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Phase Transitions in 2D Ising Model with Competing Interactions

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Phase Transitions in 2D Ising Model with Competing Interactions[#]

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Abstract

Motivation. 2D Ising model with competing interactions describes the thermodynamic properties of confined complex liquids like microemulsion films and some compounds of rare–earth metals. On the other hand there is a close relationship between critical properties of this model and peculiarities of the energy spectra of some one–dimensional quantum models. Therefore correct description of model phase diagram is of wide interest.

Method. We have used the density matrix renormalization group method for two–dimensional classical systems.

Results. A new modification of density matrix renormalization scheme for 2D Ising model with competing interactions has been presented. The estimations for critical temperatures of second order phase transitions in the model were obtained.

Conclusions. 2D Ising model with competing interactions has a complicated phase diagram and can be described by means of corresponding version of DMRG method at least in the vicinity of some critical points.

Keywords. DMRG; Ising model; phase transitions.

Abbreviations and notations

DMRG density matrix renormalization group	IRF, interaction round a phase model
ANNNI, axial next–nearest neighbor Ising model	2D, two–dimensional
α, parameter of diagonal interactions	β, parameter of axial next–nearest–neighbor interactions
MC, Monte Carlo	

1 INTRODUCTION

The theoretical analysis of the thermodynamics of lattice models with competing interactions is usually restricted to mean–field calculations and Monte Carlo simulation. First approach does not describe correctly the critical properties of low–dimensional systems. Application of Monte Carlo (MC) methods requires rather powerful computers.

In this respect, a good alternative to the traditional approaches is the density matrix renormalization group method (DMRG) proposed by White [1]. For classical 2D lattice models like

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Ising model this method is superior to the classical MC method in accuracy and has the potential of handling much larger systems [2,3].

One of the simplest lattice models of a ternary system, consisting of oil, water and surfactants is Widom model [4]. In terms of spin –½ variables it is equivalent to the Ising model with competing interactions between spins in adjacent and next–nearest neighbor lattice sites. This model can be considered as variant of so called axial next–nearest neighbor Ising model (ANNNI model) which was introduced for the explanation of ordered magnetic phases in CeSb [5]). The equilibrium thermodynamics of 3D Widom model has been studied extensively despite the complicated phase diagram of this model [6]. However, there is relatively little information about critical properties of similar two dimensional spin systems. Nevertheless, the results of such a simulation are of special interest in the context of complex fluids in porous media [7]. They may find practical application for the increase of effectiveness of the extraction processes, for example, in oil extraction technology. 2D ANNNI model was also applied for the simulation of adsorption processes [8].

On the other hand, critical behavior of classical two– dimensional spin systems has direct relations to the zero–temperature phase transitions in corresponding one–dimensional quantum systems. DMRG scheme for interaction round a phase model (IRF model) was already applied to the study of the properties of some quantum spin chains [9]. Therefore the investigation of the thermodynamics of classical two–dimensional spin model has a common interest.

In our previous work [10] we studied the temperature dependencies of internal energy and specific heat of 2D Ising model on square lattice with competing interactions: the ferromagnetic interactions of nearest neighbors and diagonal antiferromagnetic interactions. This model belongs to class of IRF models and to study its thermodynamics we applied directly DMRG method for classical 2D lattice systems proposed by Nishino. In this paper we consider similar model with additional next–nearest neighbor interactions along one of the lattice axes (2D ANNNI model). Such an extension leads to outside of a class of IRF models and requires some modification of original DMRG scheme. We constructed modified renormalization scheme with overlapping spin blocks, which is applicable to above model and studied the dependence of critical temperatures of second order phase transitions on model parameters.

2 MATERIALS AND METHODS

Let us consider 2D Ising model with competing interactions described by the Hamiltonian

$$\mathbf{H} = -\sum_{ij}\left[\sigma(i,j)\sigma(i,j\pm1)+\sigma(i,j)\sigma(i\pm1,j)+\alpha\left(\sigma(i,j)\sigma(i\pm1,j\pm1)\right)+\beta\,\sigma(i,j)\sigma(i,j\pm2)\right]$$

Here $\sigma(i,j)=\pm1$ is a spin variable of the lattice site situated on the intersection of *i*–th row and *j*–th column of the lattice. The relative strength of the diagonal interactions is described by the

parameter α. Parameter β corresponds to the interactions of the next nearest neighbor spins along the rows of the square lattice.

For the model with β = 0 the DMRG simulation shows a monotonous dependence of the internal energy on temperature for a wide range of α values [10]. At the same time the temperature dependence of the specific heat C_v has one sharp maximum, the height of which increase with the number of iterations. For small values of α this model should behave like the exactly solvable 2D Ising model on a square lattice, which has only one second–order phase transition of type order–disorder. Therefore, this maximum should correspond to the cusp for infinite 2D lattice and its position determines the temperature of the phase transition. We found linear decrease of critical temperature in the interval $-0.5 \le \alpha \le 0$.

There is a simple method of approximate evaluation of this dependence derived on a suggestion that at critical temperature the contributions to the four–spin partition function from the ordered states equal the contribution from the disordered states [11,12]. This approach gives the exact value of critical temperature of square lattice. For small values of α, ordered states should be the same as for nearest neighbor Ising model on square lattice. Therefore the following equation for critical temperature can be derived:

$$\frac{1}{4}\cosh\left(\frac{4}{T_c}\right) = 2\exp\left(\frac{2\alpha}{T_c}\right) + \exp\left(\frac{4\alpha}{T_c}\right)$$

where T is absolute temperature in energy units. In first order in α this equation has a solution:

$$T_c = \frac{2}{\ln\left(1+\sqrt{2}\right)} + \frac{\alpha\sqrt{2}}{\ln\left(1+\sqrt{2}\right)}.$$

This dependence shows a linear decrease of critical temperature with the decrease of the value of α and qualitatively agrees with the results of DMRG simulation for α from the interval $-0.5 \le \alpha \le 0$. Widom model contains also weak next–nearest neighbor interactions along the axes of the lattice. To incorporate similar interactions in our 2D model by means of transfer matrix formalism and to construct the corresponding DMRG algorithm, let us consider a lattice strip formed by two interacting rows of spins with numbers i and $i + 1$ (Figure 1). This strip can be considered as a combination of overlapping rectangular 8–spin blocks.

Similar to the IRF model, the total partition function of the lattice is defined by the maximal eigenvalue of the corresponding 'row–to–row' transfer matrix **T** formed by product of the matrices **A** of Boltzmann weights of spin configurations of overlapping 8–spin blocks.

$$\mathbf{T} = \lim_{N\to\infty} \mathbf{T}_N$$

$$\mathbf{T}_N = \mathbf{A}\begin{pmatrix} \sigma_1 & \sigma_2 & \sigma_3 & \sigma_4 \\ \sigma_1' & \sigma_2' & \sigma_3' & \sigma_4' \end{pmatrix} \times \mathbf{A}\begin{pmatrix} \sigma_3 & \sigma_4 & \sigma_5 & \sigma_6 \\ \sigma_3' & \sigma_4' & \sigma_5' & \sigma_6' \end{pmatrix} \times \cdots \times \mathbf{A}\begin{pmatrix} \sigma_{N-3} & \sigma_{N-2} & \sigma_{N-1} & \sigma_N \\ \sigma_{N-3}' & \sigma_{N-2}' & \sigma_{N-1}' & \sigma_N' \end{pmatrix}$$

$$\mathbf{A}\begin{pmatrix}\sigma_1 & \sigma_2 & \sigma_3 & \sigma_4\\ \sigma'_1 & \sigma'_2 & \sigma'_3 & \sigma'_4\end{pmatrix} = \exp\left\{\frac{1}{2T}\left[\sum_{i=1}^{4}\sigma_i\,\sigma'_i + \frac{1}{2}\left(\sum_{i=1}^{3}\left(\sigma_i\,\sigma_{i+1} + \sigma'_i\,\sigma'_{i+1}\right) + \sigma_2\sigma_3 + \sigma'_2\,\sigma'_3\right)\right.\right.$$
$$\left.\left. + \alpha\left[\sigma_2\left(\sigma'_1 + \sigma'_3\right) + \sigma'_2\left(\sigma_1 + \sigma_3\right) + \sigma_3\left(\sigma'_2 + \sigma'_4\right) + \sigma'_3\left(\sigma_2 + \sigma_4\right)\right] + \beta\left(\sigma_1\sigma_3 + \sigma_2\sigma_4 + \sigma_1\sigma_3 + \sigma'_2\sigma'_4\right)\right]\right\}$$

Here $\sigma_j = \sigma(i+1, j)$ and $\sigma'_j = \sigma(i, j)$ are spin variables which belong to upper and lower rows of the two–row lattice fragment depicted in Figure 1.

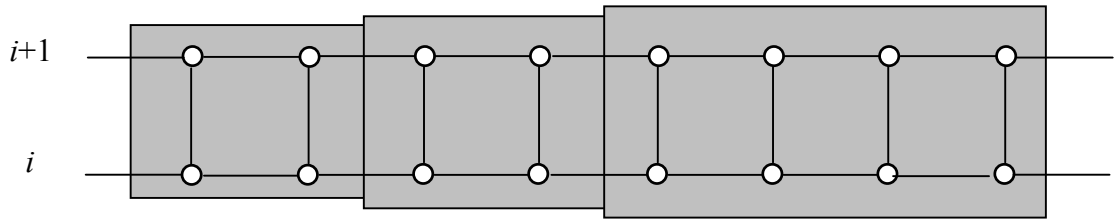

Figure 1. Block structure for the two–row transfer matrix for model with next nearest neighbor interactions along the rows. (Three overlapping 8–spin blocks are shown).

The DMRG method for classical systems is a variational approximation method that maximizes the partition function that can be expressed as a renormalization of the transfer matrix **T**. Let us start this renormalization from transfer matrix of the rectangular strip of size 2×8. The corresponding block partition is given in Figure 2.

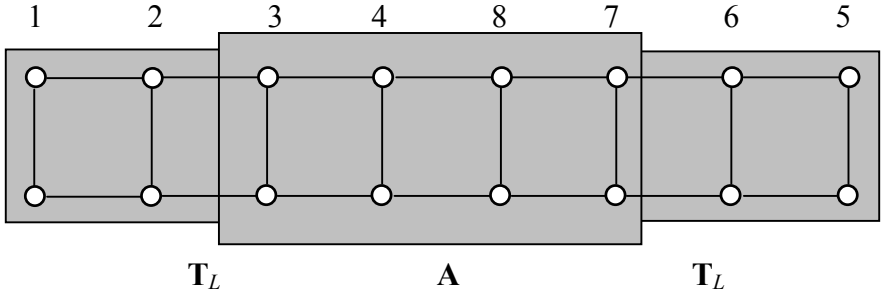

Figure 2. Factorized representation for transfer matrix of the lattice strip of size 2×8. Integer indexes enumerate columns of the strip and each index *j* corresponds to two spin variables σ_j and σ'_j.

Because of reflection symmetry a factorized representation of the model transfer matrix can be written in the form

$$\mathbf{T} = \mathbf{T}_L\begin{pmatrix}\sigma_1 & \sigma_2 & \sigma_3 & \sigma_4\\ \sigma'_1 & \sigma'_2 & \sigma'_3 & \sigma'_4\end{pmatrix} \times \mathbf{A}\begin{pmatrix}\sigma_3 & \sigma_4 & \sigma_8 & \sigma_7\\ \sigma'_3 & \sigma'_4 & \sigma'_8 & \sigma'_7\end{pmatrix} \times \mathbf{T}_L\begin{pmatrix}\sigma_8 & \sigma_7 & \sigma_6 & \sigma_5\\ \sigma'_8 & \sigma'_7 & \sigma'_6 & \sigma'_5\end{pmatrix},$$

where

$$\mathbf{T}_L\begin{pmatrix}\sigma_1 & \sigma_2 & \sigma_3 & \sigma_4\\ \sigma'_1 & \sigma'_2 & \sigma'_3 & \sigma'_4\end{pmatrix} = \mathbf{A}\begin{pmatrix}\sigma_1 & \sigma_2 & \sigma_3 & \sigma_4\\ \sigma'_1 & \sigma'_2 & \sigma'_3 & \sigma'_4\end{pmatrix} \times \exp\left\{\frac{1}{2T}\left[\sigma_1\,\sigma'_1 + \sigma_2\,\sigma'_2 + \frac{1}{2}\left(\sigma_1\,\sigma_2 + \sigma'_1\,\sigma'_2\right) + \beta\left(\sigma_1\,\sigma'_2 + \sigma_2\,\sigma'_1\right)\right]\right\}.$$

First step of renormalization procedure is described by formula

$$\mathbf{T}_L^1\begin{pmatrix} x, \sigma_5\ \sigma_6 \\ y, \sigma_5'\ \sigma_6' \end{pmatrix} = \sum_{\substack{\sigma_1',\sigma_2',\sigma_3',\sigma_4', \\ \sigma_1,\sigma_2,\sigma_3,\sigma_4}} \mathbf{Q}^+\left(y\middle|\sigma_1',\sigma_2',\sigma_3',\sigma_4'\right)\times\mathbf{T}_L\begin{pmatrix} \sigma_1,\sigma_2,\sigma_3,\sigma_4 \\ \sigma_1',\sigma_2',\sigma_3',\sigma_4' \end{pmatrix}$$

$$\times\mathbf{A}\begin{pmatrix} \sigma_3,\sigma_4,\sigma_5,\sigma_6 \\ \sigma_3',\sigma_4',\sigma_5',\sigma_6' \end{pmatrix}\times\mathbf{Q}\left(x\middle|\sigma_1,\sigma_2,\sigma_3,\sigma_4\right)$$

Here $\mathbf{Q}\left(x\middle|\sigma_1,\sigma_2,\sigma_3,\sigma_4\right)$ is projector matrix formed by *m* highest eigenvectors (optimized states) of the reduced density matrix, which corresponds to the left one–half of the transfer matrix **T**. Integer variables *x* and *y* enumerate these highest eigenvectors.

This means that total width of the lattice strip is increased by four sites after first step. This procedure is repeated up to the moment when the eigenvectors of the renormalized transfer matrix T approach their fixed–point values and local thermodynamic quantities of 2D lattice do not change their values.

In the each step of the renormalization we have a relation between $\mathbf{T}_L^{n+1}$ and $\mathbf{T}_L^n$, which is a linear transformation:

$$\mathbf{T}_L^{n+1}\begin{pmatrix} \bar{x}, \sigma_{2n+3}\ \sigma_{2n+4} \\ \bar{y}, \sigma_{2n+3}'\ \sigma_{2n+4}' \end{pmatrix} = \sum_{\substack{y,\sigma_{2n+1}',\sigma_{2n+2}', \\ x,\sigma_{2n+1},\sigma_{2n+2}}} \mathbf{Q}^+\left(\bar{y}\middle|y,\sigma_{2n+1}',\sigma_{2n+2}'\right)\times\mathbf{T}_L^n\begin{pmatrix} x,\ \sigma_{2n+1},\sigma_{2n+2} \\ y,\ \sigma_{2n+1}',\sigma_{2n+2}' \end{pmatrix}$$

$$\times\mathbf{A}\begin{pmatrix} \sigma_{2n+1},\sigma_{2n+2},\sigma_{2n+3},\sigma_{2n+4} \\ \sigma_{2n+1}',\sigma_{2n+2}',\sigma_{2n+3}',\sigma_{2n+4}' \end{pmatrix}\times\mathbf{Q}\left(\bar{x}\middle|x,\ \sigma_{2n+1},\sigma_{2n+2}\right)$$

This renormalization procedure is schematically depicted in Figure 3.

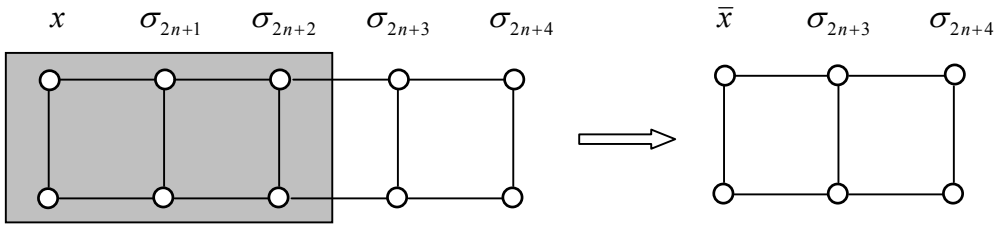

Figure 3. Renormalization scheme for the left block of the lattice. Summation is performed over variables from the shaded area.

For the evaluation of internal energy we calculated directly the thermodynamic average of energy of the configuration of 8 free spins at each iteration step of DMRG procedure. Specific heat was estimated by taking numerical derivative of internal energy with respect to temperature. At given number of optimized states *m* the dimensionality of total transfer matrix equals to $16m^2$. This can decrease the accuracy of the renormalization.

Nevertheless, for $m = 4$ the evaluation of critical temperature for the case ($\alpha = 0$, $\beta = 0$) after 100

iterations gives C_v = 2.246 (relative error is about 1%). For $\alpha < 0$, $\beta = 0$ the results of our calculations are in good agreement with the corresponding data, obtained by means of standard DMRG for IRF models.

3 RESULTS AND DISCUSSION

We studied first the temperature dependence of internal energy on temperature and the specific heat C_v at $\alpha = 0$, $\beta < 0$. For $\beta > -0.5$ a monotonous dependence of the internal energy on temperature was found. At the same time temperature dependencies of the specific heat C_v have sharp maxima similar to the case $\alpha < 0$, $\beta = 0$ (Figure 4). The temperatures of second order phase transitions were determined from the position of these maxima. It should be noted that for adequate consideration of the case $\beta = 0$ proposed modification of DMRG scheme requires more iterations then the standard method used in [10].

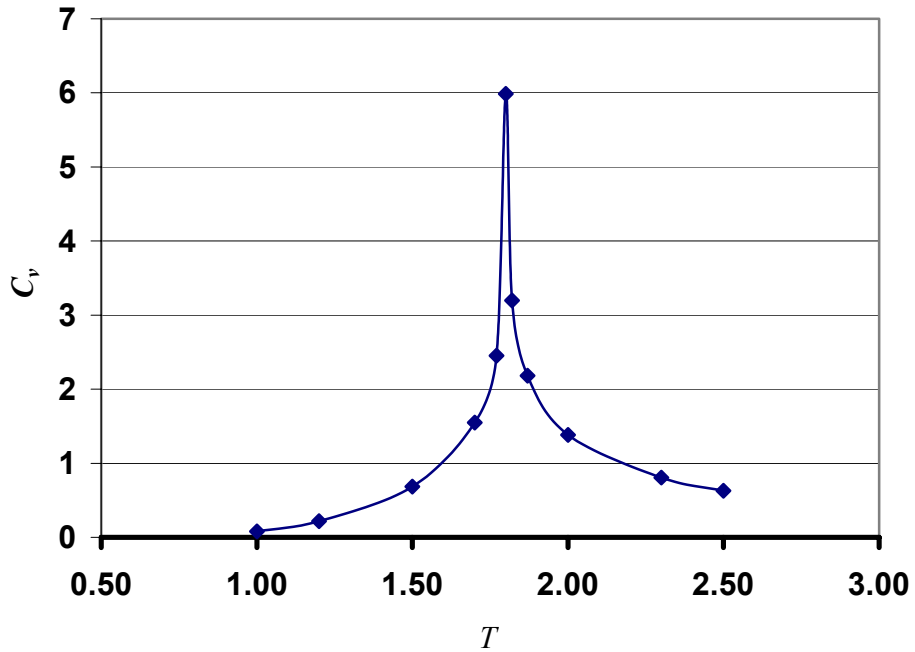

Figure 4. Temperature dependence of heat capacity C_v for $\alpha = 0$, $\beta = -0.2$ calculated at m=4, total number of iterations N = 500 and temperature step value ΔT = 0.01 in energy units.

Similar to the case $\alpha < 0$, $\beta = 0$ considered in [10], for small values of parameter β we found an approximately linear decrease of the critical temperature T_c with decreasing β value (Figure 5). At $\beta = -0.5$ we found irregular behavior of internal energy and C_v near the temperature T_c = 0.9, probably because of instability of our renormalization process and small number of states kept. Further decrease of the value of β in our simulation leads to the appearance of first order phase transition. Thus for $\beta = -0.7$ there is a first order transition near the point T_c = 1.194.

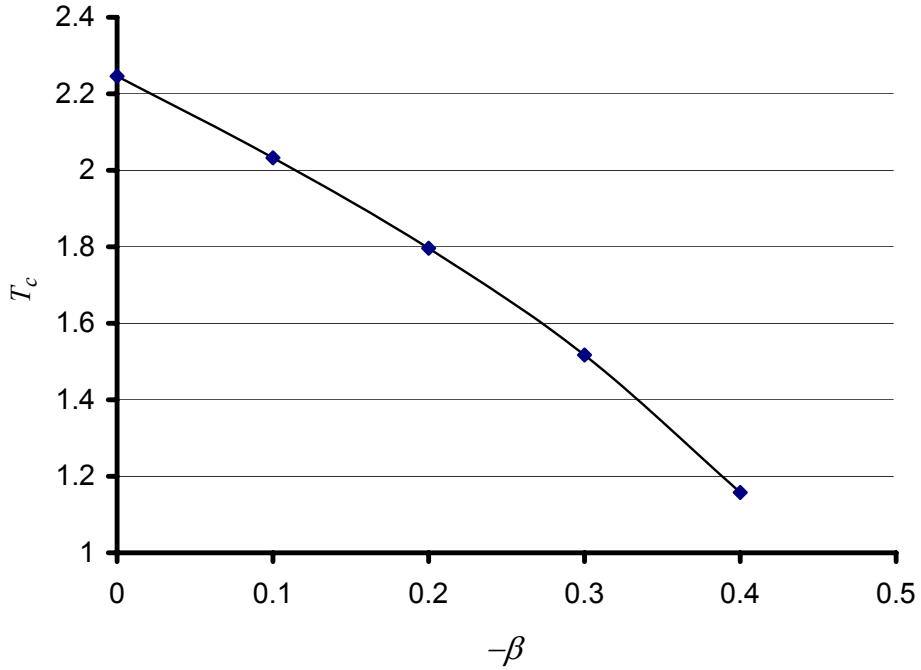

Figure 5. Dependence of critical temperature on the parameter β (α = 0).

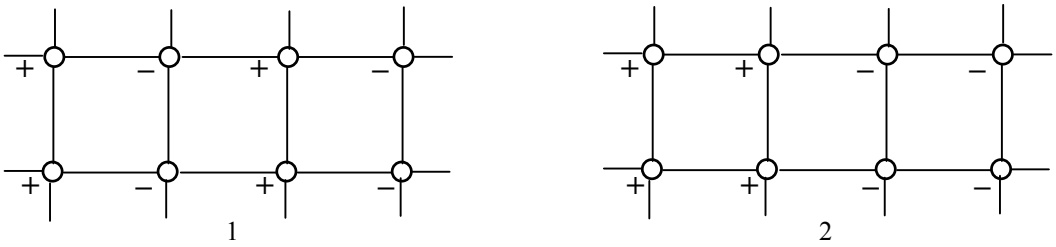

Figure 6. Layered spin configurations of infinite 2D lattice: 1) α < –0.5, β = 0; 2) α = 0, β < –0.5.

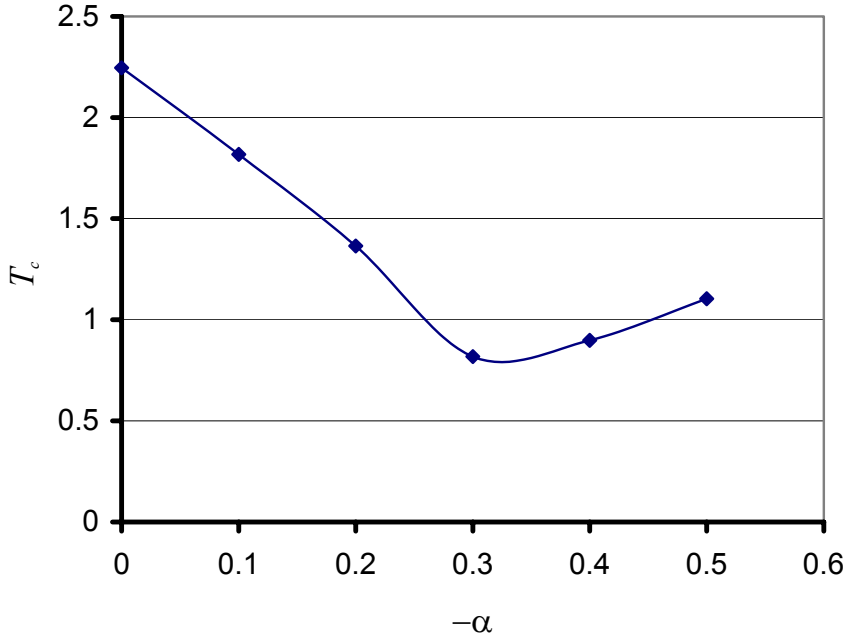

Figure 7. Dependence of critical temperature T_c on the strength of next–nearest interactions (the value of parameter α).

It is easily shown that for small temperatures the points ($\alpha = -0.5$, $\beta = 0$) and ($\alpha = 0$, $\beta = -0.5$) are critical for the model considered. In both cases there is a coincidence of the energies of the lowest ferromagnetic state and spin– layered states, which are shown in Figure 6. Let us now consider the case $\alpha = 2\beta$, which corresponds to the Widom model of microemulsion. For $-0.5 \le \alpha \le 0$ the results of DMRG calculations for T_c give clear nonlinear behavior of this value as a function of α (Figure 7). For $\alpha = -0.6$ our calculations showed the appearance of first order phase transitions but the accuracy of calculations near the corresponding critical point was rather low.

4 CONCLUSIONS

We presented a new modification of density matrix renormalization scheme for 2D Ising model with competing interactions, which is applicable to the consideration of axial next nearest–neighbor interactions. With the help of this scheme the estimations for critical temperatures of first and second order phase transitions were found. At least for small values of model parameters describing the next–nearest–neighbor interactions on 2D lattice the renormalization scheme with overlapping blocks reproduces adequately the temperatures of phase transitions.

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