Proceedings of the European Conference Physics of Magnetism 2011 (PM'11), Poznań, June 27–July 1, 2011

On Non-Ising Phase Transitions in the 3D Standard Ashkin–Teller Model

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The phase transition line near the Ising point region is studied for the 3D standard Ashkin–Teller model on a cubic lattice. This model with a multicomponent order parameter is one of the important reference points in statistical physics since it shows an interesting and complicated phase diagram. The main motivation for our study was nonuniversal behavior suggested for this line. The large-scale Monte Carlo simulations using the Binder and Challa like cumulants are performed. Accurate analysis to exclude the latent heat inherence is applied. Specific behavior of the Challa like cumulants is discovered and its interpretation is proposed. The paper is closed with preliminary conclusions concerning the continuous but non-Ising character of these phase transitions in the lower part of the mixed phase region and the possiblity of the first order on the line connecting it to the Ising point.

PACS: 75.10.Hk, 75.30.Kz, 75.40.Cx, 75.40.Mg

1. Ashkin–Teller model

Ashkin and Teller proposed their lattice model for four--component mixture [1]. The interest in this model significantly increased when Fan showed [2] that this model could be expressed in terms of two Ising models put on the same lattice with spins s_i and σ_i at each lattice site, respectively. We consider only two-spin interactions of a constant magnitude J_2 between the nearest neighbors. We can extend these independent Ising models to the Ashkin–Teller (AT) by coupling the two Ising models with a four-spin interaction of a constant magnitude J_4, also only between couples of nearest-neighboring spins. Thus, the Hamiltonian H of the AT model is of the form

$$-\frac{H}{k_{\mathrm{B}}T} = \sum_{[i,j]} [K_2(s_i s_j + \sigma_i \sigma_j) + K_4 s_i \sigma_i s_j \sigma_j], \qquad (1)$$

where $[i,j]$ denotes summation over nearest-neighboring lattice sites, $K_i = -J_i/k_{\mathrm{B}}T$, with $i = 2$ or 4, and T is the temperature of the system. We call it the standard AT model, as there are many extensions of the AT model.

The research done for this model is summarized in the caption of Fig. 1 (for details and applications of the model see e.g. [3, 4]) where the symbol $\langle \ldots \rangle$ denotes the thermal average. Thus the symbol $\langle s\sigma \rangle$ stands for the thermal average of the variable $s\sigma$, the product of the spins s and σ, both on the same lattice site.

The aim of this paper is to perform a thorough analyses of the regions of the phase diagram where the nonuniversal behavior of the 3D standard AT model was signalized (see [3] and the papers cited therein). The boundaries of the mixed phase region $\langle s \rangle$ (see Fig. 1) and the localization of the tricritical point H were investigated and the deviations from the Ising character of phase transitions on the line AHK' were reported by Musiał and Rogiers [3], whereas the localization of the remaining tricritical points K, K', F, G were examined by Musiał [5]. It is worth noting that a weakly first order phase transitions appear in the right vicinity of point A [6]. In this context the interesting question arises of a possible variation of values of critical exponents along the line AHK', like in the 2D version of this model.

We have concentrated our main attention on the line AH (see Fig. 1), but the analysis was also performed for the line HK'. We undertook a Monte Carlo (MC) study with the method developed by Musiał [5], as the latent heat occurrence should be excluded, before the further research of the universality class of phase transitions. It is absolutely clear that at the starting point A there is no latent heat, as here we have the pure Ising model with ferromagnetic interactions between the nearest neighbors.

2. The Monte Carlo simulations

To predict the behavior of a system with a large number of degrees of freedom, we perform the MC simulations. Using the tools of statistical mechanics a computer experiment is performed to predict the equilibrium behavior of a system for which the behavior is determined by the Hamiltonian (1). Equilibrium configurations of finite-size cubic spin samples of the size $L \times L \times L$ ($16 \le L \le 24$) have been generated for fixed values of the model parameters described in the Hamiltonian (1), using the Metropolis algorithm. Periodic boundary conditions were imposed and thermalization of the length of 10^5 to 10^6 Monte Carlo steps (MCS) was applied. One

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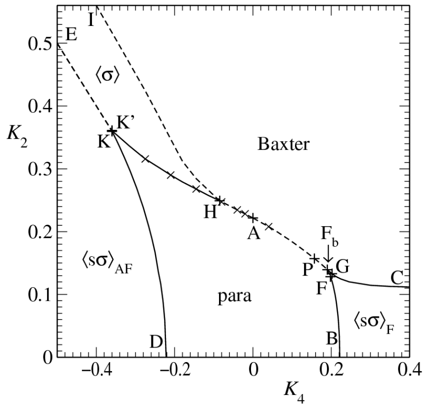

Fig. 1. The present state of knowledge about the phase diagram of the 3D Ashkin–Teller model on a cubic lattice. The broken lines denote the first order phase transitions, whereas the solid lines denote the continuous ones. In the phase labeled "Baxter" the system is ferromagnetically ordered with all order parameters $\langle s\rangle$, $\langle\sigma\rangle$ and $\langle s\sigma\rangle$ nonzero, whereas in the phase labeled "para" they are all zero. In the phases "$\langle s\sigma\rangle_{\mathrm{F}}$" and "$\langle s\sigma\rangle_{\mathrm{AF}}$" we have $\langle s\rangle = \langle\sigma\rangle = 0$, and only the parameter $\langle s\sigma\rangle$ is ferromagnetically and antiferromagnetically ordered, respectively. For the phase "$\langle s\rangle$" called the mixed phase region we have $\langle s\sigma\rangle = 0$ and either $\langle s\rangle$ or $\langle\sigma\rangle$ is ferromagnetically ordered but the other is not. The positions of labeled points inside the phase diagram are marked by $+$, whereas the results of our MC simulations are marked by $\times$.

MCS is completed when each of the lattice sites has been visited once. A 64-bit random number generator was used. Each MC run was split into k $(10 \le k \le 20)$ segments called partial averages consisting of about 10^7 MCS. In the calculation of the partial averages only every i-th MC step contributed $(8 \le i \le 10)$, to avoid correlations between sampled microstates of spins in the system and to sample microstates with the Gibbs distribution of probability.

The phase transition points were localized for particular value of K_4 coupling from the analysis of the Binder cumulant Q_L dependence on the K_2 coupling [4]:

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

where $\langle\alpha^n\rangle_L$ denotes the n-th power of the α spins order parameter, with $\alpha = s$, σ or $s\sigma$, averaged over an assembly of independent samples of the size $L \times L \times L$, as described in the previous paragraph. This is very convenient method of localization of points in the phase diagram, as it works well for both, the first order and the continuous phase transitions.

To calculate the value of the latent heat, necessary to distinguish between the first order and the continuous phase transitions, together with the above mentioned Binder cumulants we have calculated three Challa-like cumulants [5] for particular value of K_4 coupling

$$V_{\alpha,L} = 1 - \frac{\langle E_\alpha^4\rangle_L}{3\langle E_\alpha^2\rangle_L^2}, \tag{3}$$

where $\langle E_\alpha^n\rangle_L$ denotes the n-th moment of the internal energy E of α-spins ($\alpha = s$, σ or $s\sigma$) averaged over an assembly of independent samples of the size $L \times L \times L$, as described in the first paragraph of this section. These Challa-like cumulants are extremely useful to distinguish between the first order phase transitions and the continuous ones. For a continuous phase transition $V_{\alpha,L} = 2/3$ in the limit $L \to \infty$ and it remains fixed even far from the critical temperature. In contrast, for the first order phase transitions the dependence $V_{\alpha,L}(K_2)$ has a minimum. The value of this minimum $V_{\alpha,L}^{\min}$ and its localization $K_2^{\min}$ scale linearly versus L^{-3} which allows one to extrapolate the values of these two parameters to the thermodynamic limit. The limit value of $K_2^{\min}$ is the critical one (which gives the value of the critical temperature). When the value of $V_{\alpha,L}^{\min}$ remains different from $2/3$, the phase transition is of the first order [5, 7].

3. Results and conclusions

We have localized the phase-transition points at particular values of the coupling K_4 from the common intersection point of the curves $Q_L(K_2)$, given by Eq. (2), independently for order parameters $\langle s\rangle$, $\langle\sigma\rangle$ and $\langle s\sigma\rangle$ (for details see e.g. [5, 8]). We are able to achieve the accuracy of at least four decimal digits for both the first order and the continuous phase transitions. The points for which the analyses are reported in this paper are marked with $\times$ in Fig. 1. It is worth noting that the scatter of the results, as it is well known (see [5, 7, 8] and the papers cited therein), is of at least one order of magnitude greater for the first-order phase transitions when compared to the continuous ones.

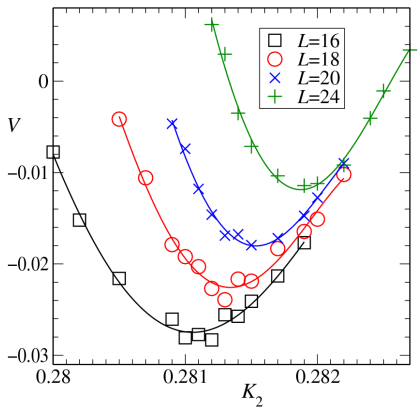

Fig. 2. The characteristic minima of the cumulant $V_{s,L}$ versus K_2 for samples with different linear sizes L, at the fixed value of the coupling $K_4 = -0.04$. The results of our MC simulations are denoted by symbols, which are explained in the legend box. Only the small regions where cumulants are minimum are shown. These curves are approximated by a polynomial of the fourth degree.

The largest effort of our large-scale MC simulations concerned the analyses of Challa-like cumulants described in detail in our previous works [5, 9] and used to analyze the tricritical behavior of the system in the vicinities of points F, G, K, and K' (see Fig. 1). The purpose of this paper is verification of the latent heat evidence on the line AHK'. The exemplary results of these analyses are shown in Fig. 2 at the fixed value of the coupling $K_4 = -0.04$ in the ferromagnetic region close to the tricritical Ising point A. For clarity we have plotted results of our MC simulations only in the regions where the cumulants $V_{s,L}$ are minimum as a function of K_2 for different system sizes L. Evidence of the deep minima can be an important signal, but is not the proof of the evidence of latent heat. We have to estimate the value of the minimum of the cumulant $V_{s,L}$ in the thermodynamic limit.

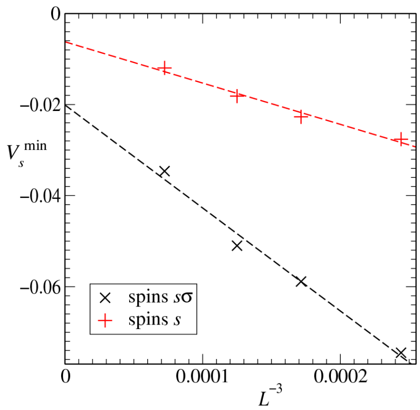

Fig. 3. The values of minima $V_{\alpha,L}^{\min}$ extrapolated to the thermodynamic limit for $\alpha = s$ and $s\sigma$, as explained in the legend box, at the fixed value of the coupling $K_4 = -0.04$. The dependences are fitted by straight dashed lines using the linear regression.

To average the scatter of the results and to determine more precisely the ordinates $V_{s,L}^{\min}$ and the abscissas $K_2^{\min}$ of these minima under consideration the MC results in Fig. 2 were approximated by a polynomial of fourth degree. The finite-size-scaling analysis of the ordinates of the minima $V_{\alpha,L}^{\min}$ is illustrated in Fig. 3 for $\alpha = s$ and $s\sigma$. The results for spins s and σ are similar because of symmetry of the Hamiltonian (1). The linear character of the plots is clearly seen.

The thermodynamic limit value of the minimum of the cumulant $V_{s,L}$ is $-0.006(4)$ and of the cumulant $V_{s\sigma,L}$ is $-0.020(6)$ at $K_4 = -0.04$. As pointed out in Sect. 2, these values different from $2/3$ within the experimental uncertainty mean that the phase transitions of all order parameters $\langle s\rangle$, $\langle\sigma\rangle$ and $\langle s\sigma\rangle$ could be of the first order. These values can be compared to the value 0.664, very close to $2/3$, for $K_4 = 0.04$ where arbitrary weak first order phase transitions can be observed [6]. The actual problem is to calculate the values of the latent heat from the estimated data of $V_{\alpha,\infty}^{\min}$ ($\alpha = s$, σ or $s\sigma$), which seems to be more complex in this region of the phase diagram and needs further study.

One can ask why these minima have hot been seen before? The reason is the unexpectedly wide region of the critical behavior of the system, as the distance from the point of the phase transition to the minima region which is about 0.1. This is probably also the cause of the specific behavior of the Challa-like cumulants in this region: although the abscissas $K_2^{\min}$ of the minima of cumulant $V_{\alpha,L}(K_2)$ scale linearly versus L^{-3}, the extrapolated values of K_2 in the thermodynamic limit are not equal to the critical ones.

We conclude that the phase transitions along the line AH in Fig. 1 could be of the first order, but still some questions remain. We observe no evidence of latent heat along the line HK'. Thus, we can confirm our conclusions from the paper [3] for the phase transitions along the line HK'.

Acknowledgments

The authors wish to thank the Poznań Supercomputing and Networking Center for the access to the supercomputers, on which a part of simulations has been performed. The research was partially supported by the European Commission under the program Human Capital POKL 4.1.1. “Integrated program supporting development of Adam Mickiewicz University in Poznań in the physical science range: innovative education, the competent staff, graduates of the future”.

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