

Scaling Regimes and the Singularity of Specific Heat in the 3D Ising Model

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Abstract. The singularity of specific heat C_V of the three-dimensional Ising model is studied based on Monte Carlo data for lattice sizes $L \leq 1536$. Fits of two data sets, one corresponding to certain value of the Binder cumulant and the other — to the maximum of C_V , provide consistent values of C_0 in the ansatz $C_V(L) = C_0 + AL^{\alpha/\nu}$ at large L , if $\alpha/\nu = 0.196(6)$. However, a direct estimation from our C_V^{\max} data suggests that α/ν , most probably, has a smaller value (e.g., $\alpha/\nu = 0.113(30)$). Thus, the conventional power-law scaling ansatz can be questioned because of this inconsistency. We have found that the data are well described by certain logarithmic ansatz.

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1 Introduction

The standard three-dimensional (3D) Ising model, as well as several models of the 3D Ising universality class, have been extensively studied by the Monte Carlo (MC) method in past (see, e.g., [1, 2] and references therein) with an aim to evaluate the critical exponents. Some cornerstone works are due to J. Chen et al. [3] and H. W. J. Blöte et al. [4]. More recent works are [5–7, 28]. In [5], the singularity of specific heat of the classical 3D

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Ising model is studied, which is also the main subject of our current MC study. In [6, 7], modified models with the so-called improved Hamiltonian are considered. The basic idea of this method is to choose such Hamiltonian, for which the leading corrections to scaling vanish. It is believed that good estimates of the critical exponents can be therefore extracted from these models by simulating even relatively small lattices. The improved Hamiltonian has to be a good approximation of the fixed-point-Hamiltonian of an exact renormalization group (RG) transformation to ensure that this method works well. Since we do not strictly know whether this condition is really satisfied, here we prefer to use a simple strategy — to simulate very large lattices. It is reasonable to choose the simplest model of the actual universality class, i.e., the classical 3D Ising model, to obtain good results (good simulation data for maximally large lattice size L) by this approach. A model including next-nearest-neighbor interactions has been considered in [4] as a good alternative to the classical Ising model, using a coupling to next-nearest neighbors as a parameter to minimize corrections to scaling. However, in some cases corrections to scaling seem to be negligible also in the classical Ising model with nearest-neighbor coupling. An example is the scaling consistency test, considered in Section 3. From this point of view, our choice of the classical 3D Ising model also could be quite good.

Usually, lattices of linear sizes L up to $L = 128$ are simulated [1]. However, much larger lattices can be well simulated on modern computers, and MC results for susceptibility and magnetization cumulant at $L \leq 1536$ have been recently reported in [8]. Some simulation results for even larger lattices have been reported in literature (see, e.g., [9] for a review). A distinguishing feature of our simulations of very large lattices is a high enough (moderately high) statistics, which is sufficient for a finite-size scaling analysis in the critical region with an aim to estimate the critical exponents. It has been found in [8] that the data can be well fit with critical exponents $\eta = \omega = 1/8$ and $\nu = 2/3$, which are consistent with the GFD (grouping of Feynman diagrams) theory of [10, 11], confirmed and appreciated also in [12], and are remarkably different from those of the perturbative RG theory, i.e., $\eta = 0.0335 \pm 0.0025$, $\omega = 0.799 \pm 0.011$ and $\nu = 0.6304 \pm 0.0013$ [13]. These results, however, are not strictly conclusive, since the fits with both sets of the exponents are quite acceptable. A minor problem for the perturbative RG scaling is that some fits of the susceptibility data of [8], assuming $\omega \approx 0.8$, give slightly larger values of η (e.g., 0.0397(28) and 0.0405(25)) than $\eta = 0.0335 \pm 0.0025$. Here we go substantially beyond the results of [8] by completing a comprehensive study on specific heat data to obtain more conclusive evidences for a better distinguishing between the two possible scaling scenario.

2 Simulation results

We have simulated the 3D Ising model on simple cubic lattice with

$$H/T = -\beta \sum_{\langle ij \rangle} \sigma_i \sigma_j, \quad (2.1)$$