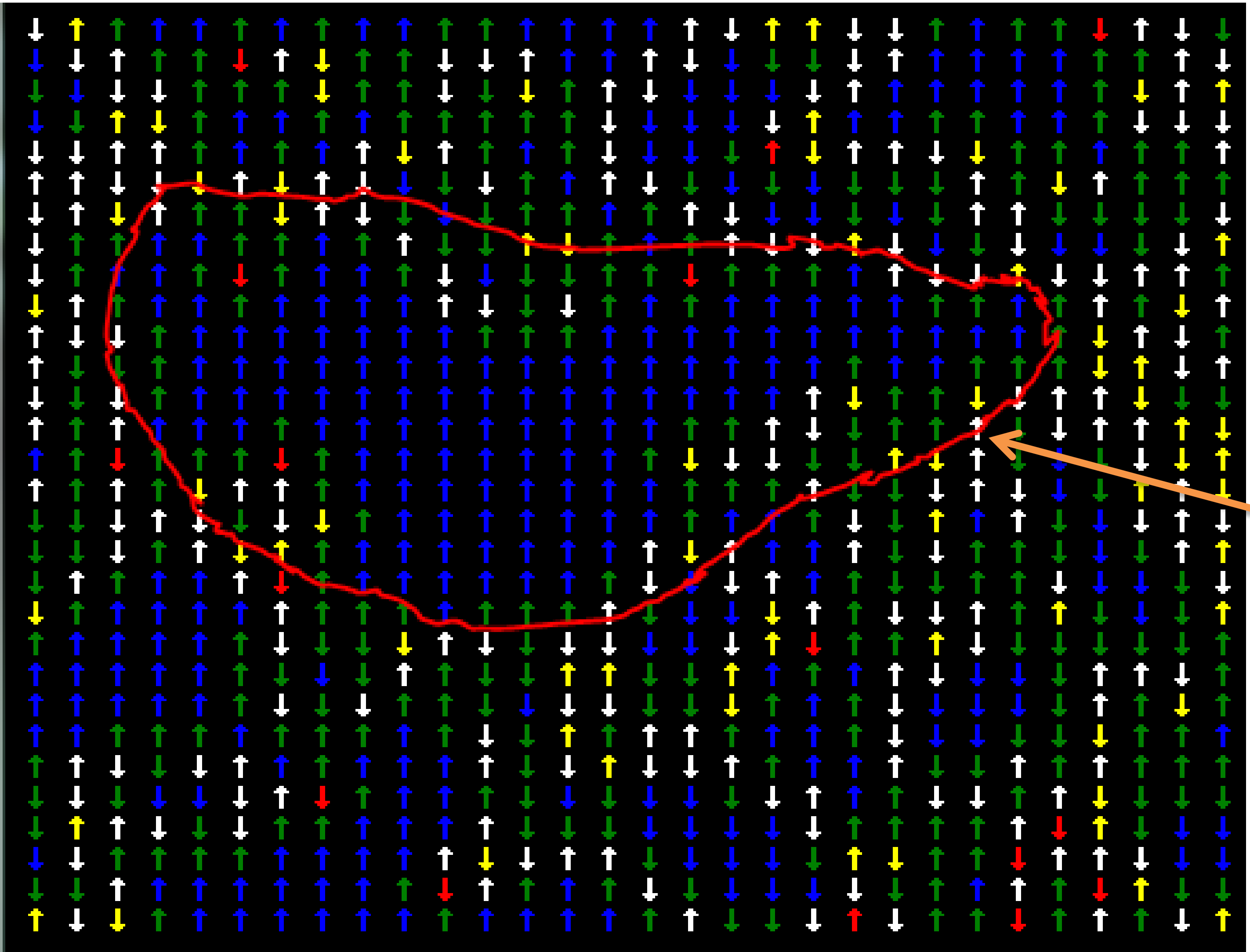

| | | Number |
|---|---|---|
| ↑ | +1 (up) | 17 |
| ↓ | -1 (down) | 8 |

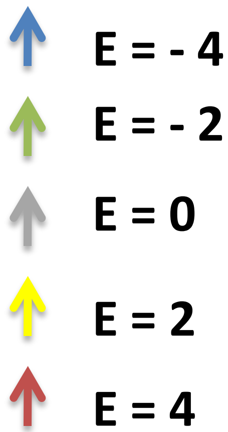
**M = 17 + (– 8) = 9**

For each atom

**M = 9/25 = 0.36**

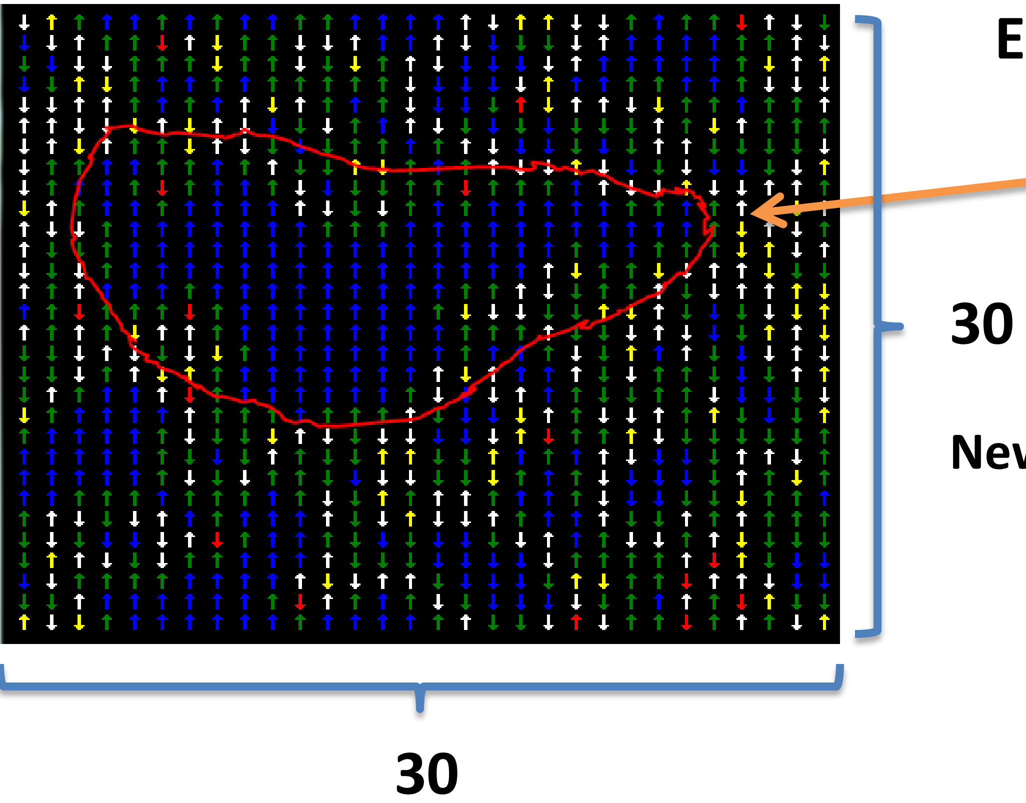
# How to calculate the new order parameter






the
largest cluster
of particles with
energy equal
to minus four

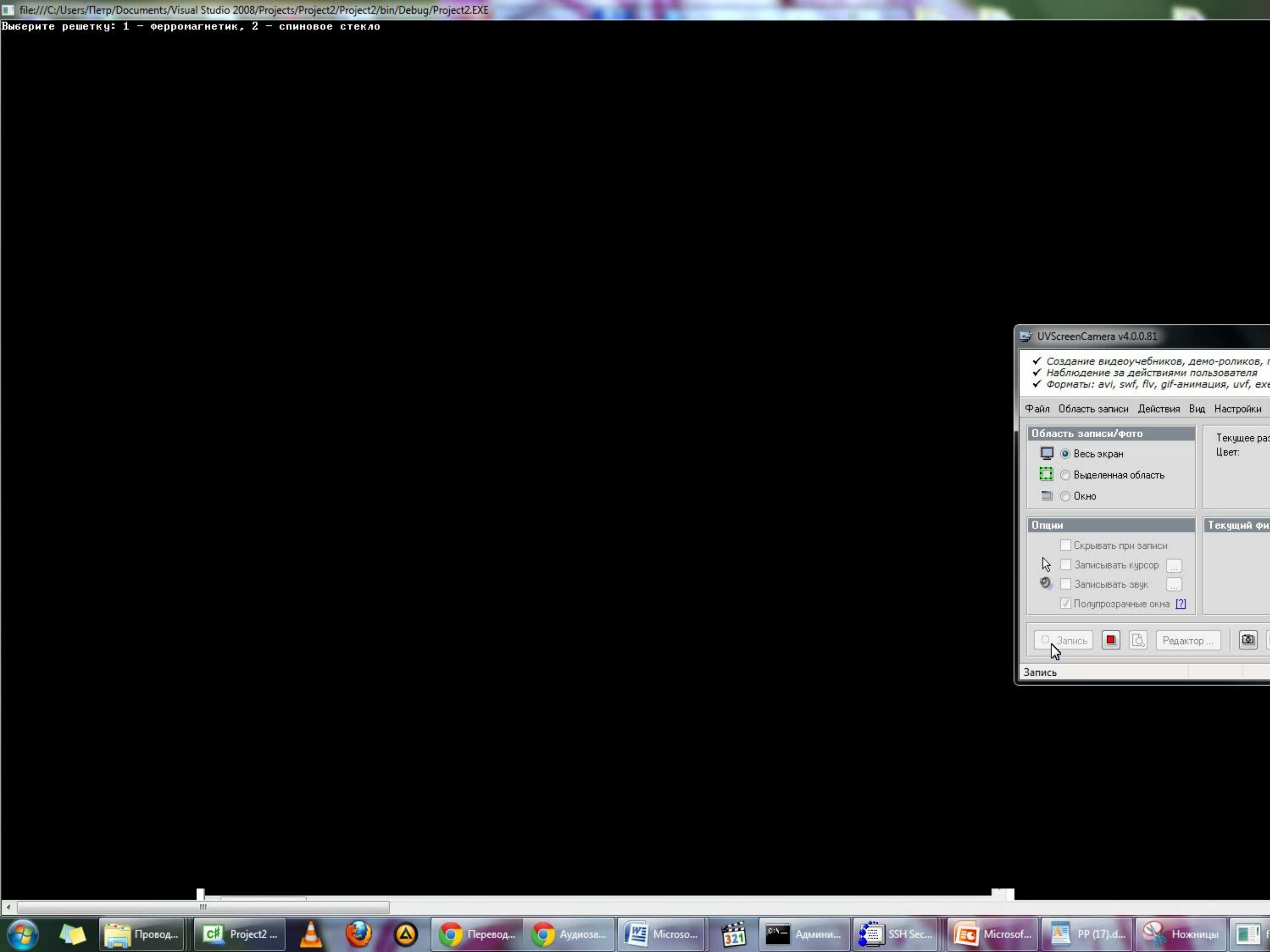
# How to calculate the new order parameter




Example

largest cluster = 120

New Order Parameter 120/900 = 0.133


file:///C:/Users/Петр/Documents/Visual Studio 2008/Projects/Project2/Project2/bin/Debug/Project2.EXE
Выберите решетку: 1 – ферромагнетик, 2 – спиновое стекло
UVScreenCamera v4.0.0.81
Создание видеоучебников, демо-роликов,
Наблюдение за действиями пользователя
Форматы: avi, swf, flv, gif-анимация, uvf, exe
Файл Область записи Действия Вид Настройки
Область записи/фото
Весь экран
Выделенная область
Окно
Опции
Скрывать при записи
Записывать курсор
Записывать звук
Полупрозрачные окна [?]
Запись
Редактор ...
Запись
Текущее ра
Цвет:
Текущий фи
Провод...
Project2 ...
Перевод...
Аудиоза...
Microso...
Админи...
SSH Sec...
Microsof...
PP (17).d...
Ножницы

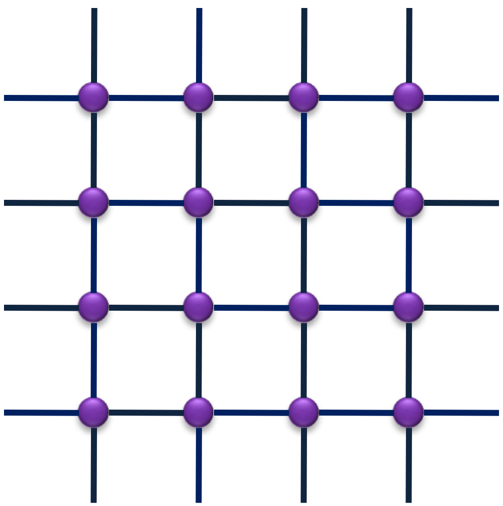
# Algorithm

**A software tool was developed for modeling the dynamics of physical quantities characterizing the system with given (including alternating) brief interaction, and studies of phase transitions in systems with different values of the exchange integral (ferromagnetic, antiferromagnetic, spin glass).**
**Algorithm implements Monte-Carlo scheme.**

# Algorithm

## 1. Creating a lattice

linear dimension = n



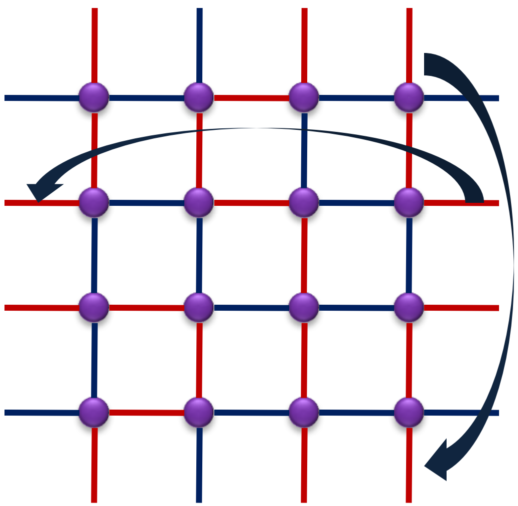
1.1 Create an array of magnetic moments (spins) $n^2$

1.2 Create an array with links $2n^2$

1.3 Creating an array of energy $n^2$

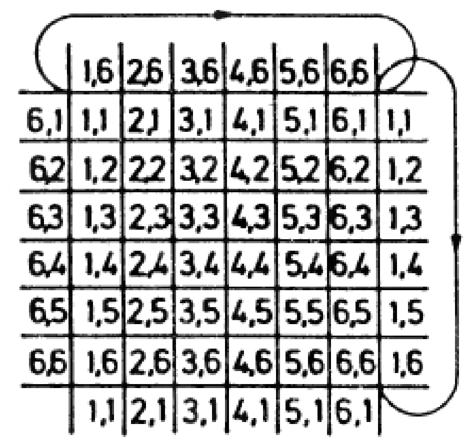
# Algorithm

## 2. Create frustrations



**Task**: Make a frustrated lattice (for the spin-glass)

**Difficulty:** necessary to comply with the boundary conditions




$$\sum_{i=1}^{z=4} J_i = 0$$

Small systems (about 5000 elements) are constructed correctly

In larger systems errors (about 0.01%)

[5]К.Биндер, Д.Хеерман. Моделирование методом Монте-Карло в статистической физике. Перевод с англ., "Наука", Москва, 1995.

# Algorithm

## 3. Monte-Carlo

**The number of Monte Carlo passes can be set in modeling.**

Each Monte Carlo pass consists of the following steps:

1. Randomly generate numbers from **1** to $n^2$. The selected number corresponds to the serial number of atom in the lattice.
2. Calculate the energy of atom **E1**, write it. Then turn over its magnetic moment and calculate **E2** energy.
3. Compare energies **E1** and **E2**. If **E1**> **E2**, the feasibility of that the spin will turn from the initial state **P** = 1, if **E1** <**E2**, then the probability is calculated by the formula:

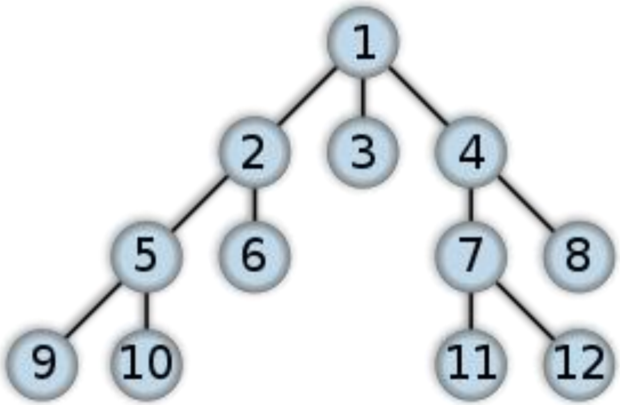
$$P = e^{\frac{E_1 - E_2}{T}}$$

4. Generate a random number **S** from **0** to **1**. We believe that the spin flipped, if **S** < **P**. Otherwise, the spin remains in its initial state.

5. Repeat steps 1-4 $n^2$ times.

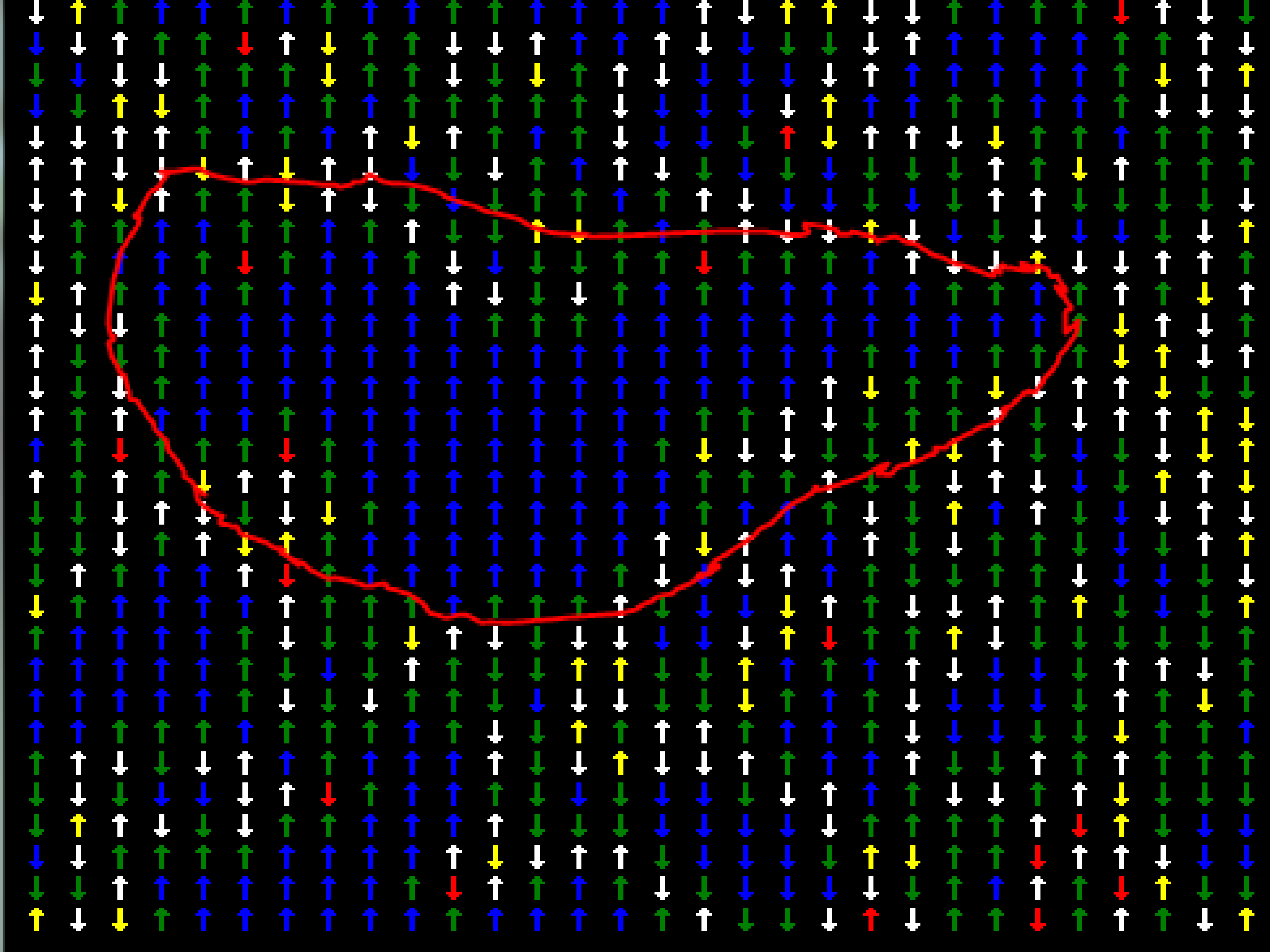
# Algorithm

## 4. How to calculate the largest cluster in the system




1. Find the atom with energy -4
2. Create a queue
3. Write it in the queue
4. Check the neighbors of the atom, if there are neighbors with energy -4, put them in the queue.
5. Consider the next in the queue, until the end of the queue.

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | … |



# Алгоритм

## 5. The implementation of the parallel parts:

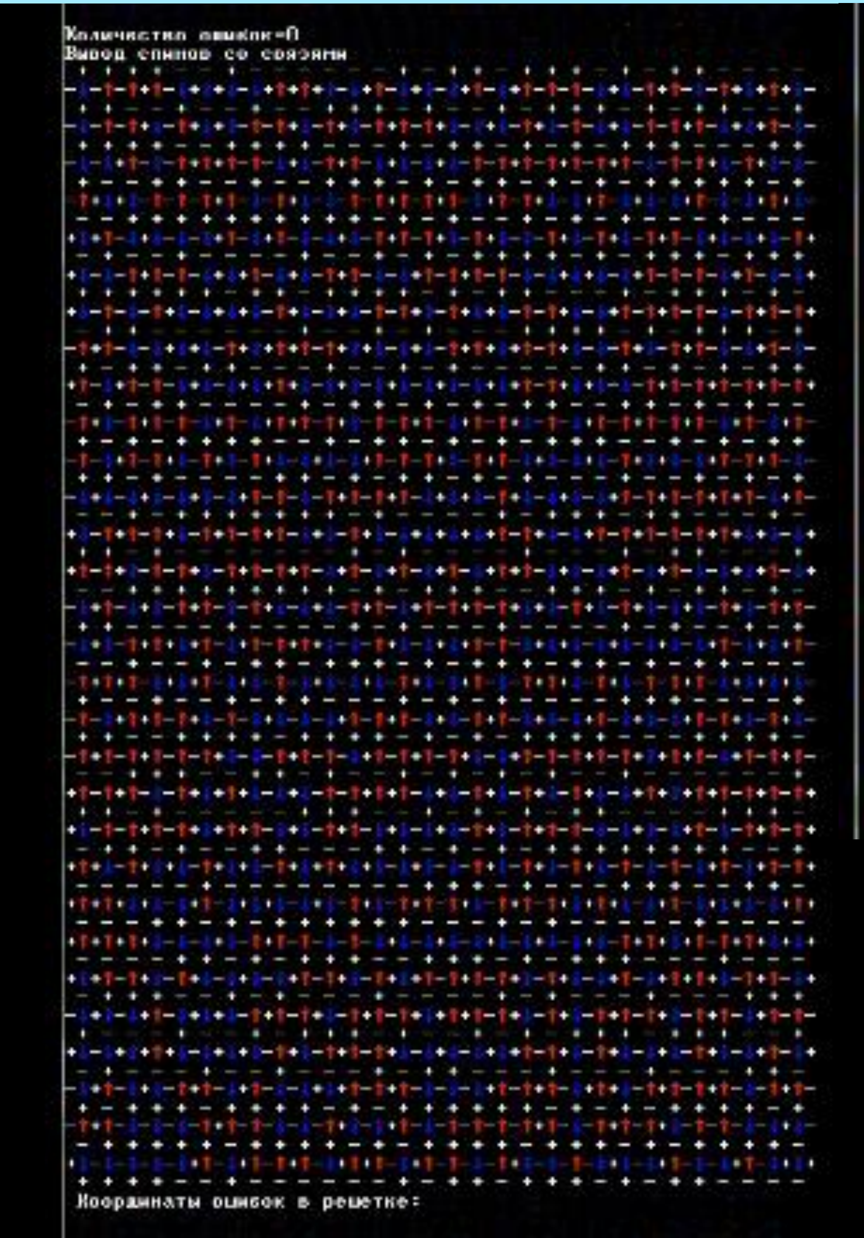
**1.** Construct frustrated links and send an array with links to each thread. (For **Spin Glass)**

**2.** Generate the initial configuration of spins and send it to each thread.

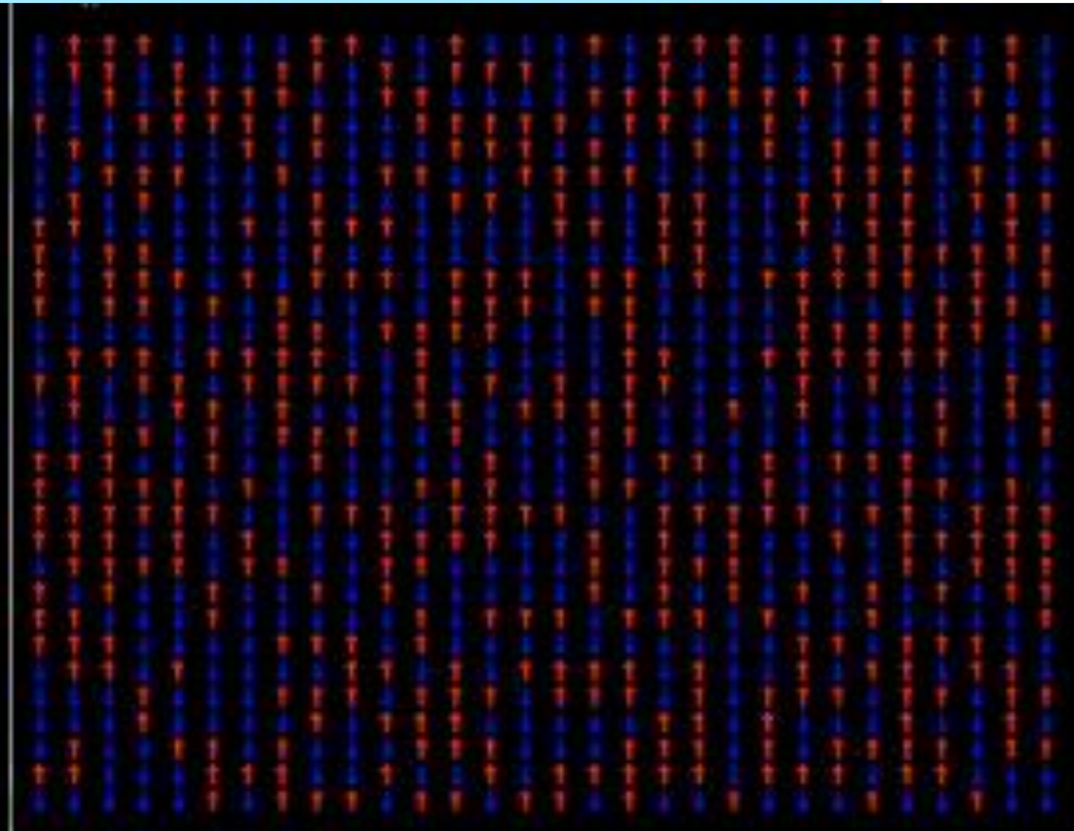
**3.** After several number of MC steps, we collect and compare the energy value of each thread

**4**. The lowest energy system is chosen and sent to all threads. So we quickly come to the system with minimum energy.

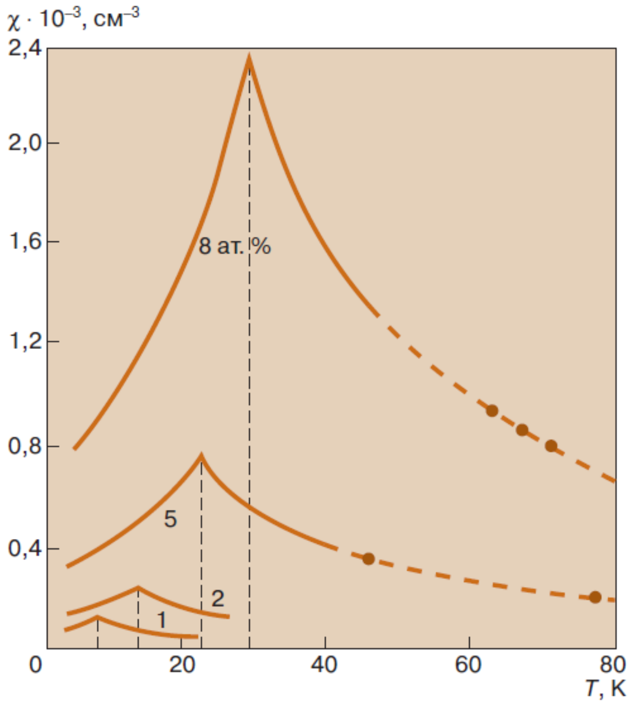
# Алгоритм

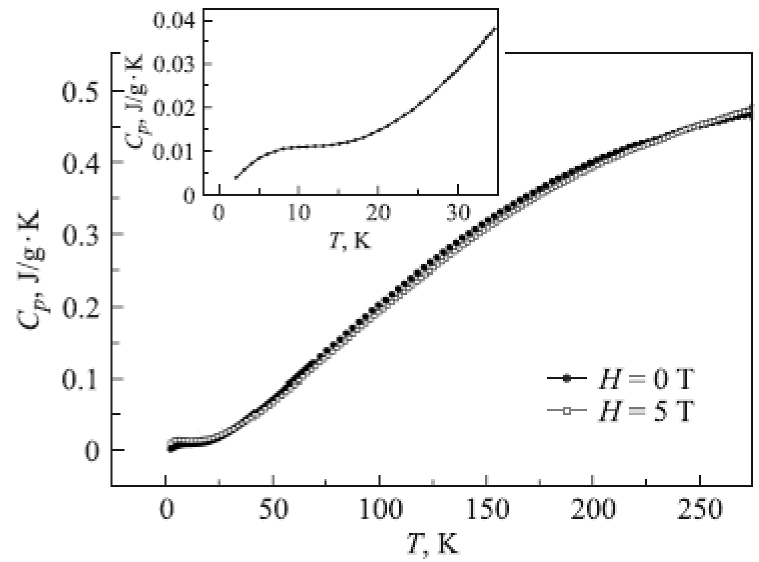


Количество ошибок=0
Вывод спинов со связями
Координаты ошибок в решетке:

# The experimental data




Low-field magnetic susceptibility χ (T) AuFe alloys with concentrations of iron
1, 2, 5 and 8 at. % [3]

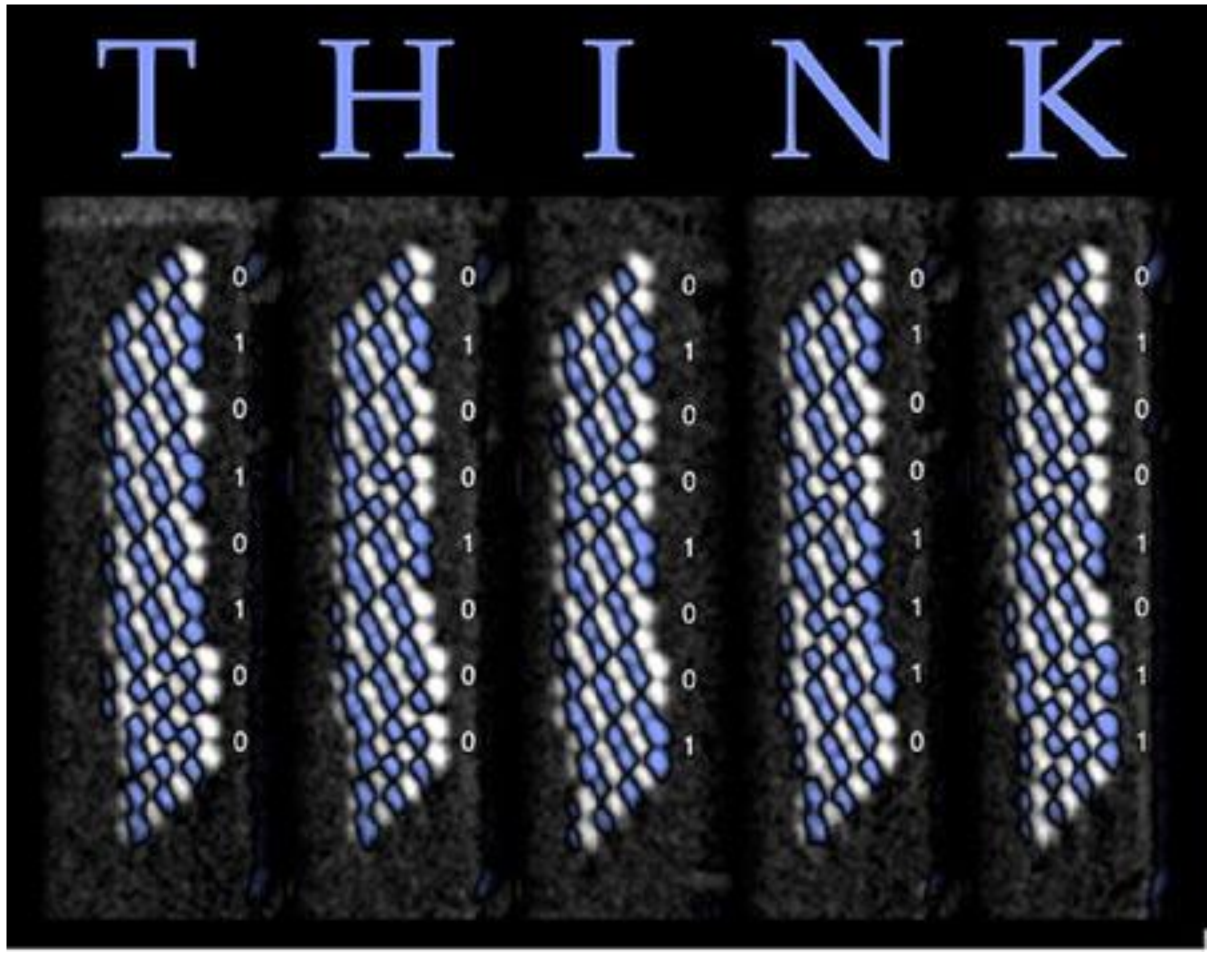
The dependence of specific heat capacity $SmFeTi_2O_7$ the temperature in fields H = 0 and 5T. The inset shows the low-temperature region at H = 0 T [4] $C_p(T)$


[3]Г. А. Петраковский, Спиновые стекла, Соросовский образовательный журнал, т. 7, №9, 2001

[4]Г. А. Петраковский, Состояние спинового стекла в $SmFeTi_2O_7$ , Физика твердого тела, 2011, том53, вып. 9

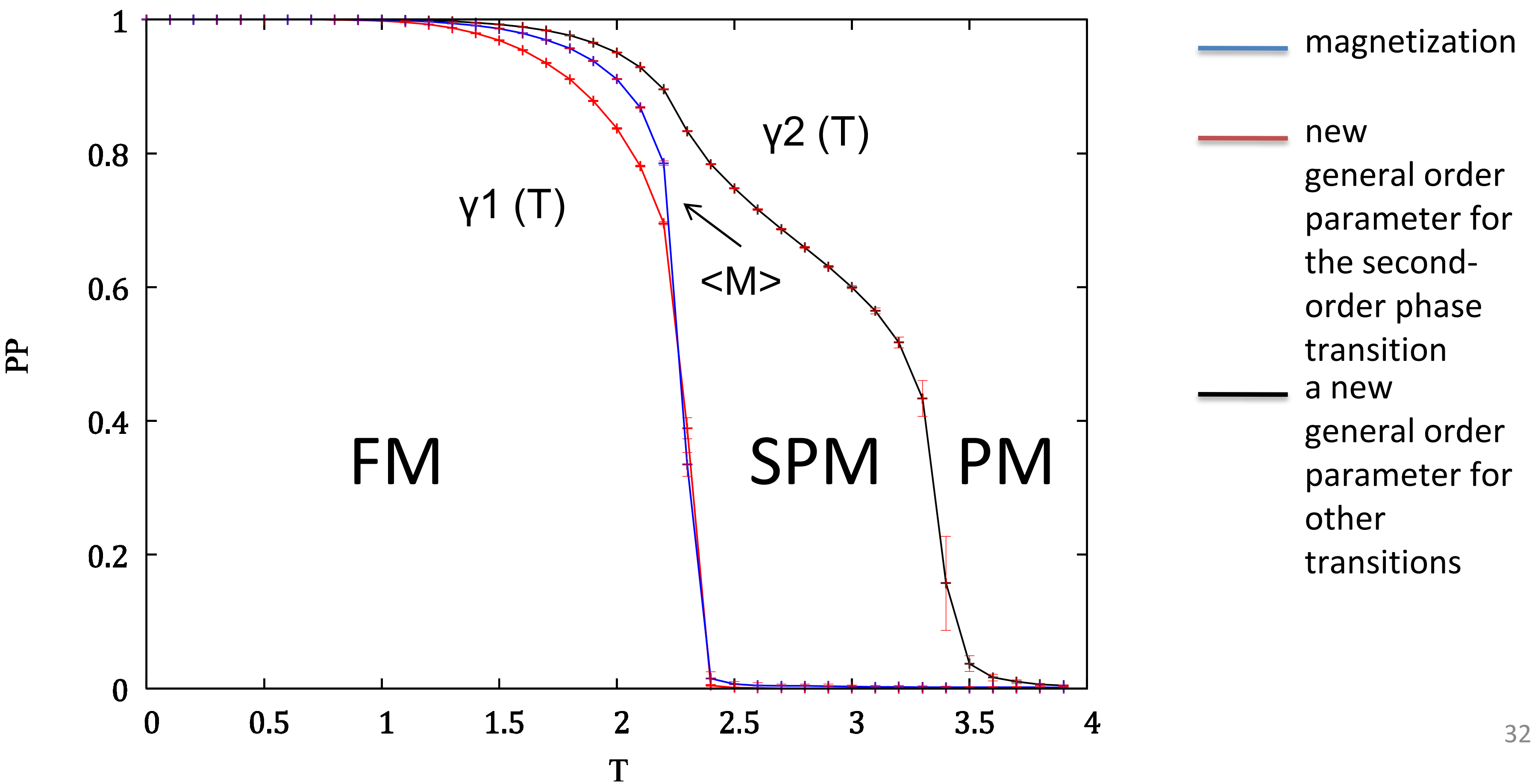
# Significance

**Example**



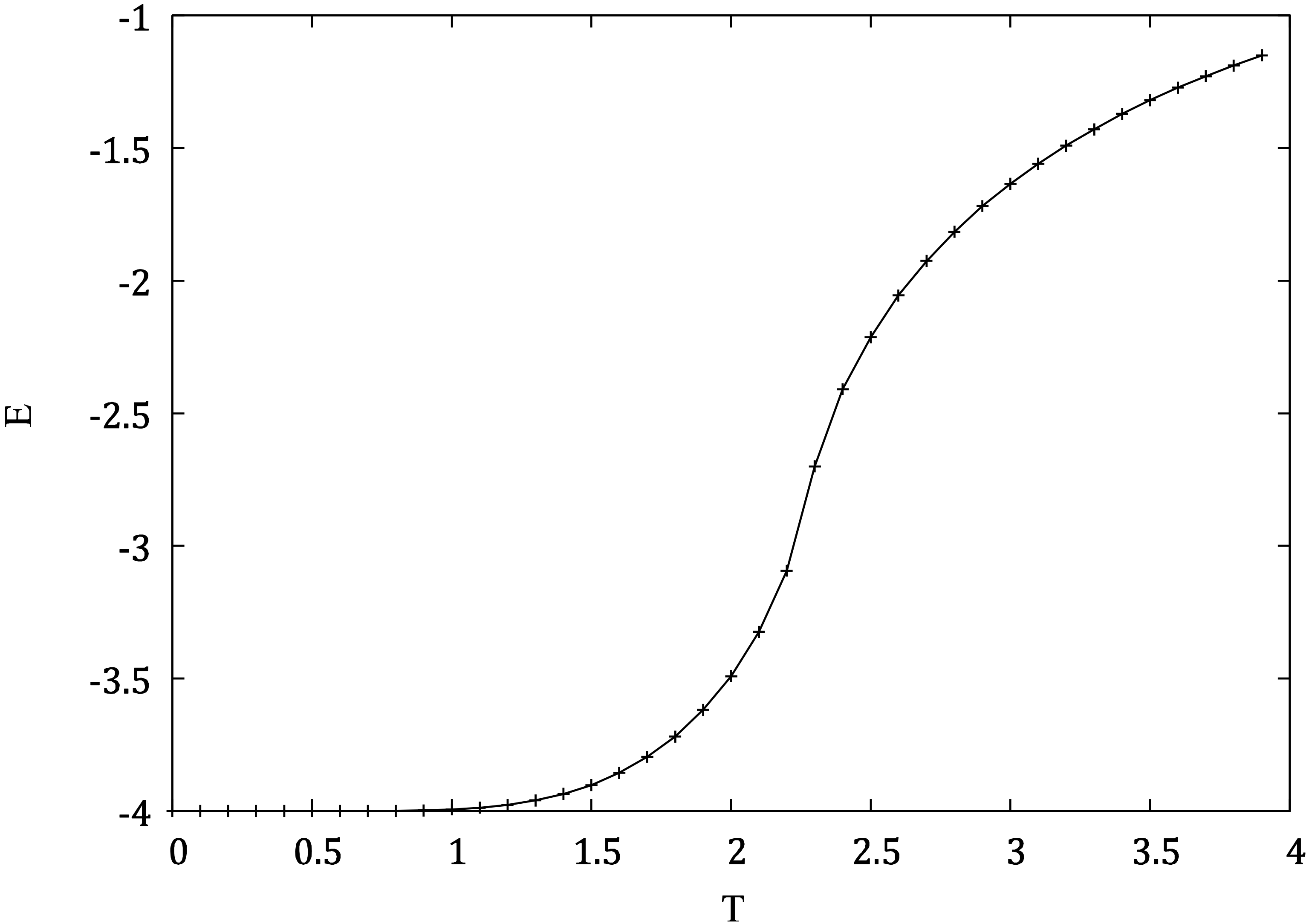
# Results

## 1. Ferromagnet 2D simple square, 4 neighbor, 1000000 elements



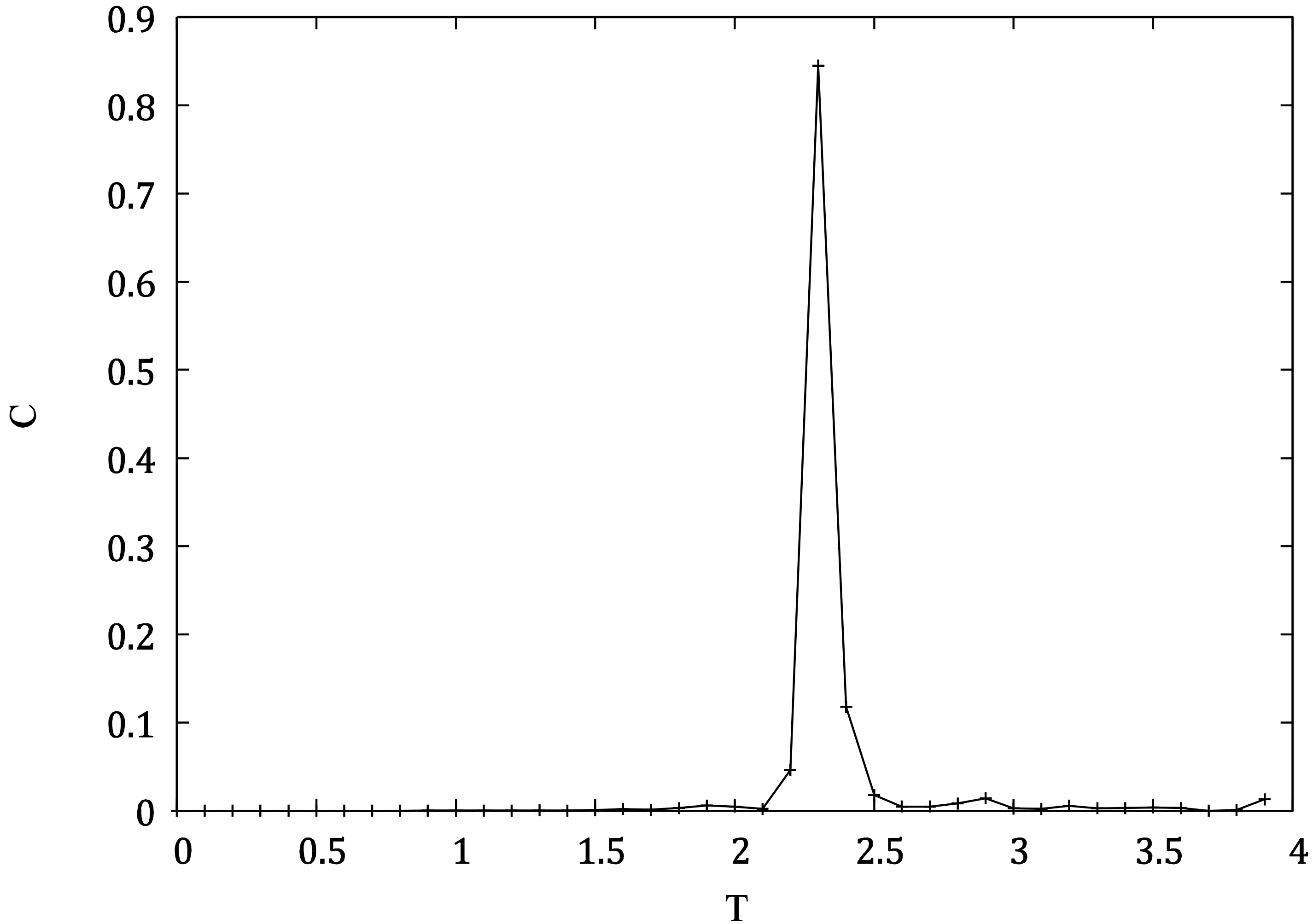
# Results

## 1. Energy of ferromagnet



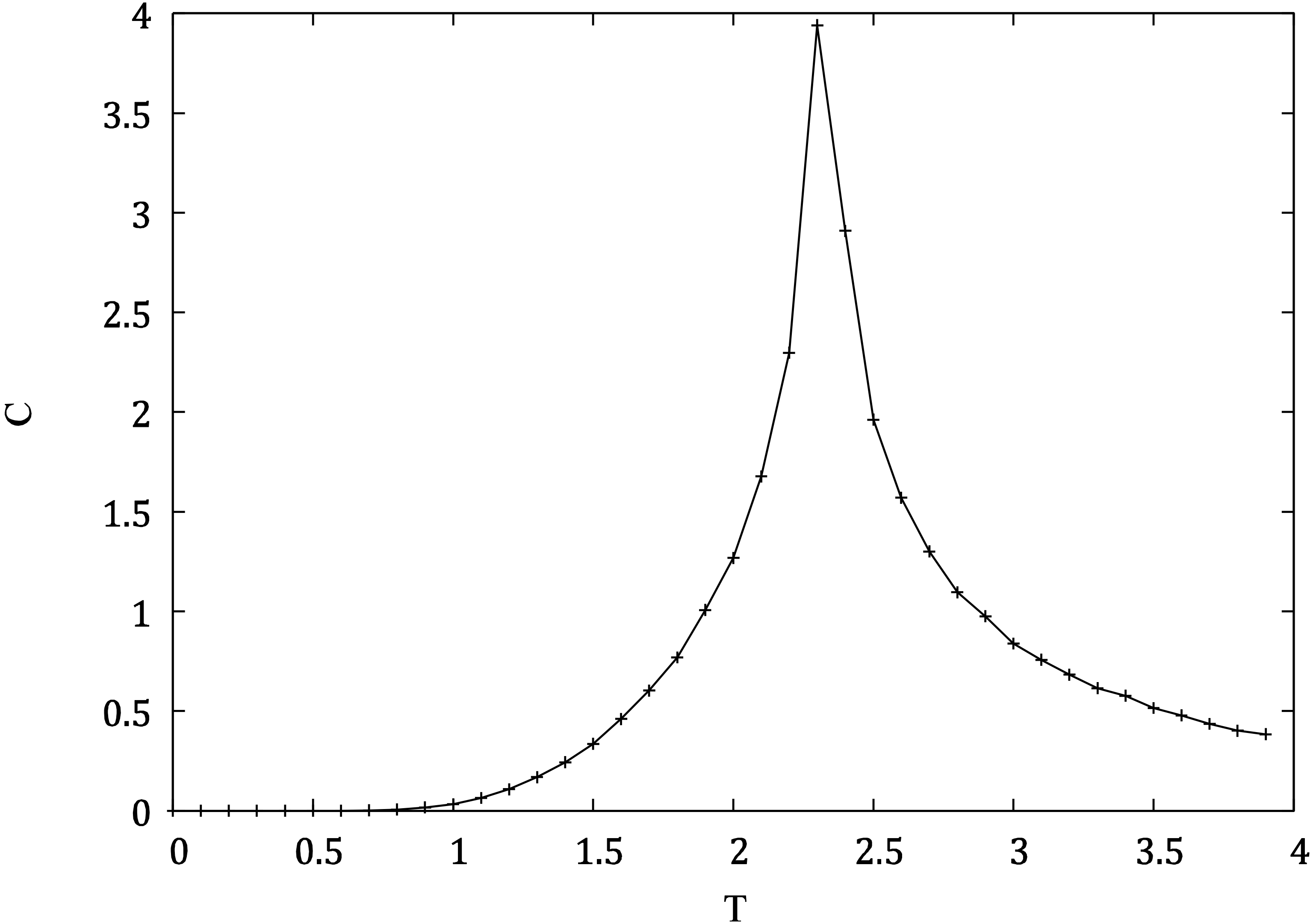
# Results

## 1. Magnetic susceptibility



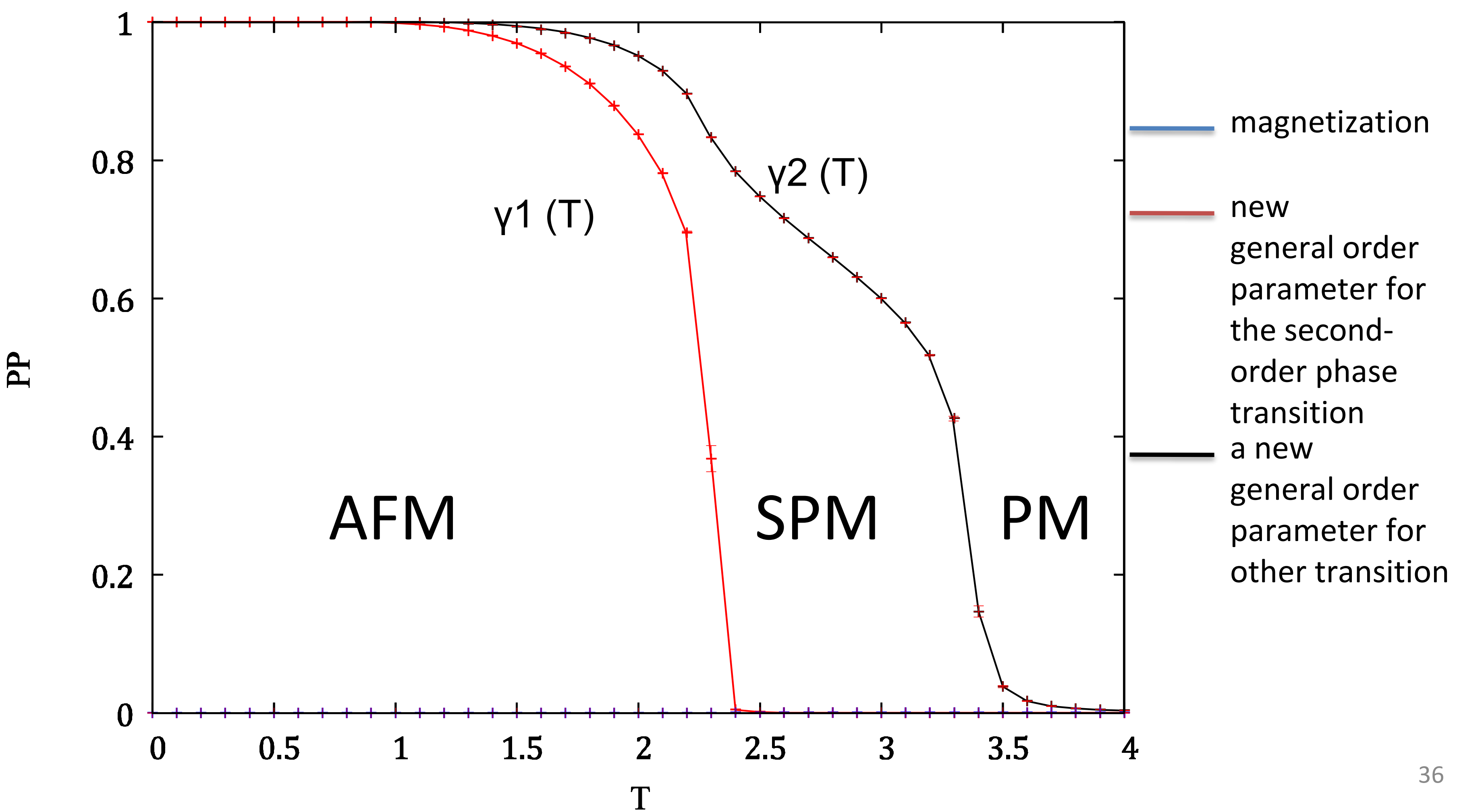
# Results

## 1. Heat capacity Ferromagnet



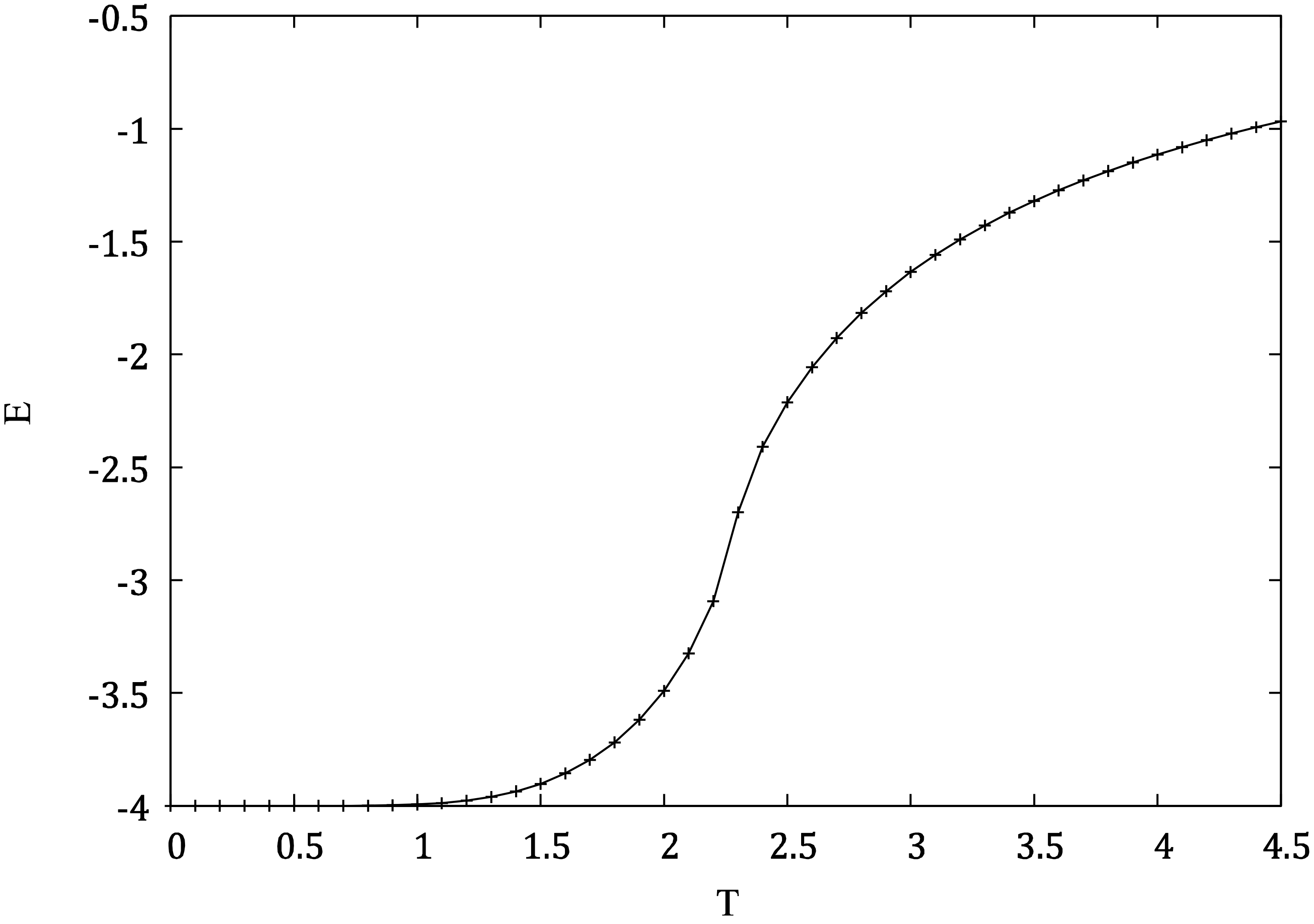
# Results

## 2. Antiferromagnet 2D simple square, 4 neighbor, 1000000 elements



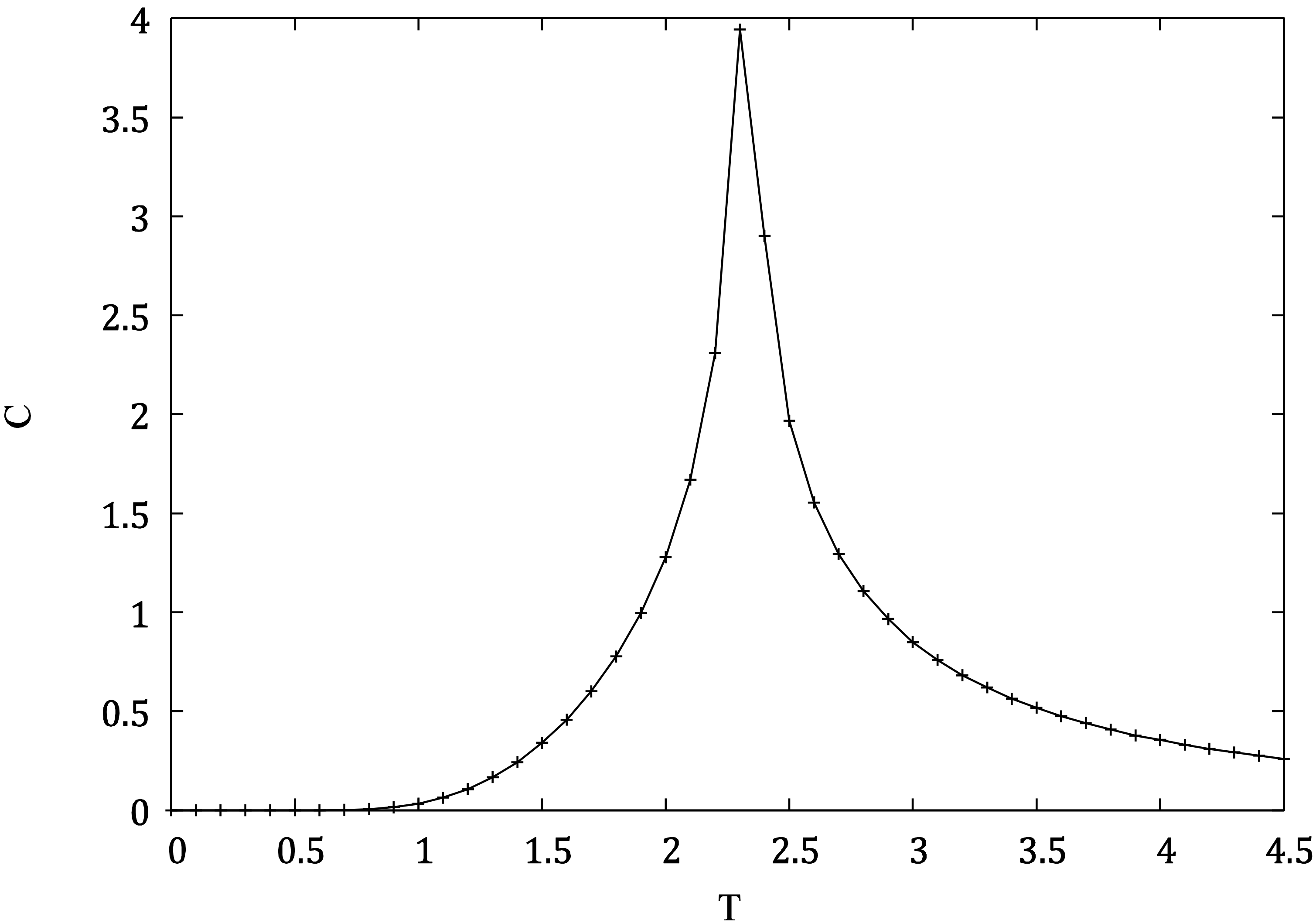
# Results

## 2. Energy of antiferromagnet



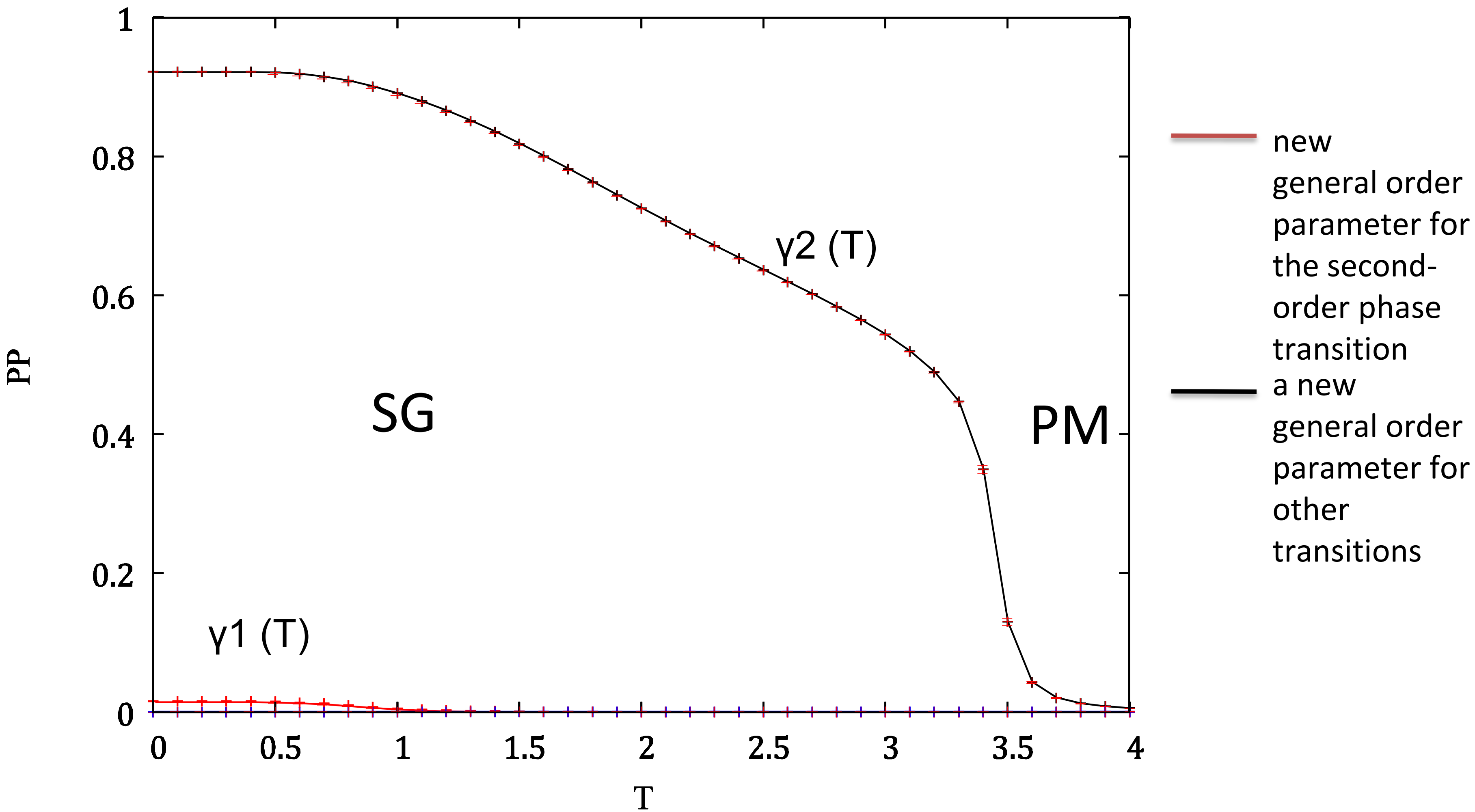
# Results

## 2. Heat capacity of antiferromagnet



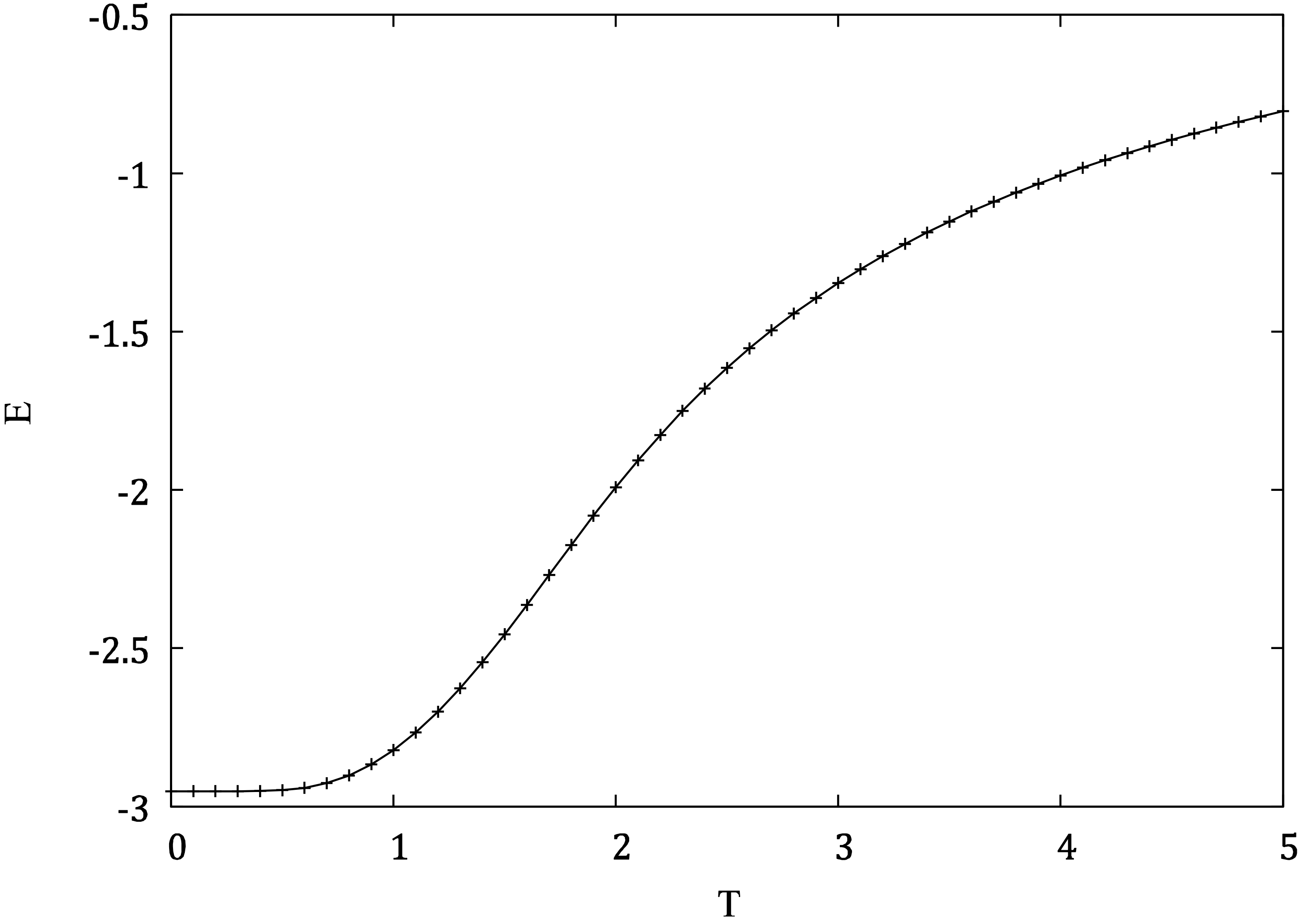
# Results

**3. Spin Glass 2D simple square, 4 neighbor, 1000000 elements**



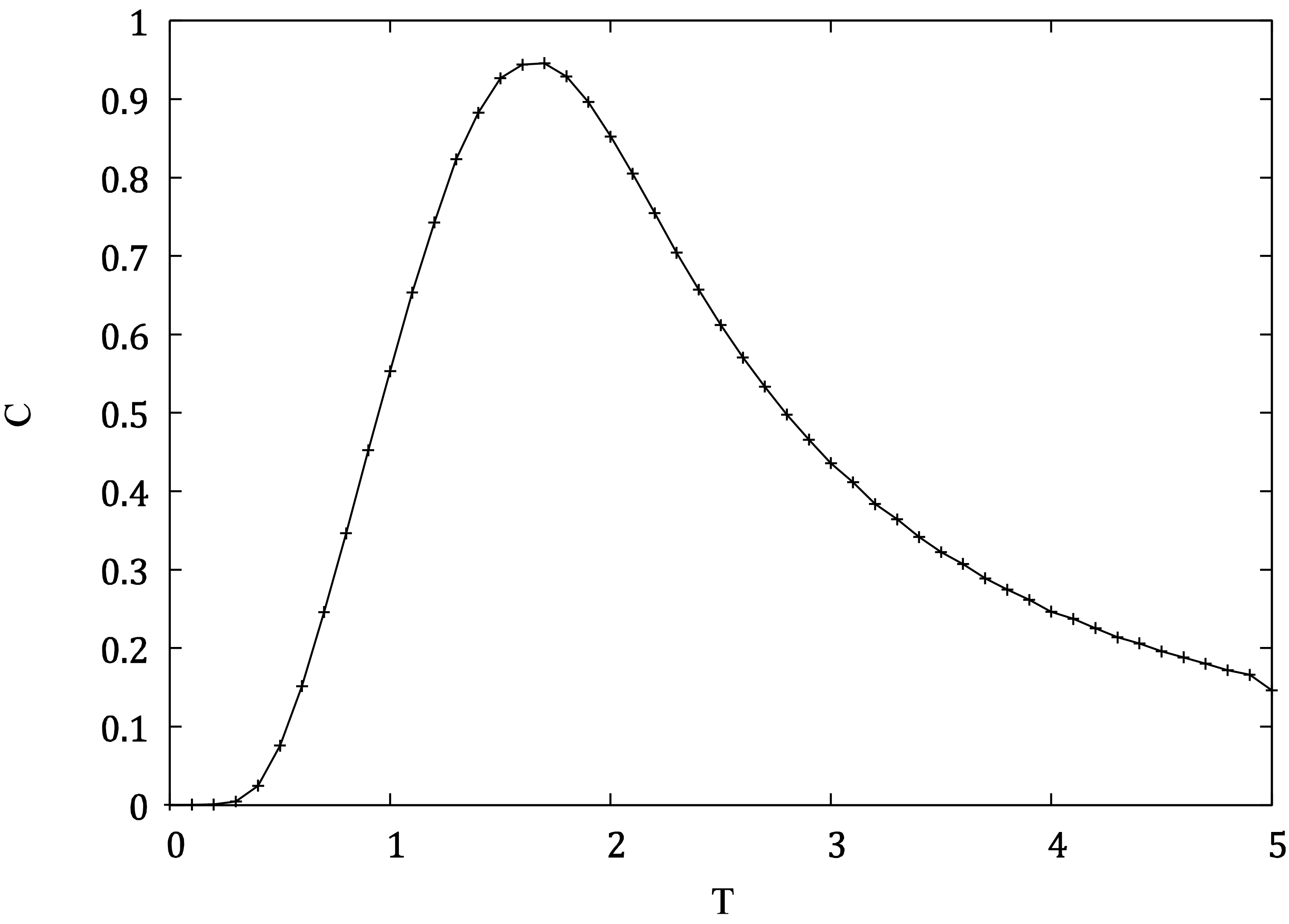
# Results

## 3. Energy of Spin Glass



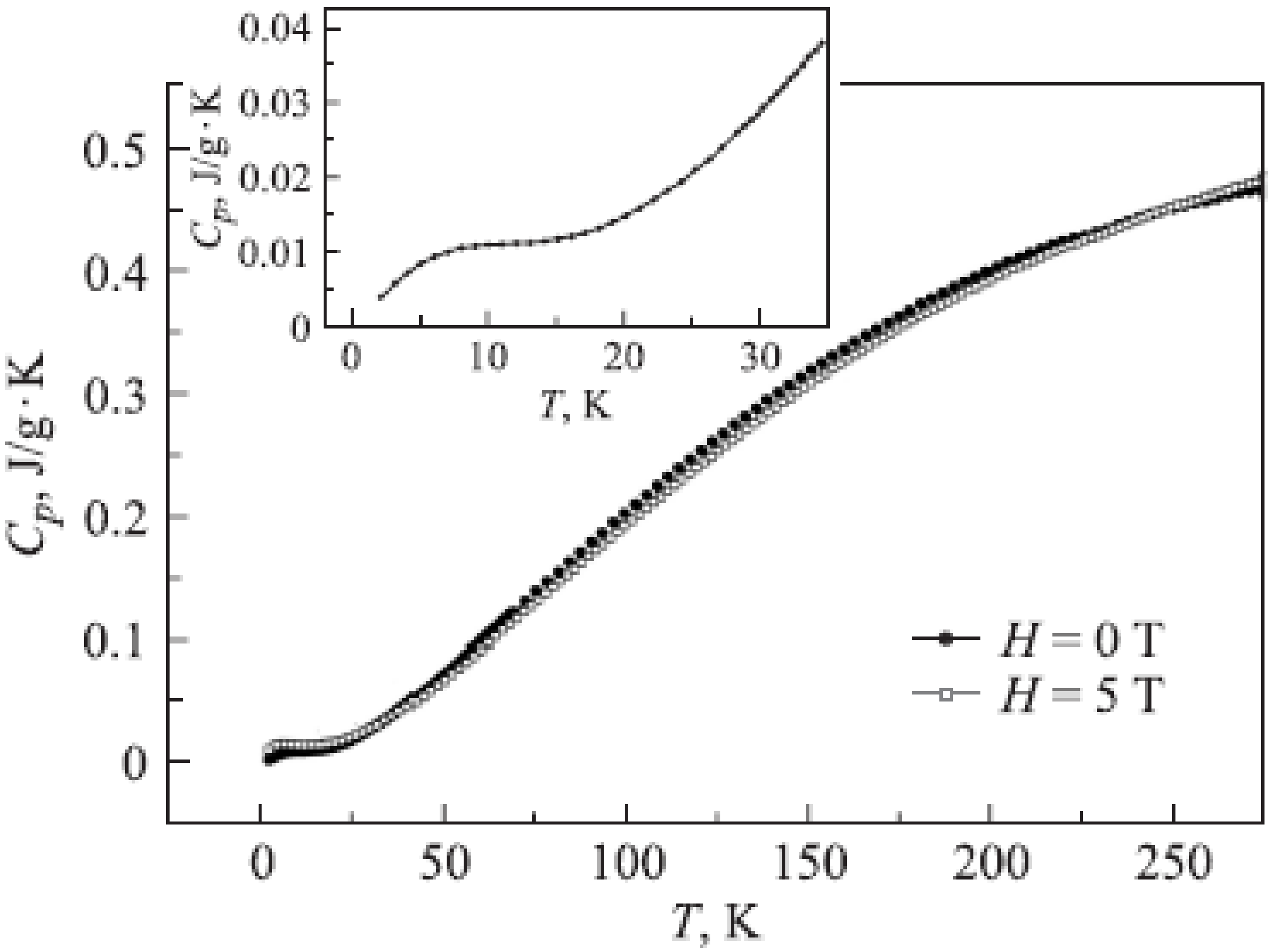
# Results

## 3. Heat capacity of Spin Glass



# Results

## 3. Heat capacity of Spin Glass



# Finding

1) Developed the algorithm, written by a computer program for a supercomputer.
2) The numerical experiments modeling behavior of ferromagnetic, antiferromagnetic and spin glass were carried out on Ising's lattice
3) Proposed a scheme for calculating order parameter. Its temperature dependence was found. And critical temperature of phase transitions in paramagnetic-spin glass, superparamagnetic-paramagnetic systems were found, too.

# Conclusion

1)The law of temperature decrease of this order parameter γ1(T) of ferromagnetic phase coincides with the law of the temperature behavior of magnetization and it’s critical index 1/8 [5]

2)The function γ1 (T) in the antiferromagnet undergoes a jump at the point of the phase transition, and it’s behavior is the same as γ1(T) in a ferromagnetic. It stands as the universality of the order parameter.

[5] Onsager L., Phys.Ref, **65**, 117 (1944)

# Conclusion

3) There is a non-analytic function in spin glass transition region – paramagnet.

Is this a phase transition PM-SG? The question remains open.

[5] Onsager L., Phys.Ref, **65**, 117 (1944)

# Thank you for your attention