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Applicability of n-vicinity method for calculation of free energy of Ising model

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HIGHLIGHTS

- The n-vicinity method is used for analyzing a D dimensional Ising model.
- The equation of state is solved for an arbitrary D and zero magnetic field.
- When $D \geq 3$ the system has a phase transition of the second kind.
- For $D \geq 3$ we obtain a simple and reliable expression for the critical temperature.

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ABSTRACT

Here we apply the n-vicinity method of approximate calculation of the partition function to an Ising Model with the nearest neighbor interaction on D-dimensional hypercube lattice. We solve the equation of state for an arbitrary dimension D and analyze the behavior of the free energy. As expected, for large dimensions ($D \geq 3$) the system demonstrates a phase transition of the second kind. In this case, we obtain a simple analytical expression for the critical value of the inverse temperature. When $3 \leq D \leq 7$ this expression is in a very good agreement with the results of computer simulations. In the case of small dimensions ($D = 1, 2$), there is a noticeable discrepancy with the known exact results.

1. Introduction

For nearly a century, the Ising model and, particularly, the calculation of its partition function has been in the focused of active research. For some important models this problem can be solved exactly [1–3]. However, in some cases, we do not know the exact solutions and the problem can be solved by means of different approximate methods only. An extensive bibliography on this subject can be found in [4,5]. Herein a numerous applications of the problem are also listed. Note that the importance of the problem goes far beyond physics, as the Ising models are often met in combinatorial optimization [6], the theory of machine learning [7] and the computer processing of images [8,9].

In [10–12] we proposed the n-vicinity method for approximate calculation of the partition function for an arbitrary connection matrix. The main idea of our method is as follows. Let us fix the initial configuration (the initial state) $\mathbf{s}_0 \in \mathbf{R}^\mathbf{N}$ and define its n-vicinity Ω_n as the set of states that differ from $\mathbf{s}_0$ by the opposite values of n coordinates ($0 \leq n \leq N$). In a general case, the distribution of the energies of the states from the n-vicinity is unknown. However, in [11,12] we found exact expressions for the mean energy E_n and the variance σ_n^2 in terms of characteristics of the connection matrix. Numerous computer simulations demonstrate that the distribution of energies from Ω_n is a single-mode and the Gaussian

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density with the parameters E_n and σ_n^2 approximates it rather accurately (see [13]). Then in the expression for the partition function $Z_N = \sum_{n=0}^{N} \sum_{\mathbf{s}\in\Omega_n} \exp\left(-\beta E(\mathbf{s})\right)$ we can replace the summation over the states from Ω_n by the integration over the Gaussian measure, and in place of the summation over n we can pass to integration over the parameter $x = n/N$. As a result the partition function takes the form of the double integral $Z_N \approx \int \mathrm{d}x \int \mathrm{d}E \exp\left[-N \cdot F(x, E)\right]$, which can be calculated with the aid of the saddle-point method. The function $F(x, E)$ depends on the inverse temperature β, the external magnetic field H (when it is present) and the characteristics of the connection matrix. In the general form the expression for $F(x, E)$ was obtained in [11,12].

In this paper, we describe an application of the n-vicinity method when analyzing the Ising model with nearest-neighbor interaction on a D-dimensional hypercube. A great variety of the obtained results for the Ising model allows us to verify our method and find the boundaries of its applicability. Below we list our results.

Assuming different interactions between the nearest-neighbors along different directions of the lattice, we obtain the equation of state (see Sections 2 and 3). It generalizes the Bragg–Williams equation. In our approach, the effective coordination number q defining the interaction of a spin with its nearest neighborhood is the main characteristic of the lattice. When interactions with all the nearest-neighbors are the same, q is equal to the number of the nearest neighbors: $q = 2D$.

We solve the equation of state in Sections 4 and 5. For the lattices of large dimensions $D > 3$, our solution reproduces all the known results for the Ising model. Namely, the presence of a phase transition of the second kind and the values of the critical exponents. We obtained an analytical expression for the critical value of the inverse temperature as function of D (Section 4). It is in a good agreement with the results of computer simulations for the dimensions $3 \le D \le 7$ [13–16]. However, for the three-dimensional Ising model ($D = 3$) our approach does not provide the correct values of the critical exponents obtained with the aid of the renormalization group method [17,18]. For small dimensions ($D < 3$) our approach is inapplicable. In the case of the one-dimensional Ising model, the same as in the mean field theory, the obtained incorrect result indicates a phase transition at a finite temperature. For the two-dimensional Ising model ($D = 2$) our approach reproduces the known quantitative results rather well. However, contrary to the exact solution, it predicts a phase transition of the first kind (Section 5).

In Section 6, we analyze the behavior of different characteristics (the magnetization, the internal energy and so on). In Section 7, we present our conclusions and discuss the obtained results. For details of calculations, see Appendices.

2. Notations and general expressions

Let $\mathbf{T} = \left(T_{ij}\right)_1^N$ be a connection matrix corresponding to the D-dimensional Ising model with the nearest-neighbor interaction. The configuration $\mathbf{s}_0 = (1, 1, \ldots, 1) \in \mathbf{R}^N$ is the ground state of the spin system and Ω_n is the n-vicinity of the ground state: $\Omega_n = \left\{\mathbf{s} : \sum_{i=1}^{N} s_i = N - 2n\right\}$ $n = 0, \ldots, N$. We based our method of calculation of the partition function on the assumption that the normal probability density approximates rather accurately the distribution of the energies from Ω_n. In [13] we discuss this question in detail, where we also presented the exact expressions for the mean energy E_n and the variance σ_n^2. Here we only use their asymptotic forms.

If $\mathbf{s} \in \Omega_n$ and H is an uniform magnetic field, the energy per one spin is

$$E(\mathbf{s}, H) = -\frac{1}{2N} \sum_{i \ne j}^{N} T_{ij} s_i s_j - \frac{H}{N} \sum_{i=1}^{N} s_i = E(\mathbf{s}) - H\left(1 - \frac{2n}{N}\right). \quad (1)$$

By E_0 we denote the energy of the ground state:

$$E_0 = E(\mathbf{s}_0) = -\frac{1}{2N} \sum_{i \ne j}^{N} T_{ij}. \quad (2)$$

Let $N \to \infty$ and let us introduce a parameter $x = n/N \in [0, 1]$. In [13] we showed that the asymptotic expressions for the mean energy and the variance are:

$$E_x = \lim_{N\to\infty} E_n = E_0(1 - 2x)^2, \qquad \sigma_x^2 = \lim_{N\to\infty} \sigma_n^2 = \frac{8 \sum_{ij} T_{ij}^2}{N^2} x^2 (1 - x)^2. \quad (3)$$

Appendix A proves that the asymptotic expression for the partition function has the form $Z_N \sim \int_0^1 \mathrm{d}x \int_{E_0}^{|E_0|} \exp\left[-N \cdot F(x, E)\right] \mathrm{d}E$, where $N \gg 1$, and the function in the exponent is equal to

$$F(x, E) = L(x) + \beta\left[E - H \cdot (1 - 2x)\right] + \frac{1}{2N}\left(\frac{E - E_x}{\sigma_x}\right)^2.$$

Here

$$L(x) = x \ln x + (1 - x)\ln(1 - x), \quad (4)$$

and $\beta = 1/T$ is the inverse temperature.

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