Phase Transition in 2D Ising Model with Next-Neighbor Interaction

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Abstract. We used a Monte Carlo method to analyze a planar Ising model taking into account a ferromagnetic interaction with next neighbors. We found that independent of the value of the additional interaction, the character of singularity of the heat capacity did not change. Namely, at the critical point the heat capacity has a logarithmic singularity. We obtained a semi-theoretical formula relating the value of the critical temperature with the value of the additional ferromagnetic interaction.

1. Introduction

Among exact solutions of statistical physics problems one of the most known result is Onsager’s equation for the critical temperature $\beta_c$ for the planar Ising model with the nearest neighbor interaction. The critical indices calculated using this equation differ from the classical mean-field values [1]. As far back as in his original work Onsager found in this system a phase transition of the second kind with a logarithmic singularity of the second derivative of the free energy at the critical point. Of course this is an asymptotic result obtained when the number of spins $N$ tends to infinity. An accurate generalization of the Onsager results to the case of a planar lattices of a finite size [3] shows that the maximal value of the heat capacity $C_{\text{max}} = \max_{\beta} C(\beta) \sim \ln N$. In other words, when the number of spins $N$ is finite but large the heat capacity increases logarithmically.

On the other hand, it was shown that in the case of hypercubic lattices of high dimensions $d > 3$ the critical indices had the classical mean-field values. When the dimension $d$ of the Ising model is equal to five or higher ($d \geq 5$) this result is known for a long time [4]. In the case of the 4D-Ising model some theoretical results were obtained in [4] and they were partly confirmed by means of computer simulations [5]. However, for the 3D-Ising model we do not know the exact values of the critical indices yet. On the other hand, there is a consensus that the heat capacity of such system has an infinite singularity at the critical point.

The classical critical indices imply in particular a finite jump of the heat capacity at the critical point but not an infinite singularity. It is believed that somewhere between the dimensions $d = 2$ and $d = 4$ the infinite singularity of the heat capacity has to be changed by a finite jump. In the present paper, we attempt to define experimentally lattice parameters for which such change of the type of singularity takes place.

2. Effective number of neighbors
In [6]-[8] we proposed a n-vicinity method for approximate calculations of the partition function. The method is based on a theoretical description of the spectral density of a spin system, which uses exact expressions for the moments of the true distribution. In the most general form the main idea and the most important equations of the method were obtained in [6]. As applied to the Ising model on the $d$-dimensional hypercube we examined this method in [7], [8].

One of the most important results of these papers is as follows: the higher the dimension $d$ the better the agreement between our theoretical estimate of the inverse critical temperature $\beta_c$ and the result of computer simulations. When $d = 3$ the relative difference between the theoretic estimate and the result of computer simulations is 2.4%. With increase of $d$ from 3 to 7 the difference decreases quickly up to the value 0.002%. However, here we would like to discuss another side of this problem.

Let $T = (T_{ij})^N$ be a connection matrix and let us define a parameter

$$\gamma = \frac{(\sum_{ij} T_{ij})^2}{N \cdot \sum_{ij} T_{ij}}. \quad (1)$$

In our problem $\gamma$ is the only parameter that contains the information about the lattice. Actually the parameter $\gamma$ characterizes an effective number of spins with which each given spin interacts. For example, in the case of the standard Ising model on the $d$-dimensional hypercube with the same interactions between all the nearest neighbors we obtain

$$\gamma = 2d. \quad (2)$$

If in our discussion, we include not the nearest neighbors only but also the next neighbors (or even the next-next neighbors) and suppose that the corresponding $T_{ij}$ can have fractional values. Then the parameter $\gamma$ can be fractional too. Let us restrict ourselves with the ferromagnetic interaction only. Then for the given dimension $d$ the value of $\gamma$ increases starting from the minimal value (2). From our previous investigations it follows that the larger the value of the parameter $\gamma$ the better our theory coincides with the results of computer simulations.

## 3. Computer simulations and obtained results

We start from the standard planar Ising model ($d = 2$) with interactions between the nearest neighbors only, where the vertical and horizontal interaction constants are the same: $J_1 = J_2 = 1$. (In what follows we use the standard notations for the matrix elements $T_{ij}$.) Then we add the interactions with the next neighbors located along the diagonals of the square cell. Let the corresponding interaction constant be $J_3$. We vary the value of $J_3$ from zero to one: $J_3 \in [0,1]$. In the same time the effective number of the nearest neighbors changes from $\gamma = 4$ to $\gamma = 8$.

We used the Monte Carlo method to examine the described model. The size of the lattice was $N = 100 \times 100$. In the course of our work for the given values of the inverse temperature we calculated the averaged magnetization $m$, the averaged energy, and its dispersion $\sigma_E^2$. The most interesting results we show in the figures 1 and 2.

Since the heat capacity is proportional to the dispersion $\sigma_E^2$, in figure 1 we show the dependence of the heat capacity on $\beta$ for different values of $J_3 = 0.268, 0.5$ and 1 ($\gamma = 4, 6, 7.2$ and 8 respectively). At each curve the point of singularity defines the critical value of the inverse temperature. Let us call it $\beta_c^{\mathrm{ex}}(J_3)$. We see that when $J_3$ increases the critical value decreases monotonically starting from the classical value $\beta_c(0) \approx 0.4407$. This is as it should be: the larger the interactions between spins the larger the value of the critical temperature $T_c \sim 1/ \beta_c$. 

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The most important conclusion following these graphs is that the type of singularity at the critical point $\beta_c^{\text{crit}}(J_\gamma)$ remains unchanged. This is a rather unpredictable result. The matter is that the planar Ising model is an idealized mathematical object. It is impossible to implement such a lattice because always there are some defects and distortions. These imperfections have an effect on macroscopic characteristics of the physical system. On the same time the results of our simulations show that even such deep distortions of the standard model as additional diagonal interaction do not change the type of singularity of the heat capacity at the critical point. Thermodynamic properties of the planar model are stable under perturbations of its parameters.

4. On estimate of critical temperature

One of our results obtained in [7], [8] is as follows. When the value of the parameter $\gamma$ exceeds $16/3$, in the spin system there is a phase transition of second kind with a finite jump of the heat capacity. The phase transition occurs when the critical value of the inverse temperature $\beta_c$ is the solution of the equation

$$1 = \beta \sum_{i,j} T_{ij} - \beta^2 \sum_{i,j} T_{ij}^2.$$

If we apply this result to the standard Ising model where only the interactions between the nearest neighbors are taken into account, we obtain an expression for the critical value $\beta_c$:

$$\beta_c = \frac{1 - \sqrt{1 - 2/d}}{2}.$$

As well as being very simple this expression describes the results of computer simulations with high accuracy. We tested the formula (4) for the values of $d = 3, 4, 5, 6$, and $7$ [7].

If the diagonal interactions $J_\gamma$ between the spins are taken into account, from Eq.(3) we obtain

$$\beta_c(J_\gamma) = \frac{1 + J_\gamma - \sqrt{2J_\gamma}}{2(1 + J_\gamma)}.$$

This result is meaningful only if $\gamma > 16/3$, which is equivalent to $J_\gamma > 0.1716$. Only such values of $J_\gamma$ we will discuss below.

Generally speaking, from our theory it follows that the phase transition is accompanied by a finite jump of the heat capacity but not the singularity shown in figure 1. This contradicts to our computer
simulations. Nevertheless, it is interesting to compare the theoretical estimate (5) of the critical inverse temperature $\beta_c(J_3)$ with its experimental value $\beta^{\text{ex}}_c(J_3)$ obtained by computer simulations. It turns out that if we scale the theoretical values multiplying them by an empiric coefficient 1.3, the obtained results are very close to the corresponding experimental values. In figure 2 we show how for $J_3 = 0.2$, 0.268, 0.369, 0.5, 0.63, 0.75, 0.85 and 1 the experimental points $\beta^{\text{ex}}_c(J_3)$ fall on the normalized theoretical curve $1.3 \cdot \beta_c(J_3)$. We would like to emphasize that we need only one coefficient to match accurately the theoretical estimates and the results of the computer simulations. The reason why there is such scaling is not clear.

5. Conclusions
For the planar Ising model we showed that account for the interactions between the next neighbors did not change the character of the singularity at the critical point. In other words, we did not obtain a finite jump in place of the logarithmic singularity. In view of this we think that there are two possible directions of future studies.

We can also include interactions with the next-next-neighbors as well as with the fourth in order of distance, then the fifth in order of distance and so on, until the conditions of the applicability of the mean-field approximation would be fulfilled. We know that in the framework of the mean-field theory the heat capacity at the critical point has a finite jump. We think that increasing the number of the interacting neighbors we will with necessity path through the value of $\gamma$ where the type of the singularity will change. At least it is interesting to implement this program.

We can discuss the problem from the other point of view. It is generally agreed that for the cubic Ising model ($d = 3$) the heat capacity at the critical point tends to infinite. On the other hand, a finite jump of the heat capacity for the 5D-Ising ($d = 5$) is an established fact [4], [9]. Maybe be it is reasonable to start our simulations from the standard 3D-Ising model (or even from the 4D-Ising model) and to increase steadily the number of interacting neighbors. Taking into account the aforesaid we can expect that when $\gamma$ reaches a certain value the finite jump will replace the infinite singularity. When the dimension of the lattice $d$ increases the number of the spins $N$ increases significantly too. In this case, the simulation has to be much more cumbersome, but we think that it is possible to realize these calculations.

We hope that the it will be possible to explain the nature of the aforesaid scaling.

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References
[1] Baxter R J 1982 Exactly solved models in statistical mechanics (London: Academic Press)
[2] Onsager L 1944 Phys. Rev. 65 117
[3] Kryzhanovsky B V, Malsagov M Yu, Karandashev I M 2018 Opt. Mem. & Neu. Net. 27 10
[4] Aizenman M, Fernández R 1986 Journal of Statistical Physics 44 393
[5] Lundow P H, Markström K 2009 Physical Review E 80 031104
[6] Kryzhanovsky B V, Litinskii L B 2014 Doklady Mathematics 90 784
[7] Kryzhanovsky B and Litinskii L Physica A 2017 468 493
[8] Kryzhanovsky B and Litinskii Leonid 2016 Journ. Phys.: Conf. Ser. 738 012064
[9] Lundow P H, Markström K 2015 Physics B 895 305