Interplay of frustrations, interaction length, and dilution on magnetic transitions in vector models

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Abstract. The research of one-dimensional Ising model with the different number of neighbors and the different sign of the exchange integral were performed. The clustered order parameter is proposed for the description of the magnetic transition in spin systems regardless of the sign of the exchange integral and the number of neighbors. The method of calculation of critical field to change the magnetic states was presented. For diluted 1D antiferromagnetic model two plateaus in magnetization behavior are observed, and explained. Influence of length of interaction plays critical role for phase transition of dipoles system. Dipoles on hexagonal lattice show the phase transition only in model of long range interaction, and there isn’t critical behavior for short range. The approach to calculation of spin system in Heisenberg model is proposed.

1. Introduction

The influence of computer modeling in the physics of condensed matter is increasing, which allows the development of new methods for the construction of complex nanostructures and which promotes the discovery of new phenomena and materials [1, 2, 3, 4, 5, 6]. The study of the collective behavior of magnetic systems will allow to predict and manage the properties of new materials, and will also make a significant contribution to the development of fundamental knowledge about the nanoworld and ongoing processes.

Today may seem from the side, that the theory of ordering reached its peak and now is reaping the fruits of their approaches on new structures, elaborating the critical indexes and the phase transition temperature. But theorists and experimenters publishing the evidence of the opposite opinion that current approaches were ill-suited to describe the order in frustrated systems or systems with quenched disorder [7, 8, 9, 10, 11]. But for better understanding the processes occurring in such complex systems, it is needed to show such processes on the simpler models. That is why finding a common approach to ordering need to start from simple models and move on to more complex ones.

Here we presented our resent results of the research well-known models of magnetism. And in our opinion, these old Ising and dipoles models of magnetics allow throwing the light on frustrations phenomena [12], description of phase transitions [13, 14], the influence of interaction length on the existence of critical phenomena [1], plateau appearance in antiferromagnetic models [5] and other interesting phenomena, which attract the attention of researchers in last time.
In this work there were used all units of temperature as dimensionless, i.e. $kT/J \rightarrow T$, and magnetic fields units were $h/J \rightarrow h$.

2. Ordering in 1D Ising model

2.1. 1D Ising model with two nearest neighbors

Ising model with two nearest neighbors is probably oldest model of magnetism. But it can be used to answer on the questions about order parameter and plateau in magnetization behavior of the diluted spin model [15].

Root mean square magnetization $<M^2>$ or its module is usually used to describe transitions in magnets models. This parameter can be used to study phase transitions in ferromagnets. However, as soon as we change the sign of the exchange integral with ”+” to ”−”, the order parameter becomes 0 for any $T$ and $N \rightarrow \infty$. Therefore, the problem of determining the universal order parameter, especially for systems with a negative or alternating exchange interaction is an actual task [16, 17].

Therefore, we have proposed an approach to the determination of the order parameter to describe the transition from a disordered phase to an ordered (or partially ordered) [13]. Order parameter can be a ratio of the maximum size of the cluster formed by spins in the ground state (lowest energy) to the total number of particles (Fig. 1).

The simplest magnetic model is the one-dimensional Ising model [18]. Classical 1D Ising model with Hamiltonian (1) was investigated, where $n$ - total number of spins, $J_{ij}$ - exchange integral and $z$ - the number of nearest neighbors, which interact with spin. The model with $z = 2, 3, 4$ considered in this paper.

$$\mathcal{H} = -\sum_{i=1}^{n} \sum_{j=1}^{z} J_{ij} S_i S_j - h \sum_{i=1}^{n} S_i$$  \hspace{1cm} (1)$$

The 1D Ising model with $n = 1000$ spins with two nearest neighbors and periodic boundary conditions (PBC) (Fig. 2) was investigated.

First of all, the ferromagnetic model with a positive exchange integral was calculated. From now on the simulation was performed with using Monte Carlo (MC), the number of MC steps for every $0.02T$ was $10^{10}$. As expected, the temperature dependence of the clustered order parameter (COP) $\gamma_1$ is almost identical to the behavior of magnetization. That is, in the case

![Figure 1. An example of calculating the clustered order parameter on ferromagnet ($J > 0$) 1D Ising spin chain with two nearest neighbors. Each spin in the chain has a different color (blue, green and red) depending on its interaction energy respectively ($−2, 0, 2$). Red line highlights the biggest cluster of spins in the lowest energy state ($−2$, that is blue). The ratio of the spins in ground state in the maximal cluster to the total number of spins in a system is the order parameter $\gamma_1$. In this sample number of the spins in ground state in the maximal cluster is 7, $n = 23$, $\gamma_1 = 7/23 \approx 0.3$](image-url)
of ferromagnetic \((J > 0)\) the COP \(\gamma_1\) describes a transition from disordered phase to ordered like magnetization.

If you change the sign of the exchange integral \(J\) to the negative, the magnetization becomes zero at any temperature, as the ground state of the system will be antiferromagnetic (Fig. 3a). Despite this, COP \(\gamma_1\) continues to describe the transition to the ordered phase (Fig.3a).

If we consider a system with alternating exchange integral (each spin has one positive link and negative second one), it becomes clear that such system is not much different from the antiferromagnet, the magnetization of such system is also equal to 0 for any \(T\), but the COP describes the ordering process (Fig.3b).

2.2. **Microstates in antiferromagnetic 1D Ising model with dilution**

Consider a chain of five magnetic moments. The field is applied perpendicular to the axis of the array. The Hamiltonian of the system:

\[
\mathcal{H} = S_1S_2 + S_2S_3 + S_3S_4 + S_4S_5 - h \sum_{j=1}^{5} S_j, \tag{2}
\]

where \(S_j = \pm 1\).
Figure 4. a) Magnetization of a chain of five magnetic moments at $T = 0.1$. b) The probability of configurations in the chain of five magnetic moments at $T = 0.1$. Blue line is probability of 3 up ([3/0]), yellow is probability of two up one down ([2/1]). c) Magnetization of diluted chain (concentration of dilution $x = 0.2$) at $T = 0.1$. d) The probability of configurations in the chain with one vacancy at $T = 0.1$. Blue line is probability of one up and one down ([1/1]), yellow is probability of two up ([2/0]).

The magnetization of the chain of five magnetic moments at a temperature $T = 0.1$ is shown in Fig. 4a. There are two plateaus in magnetization curve. Consider the reason for the appearance of the plateau of magnetization. The reversal of one spin will change the energy of interaction with the two neighboring spins. Let us consider the probability of the appearance of different configurations of three spins in a system of five spins.

As can be seen in Figure 4b, the probability of a configuration of two up one down ([2/1]) drops sharply at a field value of $h_c = 2$, while the probability of the configuration of 3 up ([3/0]) sharply increases at the same value of the field $h_c = 2$. There were no other configurations. Thus, the jump in the magnetization curve is caused by a change in the probabilities of microstates.

Let’s remove one spin from the array (concentration of dilution $x = 0.2$), then the Hamiltonian of the system:

$$\mathcal{H} = S_1S_2 + S_5S_1 - h \sum_{j=1}^{5} S_j + hS_3.$$  \hfill (3)

The magnetization curve for the “diluted” system is shown in Fig. 4c.

Consider the cause of additional magnetization plateau in the case of dilution concentration $x = 0.2$. At such a dilution concentration, a revolution of one spin will change the energy of
interaction with the two neighboring spins or only with one, in the case of proximity to the vacancy. The probability of a configuration with three spins has not changed and is shown in Fig. 4a, but at the same time a configuration appeared in which there are 2 spins and one vacancy. The probability of configurations with one vacancy is shown in Fig. 4d.

| Configuration | number of spins | Energy   |
|---------------|-----------------|----------|
| 3/0           | 3               | -2+3h    |
| 2/1           | 3               | 2+h      |
| 2/0           | 2               | -1-2h    |
| 1/1           | 2               | 1        |
| 1/0           | 1               | h        |
| 0/1           | 1               | -h       |

Using Table 1, we can calculate the values of $h_c$ at which the transition occurs from one configuration to another. For example, in the transition from 2/1 to 3/0:

$$-2 + 3h = 2 + h$$  \hspace{1cm} (4)
$$-4 = -2h$$  \hspace{1cm} (5)

$$h_c = 2$$  \hspace{1cm} (6)

Similarly, the remaining critical transition fields can be calculated.

In this way the jumps on the graph of the magnetization of the diluted sample coincide with the jumps in the probability curves of the configurations. The appearance of an additional plateau on the magnetization schedule is caused by an increase in the number of possible microstates.

2.3. 1D Ising model with three nearest neighbors

![Figure 5. 1D Ising model with three close neighbors and PBC.](image)

Also, the 1D Ising model with $n = 1000$ spins with three nearest neighbors and PBC (Fig. 5) was investigated. As in the model with two neighbors, the ferromagnetic model (all exchange integrals are positive $J > 0$) shows the coincidence of the temperature behavior of the magnetization and COP $\gamma_1$ (Fig. 6a). At the same time in the model with $J < 0$ the average magnetization is equal to 0, but COP $\gamma_1$ showed the transition to order. As well as in model with alternating exchange integral (all vertical $J_v < 0$, and horizontal $J_h > 0$, or vice versa) COP $\gamma_1$ showed transition to order while magnetization is equal to 0 (Fig. 6b).
Figure 6. The temperature behavior of COP $\gamma_1$ and magnetization of 1D Ising model (1000 spins) with three nearest neighbors and PBC. a) Blue denotes the magnetization of the ferromagnetic model with $J > 0$, green - magnetization of the antiferromagnetic model with $J < 0$, orange - COP (the same for both models). b) Blue denotes the magnetization with alternating exchange integral (each horizontal bonds of the spins are positive $J_h > 0$, and the vertical are negative $J_v < 0$ or vice versa), orange - the same COP $\gamma_1$ for such model.

2.4. 1D Ising model with four nearest neighbors

Figure 7. 1D Ising model with four close neighbors and PBC.

The 1D Ising model with $n = 1000$ spins, with four nearest neighbors and PBC (Fig. 7) was investigated. In case of ferromagnet interaction ($J > 0$) COP $\gamma_1$ coincides with the magnetization (Fig. 8a). In model with alternating exchange integral $J_h > 0$ and $J_v < 0$ magnetization equal to 0, but COP $\gamma_1$ shows the ordering (the same for both model).

But when we change the exchange integral to negative $J < 0$ or to alternating with negative horizontal $J_h < 0$ and positive vertical $J_v > 0$ the frustration appears (Fig. 9).

The COP $\gamma_1$ does not working for frustrated systems because spins can not minimize its energy, which results to the impossibility of ground state cluster formation. However, under the proposed approach a more general clustered order parameter $\gamma_2$ for frustrated systems has been proposed. COP $\gamma_2$ represents a ratio of the maximum size of the cluster formed by spins not only in the ground state but also with energy closest to the ground state to the total number of particles (highlighted by the green line in Fig. 1).

Figure 8b shows that $\gamma_2$ describes ordering process in frustrating systems. The behavior of $\gamma_2$
Figure 8. The temperature dependencies of COP $\gamma_1$, $\gamma_2$ and magnetization of 1D Ising model (1000 spins) with four nearest neighbors and PBC. a) Blue denotes the magnetization of the model with $J > 0$, green - the magnetization of the model with $J_h > 0$ and $J_v < 0$, orange - COP $\gamma_1$ same for these two models. b) Orange denotes COP $\gamma_2$ of frustrated systems with negative exchange integral $J < 0$ and with alternating exchange integral with $J_h < 0$ and $J_v > 0$. Magnetization of these model is denoted as blue.

Figure 9. Frustrations in 1D Ising model with four nearest neighbors a) in the antiferromagnet model with $J < 0$ b) in the model with alternating exchange integral $J_h < 0$ and $J_v > 0$.

is the same for two frustrated systems mentioned previously. Also, the clustered order parameter $\gamma_2$ can describe the ordering in other frustrated systems. A more detailed description of the approach can be found in the paper [13].

3. Honeycomb Spin Ice Heat Capacity

As was shown above, frustrations introduce new interesting effects and unusual behavior of the system. The most interesting frustrated system is artificial spin ice (ASI) of various geometries and one of the most discussed - a model of hexagonal artificial spin ice. Depending on the Hamiltonian, there are different approaches to modeling such systems. Some calculate the model including only the interactions of the nearest neighbors with Hamiltonian (1) [19]. Others taking into account only the dipole-dipole interaction with (or without) cut-off radius [20, 21]. And some taking into account both the interaction of the nearest neighbors and the dipole-dipole interaction, trying to find the correct coefficient of their proportionality [22, 23, 24].

$$\mathcal{H} = D a^3 \sum_{i<j} \frac{\vec{m}_i \cdot \vec{m}_j}{r^{3/2}} - 3 \frac{(\vec{m}_i \cdot r_{ij}')(\vec{m}_j \cdot r_{ij}')}{r^{5/2}}$$

(7)

We decided to consider a model with a pure dipole interaction (7). Effect of long- and short-range interactions on the thermodynamics of dipolar spin ice with different geometries was considered here [1].
Two series of samples which are consisting of various numbers of particles formed in hexagonal spin ice arrays, square and hexagonal ("from the center") forms with the different radius of interaction were simulated. Models were considered with long-range (LR) and short-range (SR) dipole-dipole interaction. At LR interaction, every spin interacted with everyone. At SR interaction, every spin interacted with the 4 nearest neighbors (less on the borders). The simulation was performed by Wang-Landau method [25, 26, 27]. Thermodynamics of the samples was calculated using 24 WL-steps. The heat capacity temperature behavior of the hexagonal spin ice (hexagon sample) with the number of particles (N) = 30, 72, 132, 210, 306 with LR and SR interactions shown in fig.10.

![Figure 10](image)

**Figure 10.** The heat capacity temperature behavior of the hexagonal spin ice (hexagon sample) with LR (a) and SR (b) interactions. (c) Comparing of the heat capacity peaks depending on the number of particles in the system for honeycomb spin ice with square and hexagonal shapes. At $N \rightarrow \infty$ with LR interaction the temperature behavior of the heat capacity reveals the singularity, the second peaks converge to $0.133D/k_B$, and with SR peaks converge to $0.119D/k_B$.

In LR (Fig. 10a) interaction models the temperature dependence of the heat capacity shows anomalous character, there are two temperature peaks, ie, critical behavior of the system of dipoles in the region of $T_c$ significantly changes. The first peak with increasing number of particles increases and the second peak reduces. As can be seen from Fig. 10b, the heat capacity peak of models with SR interaction with increasing number of particles is reduces. The temperature behavior of the specific heats square shape samples with LR and SR interactions repeats the behavior of the specific heats hexagonal shape samples, described above. The comparing of the heat capacity peaks depending on the number of particles in the system for honeycomb spin ice with square and hexagonal shapes shown in Fig. 10c. The solid lines in this figure show the approximation. From Fig. 10c follows that at $N \rightarrow \infty$ the influence of the boundaries on the critical phenomena in $T_c$ can be neglected. There is the convergence of specific heat peaks for square and hexagonal shapes. At SR interaction, peaks values converge to $0.119D/k_B$. At LR interaction heat capacity reveals the singularity at low temperatures and the height of the second peak with increasing system size convergences to the $0.133D/k_B$. In models with SR interaction, the phase transition is absent, while models with LR interactions show phase transition. The question of how much neighbors should be taken into consideration to not lose the basic thermodynamic properties of the system is necessary to investigate further.

4. 3D Heisenberg model

A further development of this study may be the transition to the use of the classical Heisenberg model. The Hamiltonian of the spin system in frame of Heisenberg model was set as follows:

$$
\mathcal{H} = -J \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j - A_z \sum_i \mathbf{S}_i \cdot \mathbf{z} - h \sum_i \mathbf{S}_i
$$

(8)
where $\vec{S}_i$ is the atomic spin at the $i$-th lattice site, $J$ - ferromagnetic short-range exchange interaction, $|A|$ - constant of magnetic anisotropy, $h$ - external magnetic field. The sum is multiplied by $1/2$ in order to avoid double summation, but some write it without the $1/2$ factor; it’s alright as long as one remembers that the summation is over $i$ and $j$ so that $i<j$. A spin $\vec{S}_i = \{S_x^i, S_y^i, S_z^i\}$ is introduced as a three-dimensional unit vector in accordance with formulas:

$$
\begin{align*}
    x &= r \sin(\phi) \cos(\theta) \\
    y &= r \sin(\phi) \sin(\theta) \\
    z &= r \cos(\phi)
\end{align*}
$$

(9)

One may note that in the case of ferromagnets the above Heisenberg Hamiltonian (8) predicts the parallel alignment of atomic spins, but does not specify a preferential direction of alignment, see the first two terms in Eq. 8. Thus, in such case the Heisenberg Hamiltonian is called the isotropic Heisenberg Hamiltonian. However, in real crystals the isotropy is broken by other magnetic effects that were neglected in the original Hamiltonian, like the dipolar interactions and spin-orbit coupling. Also, an external magnetic field can be applied so that the isotropy is broken by introducing a certain direction (the direction of the field). Thus, the whole Eq. 8 describes the anisotropic Heisenberg Hamiltonian.

The developed software for simulation of systems in frame of Heisenberg model is based on the new, promising programming language Rust. Rust is a new experimental programming language developed by Mozilla. Rust supports functional, parallel, procedural and object-oriented programming, that is, almost the entire range of paradigms actually used in applied programming. From the above, it could be concluded that this language combines all the properties needed for numerical simulation. Also this language supports MPI for high performance computing.

The results obtained by the created software was verified in comparison with known results for the Heisenberg model [28], e.g. convergence of critical temperature $T_c = 1.44(2)$ has been reached.

5. Summary
In this paper, the investigation of some Ising spins and dipoles models was performed.

We show that the COP is more universal than magnetization. In general, these models show similar results. Magnetization shows the transition only at positive $J$, but COP describes the transition, regardless the exchange integral sign and the number of neighbors.

The open question is leave for us to develop the approach of the cluster order parameter on ASI systems with dipolar Hamiltonian (7). In such systems there are a lot of neighbors for each dipole, that can present some troubles for approach. But knowing the order parameter is necessary for calculation of critical indexes of phase transition.

The observed anomalous behavior of the heat capacity in the arrays must be investigated in detail to find out the reason behind the variation of critical behavior near the critical phase transition temperature. Here two directions of research are possible with the purpose of theoretical description of the second-order phase transition.

The first can obviously be due to the fact that the classical concept of a second-order phase transition assumes a mutual transformation of the two phases, which is usually explained in terms of percolation theory, i.e. the appearance of the ”percolation cluster”. The presence of one or several peaks in $T_c$ region can be due to the existence of several transitions between possible coexisting phases, the creation and sequential transformation of a percolation cluster under the conditions of long-range dipole interaction. The question of the concept of “percolation cluster” in systems with alternating long-range interaction also remains open.
The second direction of research can be connected with the definition of critical behavior, which is no longer described in the framework of universal and simple power laws, i.e. the hypothesis of the universality of the critical behavior of second order phase transitions requires verification.

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