

A Study of XY Model by Spin-dynamic simulation

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We studied the 2-dimensional XY model through a spin-dynamic simulation, by introducing a classical rotation. The magnetization, energy, susceptibility, heat capacity and correlation length are derived and well consistent with Monte Carlo simulation results. We also studied the mean square displacement $\langle (\phi(t) - \phi(0))^2 \rangle$ for the individual spin. It was found that under low temperature $T < 1.2$, the spin is oscillating around the balance point and the mean square displacement is zero. Under high temperature $T > 1.2$, however, the spin is rotating along the same direction. A linear relation $\langle \phi(t)^2 \rangle \propto t$ was found, which is consistent with Einstein diffusion equation.

INTRODUCTION

The 2 dimensional XY model is defined by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \cos(\phi_i - \phi_j) \quad (1)$$

J represents the interaction strength between neighboring spins, and ϕ_i describes the angle of spin i . Based on the Hamiltonian, a lot of Monte Carlo (MC) simulations have been employed to study the phase transition of the system ([1, 2] and references therein). However, as an equilibrium states sampling method, MC simulation can not provide time related properties, i.e. the dynamic behavior of the system. It is therefore important to conduct a dynamic simulation, as a supplementary to MC study.

In this paper, we studied the dynamics by introducing a classical kinetic energy into the Hamiltonian ([3])

$$H = \sum_i \frac{1}{2} I \dot{\phi}_i^2 - J \sum_{\langle i,j \rangle} \cos(\phi_i - \phi_j) \quad (2)$$

I is the inertia of the spin. The dynamics of the system is thus controlled by Hamilton's equation. According to Velocity-Stormer-Verlet method, the motion of spin can be integrated out by

$$\phi_i(t + \delta t) = \phi_i(t) + \dot{\phi}_i(t)\delta t + \frac{M_i(t)}{2I} \delta t^2 \quad (3)$$

$$\dot{\phi}_i(t + \delta t) = \dot{\phi}_i(t) + \frac{(M_i(t) + M_i(t + \delta t))}{2I} \delta t \quad (4)$$

where $M_i = -J \sum_j' \sin(\phi_i - \phi_j)$ represents the torque on spin i . In our simulation, the interaction strength J and time step δt were both set to be 1. The inertia I was set to be 1.1×10^3 , which guarantees that the angular variation during each step neither too small to low down the simulation efficiency, nor too large to be inaccurate. To simulate the canonical ensemble, the angular velocities are rescaled by $\sum_i \frac{1}{2} I \dot{\phi}_i^2 = \frac{1}{2} N k_B T$, to satisfy the equipartition theorem. The system consists of 2500 spins (50×50), and periodic boundary conditions are applied. To avoid the rotation of whole system, the angular of the first spin was always set to be spin-up, i.e. $\phi_1 = 0$. The initial configuration of the system was set spin-up, and the

simulation were conducted under different temperatures. To be statistically reliable, 20 simulations were employed under each temperature. The total time steps for each simulation is 1000000, and all the properties calculated came from the data after 200000 time steps, to eliminate the non-equilibrium effects.

RESULTS

Magnetization and Susceptibility

The magnetization of the system at time t was defined by

$$m(t) = \frac{1}{N} \sum_i \cos \phi_i(t) \quad (5)$$

Fig. 1 shows that the variation of magnetization as function of

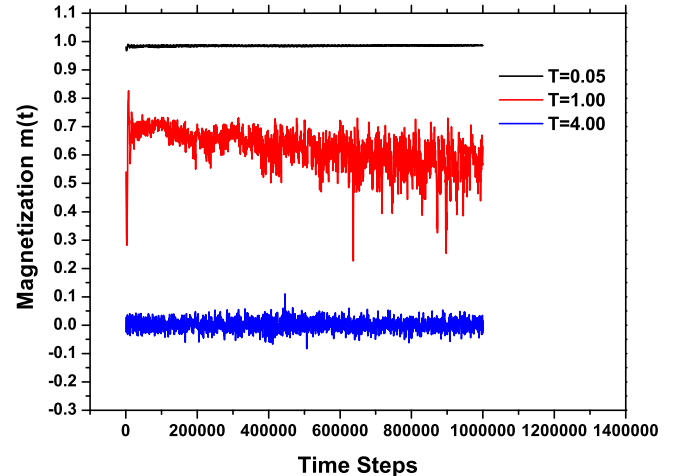


FIG. 1: Instantaneous magnetization $m(t)$ under three different temperatures: $T = 0.05$, $T = 1.00$ and $T = 4.00$, respectively (J has been set to 1).

time, under different temperatures. It can be seen that under low or high temperature, the magnetization is stable and has

very small fluctuation. Under intermediate temperature ($T \sim 1.0J/k_B$), however, there is a large fluctuation for $m(t)$. The average magnetization of the system is further defined by

$$\langle m \rangle = \frac{1}{\tau_{tot} - \tau_{eq}} \int_{\tau_{eq}}^{\tau_{tot}} m(t) dt \quad (6)$$

In Eq. (6), τ_{eq} represents the equilibrium time (200000 in our study), and τ_{tot} represents the total simulation time (1000000 steps). The susceptibility χ can be derived from the fluctuation of magnetization:

$$\chi = \frac{1}{k_B T} (\langle m^2 \rangle - \langle m \rangle^2) \quad (7)$$

As illustrated as in Fig. 2, there is a spontaneous magne-

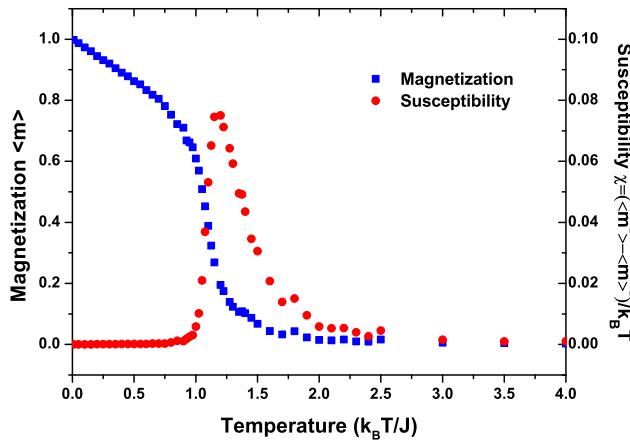


FIG. 2: Magnetization $\langle m \rangle$ and susceptibility χ under different temperatures.

tization under low temperature. Correspondingly, there is a peak for susceptibility around the temperature $1.1J/k_B < T < 1.2J/k_B$, which is well consistent with prior MC simulation.

Energy and Capacity

Similar to the derivation of magnetization, the energy of the system can be calculated by

$$\langle E \rangle = \frac{1}{\tau_{tot} - \tau_{eq}} \int_{\tau_{eq}}^{\tau_{tot}} [-J \sum_{\langle i,j \rangle} \cos(\phi_i(t) - \phi_j(t))] dt \quad (8)$$

Consequently, the heat capacity can be derived from the fluctuation of the energy

$$C_V = \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2) \quad (9)$$

The energy was found monotonically increase as a function of temperature. The slope changes fast around $\langle E \rangle \sim -1.0$ and there is correspondingly a maximum for the heat capacity (Fig. 3). The position of the peak is the same as in susceptibility. This behavior is also well consistent with MC results.

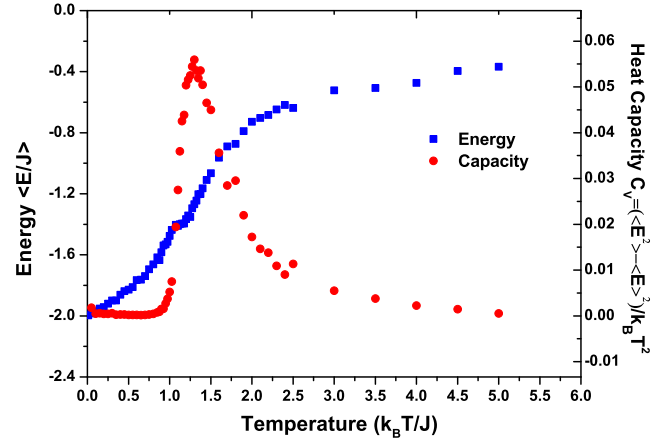


FIG. 3: Average energy per spin $\langle E \rangle$ and heat capacity C_V under different temperatures.

Correlation Function

It is known that there is a Kosterlitz-Thouless-Berezinskii (KBT) transition ([4] and references therein) for the 2-dimensional XY model. There exist two phases: (i) Under low temperature, there is a quasi-long range order phase. (ii) Under high temperature, there is a disordered phase. The correlation function is defined by

$$C(r) = \langle \vec{s}(0) \cdot \vec{s}(r) \rangle = \langle \cos(\phi(0) - \phi(r)) \rangle \quad (10)$$

The evolution of the correlation function with increasing tem-

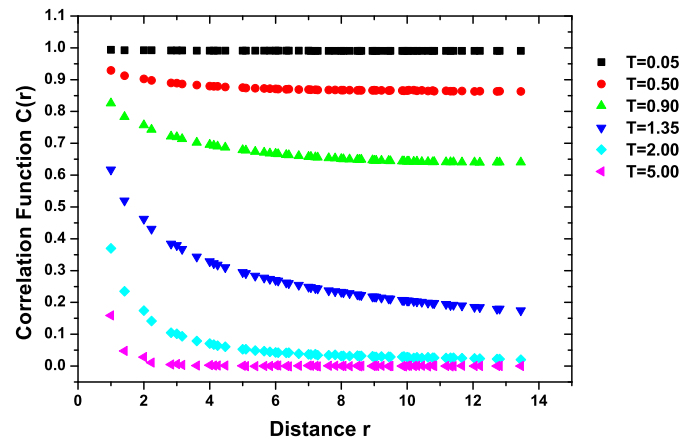


FIG. 4: The correlation function under different temperatures.

perature is shown in Fig. 4. It can be seen that under low temperature, the decaying rate of correlation function is slow, while under high temperature, the correlation decays very fast

as distance increasing. According to the theory of XY model: For low temperature phase, most spins are aligned and the correlation-function decays with a power law $C(r) \propto r^{-\eta}$. (ii) For high temperature phase, the correlation-function decays exponentially as $C(r) \propto \exp(-\frac{r}{\xi})$, where ξ is the correlation length. The critical temperature has been given by many MC simulations with the value of $T_c \approx 0.9J/k_B$. We thus derived the exponent η and correlation length ξ below and above the critical temperature, respectively. It can be seen from Fig. 5 that the exponent η slowly increases as a function of temperature and reaches the value $\eta \sim 0.1$ at the critical temperature. On the other hand, the correlation length was found diverges when approaches to critical point. The divergence exponent was fitted by -0.48 , which is well consistent with the theoretical results of -0.5 .

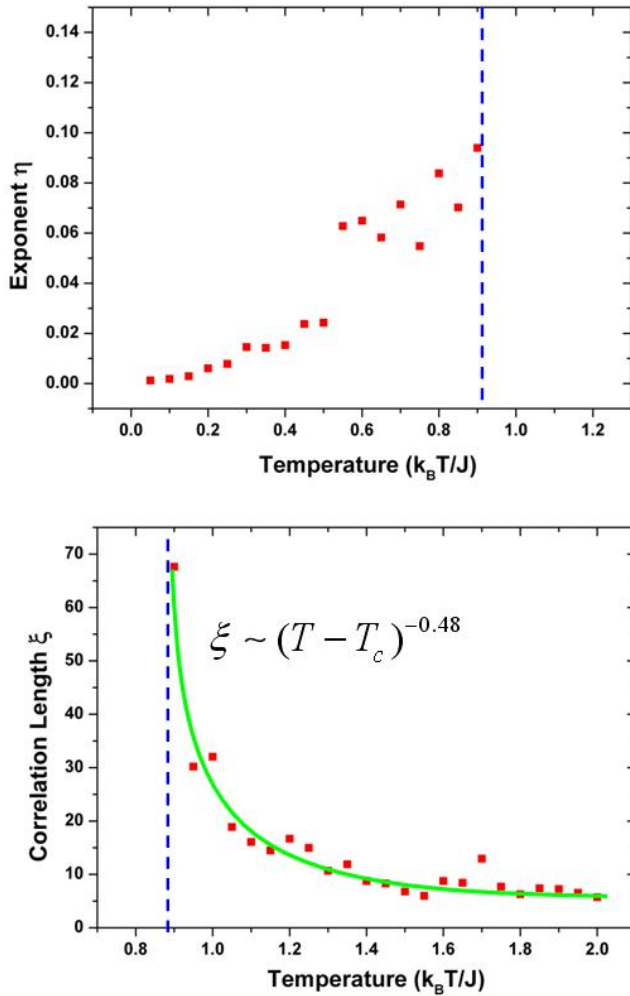


FIG. 5: Above: The relation between exponent η in the power law decay and temperature; Below: The divergence of correlation length ξ , when approaches to the critical temperature.

Mean Square Displacement

Self-correlation is an important property in the condensed matter area. In this paper, we focused on the mean square displacement (MSD). The MSD here is defined by

$$R^2(t) = \frac{1}{N} \sum_i \langle (\phi_i(0) - \phi_i(t))^2 \rangle \quad (11)$$

As described in Fig. 6, the MSD is oscillating under low tem-

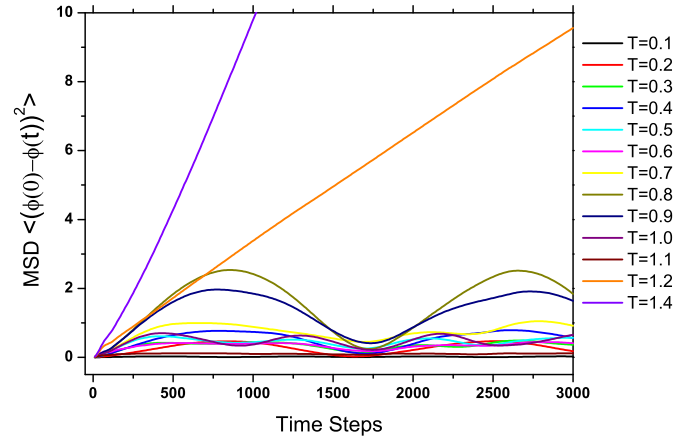


FIG. 6: The mean square displacement variations under different temperatures.

perature ($T < 1.2J/k_B$), which indicates that the spins are constrained around the balance positions. Under high temperature, on the other hand, the MSD almost linearly increases as a function of time, which is consistent with Einstein's diffusion equation $R^2(t) = 2Dt$. This behavior is very similar to the MSD in solid-liquid phase transition. It is interesting to point out that, the MSD behavior changes at $T \sim 1.2J/k_B$, the same position where susceptibility and heat capacity reach their maximum. However, this value differs from critical temperature of $T_c \approx 0.9J/k_B$

CONCLUSION

We studied the XY model by a dynamic simulation. A classical rotation energy was introduced into the traditional XY-Hamiltonian (Eq. (2)). The motion of spins are integrated according to the Velocity-Stormer-Verlet algorithm. We studied the equilibrium properties such as magnetization, susceptibility, energy and heat capacity. The correlation function was also investigated, and the corresponding exponent η and correlation length ξ were derived. All these results are consistent with prior MC simulations.

In addition, we studied the dynamic properties of XY model, which can not provided by equilibrium sampling

method, e.g. the MC simulation. Specifically, we studied the mean square displacement behavior of the system. It is found that under low temperature, the spins are oscillating around the balanced points; under high temperature, however, the MSD linearly increases as a function of temperature. The transition temperature is consistent with the peak position for susceptibility and heat capacity, however differs from the critical temperature for KBT transition. The behavior is very similar to the solid-liquid phase transition and well satisfies the Einstein diffusion relation.

The topological defects in XY model is of great importance, and is strongly related to the underlying potential energy surface of the system. There is a recent developed approach, named Autonomous Basin Climbing (ABC) Method has been proved powerful in exploring the multi-dimensional potential energy surface ([5]). Applying the ABC method to study the excitation states and associated topology will be the future work.

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