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Arbitrarily Weak First Order Phase Transitions in the 3D Standard Ashkin–Teller Model by MC Computer Experiments

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The first order phase transition line in the vicinity of the tricritical Ising point region is studied in the 3D standard Ashkin–Teller model on a cubic lattice. The large-scale Monte Carlo computer experiments using the Binder- and Challa-like cumulants, the latter modified by Musial, are proposed and performed. Specific behavior of the Challa–Musial cumulants for weak first order phase transitions is discovered and its interpretation is proposed. The paper proves the arbitrarily weak first order character of phase transitions when approaching to the Ising point.

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1. The standard Ashkin–Teller model

Ashkin and Teller have proposed their lattice model for four component mixture [1]. The range of applications of this model substantially increased after Fan's work [2] in which this model is expressed in terms of two Ising models put on the same lattice with spins s_i and σ_i at each lattice site, respectively. As in standard Ising model, only two-spin interactions of a constant magnitude J_2 between the nearest neighbors are considered. Fan extended these independent Ising models to the Ashkin–Teller (AT) one by introducing the four-spin interaction of a constant magnitude J_4 also only between couples of nearest-neighboring spins. Thus, we have the Hamiltonian H:

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

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 consider the standard AT model in 3D put on the cubic lattice.

The research done for this model and its applications can be found in many papers, e.g. [3–6]. The $K_2(K_4)$ phase diagram of the AT model is very diversified as three components of the order parameter can order independently: $\langle s \rangle$, $\langle \sigma \rangle$ and $\langle s\sigma \rangle$ where the symbol $\langle \ldots \rangle$ denotes the thermal average.

The aim of our paper is to verify the existence of arbitrarily weak temperature-driven first order phase transitions when approaching the Ising point situated at $K_4 = 0$ where obviously there is continuous Ising phase transition, as from Eq. (1) follows that here we have the pure Ising model with ferromagnetic interactions between the nearest neighbors. It has been signalized [3, 4] that for $K_4 > 0$ up to the Potts point situated at $K_4 = K_2 \approx 0.157154$ the phase transitions are of the first order but Arnold and Zhang suggested also that they are arbitrarily weak when approaching an Ising point [3].

For this purpose in the next section we propose the large-scale Monte Carlo (MC) computer experiments to measure precisely the latent heat for the phase transitions under consideration.

2. The Monte Carlo experiment

We consider a finite-size cubic samples of the standard AT model to go next to the thermodynamic limit and in consequence to obtain the results suitable for a macroscopic system. The number of degrees of freedom in our system is too large to be able to take into account all the states of the system. Therefore, we have to use the tools of statistical mechanics including MC method with importance sampling of states.

In contrast to simple MC simulations, we propose the MC computer experiment in which one not only calculates the thermodynamic quantities but also precisely determines their uncertainties. Such a way of obtaining of the results should be called a measurement. Therefore, we refer to it as the computer experiment which is situated somewhere between a theory and a real experiment. Computer experiments play still increasing role in modeling of any kind.

According to the statistical mechanics methodology, we perform our computer experiments to predict the equilibrium behavior of the standard AT model. This behavior is fully determined by the Hamiltonian (1). Therefore, we generate equilibrium configurations (microstates) of finite-size cubic spin samples of the size $L \times L \times L$ ($16 \leq L \leq 34$) for fixed values of the model parameters, which are described above at the Hamiltonian (1), using the Metropolis algorithm. As we obtain our final results in the thermodynamic limit, we assume convenient periodic boundary conditions. To bring the system to the thermodynamic equilibrium, we apply thermalization of the length of order of 10^6 Monte Carlo

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steps (MCS). One MCS in our computer experiment is completed when each of the lattice sites has been visited once. We use a 64-bit random number generator.

To determine uncertainties of the measured quantities, each MC run is split into k ($10 \leq k \leq 20$) segments called partial averages. Each partial average consists from 0.4×10^7 MCS for smaller L values up to 3.6×10^7 MCS for the largest L's. In the calculation of the partial averages only every i-th MC step contributed (with $8 \leq i \leq 10$) to avoid correlations between sampled microstates of spins in our system and to sample microstates with the Gibbs distribution of probability. In this way our program spends most of time working with states which give the largest contribution to the quantities under computation.

To localize a temperature-driven phase transition point, we fix the particular value of K_4 coupling and analyse the Binder cumulants $Q_{\alpha,L}$ dependences on the K_2 coupling (see e.g. [5, 7]):

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

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 ensemble of independent samples of the size $L \times L \times L$. This method allows us to localize both, continuous and first order phase transition points.

To distinguish between the first order and the continuous phase transitions, simultaneously with the above mentioned Binder cumulants we calculate three Challa cumulants [8] modified by Musial [4] 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 α-spins order parameter interaction energy averaged over an ensemble of independent samples of the size $L \times L \times L$.

These Challa–Musial cumulants are extremely useful to distinguish between the first order and the continuous phase transitions in a system with a multi-component order parameter. For a continuous phase transition $V_{\alpha,L} = 2/3$ in the thermodynamic limit and it remains fixed even far from the critical coupling K_2 value. In contrast, for the first order phase transitions the dependence $V_{\alpha,L}(K_2)$ has a characteristic local minimum. The value of this minimum $V_{\alpha,L}^{\min}$ and its localization $K_2^{\min}$ scale linearly versus L^{-3} [4, 8] which allows one to extrapolate the values of these two parameters to the thermodynamic limit. In addition the $K_2^{\min}$ limit value is the better estimation of the critical one than that obtained from the above mentioned analysis of the behavior of the Binder cumulant (2). Thus, we have the important criterion: when $V_{\alpha,L}^{\min}$ value with its uncertainty remains different from $2/3$, a phase transition is of the first order [4, 8].

We determine the partial latent heat related to above mentioned α-spins interaction energy E_α in the limit $L \to \infty$ ($E_\pm = E_\alpha(T \to T_c|_\pm)$) from the formula [8]:

$$V_{\alpha,\infty}^{\min} = 1 - \frac{2(E_+^4 + E_-^4)}{3(E_+^2 + E_-^2)^2} \tag{4}$$

and using the method proposed by Musial [4]. According to the latter we compute the value E_- from Eq. (4) using $V_{\alpha,\infty}^{\min}$ value determined from the analysis explained below Eq. (3) and the value E_+ estimated from the E_α energy plot for the finite-size samples. Obviously, the latent heat of the whole system is the sum of the partial ones.

It is worth noting that when the latent heat $E_+ - E_-$ tends to zero, $V_{\alpha,\infty}^{\min}$ approaches the value $2/3$, as described above for the continuous phase transitions.

3. Results and conclusions

The temperature-driven phase transition points at particular values of the coupling K_4 have been localized from the common intersection point of the curves $Q_{\alpha,L}(K_2)$ specified by Eq. (2) independently for $\langle \alpha \rangle$ order parameters with $\alpha = s$, σ and $s\sigma$ (see e.g. [4, 7]). This analysis has allowed us to achieve the accuracy of at least four decimal digits for the K_2 coupling critical value.

The essential element for the aim of this paper is the computation of the latent heat using the Musial method [4]. For this purpose we have analysed the behavior of the Challa–Musial cumulants specified by Eq. (3). The limited volume of this paper allows us to present this analysis for spins s only. We obtain similar values for spins σ for Hamiltonian (1) symmetry reasons.

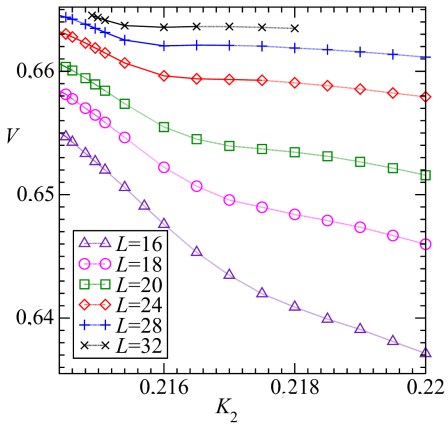

Fig. 1. The characteristic minima of the cumulant $V_{s,L}$ versus K_2 for samples with different linear sizes $L \geq 24$ at the fixed value of the coupling $K_4 = 0.02$. The results of our MC computer experiments are denoted by symbols, which are explained in the legend box. The uncertainties are less than magnitudes of symbols. Within the small minimum region an experimental curve is approximated by a polynomial of the fourth degree and represented by solid lines. For clarity, the results for selected L values are presented only.

The example of such analyses is shown in Fig. 1 at the fixed value of the coupling $K_4 = 0.02$ in the region close to the tricritical Ising point where takes place the temperature-driven transition from ferromagnetically ordered phase to the disordered one. For clarity we have

plotted our results only for selected values of system linear size L. Surprisingly, a characteristic local minima as a function of K_2 coupling are observed only for system sizes $L \geq 24$. For smaller L's the curves in Fig. 1 manifest only the inflection point.

This specific behavior of the Challa–Musial cumulants has to be attributed to weak first order phase transitions, as for $K_4 = 0.01$, where the smaller latent heat value is expected, the minima are observed for $L \geq 28$. This rule is also fulfilled when the latent heat values should become greater and greater: for $K_4 = 0.03$ these minima start from $L = 22$, for $K_4 = 0.04$ from $L = 20$, for $K_4 = 0.05$ from $L = 18$, and for $K_4 = 0.06$ from $L = 16$.

It is worth noting that the presence of the minima is an important signal, but not the proof of the existence of latent heat [6]. To compute the latent heat, we now have to estimate the value of the cumulant $V_{s,L}$ minimum in the thermodynamic limit.

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 in Fig. 1, the MC computer experiment data were approximated by a polynomial of fourth degree as explained in the caption. Nevertheless, the uncertainties of the ordinates $V_{s,L}^{\min}$ in Fig. 2 (and of the abscissas $K_2^{\min}$ not analyzed here) of these minima fully take into account this scatter as the uncertainties should always be rounded up.

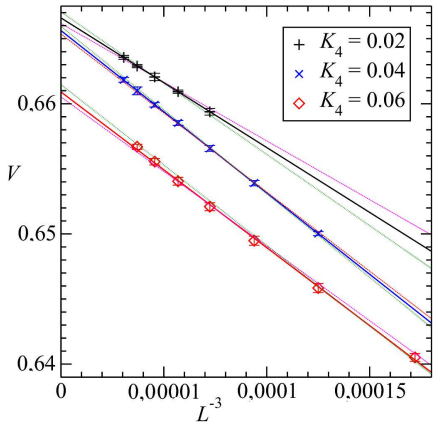

Fig. 2. The values of Challa-Musial cumulant $V_{\alpha,L}^{\min}$ minimas extrapolated to the thermodynamic limit for $\alpha = s$ (the line for $\alpha = \sigma$ falls within the line thickness) at the fixed values of the coupling K_4 explained in the legend box. The dependences are fitted by straight solid lines using the linear regression. For clarity, the results for selected K_4 values are presented only. The role of the broken and dotted lines is explained in the text.

The finite-size-scaling analysis of the ordinates of the above mentioned Challa–Musial cumulant minima is illustrated in Fig. 2 for spins s (also here the results for spins σ are similar because of the symmetry of the Hamiltonian (1)). One can see the clear linear character of the MC computer experiment data which are inter- and extrapolated by the solid lines using linear regression. The thermodynamic limit values of the minima of the cumulant $V_{s,L}$ for particular K_4 coupling values are found at the intersection points of these solid lines with the ordinate axis. Passing through uncertainty bars, the dotted and broken lines in Fig. 2 are deflected to the maximum degree up and down from the solid one, respectively. Their intersection points with ordinate axis determine $V_{s,\infty}^{\min}$ uncertainties.

We have determined the partial latent heat connected with $\langle s \rangle$ order parameter for particular K_4 coupling value using formula (4), the Challa–Musial cumulant $V_{s,\infty}^{\min}$ value, and the value E_+ estimated from the E_s energy plot for the finite-size samples. The results of our analysis for latent heat $E_+ - E_-$ in $k_{\mathrm{B}}T$ units are presented in Table. It is important that $(E_+ - E_-)/(k_{\mathrm{B}}T)$ value weakly depends on the precision of estimation of E_+ value varying by 1 or 2 on the last decimal digit only.

TABLE

The latent heat $(E_+ - E_-)/(k_{\mathrm{B}}T)$ computed for the spins s phase transitions at the specified values of K_4 coupling for the standard 3D AT model on a cubic lattice.

K_4	0.01	0.02	0.03
$(E_+ - E_-)/(k_{\mathrm{B}}T)$	0.0016(55)	0.0030(51)	0.0066(15)
K_4	0.04	0.05	0.06
$(E_+ - E_-)/(k_{\mathrm{B}}T)$	0.0111(19)	0.0176(12)	0.0247(12)

The results presented in Table unequivocally prove that when one approaches the Ising point situated at $K_4 = 0$ for the positive values of K_4 the temperature-driven phase transitions of spins s and σ from the ordered to the unordered phase are of the first order. Moreover, these phase transitions become arbitrarily weak when one comes closer and closer to the value $K_4 = 0$. We have obtained similar conclusions for $\langle s\sigma \rangle$ order parameter.

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References

[1] J. Ashkin, E. Teller, *Phys. Rev.* **64**, 178 (1943).
[2] C. Fan, *Phys. Lett.* **39A**, 136 (1972).
[3] P. Arnold, Y. Zhang, Nucl. *Phys. B* **501**, 803 (1997).
[4] G. Musiał, *Phys. Rev. B* **69**, 024407 (2004).
[5] G. Szukowski, G. Kamieniarz, G. Musiał, *Phys. Rev. E* **77**, 031124 (2008).
[6] D. Jeziorek-Knioła, G. Musiał, L. Dębski, J. Rogiers, S. Dylak, *Acta Phys. Pol. A* **121**, 1105 (2012).
[7] G. Musiał, L. Dębski, G. Kamieniarz, *Phys. Rev. B* **66**, 012407 (2002).
[8] M.S.S. Challa, D.P. Landau, K. Binder, *Phys. Rev. B* **34**, 1841 (1986).