Critical behaviour of a heat capacity for three-dimensional Ising model

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Abstract
We investigated the behavior of a heat capacity near the critical temperature for the three-dimensional Ising model. The calculations were carried out by the Metropolis algorithm. The simulation results indicate that the specific heat has an infinite singularity at the critical point.

Keywords
Ising model, cubic lattice, critical temperature, heat capacity, Monte-Carlo methods

1. Introduction

It is well-known that in the two-dimensional (d = 2) Ising model the heat capacity at critical temperature has a logarithmic discontinuity. Results of Monte Carlo simulations [1] and theoretical estimations [2, 3] gives us a clear evidence that the critical value of the specific heat in d ≥ 5 Ising model tends to a limit value with increasing lattice sizes. Meanwhile, the critical behavior of the heat capacity in d = 3, 4 cases remains unclear [4, 5]. In works [6, 7], the n-vicinity method was proposed to approximate the partition function of the Ising model. The values of critical temperatures obtained by this method have a good agreement with experimental data. However, the n-vicinity method predicts a finite scaling behavior of the heat capacity. In this work, we studied the scaling behavior of the heat capacity in the three-dimensional Ising model. The calculations were performed by Metropolis algorithm.

2. Simulation results

The Metropolis algorithm was used to calculate the average energy and the energy variance at the temperatures near the critical point. We carried out simulations for cubic spin lattices with different linear sizes L ranging from 16 to 256. Initially, the system was set to the ground state. The spins were updated in typewriter order and after each sweep the energy was measured. The first 10^5 Monte-Carlo steps were carried out without accumulating the statistical data in order to achieve the equilibrium state of the system. The total number of Monte Carlo steps were $3\cdot10^5L^3$. The inverse temperature $\beta = 1/k_BT$ was varied within a step $2\cdot10^{-5}$.

The simulation results are presented in Fig. 1. With increasing the lattice size, the displacement of the maximal specific heat to higher temperatures is observed. As seen in Fig. 1(b), the dependence of the critical specific heat on the logarithm of the linear lattice size is linear and it can be approximated by the next expression:

$$C_{max} = -0.3075 + 0.9428 \ln L, \quad (1)$$

The average error of this approximation is 0.94%. Hence, the simulation results justify that the specific heat has infinite logarithmic scaling behavior.

3. Conclusion

The results of simulations confirmed that the specific heat has a discontinuity in the critical point. The logarithmic approximation of dependence of critical specific heat on the lattice size is in a good agreement with simulation data. However, it is quite possible that this discontinuity is not logarithmic and the critical heat capacity changes as a power function with a very small exponent if a deviation from the logarithmic scale would be found above L = 256. Though, it is clear that the heat capacity increases unlimitedly at the critical point in three-dimensional case.

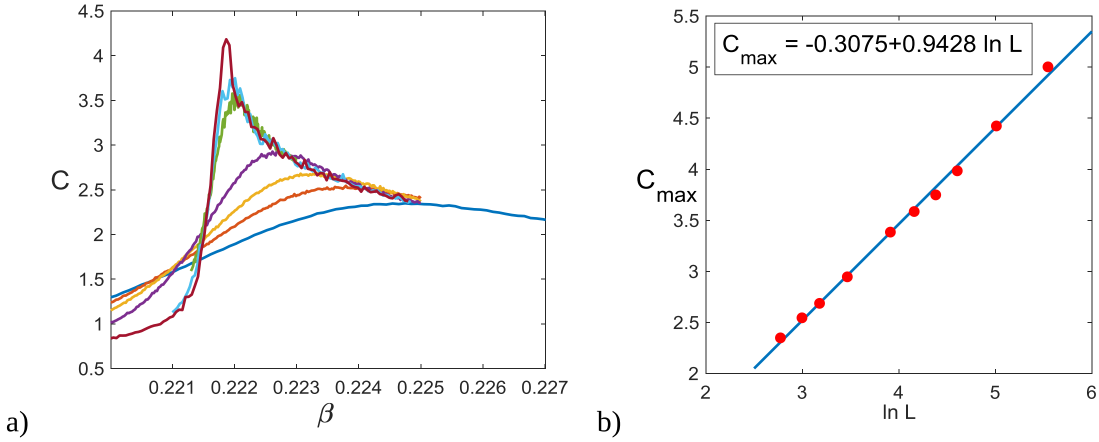

Figure 1: The simulation results. (a) The specific heat C vs. the inverse temperature $\beta=1/k_BT$ for lattices with different linear sizes L = 16, 20, 24, 32, 64, 80, 100 (from down to up). (b) Critical values of the specific heat C_{max} vs. linear size of lattice L

4. References

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