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IMPROVED PHASE DIAGRAMS OF ASHKIN–TELLER MODEL

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The phase diagram of the Askhin–Teller model in two dimensions is determined. Numerical calculations are performed for the simple square $L \times L$ lattice using transfer matrix technique. Exploiting finite-size scaling all unknown critical lines were obtained with good accuracy. An extended version of the Ashkin–Teller model is also considered within the molecular field renormalization group method and the critical surface for three-parameter odd-parity Hamiltonian is calculated.

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The Askhin–Teller (AT) model has first been proposed as a model of a four--component alloy [1]. It has attracted a lot of theoretical interest for years because it is a quite simple but a non-trivial generalization of the Ising and four-state Potts models. Fan [2] has shown that the Hamiltonian of the AT model can also be written with two Ising variables located at each site of the lattice

$$\mathcal{H} = -\sum_{\langle i,j \rangle}(K_1 S_i S_j + K_2 \sigma_i \sigma_j + K_4 S_i \sigma_i S_j \sigma_j). \tag{1}$$

We consider only nearest neighbour couplings between sites of the simple square lattice and we assume that $K_1 = K_2$ (isotropic case). S and σ are Ising variables which can take values ± 1. The Boltzmann factor $1/k_B T$ is absorbed in thus defined K_i coefficients.

In our numerical approach we exploit the finite-size scaling for the ratio

$$Q_L = \frac{\langle M^2 \rangle_L^2}{\langle M^4 \rangle_L}, \tag{2}$$

where $\langle \ldots \rangle$ means the thermal average, M stands for the total magnetization (in our case $M = \sum_{i=1}^{N} S_i \sigma_i$) and the index L indicates the finite size of the system $(L \times L)$. $Q = \lim_{L \to \infty} Q_L$ is universal at the critical point and depends only on the

general class to which the system belongs (the universality class). Three unknown critical lines of the isotropic AT model (two of them are related with each other by a duality relation: knowledge of one of them is equivalent to knowledge of the other) are believed to belong to the Ising universality class [3, 4]. It is supposed that these lines whose positions are not known exactly correspond to Ising-like continuous transitions. Therefore, we derive a scaling formula

$$Q_L(t) = Q_L(0) + \left.\frac{\partial Q_L(t)}{\partial t}\right|_{t=0} t + \ldots \tag{3}$$

The term $Q_L(0)$ was evaluated previously [5] and the second term is of the form

$$\left.\frac{\partial Q_L(t)}{\partial t}\right|_{t=0} = \alpha_1 L + \alpha_2 + \alpha_3 L^{3-2y_H} + (\alpha_4 + \alpha_5 \ln L) L^{2-2y_H} \ldots \tag{4}$$

where $y_H = \frac{15}{8}$ is the magnetic critical exponent, α_i $(i = 1, \ldots, 5)$ are unknown amplitudes and t is the thermal scaling field.

We followed the transfer matrix technique which for the Ising model was explained in [5]. Firstly, we calculated the ratio Q_L with $L = 2, 3, \ldots, 9$ (in the antiferromagnetic region $L = 2, 4, 6, 8$ only) for $K_2 = 0$ (corresponding to the Ising model in $S\sigma$) and a few values of K_4 close to the exactly known critical value $K_{4c} = \frac{1}{2}\ln(1 + \sqrt{2})$. In this case we know that

$$t = \frac{K_{4c} - K_4}{K_4} \tag{5}$$

and from Eqs. (3) and (4) we solved the set of linear equations for the unknown coefficients α_i.

Then, knowing α_i ($i = 1, 2, 3$ is sufficient) and $Q_L(0)$, we calculated Q_L for $K_2 \neq 0$ and from (3) and (4) we found the values of t and from (5) the values of K_{4c}.

Our final results are presented and compared with other results and predictions in Fig. 1. The numerical uncertainties do not exceed the size of the symbol. As can be seen (Fig. 1) our results are in good agreement with MCRG [6] approach, but are quite different from Baxter's predictions [4] in the antiferromagnetic region. The latter are based on some renormalization-group calculations and the line representing them crosses the line $K_2 = -K_4$, which seems incorrect [3]. Our accuracy is really very good: near the Ising point it is about 2×10^{-4} % although it becomes less precise in the neighbourhood of the Potts point. The accuracy in the antiferromagnetic region is not worse. The curve plotted by the solid bold line is the only one known exactly [4].

In Ref. [7] we considered possible extensions of the Ashkin–Teller model in order to reduce degeneracy of the energy levels. Assuming six order parameters we calculated a phase diagram within the MFA. However, MFA is a good approximation in three or more dimensions but not in two [3]. Plascak and Barreto [8] performed the calculations of the phase diagram of the symmetric AT model within the mean field renormalization group approach (MFRG) in two dimensions. Here we generalize their approach to our extended case in order to obtain three-dimensional phase diagram for a two-dimensional square lattice. The Hamiltonian contains now an additional term

$$-K \sum_{i,j} (S_i + S_j)(\sigma_i \sigma_j + 1). \tag{6}$$

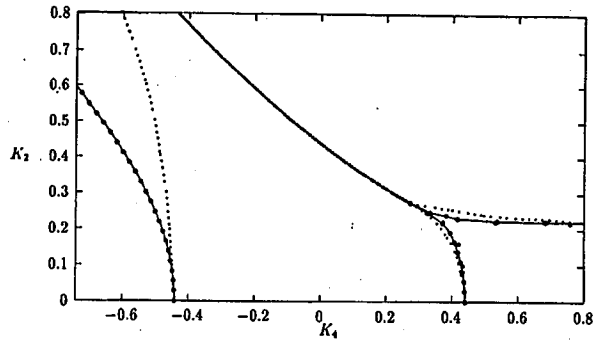

Fig. 1. Phase diagram of the symmetric AT model in two dimensions. Solid bold line stands for the exactly known critical line, dotted lines for Baxter's predictions, empty circles with line describe our results, solid circles stand for MCRG results [6].

We begin splitting the lattice into blocks, and then replacing each block by just one single site, so as to produce a lattice like the one we started with, except for an increase in the lattice spacing. We consider the simplest two-site blocks. As a next step we write down the molecular field equations for one and two-site clusters. The mean-field Hamiltonian for the one-site cluster is

$$H_1 = ZSh'_s + Z\sigma h'_\sigma + ZS\sigma h'_{s\sigma}. \tag{7}$$

Here Z denotes the number of the nearest neighbours while h'_σ, h'_s and $h'_{s\sigma}$ are the symmetry breaking fields simulating the effect of the infinite system. The Hamiltonian for the two-site cluster contains also three boundary fields: h_s, h_σ, $h_{s\sigma}$. Now the equations for the order parameters m'_s, m'_σ, $m'_{s\sigma}$, m_s, m_σ, $m_{s\sigma}$ can be calculated and linearized. In order to apply the MFRG method we assume that the magnetizations scale as $m'_i = \xi_i m_i$ ($i = \sigma$, s or $s\sigma$) and impose the similar relations for the fields, i.e. $h'_i = \xi_i h_i$. Since m_s is not critical, we put $m'_s = m_s$ and $h'_s = h_s$ which gives a self-consistent equation for h_s. It is not possible to eliminate all ξ and h from the resulting set of equations, as in the approach of Plascak and

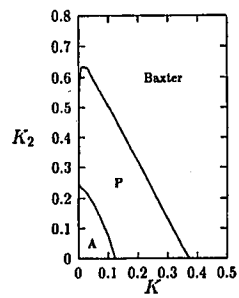

Fig. 2. Cross-section of the three-parameter critical surface for $K_4 = -0.4$. *A* denotes phase where $\langle S\sigma \rangle$ is ordered antiferromagnetically, *P* stands for a paramagnetic phase, *Baxter* denotes Baxter (ferromagnetic) phase.

Barreto. It is still possible, however, to obtain a single flow equation as a condition for unambiguity of solutions.

This condition gives a critical surface in a three-dimensional space of parameters K_2, K_4 and K, for $K_2 > 0$. The left part of the diagram (see Fig. 1, $K_2 < 0$) requires a separate but similar treatment. An example of a two-dimensional section of the critical surface is shown in Fig. 2.

This method allows us also to find lines of tricritical points which may be identified with saddle points of the function $\Delta(K_2, K)$ for fixed values of K_4. For $K_2 < 0$ this simplest MFRG scheme does not work, because we have six order parameters which lead to six equations with twelve unknown variables h_i and ξ_i. Even for $K_2 > 0$ it will be difficult to go beyond MFRG presented here, because at first, all existing approaches work for two parameter Hamiltonians, and at second, odd Hamiltonians require a special treatment as follows from our work.

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