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Phase Transitions in 2D Ising Model with Competing Interactions#

V.O.Cheranovskii[1,2,*], T.O.Kuznetsova[2], I.Ozkan[1]

[1] Middle East Technical University, Department of Chemistry,
06531 Ankrara, Turkey
[2] Kharkov National University, Institute of Chemistry,
610077 Svoboda Sq.4, Kharkov, Ukraine

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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. 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.

Availability..

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
MC, Monte Carlo methods	α - papameter of diagonal interactions
MC, Monte Carlo methods	β parameter of axial next-nearest-neighbor interactions

1 INTRODUCTION

The thermodynamics of the lattice spin models is investigated usually by the mean-field approximation and Monte Carlo simulation (MC). The mean-field approximation does not describe correctly the critical properties of low-dimensional systems. MC simulations, on the other hand, require 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 Ising model this method is superior to the classical MC method in accuracy and has the potential of handling much larger systems [2-4].

One of the simplest lattice model of a ternary system, consisting of oil, water and surfactants is the Widom model [5]. In terms of spin-½ variables it is equivalent to the Ising model with competing interactions (e.g. so called axial next-nearest neighbor Ising model (ANNNI model)

Dedicated on the occasion of the 65th birthday to Professor Nenad Trinajstić.

which describes thermodynamics of some compounds of rare-earth metals). The equilibrium thermodynamics of 3D Widom model has been studied extensively despite the complicated phase diagram of this model. However, there is relatively small 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. They may find practical application for the increase of effectiveness of the extraction processes, for example, in oil extraction technology.

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 [4]. Therefore the investigation of the thermodynamics of classical two-dimensional spin model have a common interest.

In our previous work [6] 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. 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

$$\mathbf{H} = -\sum_{ij} \sigma(i,j)\sigma(i,j\pm 1) + \sigma(i,j)\sigma(i\pm 1,j) + \alpha\left(\sigma(i,j)\sigma(i\pm 1,j\pm 1)\right) + \beta\,\sigma(i,j)\sigma(i,j\pm 2), \quad (1)$$

is a spin variable of the lattice site situated on the intersection of i-th row and j-th column of the lattice ($\sigma(i,j) = \pm 1$); the relative strength of the diagonal interactions is described by the parameter α, and parameter β corresponds to the interactions of next nearest neighbor spins along the rows of the square lattice.

For model with β=0 the DMRG simulation shows a monotonous dependence of the internal energy on temperature in wide region of the values of α. At the same time the temperature

dependence of the specific heat C_v has a sharp maximum. From the position of this maximum the temperature of second order phase transition was determined and linear decrease of critical temperature as a function of the value of α from the interval $-0.5 \le \alpha \le 0$ was found.

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 [7]. 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:

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

where T is absolute temperature in energy units.

In first order in α this equation has a solution:

$$T_c = \frac{2}{\ln\left(1+\sqrt{2}\right)} + \frac{\alpha\sqrt{2}}{\ln\left(1+\sqrt{2}\right)} \tag{3}$$

This dependence qualitatively agrees with the results of DMRG simulation.

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 lattice strip formed by two interacting rows of spins with numbers *i* and *i*+1 (Fig.1). This strip can be considered as a combination of overlapping rectangular 8-spin blocks.

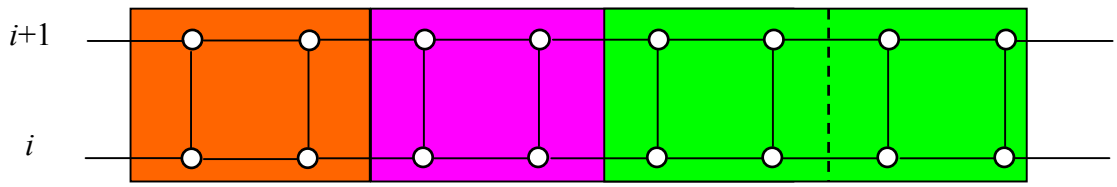


Figure 1. Block structure for the two-row transfer matrix for model with next nearest neighbor interactions along the rows. (Three overlapping 8-spin blocks are shown).

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.

$$\mathbf{T} = \lim_{N\to\infty} \mathbf{T}_N \tag{4}$$

$$\mathbf{T}_N = \mathbf{A}(1,2,3,4)\times \mathbf{A}(3,4,5,6)\times\ldots\times \mathbf{A}(N-3,N-2,N-1,N)$$

where

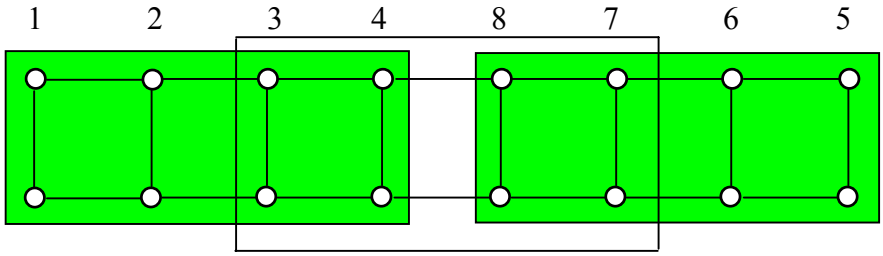
$$\mathbf{A}(1,2,3,4) = \exp\left\{\frac{1}{2T}\left[\sum_{i=1}^{4}\sigma_i\sigma_i^* + \frac{1}{2}\sum_{i=1}^{3}\left(\sigma_i\sigma_{i+1} + \sigma_i^*\sigma_{i+1}^*\right) + \sigma_2\sigma_3 + \sigma_2^*\sigma_3^*\right.\right.$$

$$+\alpha\left[\left(\sigma_2\left(\sigma_1^* + \sigma_3^*\right) + \sigma_2^*\left(\sigma_1 + \sigma_3\right) + \sigma_3\left(\sigma_2^* + \sigma_4^*\right) + \sigma_3^*\left(\sigma_2 + \sigma_4\right)\right)\right]$$

$$\left.\left.\beta\left(\sigma_1\sigma_3 + \sigma_2\sigma_4 + \sigma_1^*\sigma_3^* + \sigma_2^*\sigma_4^*\right)\right]\right\}$$

Here $\sigma_j = \sigma(\imath+1, j)$ and $\sigma_j^* = \sigma(i, j)$ are spin variables which belong to upper and lower rows of the two-row lattice fragment depicted in Fig.1.

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 Fig.2.



$\mathbf{T}_L$ **A** $\mathbf{T}_L$

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

$$\mathbf{T} = \mathbf{T}_L(1,2,3,4) \times \mathbf{A}(3,4,6,5) \times \mathbf{T}_L(8,7,6,5) \tag{5}$$

where

$$\mathbf{T}_L(1,2,3,4) = \mathbf{A}(1,2,3,4) \times \exp\left\{ \frac{1}{2T} \left[\sigma_1\sigma_1^* + \sigma_2\sigma_2^* + \frac{1}{2}\left(\sigma_1\sigma_2 + \sigma_1^*\sigma_2^*\right) + \beta\left(\sigma_1\sigma_2^* + \sigma_2\sigma_1^*\right) \right] \right\}$$

Renormalization procedure is described by formula

$$\mathbf{T}(1',2',5,6) = \mathbf{Q}^{+}(1',2'|1,2,3,4) \times \mathbf{T}_L(1,2,3,4) \times \mathbf{A}(3,4,5,6) \times \mathbf{Q}(1',2'|1,2,3,4)$$

Here $\mathbf{Q}(1',2'|1,2,3,4)$ 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**. The renormalization procedure is schematically depicted in Fig.3

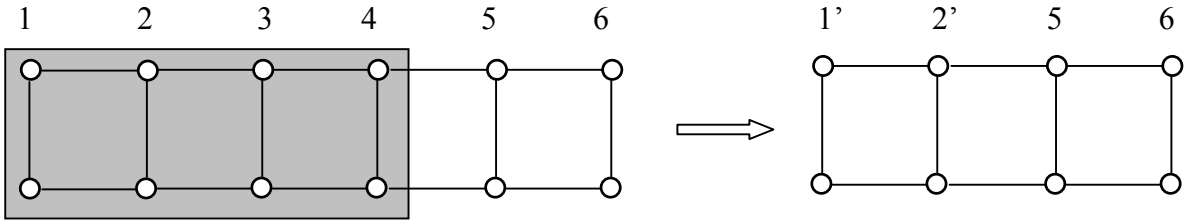


Figure 3. Renormalization scheme for the left block of the lattice. Summation is performed over the spin variables from the shaded area.

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 T_c=2.246 (relative error less than 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 α=0, β<0. For β>-0.5 a monotonous dependence of the internal energy on temperature was defined. At the same time the temperature dependencies of the specific heat C_v had sharp maximums. The temperatures of second order phase transitions were determined from the position of these maximums.

Similar to the case $\alpha < 0, \beta = 0$ considered in [7] for small values of parameter β we found approximate linear decrease of the critical temperature T_c at the decrease of the value of β (Fig.4). At β=-0.5 we found irregular behavior of inner energy and C_v near to 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 β=-0.7 there is a first order transition near the point T_c=1.194 and, probably, second order transition at T_c=1.721 (it corresponds to very weak maximum on the graph of temperature dependence of C_v).

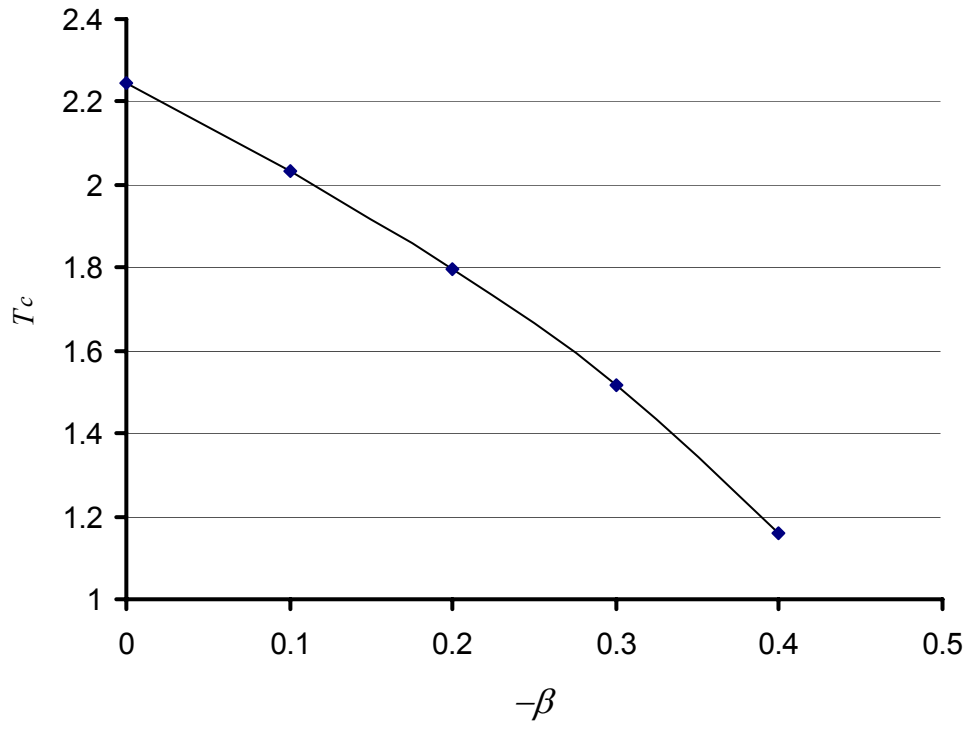


Figure 4. Dependence of critical temperature on parameter β (α=0).

At $\alpha < -0.5$, β=0 there was a rapid increase of the critical temperature. In [6] this effect was interpreted as a second order phase transitions associated with the destruction or change of the periodic structures in the liquid film.

It is easily shown that for small temperatures the values α=-0.5 and β=-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 Fig.5.

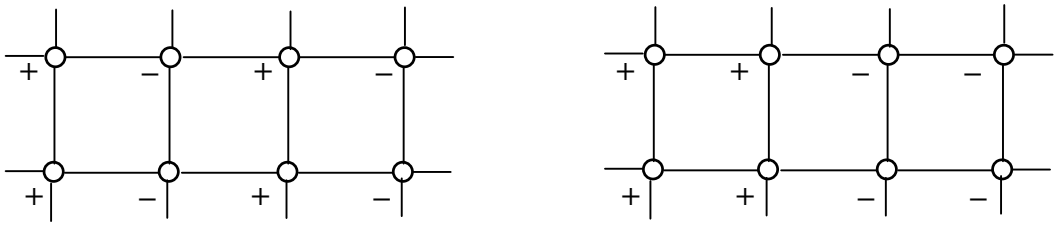


Figure 5. Layered spin configurations of infinite 2D lattice: 1) α<-0.5, β=0; 2) α=0, β<-0.5

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 (Fig.6).

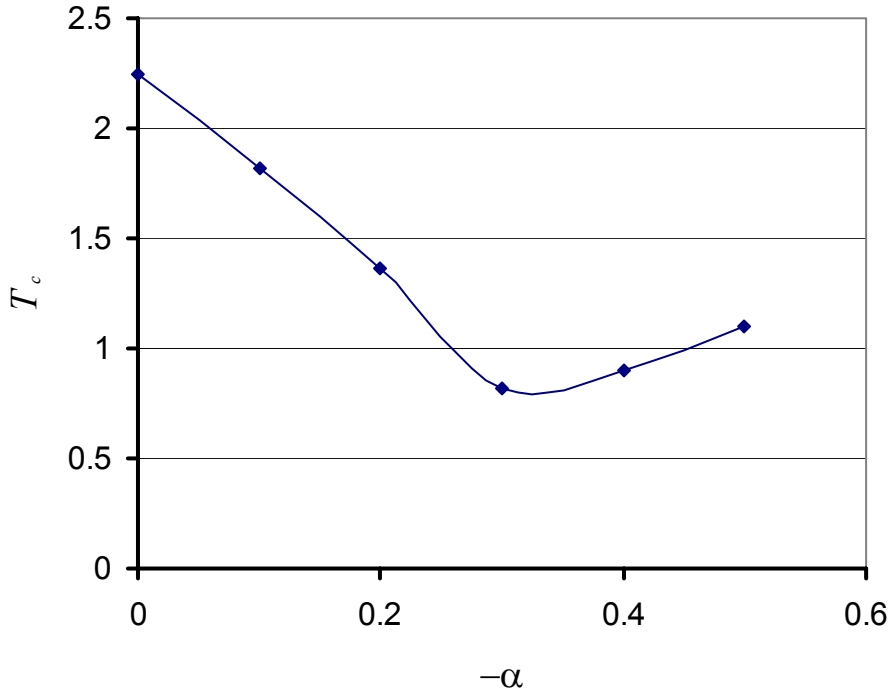


Figure 6. Dependence of critical temperature T_c on the strength of next nearest neighbor interactions (value of the parameter α).

For $\alpha = -0.6$ our calculations had shown 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 special type of axial next nearest-neighbor interactions. With the help of this scheme the estimations for critical temperatures of second order phase transitions were found. At least for small values of model parameters describing the next-nearest-neighbor interactions the modified renormalization scheme works adequately. We hope this approach can be also extended to the case of a standard ANNNI model on square lattice.

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