Monte Carlo simulation of the one-dimensional $N$-state clock model with long range inverse square interaction

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Abstract.

Using Monte Carlo simulation, the one dimensional $N$-state clock model with long range inverse square interaction has been studied. In the case of $N = 6$, the temperature dependence of the specific heat shows two peaks at $T_1$ and $T_2$ ($< T_1$). The critical exponent $\eta$ calculated from the system size dependence of magnetization changes with temperature in the region between $T_1$ and $T_2$. The behaviors are very similar to those of the two-dimensional 6-state clock model with the nearest neighbor interaction which shows two steps of phase transition, Berezinskii-Kosterlitz-Thouless transition and ordinary long range order. We have also confirmed that the temperature $T_2$ shift toward zero with the increase of $N$.

1. Introduction

It is well known that the one-dimensional classical spin system has no long range order. However, when the long-range interactions decaying with distance $r$ as $r^{-\sigma}$ ($1 < \sigma \leq 2$) are included, the critical behavior changes greatly.

In the case of XY-model, Fisher et.al have studied the system by using the renormalization group approach [1]. They predicted that it has mean-field type long range order (LRO) for $1 < \sigma < 1.5$ and non-trivial LRO in which the critical exponent continuously varies with $\sigma$ for $1.5 < \sigma < 2$.

On the other hand, for the case of inverse square interaction ($\sigma = 2$), Brown and Šimánek performed Monte Carlo (MC) calculation and found that the nature of the phase transition is just like Berezinskii-Kosterlitz-Thouless (BKT) transition which has been well known for the two-dimensional XY model with the nearest neighbor interactions. Then, it is called as the (one-dimensional) BKT-like transition while the one-dimensional continuous symmetry spin model has no topological defects [2].

Another example showing the BKT transition is the $N$-state clock model which has discrete and rotational symmetry. Various numerical calculations have been performed for the two-dimensional $N$-state clock model with the nearest neighbor interactions. For the case of $N \leq 4$ it has only one transition with an well defined finite value for the exponent $\nu$, but for the case
of $N \geq 5$ there appear two phase transitions producing the intermediate BKT phase where exponent $\eta$ varies with temperature [3-5].

In the present paper, we perform the MC calculation for the $N$-state clock model with long range inverse square interaction. Our aim is to check the BKT-like transition in the present system, i.e. to confirm in the discrete model whether similar type of phase transition occurs for the long range one-dimensional system and the nearest neighbor two-dimensional system as confirmed in the continuous $XY$ model.

2. Method

The Hamiltonian for the one dimensional $N$-state clock model with long range inverse square interaction is given by

$$H = -\sum_{<ij>} J_{ij} \cos \frac{2\pi(p_i - p_j)}{N},$$

where $p_i(= 1, 2, \cdots, N)$ denotes the clock state of the $i$th site and $J_{ij} = J_0 r_{ij}^{-2}$ is a coupling constant between sites $i$ and $j$ separated by distance $r_{ij}$. In the calculation, we assumed ferromagnetic coupling $J_0 > 0$ and periodic boundary condition for the system of the chain length $L = 2^8 \sim 2^{15}$ and $N = 4 \sim 9$.

Because of the infinite long range interaction in the present system, we need the calculation time proportional to the square of the system size $L$. In order to reduce the calculation time, we used a discrete update (DUD) MC method. In the DUDMC method, we divide the effective field acting on the $i$th site into two parts: $H_i = H_{\text{near}} + H_{\text{far}}$ where $H_{\text{near}}$ is the effective field from spins near to the site $i$, and $H_{\text{far}}$ is that from spins in the far sites. When the thermal equilibrium is realized, the field $H_{\text{far}}$ does not vary so much during the spin update process. Then we update $H_{\text{far}}$ only for par $m$ MC steps (discrete update), while we update $H_{\text{near}}$ in every update trial since it is strongly affected by each spin configuration. In the present study we have included up to the 8th nearest neighbor sites in $H_{\text{near}}$ and considered the case of $m = 1$ or 2. Furthermore, we made use of the Fast Fourier Transform algorithm (FFT) to calculate $H_{\text{far}}$ with the aid of the convolution theorem in $k$-space. The FFT can reduce the calculation time from the order $L^2$ to $L \log_2 L$. By these reduction of the calculation time, we can treat fairly large system size leading a qualitatively and also quantitatively far reliable result. The validity of this method is explained in reference [6]. When we need more precise calculation, we also adopted the Swendsen’s histogram MC method [7].

Thermal averages are calculated using $5 \times 10^5$ MC steps after equilibrating over $1 \times 10^5$ MC steps, and for more precise calculation with histogram MC method, we take $8 \times 10^5$ MC steps for making energy histogram.

3. Results

In figure 1, we showed the temperature dependence of the specific heat $C$, for the case of $N = 6$. The specific heat exhibits two anomalies; the rather sharp peak at low temperature, $T_2$, and the broad maximum at high temperature, $T_1(> T_2)$. We can estimate the precise positions of $T_1$ and $T_2$ by using the histogram MC method, and determined as $T_1 = 0.862 \pm 0.003$ and $T_2 = 0.457 \pm 0.003$. In the inset, we showed the size dependence of the peak height of the specific heat at $T_1$ and $T_2$. As expected for the BKT transition, both peaks have no evident size dependence. All those behaviors of $C$ are very similar to those found in the two-dimensional 6-state clock model with the nearest neighbor interactions. Then it is considered that two-step phase transition occurs, i.e. BKT at $T_1$ and ordinary LRO at $T_2$ leading intermediate BKT phase for temperatures $T_2 < T < T_1$.

The temperature dependences of the specific heat for the case of $N = 4 \sim 9$ are shown in figure 2. In the case of $N = 4$, the curve exhibits only one peak probably corresponding to
Figure 1. Temperature dependence of the specific heat for several system size $L$ ($N = 6$). Inset shows the size dependence of the peak height at $T_1$ and $T_2$ calculated by the histogram method.

Figure 2. Temperature dependence of the specific heat for several values of $N$ ($L = 2^{14}$). Inset shows the $N$ dependence of the temperature $T_2$ and its peak height calculated by the histogram method.

Figure 3. Temperature dependence of the magnetization for several system size $L$ ($N = 6$).

Figure 4. Log-Log plotting of the relation between $M$ and $L$ for some selected temperatures between $T_1$ and $T_2$ ($N = 6$).

$T_2$. This behavior is similar to that of the two-dimensional 4-state clock model with the nearest neighbor interactions. For the case of $N = 5$, the peak begins to split into two peaks, and there appear two separate peaks for the case of $N = 6$. With further increase of $N$, $T_2$ is shifted to the lower temperature. By using the histogram MC method we have estimated the $N$ dependence of the temperature $T_2$ and the peak height of $C$ at $T_2$. The results are shown in the inset. We may be able to expect that the sharp peak at $T_2$ is shifted to the zero temperature and disappears in the limit of $N \to \infty$. The position of the peak at higher temperature does not depend on the value of $N$ and consistently coincides with that of the single peak found for long range XY chain model in reference [2].
In figure 3, we showed the temperature dependence of the magnetization $M$, for the case of $N = 6$. As discussed before, the low temperature phase at $T < T_2$ is expected to be ordinary LRO phase and the phase at $T_2 < T < T_1$ is the intermediate BKT phase. It seems that a comparatively large magnetization observed for the intermediate region $T_2 < T < T_1$ is caused by the infinite correlation length of the BKT like phase. The finite size scaling theory for the BKT phase transition predicts that the size dependence of $M$ should be as follows

$$M \sim L^{-(d-2+\eta)},$$

where $d$ is the lattice dimensionality.

| $T$ (K) | $d - 2 + \eta$ | $\eta$ (d = 1) |
|--------|----------------|----------------|
| 0.70   | 0.503          | 1.503          |
| 0.65   | 0.452          | 1.452          |
| 0.60   | 0.448          | 1.448          |
| 0.55   | 0.418          | 1.418          |
| 0.50   | 0.406          | 1.406          |
| 0.45   | 0.345          | 1.345          |

We show the size dependence of magnetization for various temperature between $T_1$ and $T_2$ in figure 4 for the case of $N = 6$. Because of the large finite size effect in the long range system, there are large deviation from the liner behavior even for the case of fairly large value of $L$. Then, for the estimation of the slope, $d - 2 + \eta$, we used the largest two sizes available in the present calculation. The results are shown in table 1 for some selected values of temperatures in the region of $T_2 < T < T_1$. The value of $\eta$ varies with temperature. Though the value of $\eta$ differs from that obtained for the two dimensional nearest neighbor clock model, the tendency of the temperature dependence is quite similar to each other. Thus we conclude that there is intermediate phase (BKT-like phase) in one dimensional 6-state clock model with long range inverse square interactions.

4. Conclusion

In the present study, we discussed the one dimensional $N$-state clock model with long range inverse square interaction by using the method of the MC simulation. We have calculated the temperature dependence of the specific heat and magnetization, and their system size dependences. For the case of $N \leq 4$, it shows only one LRO phase transition, but for the case of $N \geq 5$, it shows the two-step phase transition giving the intermediate BKT phase with temperature dependent exponent $\eta$. With the further increase of $N$, the peak of the specific heat corresponding to the LRO is shifted to zero temperature and expected to disappear in the limit of $N \to \infty$, leaving only one peak of the BKT-like transition found in reference [2]. Then, we could confirm in the $N$-state clock model that the one-dimensional system with inverse square interaction shows similar type of phase transition to that of the two-dimensional system with nearest neighbor interaction.

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