Verification of the new Baxter phase in the 3D Ashkin-Teller model

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Although the lattice Ashkin-Teller (AT) model is one of the most important in statistical physics and is being studied for decades [1,2], it still attracts a great interest, raises many applications and intriguing questions that have not found satisfactory answers, as it is a non-trivial generalization of the widely used Ising model. The effective Hamiltonian H of the AT model is of the form: $-H/(k_{\rm B}T) = \sum_{[i,j]}\{K_2(s_is_j + \sigma_i\sigma_j) + K_4 s_i\sigma_i s_j\sigma_j\}$, where the summation occurs over the pairs of nearest neighbors, Ising spins s_i and σ_i reside on the same cubic lattice site, k_B is the Boltzmann constant, and T is the temperature of the system. As a result, the order parameter contains three components $\langle s\rangle$, $\langle\sigma\rangle$, and $\langle s\sigma\rangle$, each of which can order independently. Here, the symbol $\langle ...\rangle$ denotes the thermal average. The 3D AT model demonstrates an interesting and complex phase diagram [2] which contains weakly to strong first-order phase transitions, continuous ones, many tricritical and bifurcation points, as well as the wide crossover region. Here we concentrate on the interesting mixed phase region, where $\langle s\sigma\rangle = 0$ and either $\langle s\rangle \neq 0$ and $\langle\sigma\rangle = 0$ or $\langle s\rangle = 0$ and $\langle\sigma\rangle \neq 0$ with ferromagnetic order, which is the most complex and least recognized one [1,2]. In particular, the subject of our research is the border region with the Baxter phase, in which all three components are ordered ferromagnetically and $\langle s\rangle = \langle\sigma\rangle$. Ditzian *et al.* observed a narrow region here where $\langle s\rangle$, $\langle\sigma\rangle$, and $\langle s\sigma\rangle$ are nonzero, but $\langle s\rangle \neq \langle\sigma\rangle$, despite the symmetry of both components resulting from the Hamiltonian. Recently, Santos *et al.* [1] presented the MFT results from the Bogoliubov inequality for the 3D AT model on a cubic lattice for clusters with 1-, 2-, 4-, and 8-sites and they identified this region as the new Baxter$^{(2)}$ phase for the first time. In this paper, we use our extensive Monte Carlo computer experiments [2] to explore this intriguing Baxter$^{(2)}$ phase region in a 3D AT model. Due to the existence of metastable and unstable phases in this region, we based our computer experiments not only on the Metropolis algorithm, but also on our recently discovered cluster one [2]. At the transition of the system from the mixed phase region to the Baxter one, a step energy change is observed for all three components of the order parameters, however, two of them order by reducing their internal energy, at the expense of the step change in the internal energy of the already ordered component. The sum of the latent heat of the entire system is different from zero, and we demonstrate that it is equal to the sum of the latent heat of individual components of the order parameter computed separately. Our results show that as the system size increases, this region indicated as Baxter$^{(2)}$ phase is becoming narrower and disappears in the thermodynamic limit.

References:

[1] J. P. Santos *et al.*, Phys. Lett. A 272 (2018) 382; J. Magn. Magn. Mater. 469 (2019) 35

[2] Z. Wojtkowiak *et al.*, Physica A 513 (2019) 104; J. Magn. Magn. Mater. 500 (2020) 166365