Reweighting in Monte-Carlo calculation
Renormalized Coupling Constant for the Three-Dimensional Ising Model

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Abstract. We investigated the thermodynamic behaviour of the three-dimensional Ising model near the critical temperature region using Monte Carlo calculations. The magnetic susceptibility, the correlation-length and renormalized coupling constant were calculated using the reweighting method.

1. Introduction

The order-parameter fluctuations with the long-range interactions are one of the key points of the second-order phase transitions theory. The only way to obtain precise critical properties was the analysis of perturbation series for the critical behaviour, which was not efficient for the hyperscaling violations resolution [1].

Renormalized coupling constant is the key parameter of the renormalization group theory and it is defined as

\[ g^* = \lim_{K \to K_c} g(K) = -\lim_{K \to K_c} \frac{\partial^2 \chi(K)/\partial H^2}{\chi^2(K)\xi^d(K)^{1/2}}, \]

where \( K_c \) is the critical value of the inverse temperature \( K = \beta J \), with the exchange energy \( J \), magnetic susceptibility \( \chi \) and second-moment definition correlation-length \( \xi \). This means the renormalized coupling constant is related to the magnetic moments by

\[ g \equiv \left( \frac{L}{\xi} \right)^d \frac{3\langle M^2 \rangle^2 - \langle M^4 \rangle}{\langle M^2 \rangle^2}, \]

where \( \chi = \langle M^2 \rangle / L^d \), M is the total magnetization. Being the fixed point, the renormalized coupling constant defines the critical properties of a system and critical exponents. It is highly expected to obtain more reliable results of the critical properties using non-perturbative Monte Carlo method.

One of the crucial points of Monte Carlo methods is the efficiency of the simulation. It is important to find an approach where the data obtained from a single simulation can be used to study the entire region near the critical point. Reweighting method, described in [3], is used to extract more information from the simulation. In this study we used a single histogram method, where a Monte Carlo simulation performed at \( T \) generates a histogram \( H(E, M) \), which provides
the normalized probability distribution.
In this paper we consider 3D Ising model, defined by the Hamiltonian
\[ H = -J \sum_{\langle i,j \rangle} S_i S_j, \] (3)
where \( J \) is the nearest-neighbour sites interaction exchange, \( S_i = \pm 1 \) is the sum of the sites sit on three-dimensional cubic lattice of linear size \( L \) with periodic boundary conditions. In our case \( J > 0 \), which stands for ferromagnetic state. A particular microstate of the lattice is specified by the set of variables \( \{s_1, s_2, \ldots, s_N\} \) for all lattice sites, and macroscopic states of the system are determined by its microstates properties.

Our goal is to calculate the renormalized coupling constant (2), hence we have to calculate other quantities, such as:

- the total magnetization of the system
  \[ M = \sum_i S_i, \] (4)
- the magnetic susceptibility
  \[ \chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{kT}, \] (5)
- the correlation-length
  \[ \xi = \frac{1}{2 \sin(\pi L)} \sqrt{\frac{\chi}{F} - 1}, \] (6)
where \( F = \frac{\langle \Phi \rangle}{L^3}, \)
\[ \Phi = \frac{1}{3} \left( \left| \sum_i S_i \exp \frac{2\pi i x_{1,i}}{L} \right|^2 + \left| \sum_i S_i \exp \frac{2\pi i x_{2,i}}{L} \right|^2 + \left| \sum_i S_i \exp \frac{2\pi i x_{3,i}}{L} \right|^2 \right). \] (7)

2. Monte Carlo reweighting method
The second-order phase transition is able to happen only with the use of thermodynamic limit \([2]\), when \( N \to \infty \) and \( V \to \infty \), but \( \frac{N}{V} \) is finite. At the critical point (or the transition point) the thermodynamic quantities display singular behaviour. Thus, the finite-size scaling methods are used to define such quantities in the vicinity of the critical point. However, these methods did not give reliable answers in the thermodynamic limit, because of this coupling constant behaviour
\[ g_R^\infty \equiv \lim_{\beta \to \beta_c} \lim_{L \to \infty} g_R(L, \beta) \neq \lim_{L \to \infty} \lim_{\beta \to \beta_c} g_R(L, \beta) \equiv \tilde{g}_R, \] (8)
where \( \beta = 1 \) is the inverse temperature.
Hence we used the reweighting method for the calculations of the thermodynamic quantities, which allows to obtain the averages of the physical quantities at nearby temperatures from a simulation performed at the temperature \( \beta \).

\[ \langle O \rangle_{\beta} = \frac{\sum_E O(E) h_{\beta}(E)}{\sum_E h_{\beta}(E)} = \frac{\sum_E O(E) h_{\beta}(E) \exp(-(\beta - \beta_c))}{\sum_E h_{\beta}(E) \exp(-(\beta - \beta_c))}, \] (9)
where \( E \) is the energy of the system, \( h_{\beta} \) is the amount of states with the energy \( E \).

In the vicinity of the critical point the relaxation time and the correlation time diverge, so to reduce the critical slowing down effects we used the Wolff cluster algorithm\([4]\). Monte Carlo algorithm in Wolff edition:
Table 1. The coupling constant $g_R$ dependence of the temperature

|   |   |
|---|---|
| $T$ | $g_R$ |
| 4.5242 | 27.39(2) |
| 4.5241 | 27.32(3) |
| 4.5240 | 27.25(3) |
| 4.5239 | 27.18(2) |
| 4.5238 | 27.12(4) |
| 4.5237 | 27.07(2) |
| 4.5317 | 28.23(4) |
| 4.5316 | 28.06(4) |

(i) Choose random site $i$, label it as the center, then flip it.
(ii) Study neighbouring sites $j$. If $s_j = s_i$, join site $j$ to cluster with probability $p = 1 - \exp(-2\beta)$.
(iii) Repeat step (ii) for site $j$, if it was joined to the cluster. Keep on doing this as long as the cluster grows.
(iv) When the cluster is finished, invert the spins which belong to it and empty the stack.

This process is called the cluster flip and it is equal to 1 Monte Carlo step.

3. Results

We have carried out $2 \times 10^6$ elementary Monte Carlo steps for lattices with linear sizes $L = 32, 48, 64, 96, 128$ near the critical temperature $T_c = 4.5115$. The Monte Carlo step was composed of 10 Wolff cluster flips. Since the condition for reaching the thermodynamic limit is $L/\xi > 4$, we have specified the information, when $L/\xi = 6$. The results of our computations are listed in Table 1.

4. Discussion

Based on the obtained data from tab. 1 it is possible to determine the critical point corresponding to the fixed point of renormalization group transformation $g_R^\infty$

$$g_R(\tau) = g_R^\infty(1 + \alpha\tau^\theta),$$

where $\tau = (T - T_c)/T_c$ is the temperature, $\theta = 0.504$ [5] is the correction scaling index for 3D Ising model. Using the method of least squares we have calculated $g_R^\infty = 23.85(3)$, which corresponds well with the mean-field theory solution [6] $g_R^\infty = 23.73(2)$ and Monte Carlo simulations results [5] $g_R^\infty = 23.3 - 26.4$.

Reweighting method proves itself in the computation of the renormalized coupling constants, especially relevant it appears for the strongly disordered systems.

References

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