The critical behaviour of the 1-dimensional XY model with power law decay long range interactions

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Abstract. We discuss the critical behaviour of the 1-dimensional classical XY model with power law decay long range interactions by using Monte Carlo simulation. It has been predicted by renormalization group calculation that the critical behaviour changes with the power of interactions. From the simulation result of temperature dependence of the specific heat, we confirm that the system shows the critical behaviour of the mean field type and the non-trivial long range order. We also estimate the critical exponent η for the system with the inverse square long range interactions, and by using the phenomenological renormalization group plot, we confirm the ‘Berezinskii-Kosterlitz-Thouless (BKT)-like’ transition which has been predicted by the spin wave calculations.

1. Introduction
The 1-dimensional classical spin system with the nearest-neighbour interactions has no long range order at finite temperature. However, it is well known that the introduction of long range interactions decaying with distance r as \( r^{-(1+\sigma)} \) (0 < \( \sigma \) < 1) greatly changes its critical behaviour.

In the case of XY model, Fisher et al. studied the system by using the renormalization group (RG) approach [1]. They predicted that it has mean field type long range order (LRO) for 0 < \( \sigma \) < 0.5 and non-trivial LRO in which the critical exponent continuously varies with \( \sigma \) for 0.5 < \( \sigma \) < 1. This behaviour induced by the long range interactions commonly appears in many other spin systems such as Ising model or the spherical model [2].

On the other hand, in the case of inverse square interactions (\( \sigma = 1 \)), the situation is more complicated. The system is generally believed to have no LRO. Šimánek [3] confirmed that there was no spontaneous magnetization by the spin wave calculation, but also predicted that it has a power law decay spin correlation function and the divergence of susceptibility at low temperatures.

The nature of this phase transition is just like BKT transition that has been well known for the 2-dimensional XY model with the nearest-neighbour interactions. There are no topological defects in the ordering of the 1-dimensional continuous symmetry spin model. Therefore, it is called (1-dimensional) ‘BKT-like’ transition.

As for Ising model, a number of theoretical and numerical calculations have been performed and its behaviour has been well understood. On the other hand, few simulation results have
been reported on XY model. Brown and Šimánek [4], and Romano [5] reported the infinite susceptibility and non-divergent specific heat. They estimated the critical temperature $T_c$, but the critical exponents have been still unknown.

In this paper, we present the MC calculation result for the 1-dimensional XY model with long range power law decay interactions. First, we estimate the critical exponents from the finite size scaling for $0 < \sigma \leq 1$ and then compare our MC result with the predictions of RG calculations. Next, we perform the phenomenological renormalization group plot and confirm whether the ‘BKT-like’ transition occurs or not at $\sigma = 1$.

2. Method
The Hamiltonian for the 1-dimensional XY model with long range power law decay interactions is given by

$$ H = - \sum_{< i,j>} J_{ij} \cos(\theta_i - \theta_j), $$

where $\theta_i$ denotes an angular variable at site $i$ and $J_{ij} = J_0 r_{ij}^{-(1+\sigma)}$ is a coupling constant between site $i$ and $j$ separated by distance $r_{ij}$.

In this calculation, we assume ferromagnetic coupling $J_0 > 0$ and periodic boundary condition for the system of the chain length $L = 2^n$ ($n = 7 \sim 14$).

Because of the infinite long range interactions in the present system, we need the calculation time proportional to the square of the system size $L$. Recently, many methods based on the cluster algorithm are proposed to shorten the computing time [6]. In this study, we use the simplest discrete update (DUD) MC method. In the DUDMC method, we divide the effective field acting on the site $i$ 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 at 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 every $m$ MC steps (discrete update), while we update $H_{\text{near}}$ in every update trial since it is strongly affected by each spin configuration. In this study, we include up to the 8th nearest neighbour sites in $H_{\text{near}}$ and consider the case of $m = 1$ or 2. Furthermore, we make 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 $L \log_2 L$. The validity of this method is explained in reference [7]. When we need more precise calculation, we also adopt the Swendsen’s histogram MC method [8].

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. Result
3.1. The $\sigma$-dependence of critical behaviour
It has been predicted that the critical behaviour of this system is the mean field type for $0 < \sigma < 0.5$ and non-trivial $\sigma$-dependent type for $0.5 < \sigma < 1$. At $\sigma = 0.5$, the essentially singular type critical behaviour has been predicted.

Figure 1 shows the temperature dependence of the specific heat $C$ in the cases of $\sigma = 0.4$ and $\sigma = 0.7$. In the mean field approximation, the specific heat jumps to finite value at $T = T_c$. For $\sigma = 0.4$, the specific heat shows the tendency of mean field type critical behaviour as system size increases. On the other hand, for $\sigma = 0.7$, the specific heat shows no jump, and obviously the system has the critical behaviour which is different from the mean field type.

We estimate the critical exponent $\gamma/\nu$ from the susceptibility $\chi$ by using the finite size scaling

$$ \chi \propto L^{\gamma/\nu}. $$
The $\sigma$-dependence of the critical exponent $\gamma/\nu$ is shown in figure 2. In the region $0.5 < \sigma < 1$, the critical exponent $\eta$ is calculated from the relation $\eta = 2 - \gamma/\nu$. Our result is well fitted with the relation $\eta = 2 - \sigma$ predicted by Fisher et al. [1].

The value of $\gamma/\nu$ expected by the mean field calculation is $\gamma/\nu = 2$. Our estimation of $\gamma/\nu$ is almost $\gamma/\nu = 0.5$ in the area of $0 < \sigma < 0.5$. At present we cannot explain this large deviation from the expected mean field value. The smaller $\sigma$ means the longer range interactions. In order to elucidate the situation, more careful scaling correction is necessary for $0 < \sigma < 0.5$ by using larger $L$ systems.
3.2. The case of $\sigma = 1$

Figure 3 shows the temperature dependence of the specific heat $C$ for $\sigma = 1$ where the BKT-like transition is expected. These curves show no system size dependence. On the other hand, the susceptibility $\chi$ has the system size dependence and we obtain no clear curve at low temperature region (not reported here). These behaviours commonly appear on the MC simulations for the 2-dimensional XY model that shows BKT transition. In the inset, we show $T_c$ obtained from the maximum of $\chi$, and we got $T_c \approx 0.6$.

Figure 4 shows the phenomenological renormalization group plot of the magnetization $M$ [9]. We calculate the temperature dependence of the following quantity $R$ with

$$R = -\frac{\ln(M/M')}{\ln(L/L')}$$

where $L$ and $L'$ denote the different two lattice size ($L, L' = 2^{10}, 2^{11}, 2^{12}$) and $M$ and $M'$ are corresponding magnetizations.

If $M$ is proportional to $L^{-\beta/\nu}$ at critical temperature, $R$ should take the only one value of $\beta/\nu$ independent of $L$ and $L'$. For ordinary LRO, therefore, the curves of the temperature dependence of $R$ should cross only at critical temperature (point) $T_c$. On the other hand, in the BKT transition which has the critical line, $R$ should lap over one curve for $T < T_c$.

Our result at lower temperature than $T_c \approx 0.6$ collapse on the one curve and this shows a one evidence supporting the BKT transition.

The critical exponent $\eta$ estimated from the finite size scaling using the relation $\gamma = \nu (2 - \eta)$ gives $\eta = 0.977 \approx 1$. In the BKT transition of 2-dimensional XY model, the system has $\eta = 1/4$ at higher temperature. In our case, only the critical exponent $\eta$ is different from the ordinary BKT transition. But our results generally support that the system has the ‘BKT-like’ transition.

4. Conclusion

We have discussed the critical behaviour of the 1-dimensional XY model with power law decay interactions $r^{-(1+\sigma)}$ by using the MC simulations. For $0 < \sigma < 1$ we have calculated the temperature dependence of the specific heat, and also estimated the critical exponent $\gamma/\nu$ from the finite size scaling analysis of the susceptibility $\chi$.

For $0 < \sigma < 0.5$, we have obtained the mean field type transition from the temperature dependence of the specific heat, while the value of the critical exponent is different from the expected value probably because of the insufficiency of the system size. We would like to make more accurate scaling correction by using larger systems in the future studies.

For $0.5 < \sigma < 1$, we have confirmed the RG prediction of $\eta = 2 - \sigma$. In the case of $\sigma = 1$, the specific heat shows no system size dependence. From the result of phenomenological renormalization group plot, we can confirm the existence of some ‘BKT-like’ transition with the exponent $\eta = 1$.

References

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