Influence of long-range interactions on the critical temperature of the Ising model phase transition

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The article deals with the two-dimensional and three-dimensional Ising models with the long-range spin interactions. The intensity of the interaction between the spins is considered decreasing with distance r in accordance with the power law $r^{-d-\sigma}$ with dimensionality d and parameter σ. The research was conducted by the Monte Carlo method with Metropolis algorithm using parallel computing techniques. On the basis of numerical simulation the dependence of the phase transition temperature upon the parameter σ is found. The phase transition temperature is shown to decrease with increasing σ.

1 Introduction

The magnetic properties of a substance and the problem of phase transitions between paramagnetic and ferromagnetic states has been studied up to the present day. In 1924 E. Ising proposed a model of the magnetic as a system of the spins interacting by pairs and described magnetic properties of the system for the one-dimensional chain. He proved the absence of a phase transition in this case [1]. In 1944 the two-dimensional Ising model was examined by L. Onsager [2] who proved the phase transition existence and calculated its temperature. In 1952 C. N. Yang found the spontaneous magnetization in the two-dimensional Ising model [3]. However, attempts to explore three-dimensional Ising model, as well as a two-dimensional model in an external magnetic field by analytical methods were unsuccessful, leading to the development of numerical methods for its study.

Computer modeling has allowed to study the critical behavior of systems of any complexity and with different external conditions [4]. For example, studies have been carried out of two-dimensional and three-dimensional Ising models with different configurations of lattices (triangular, simple cubic, hexagonal, pentagonal) with the presence of defects [5, 6].

In papers [7, 8] phase diagrams of equilibrium between the paramagnetic and ferromagnetic states of the Ising model on a simple cubic lattice taking into account the interaction of both the first and second nearest neighbors were constructed numerically. In paper [9] the exchange interaction in a variety of configurations of two-dimensional lattices were considered including second neighbor spins, and long-range interactions added has been proved to increase the phase transition temperature.

In [10] we considered the Ising models with different values of the interaction between the spins and analyzed the dependence of the phase transition temperature of the coupling constants, while linearly decreasing the distance between the spins.

In paper [11] we considered the Ising models with different interaction radii of the spins in the presence and absence of an external magnetic field with a nonlinearly decreasing interaction constant. It has been

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shown that the phase transition temperature increase is a process having saturation at the large interaction radii between spins.

To allow for long-range interactions in the Ising model M. Fisher offered to consider the intensity of the interaction between the spins decreasing with distance according to the power law [12]:

$$J \propto r^{-d-\sigma}, \tag{1}$$

where d is the lattice dimensionality, σ is the phenomenological parameter, r is the distance between spins.

Parameter σ influences the values of the critical exponents of the phase transition in the Ising model significantly. For example, it has been shown [13, 14] critical exponents are approaching the values predicted by the renormalization-group analysis for the two-dimensional Ising model with the nearest-neighbour spin interaction with increasing parameter σ.

Paper [15] is devoted to the two-dimensional and three-dimensional Ising models with long-range interactions having the magnitude of the interaction varying according to the law (1). A function was found approximating the dependence of the phase transition temperature on the parameter σ.

In this paper we defined phase transition temperature between the paramagnetic and ferromagnetic states in two-dimensional and three-dimensional Ising models with long-range interactions for different values of σ basing on the Monte Carlo method. The form has been proposed of an analytic function that approximates the relationship between the phase transition temperature and the parameter σ.

2 The Ising model with long-range interactions

Consider the Ising model, which is described by a simple square or cubic lattices (all edges have the same length which is equal to unity) with periodic boundary conditions. Spins are taking one of two possible values: +1 or -1 and situated in each lattice site. To describe the position of each spin we introduce a rectangular coordinate system, the axis x, y, z are parallel to the sides of the lattice.

For a two-dimensional model, the position of the spins is determined by two integers (i, j), which are 1, 2, 3, etc. The hamiltonian of the spin with coordinates (i, j) is given by:

$$H(S_{ij}) = \sum_{l=i-N}^{i+N} \sum_{m=j-N}^{j+N} \frac{J_0}{r_{lm}^{2+\sigma}} S_{ij} S_{lm} \tag{2}$$

where $r_{lm} = \sqrt{(i-l)^2 + (j-m)^2}$ is the distance between spins S_{ij} and S_{lm}, J_0 is the interaction constant, $S_{ij} = \pm 1$ for all i, j.

The summation in the expression (2) is carried out over all the points (l, m), which are in a circle of radius R with the center at the spin with the coordinates (i, j), where

$$r = \sqrt{(l-i)^2 + (m-j)^2} \le R = N.$$

While the self-interaction of spin is excluded, i.e. equalities $l = i, m = j$ can not be satisfied simultaneously.

The intensity of the interaction between the spins of S_{ij} and S_{lm} $J_l m$ decreases with distance r_{lm} according to the power law:

$$J_l m = \frac{J_0}{r_{lm}^{2+\sigma}}$$

Similarly, the position of the spin in the three-dimensional model is determined by three integers i, j, s. The hamiltonian of the spin S_{ijs} with coordinates $(i, j, s), i, j, s = 1, 2, 3...$ takes the form

$$H(S_{ijs}) = \sum_{l=i-N}^{i+N} \sum_{m=j-N}^{j+N} \sum_{n=s-N}^{s+N} \frac{J_0}{r_{lmn}^{3+\sigma}} S_{ijs} S_{lmn} \tag{3}$$

where $r_{lmn} = \sqrt{(i-l)^2 + (j-m)^2 + (s-n)^2}$ is the distance between spins S_{ijs} and S_{lmn}.

As well as in the case of a two-dimensional model of the summation is carried out over all the points (l, m, n), located in the a sphere of radius R, where

$$\sqrt{(l-i)^2 + (m-j)^2 + (n-s)^2} \leq R = N,$$

and the equalities $l = i, m = j, n = s$ can not be satisfied simultaneously. The intensity of the interaction between the spins of S_{ijs} and S_{lmn} J_lmn decreases with distance r_{lmn} according to the law:

$$J_lmn = \frac{J_0}{r_{lmn}^{3+\sigma}}.$$

Summation in expressions (2), (3) is done over all l, m, n with the periodic boundary conditions.

The average value of the magnetic moment per one spin for the two-dimensional and three-dimensional lattices respectively is found by the formulas:

$$\langle M \rangle = \frac{1}{L^2} \sum_{i,j=1}^{L} S_{ij} Z^{-1} \exp\left(-\frac{1}{kT} H(S_{ij})\right) \tag{4}$$

$$\langle M \rangle = \frac{1}{L^3} \sum_{i,j,s=1}^{L} S_{ijs} Z^{-1} \exp\left(-\frac{1}{kT} H(S_{ijs})\right) \tag{5}$$

where

$$Z = \exp\left(-\frac{1}{kT} H(+1)\right) + \exp\left(-\frac{1}{kT} H(-1)\right) \tag{6}$$

is the normalization constant, k is the Boltzmann constant, T is the absolute temperature of the system, L is the linear size of the lattice, that is the number of intervals between spins along each axis of x, y, z.

In the proposed model the values of the phenomenological parameters J_0, L, N, σ are given. We call the introduced radius R the radius of the spin interaction area.

3 Ising models numerical simulations

It is very difficult to calculate the $< M >$ and its dependence upon the temperature T in the proposed models by the analytical methods with formulas (4) - (6). To solve this problem it is proposed to use the Monte Carlo method of numerical simulation.

For the numerical study of the Ising model by the formulas (2) - (6) it is necessary in these expressions to go over to dimensionless quantities. For this purpose we measure the distance between the spins in terms of the distance between neighboring spins along the axis of coordinates, the energy of interaction between the spins of J - in terms of the energy of interaction between the nearest spins J_0, the value kT is equated to a dimensionless parameter T assumed as the reduced temperature. We choose the parameter N determining the interaction area radius between the spins to be 10.

To calculate the average value of the magnetic moment with the formulas (4) - (6) by the Monte Carlo method with a small error it is necessary to consider a large number of lattice sites and carry out a large number of statistical tests. However, in this model the method becomes resource consuming, since the calculation time exponentially increases with the number of nodes and the number of tests. Therefore, to study the model the Monte Carlo algorithm was developed, using parallel computing techniques. The lattice was divided into subregions, each subregion was processed separately by its own processor. This approach is based on the additive property of the magnetic moments of the lattice spins.

Figure 1 shows plots of the average magnetic moment $< M(T) >$ on the temperature for different values of σ for two-dimensional (a) and three-dimensional (b) Ising model. Plot $< M(T) >$ experiences a jump at the phase transition temperature T_c. From the analysis of the graphs we can conclude that the value of T_c decreases with increasing value of the parameter σ.

Note that the accuracy of the phase transition temperature T_c of the plots in Fig. 1 - 2 is too low. The accuracy of determining the temperature T_c is significantly affected by the effect of the finite size of the system [16], [17].

For a more precise determination of the phase transition temperature, we used a fourth-order cumulants method proposed by K. Binder and it has proved very effective [18], [19], [20], [21]. It is the construction of the temperature dependence of the cumulants $U_N(T)$

$$U_L(T) = 1 - \frac{< M^4(T) >}{3 < M^2(T) >^2}, \tag{7}$$

for the various linear sizes of the lattice L. T_c is picked from a common crossing point of the plots of these dependencies.

On the basis of numerical simulation were obtained graphs of the temperature dependence of the Binder cumulant equation (7). Calculations were performed for two-dimensional lattices of 100×100 and 60×60 and three-dimensional lattices of size $90 \times 90 \times 90$ and $72 \times 72 \times 72$. The values of the parameter σ were taken from 0 to 10.

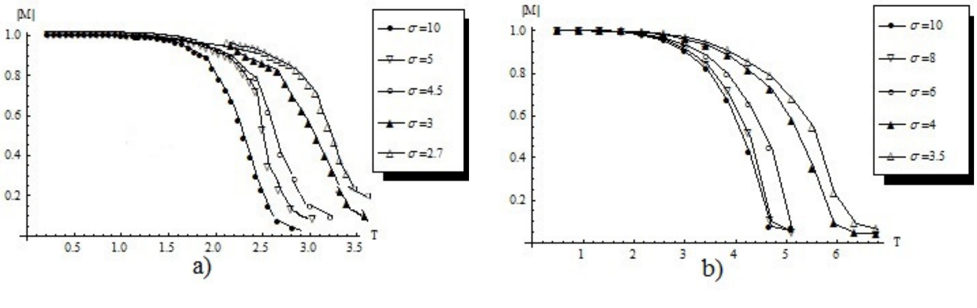

Figure 1: $< M >$ dependence from T for different σ values:
(a) two-dimensional Ising model; (b) three-dimensional Ising model

The values of the critical temperatures for different values of σ for two-dimensional and three-dimensional models are presented in figures 2-3 by points. The graphs show that the critical temperature in the two-dimensional and three-dimensional cases decrease with increasing values of the parameter σ exponentially.

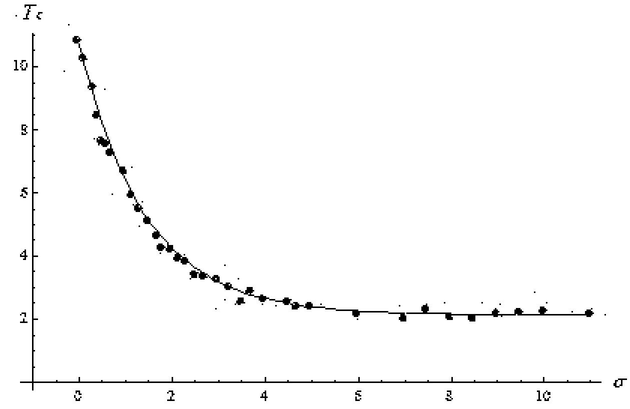

Figure 2: $T_c(\sigma)$ dependence for the two-dimensional Ising model

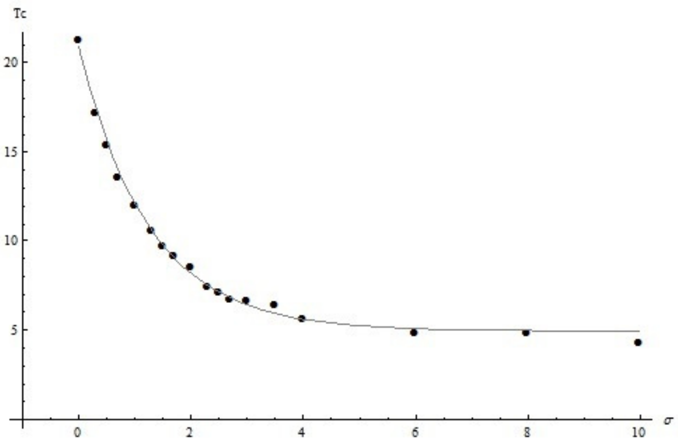

Figure 3: $T_c(\sigma)$ dependence for the three-dimensional Ising model

The dependence of $T_c(\sigma)$ upon the parameter σ was obtained in analytical form, basing upon the results of numerical modeling of the least squares. These functions have the form:

$$T_c(\sigma) = 2.233 + 8.672 \exp(-0.73\sigma) \tag{8}$$

for two-dimensional model and

$$T_c(\sigma) = 4.511 + 15.863 \exp(-0.7\sigma) \tag{9}$$

for three-dimensional model. Their plots are presented in figures 2-3 by the full line.

The proposed formulas (8), (9) can be written as a single equation

$$T_c(\sigma) = A + B\exp(-c\sigma), \tag{10}$$

where $A = 2.233$, $B = 8.672$, $c = 0.73$ for two-dimensional model and $A = 4.511$, $B = 15.863$, $c = 0.7$ for three-dimensional model.

Note, that in the proposed model the relative change in the intensity of the interaction $J(R)$ between the spins located at the distance R, and spins at a distance $R = 1$ is represented by the expression

$$\delta = \frac{J(R)}{J_0} = \frac{1}{R^{(d+\sigma)}}, \tag{11}$$

that is, for small σ the interaction constant $J(R)$ between the spins for the particular value R has a bigger value than that for large σ.

Basing on (11) we construct the dependence σ from R and δ as the function $\sigma(R, \delta)$

$$\sigma = -\left(d + \frac{\ln\delta}{\ln R}\right). \tag{12}$$

Formula (12) defines σ value, where $J(R) = \delta J_0$ with the chosen values of R and δ.

We assume that with $\delta = 10^{-d}$ (where d is the dimension of the lattice) the intensity of the interaction between the spins is taken into account before the distance between the spins becomes R_k, where $J(R_k) = 10^{-d}J_0$. It is possible to assume $J(R_k + 1) = 0$. In the proposed model, this condition will be satisfied, if in accordance with the expression (12) we take σ as σ_k

$$\sigma_k = -\left(d + \frac{-d\ln 10}{\ln R_k}\right), \tag{13}$$

with $k = 2, 3, ..., 10$.

Thus, formula (13) associates the parameter σ_k and a selected radius of the spin interaction area R_k. Substituting the expression for σ_k defined by the equation (13) into the expression (10), we obtain a formula that determines the dependence of the phase transition temperature T_c upon the radius of the spin interaction area R_k, i.e. $T_c(R_k)$, for both two-dimensional and three-dimensional models

$$T_c(R_k) = A + B\exp\left[-cd\left(\frac{\ln 10}{\ln R_k} - 1\right)\right], \tag{14}$$

where A, B, c are coefficients specified in accordance with the expressions (8), (9) for a two-dimensional or three-dimensional models.

The logarithm of the critical temperature $\ln T_c$ from the radii of the interaction R_k according to the equation (14) are represented by points in fig. 4.

The plot in the figure, represented by a point, for clarity, can be approximated by a continuous line, which is defined by the equation derived on the basis of (14) provided that R_k replaced by R receives continuous values.

$$\ln T_c(R) = \ln\left[A + B\exp\left[-cd\left(\frac{\ln 10}{\ln R} - 1\right)\right]\right], \tag{15}$$

The plots presented in fig. 4 show that the critical temperature increases with radius R_k of the spin interaction area, approaching a limit value for large R_k.

Note, that these plots are in qualitative agreement with the plots obtained earlier in [11], in which we investigated the Ising model with another form of interaction between the spins.

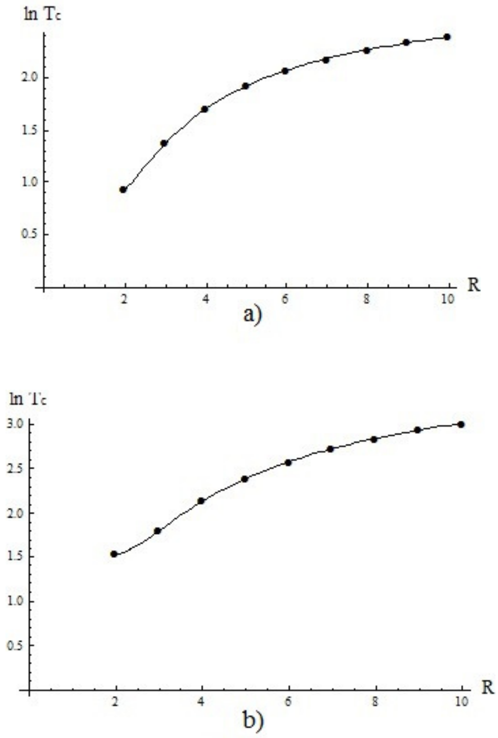

Figure 4: The logarithmic dependence of the critical temperature $\ln T_c$ from the interaction radius area R_k: (a) two-dimensional Ising model; (b) three-dimensional Ising model

4 Conclusions

Monte Carlo calculations of the phase transition temperature in two-dimensional and three-dimensional Ising models with long-range interactions have shown that temperature increases with the increase of the radius of the lattice spins interaction. In the proposed model in which the interaction is inversely proportional to the distance between the spins raised to a certain power, the temperature depends strongly on the exponent and increases with σ decreasing. These results, obtained on the particular Ising model, are the basis for the description of phase transitions in more complex models.

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