MONTE CARLO SIMULATIONS OF PHASE TRANSITIONS IN THE THREE-DIMENSIONAL ASHKIN–TELLER MODEL*

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The Monte Carlo simulations allowing a distinction between the 1st and the 2nd order phase transitions in the three-dimensional Ashkin–Teller spin-lattice model, a system with three order parameters, are described. The applied method allows a precise location of points on the phase diagram. Some critical points on the phase boundaries have been calculated in the regions complementary to the results recently described in literature.

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Ashkin and Teller [1] have introduced a model of a four-component system by generalization of Ising model, which can be interpreted as a two-component system. Fan [2] has shown, that this four-component model can be expressed in terms of Ising spins, with two spins s_i and σ_i at each lattice site (*i.e.* s_i and σ_i are variables that can take values $+1$ or -1), so can be interpreted as two superimposed Ising models. One of them is described in spin variables s_i and the other in variables σ_i and in both models there are exclusively two-spin interactions of a constant magnitude J_2 between the nearest neighbors only. Simultaneously, these two different models are coupled by four-spin interaction of a constant magnitude J_4, also only between couples of spins residing at the nearest neighboring lattice sites. Thus, the Hamiltonian of this model is

$$-\beta\mathcal{H} = H = \sum_{[i,j]} \{K_2(s_i s_j + \sigma_i \sigma_j) + K_4 s_i \sigma_i s_j \sigma_j\}, \tag{1}$$

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where $\beta = (k_{\mathrm{B}}T)^{-1}$, $[i,j]$ denotes summation over nearest neighboring lattice sites and $K_i = -J_i/k_{\mathrm{B}}T$, with $i = 2$ or 4 and T is the temperature. This is a model with three order parameters: $\langle s\rangle$, $\langle\sigma\rangle$ and $\langle s\sigma\rangle$ where the symbol $\langle\ldots\rangle$ denotes the thermal average.

The standard Ashkin–Teller (AT) model in three-dimensions has been analyzed by the short series analysis and (for the first time) by the Monte Carlo (MC) method by Ditzian *et al.* [3] to obtain the approximate phase diagram. Besides Ditzian's results at present we have more precise results of Arnold *et al.* [4] and Dębski [5] in the narrow ranges of the model parameters. For the detailed discussion of the 3D AT phase diagram we refer the reader to these papers.

The aim of this paper is to present the Monte Carlo simulations and some results for the 1st and 2nd order phase transition points in the (K_4, K_2) diagram. The positions of these points should be calculated with a sufficient precision (comparable to that in [4]) because of the appearance of tricritical and bifurcation points in the diagram. The applied MC method based on Binder cumulants [6] analysis enables us to distinguish transitions of the 1st order from these of the 2nd order in the three-dimensions system with many order parameters.

We have generated equilibrium configurations of the finite-size cubic samples of spins of the volume L^3 $(10 \leq L \leq 26)$ for fixed values of the model parameters. Periodic boundary conditions were imposed and thermalization of the initial configurations was applied. The 48- and 64-bit random number generators were used.

Gibbs distribution was sampled using the Metropolis algorithm [7]. We started with some initial configuration τ of spins, and a new configuration τ' of the system was generated from τ by the repetitive application of the importance sampling procedure when flipping successive spins on the lattice. In order to decide whether to accept a single spin–flip or not, we compared the energies of the new and old configurations. If the energy change $E_{\tau'}$–E_τ was negative, then the new configuration was automatically accepted; if, however, it was positive, the new configuration was accepted with a probability $\mathrm{e}^{-\beta(E_{\tau'}-E_\tau)}$. Physically it means that both configurations are in equilibrium and none of them arises at the expense of another. When each spin of the sample has been visited once, we carried out one Monte Carlo Step (MCS). This procedure ensures the satisfaction of the accessibility criterion.

Using this method, we generated configurations which allowed us to calculate physical quantities in a direct way. The phase transition point T_{c} was determined [6,8,9] from the analysis of the fourth order cumulant

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

where $\langle M_\alpha^n \rangle_L$ denotes the n-th power of the order parameter $\langle \alpha \rangle$, with $\alpha = s$, σ or $s\sigma$, averaged over an assembly of independent samples of the size $L \times L \times L$. For $T > T_c$ and $L \gg \xi$, where ξ denotes the correlation length, Q_L tends towards 1/3 which corresponds to a Gaussian distribution. For $T < T_c$ and $L \gg \xi$, Q_L tends to 1. For $L \ll \xi$, Q_L varies only weakly with temperature and linear dimension, and stays very close to the constant value Q. For the three-dimensions Ising model $Q = 0.6233(4)$ [9, 10], the value achieved at the critical point in the limit $L \to \infty$. This behavior of the cumulant is useful for determination of T_c. One may plot Q_L *versus* T for various L's and estimate T_c from the intersection point of these curves (see [6, 9] and the papers cited therein).

Since T appears in our Hamiltonian only in couplings K_i, i=2 or 4, for 2nd order phase transitions it is convenient to use the following form of the finite-size expansion of $Q_L(K)$ [9, 10]

$$Q_L(K) = Q + a_1(K - K_c)L^{y_t} + a_2(K - K_c)^2 L^{2y_t} + \ldots + b_1 L^{y_i} + b_2 L^{y_2} + \ldots \quad (3)$$

where a_i and b_i are non-universal coefficients, $y_2 = d - 2y_h$, $d = 3$ is the dimensionality and $y_t = 1.587(2)$, $y_h = 2,4815(15)$, $y_i = -0.82(6)$ are the pertinent renormalization exponents. This formula allows a precise location of a continuous phase transition points.

To confirm the 1st order character of the transition point (together with the above mentioned cumulant Q_L) we calculate another fourth order cumulant V_L defined by [6]

$$V_L = 1 - \frac{\langle E^4 \rangle_L}{3\langle E^2 \rangle_L^2}, \quad (4)$$

where $\langle E^n \rangle_L$ denotes the n-th moment of the internal energy E averaged over an assembly of independent samples of the size $L \times L \times L$. The cumulant V_L is extremely useful in distinguishing the 1st order phase transitions from these of the 2nd order. For the 2nd order phase transition $V_L = 2/3$ in the limit $L \to \infty$ and it remains fixed even for $T \neq T_c$ [6], whereas varying T for the 1st order phase transitions, V_L has a minimum $V_L^{\min}$ at $T = T_c(L)$. Moreover [6]

$$V_L^{\min} = 1 - \frac{2(E_+^4 + E_-^4)}{3(E_+^2 + E_-^2)^2}, \quad (5)$$

in the limit $L \to \infty$. Here $E_\pm = E(T \to T_c|_\pm)$. Thus when the latent heat $E_+ - E_-$ tends to zero, $V_L^{\min}$ approaches a value 2/3, as described above for the continuous phase transitions. It is also important that the functions $V_L^{\min}$ and $K_i(T_c(L))$ *versus* L^{-d} are linear [6], which allows a determination of the limit value $V_\infty^{\min}$ and the true critical value of the couplings K_i. These considerations were carried out for a system with a single order parameter.

We have generalized the use of the cumulant V_L for a system with many order parameters. To determine the phase transition connected with the order parameter $\langle s\rangle$, the moments $\langle E^n\rangle_L$ in the cumulant (4) should be calculated only for the interactions between spins s (the first term in the Hamiltonian (1)). Analogously, we investigate the phase transitions connected with the order parameter $\langle\sigma\rangle$, whereas when calculating the moments $\langle E^n\rangle_L$ in (4) for the transitions connected with the order parameter $\langle s\sigma\rangle$, we have to take into account only interactions between the spins $s\sigma$ (the third term in the Hamiltonian (1)). It is worth noting that when one takes into regard all the interactions included in the Hamiltonian (1) then the quantity V_L manifests the averaged behavior of all order parameters in the system.

In the simulations we have always applied thermalization of the initial configurations and it is enough to take 10^5 to 10^6 MCS for this purpose. Then we calculate k partial averages of the moments $\langle M_\alpha^n\rangle_L$ and $\langle E_\alpha^n\rangle_L$ for $\alpha=s$, σ and $s\sigma$ usually after each $10\times k\times 10^6$ MCS with $k=6$ to 30 depending on L and how far from the critical value of K_i we are. The factor 10 reflects the fact that for the calculation of a partial average we take results only every 10th MCS to avoid correlations between sampled configurations of spins in the system.

To illustrate the MC method performance, we have carried out our simulations for the AT model on the three-dimensions simple cubic lattice and for the regions of the parameter space (K_4, K_2) where the phase transitions are expected to be of the 1st and of the 2nd order, obtaining some preliminary results. To investigate the positions of the phase transition points we have used $\langle s\rangle$, $\langle\sigma\rangle$ and $\langle s\sigma\rangle$ as an order parameter. In practice, as suggested by Binder [11], we calculated Root Mean Square (RMS) value of an order parameter to avoid trouble with a restricted ensemble.

Our results are presented in Table I and they are more accurate than those of Ditzian *et.al.* [3]. We have observed the presence of the latent heat on the line of the transitions from the $\langle s\sigma\rangle_{\text{ferro}}$ to the paramagnetic phase for $K_4 < 0$, what is the main difference when compared to the results in [3]. Moreover, the results for $K_4 = 0.19$ clearly show that there are two tricritical points in this region: one on the line of the transitions from the $\langle s\sigma\rangle_{\text{ferro}}$ to the paramagnetic phase and another one on the line of the transitions from the $\langle s\rangle_{\text{ferro}}$ to the paramagnetic phase.

Our results are complementary to those recently obtained in literature [4,5]. Moreover, our results in the vicinity of the bifurcation and tricritical points for $K_4 > 0$ shift the former to smaller values of K_4 than indicated in [3], probably to the Potts point. In the vicinity of these points, the simulations have to be performed extremely carefully. Using the method presented here, we plan to consider the rest of the phase diagram of the 3D AT model, which is still not fully resolved and rises many interesting points.

TABLE I

The couplings K_4, K_2 and the order of the phase transition points in the 3D Ashkin–Teller model obtained from our Monte Carlo simulations.

K_4	K_2	Order
The line of the transitions from the $\langle s\sigma\rangle_{\text{ferro}}$ to the paramagnetic phase:		
−0.085	0.2492(3)	1st
−0.055	0.2394(3)	1st
0.175	0.14791(3)	1st
0.190	0.13947(3)	1st
0.203	0.1184(2)	2nd
0.210	0.0991(2)	2nd
0.217	0.0663(3)	2nd
The line of the transitions from the $\langle s\rangle_{\text{ferro}}$ to the paramagnetic phase:		
−0.162	0.2736(3)	2nd
−0.145	0.268(2)	2nd
−0.085	0.2492(3)	2nd
−0.055	0.2394(3)	2nd
0.175	0.14791(3)	1st
0.190	0.13949(3)	2nd
0.246	0.12003(3)	2nd
0.440	0.11142(3)	2nd
The line of the transitions from the $\langle s\sigma\rangle_{\text{antiferro}}$ to the paramagnetic phase:		
−0.340	0.3345(2)	2nd
−0.313	0.2957(2)	2nd
−0.266	0.2078(5)	2nd
−0.230	0.0912(5)	2nd

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REFERENCES

[1] J. Ashkin, E. Teller, *Phys. Rev.* **64**, 178 (1943).

[2] C. Fan, *Phys. Lett.* **39A**, 136 (1972).

[3] R.V. Ditzian, J.R. Banavar, G.S. Grest, L.P. Kadanoff, *Phys. Rev.* **B22**, 2542 (1980).

[4] P. Arnold, Y. Zhang, *Nucl. Phys.* **B501**, 803 (1997).

[5] L. Dębski, *Acta Phys. Pol.* **A97**, 859 (2000).

[6] M.S.S. Challa, D.P. Landau, K.Binder, *Phys. Rev.* **B34**, 1841 (1986).

[7] N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller, E. Teller, *J. Chem. Phys.* **21**, 1087 (1953).

[8] P. Pawlicki, G. Kamieniarz, L. Dębski, *Physica* **A242**, 290 (1997).

[9] G. Kamieniarz, H.W.J. Blöte, *J. Phys. A: Math. Gen.* **26**, 201 (1993); H.W.J. Blöte, E. Luijten, J.R. Herringa, *J. Phys. A: Math. Gen.* **28**, 6289 (1995).

[10] A.L. Talapov, H.W.J. Blöte, *J.Phys. A: Math. Gen.* **29**, 5727 (1996).

[11] K. Binder, D. W. Heerman, *Monte Carlo Simulation in Statistical Physics*, Springer Series in Solid State Physics, Springer–Verlag, Berlin, Heidelberg 1988.