Nonequilibrium relaxation analysis of Kosterlitz-Thouless phase transition

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A simple and efficient numerical analysis is proposed for the Kosterlitz-Thouless (KT) phase transition. The nonequilibrium relaxation method is applied to it. The two-dimensional ferromagnetic XY models are investigated to show the efficiency. At the KT transition point as well as inside the KT phase, the nonequilibrium relaxation of magnetization from the all-aligned state shows an asymptotic power-law decay, $m(t) \sim t^{-\lambda(T)}$. Only outside the KT phase, an asymptotic single exponential decay is observed. Using a standard scaling form $m(t) = \tau^{-\lambda}\overline{m}(t/\tau)$ in this regime, where τ is the relaxation time at each temperature, we find a simple and efficient numerical estimation of the KT transition point and dynamical exponent. This method can be applied to various kinds of models which show the KT-like behavior.

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I. INTRODUCTION

The equilibrium Monte Carlo simulation (EMCS) is widely used in statistical physics. It has revealed much helpful information on phase transitions and critical phenomena. In most cases, analyses are made with the finite size scaling hypothesis and resulting scaling plots providing the transition temperature as well as critical exponents. However, the EMCS is sometimes confronted with difficulties in the analysis of so-called slowly relaxing systems. In low-temperature regime of frustrated systems or in critical regime of some low-dimensional systems, the relaxation becomes tremendously slow, and the simulation takes much time for equilibration [31]. This restricts the available system sizes as too small and prevents accurate estimations for the critical point and critical exponents. The development and improvement of simulation technique in past decades are mainly devoted to overcome this difficulty.

The Kosterlitz-Thouless (KT) transition [1,2] is one example to show such difficulty. In two dimensions, there exists no long range order in continuous spin systems [3], while the KT phase appears in the XY model. In this phase, there is no spontaneous magnetization but the correlation length always diverges. Since the correlation length increases exponentially as T approaches T_{KT} from the disordered phase, it is difficult to analyze large systems easily by the EMCS [4–8].

In the KT transition, another difficulty arises in the analysis of EMCS. Let us consider finite size scaling analyses with the domain-wall free energy [9], the Roomany-Wyld's β function [10] or the Binder's cumulant [11], which have been standard methods for second-order transitions. These functions change the size dependence and become scale invariant at the critical point. Therefore, data curves for several sizes plotted with respect to temperature show crossing at the transition point, and one can estimate it. On the other hand, these quantities show scale invariance in the whole KT phase as well as at the KT transition point, since the correlation length always diverges there. Then, the data curves merge below the transition point, and it becomes difficult to estimate it.

Recently, efficient Monte Carlo technique is proposed to study critical phenomena using nonequilibrium relaxation process [12–24]. It is called the nonequilibrium relaxation (NER) method. One may observe the relaxation of the order parameter (e.g., the magnetization in the ferromagnet) in the thermalization process from the complete ordered state. It provides the critical temperature and critical exponent accurately [18,21]. This analysis has been used successfully to study various problems including frustrated and/or random systems [15–18,22–24]. The NER analysis is advantageous over the EMCS in two features: First, for a fixed time t, system-size dependence of the NER function is exponentially small even at the critical point. This feature is understood from the fact that the correlation length $\xi(t)$ keeps finite at finite time. So the value in the thermodynamic limit is easily estimated. Second, equilibration step is not necessary. Simulation is made only up to the steps when the first trace of equilibrium state is caught with required accuracy. These advantages become more effective for slowly relaxing systems.

In the present paper, we investigate the NER analysis of

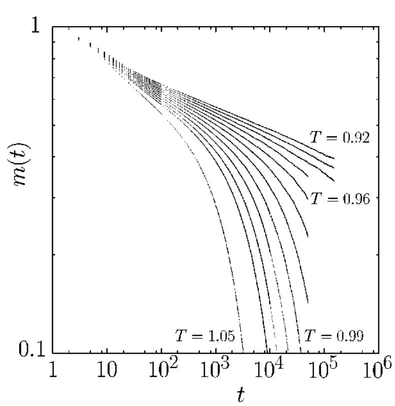

FIG. 1. The relaxation of magnetization $m(t)$ for $T = 0.92$, 0.93, 0.94, 0.95, 0.96, 0.97, 0.98, 0.99, 1.00, 1.01, 1.02, 1.05 in double-log plot.

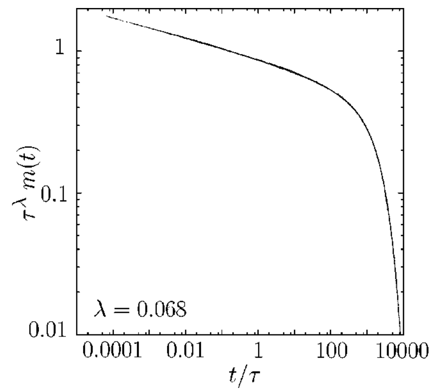

FIG. 2. Scaling plot of magnetization curves for all the temperatures in $1.05 \geqslant T \geqslant 0.92$ to Eq. (2) with appropriately chosen $\tau(\varepsilon)$ (see Fig. 3) and λ.

the KT transition. A similar analysis has already been attempted [19,20] in a different manner. Our method is simple and easy to apply to various systems. Here, we propose a scaling analysis to estimate accurate transition point and exponent with a simple and systematic procedure for very large systems. In the following section, the method is explained and is applied to the *XY* (plane rotator) model in two dimensions [1,2,4–8] to check the efficiency. It is also applied to the six-state clock model [8,25–28] in Sec. III, in which the ferromagnetic (FM)-KT transition appears, as well as the paramagnetic (PM)-KT one. Section IV is devoted to remarks.

II. NER ANALYSIS OF KT TRANSITION

The Hamiltonian of both models is written as

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j), \qquad (1)$$

where the variable θ_i takes any values in $[0,2\pi)$ for the former case and $\{(n\pi/3)\ n=0,1,\ldots,5\}$ for the latter case. We observe the relaxation of magnetization from the all-aligned state as in the analysis of the FM case. For each model, calculations are carried out mainly on the 1001×1000 square lattice with the screw boundary condition up to the observation time 1.5×10^5 MCS. About 192–640 independent runs are performed for averaging. The size dependence is checked to be negligible when we compare the data with those for 1501×1500 for some temperatures.

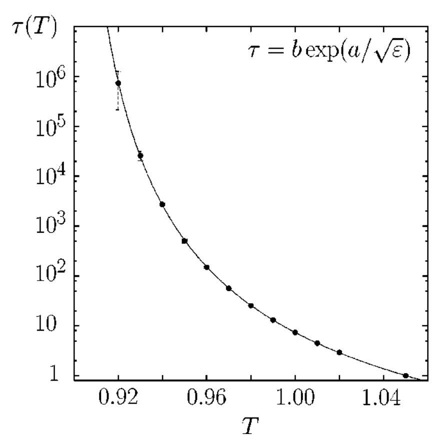

FIG. 3. Relaxation times $\tau(\varepsilon)$ in a unit of τ at $T=1.05$. The curve fitted to Eq. (3) with $T_{\mathrm{KT}}=0.894$ is shown.

TABLE I. Transition temperature T_{KT} and exponents η and λ for the *XY* model.

Ref.	T_{KT}	η	λ
[4]	0.89		
[5]	0.89(2)	0.24(3)	
[6]	0.898(2)	0.34	
[19]	0.894	0.238(4)	
[7]	0.893(8)	0.251	
[8]	0.8933(6)	0.243(5)	
Result	0.894(4)		0.068(6)

A. NER function of *XY* model

First, we show the analysis of the *XY* model. The transition of the PM and KT phases occurs at $T=T_{\mathrm{KT}}$. For efficiency of calculation, we discretize the spin state and use the 1024-states clock model. This discretization is checked to be negligible when we compare the data with the 2048-state model. The result for $1.05 \geqslant T \geqslant 0.92$ is plotted in Fig. 1; hereafter, we measure the temperature T in the unit of J/k_{B}. Similar to the scaling analysis in the EMCS, we cannot distinguish the transition point and the KT regime from the relaxation behavior directly, since it is always power-law inside the KT phase. It is much different from the NER analyses for standard second-order-transition systems. Due to the critical relaxation in the KT phase, it is not apparent whether the observed power-law behavior stays in a longer time scale. In fact, in $0.94 \geqslant T \geqslant 0.92$ in Fig. 1, which is higher than the expected T_{KT}, the relaxation behavior keeps an almost power law within the observed time $t=1.5\times 10^5$.

B. Scaling form

In Fig. 1, one can see a coherent behavior of the relaxation function $m(t)$ in the regime of $T>T_{\mathrm{KT}}$. After some

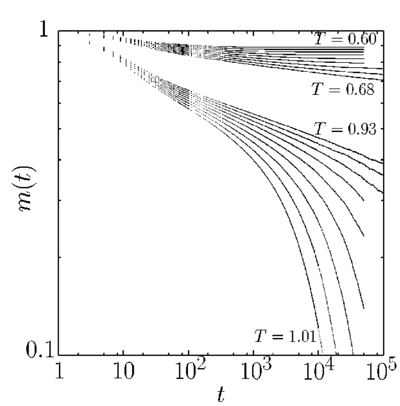

FIG. 4. The relaxation of magnetization $m(t)$ for $T=0.60$, 0.61, 0.62, 0.63, 0.64, 0.65, 0.66, 0.67, 0.68, and for 0.93, 0.94, 0.95, 0.96, 0.97, 0.98, 0.99, 1.00, 1.01 in double-log plot.

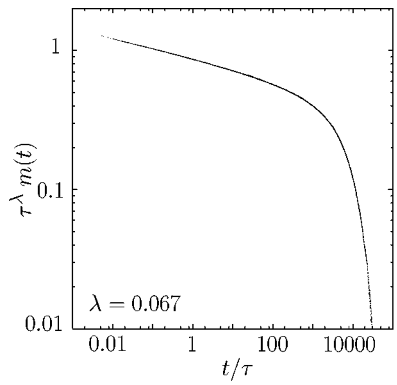

FIG. 5. Scaling plot of magnetization curves for all the temperatures in $1.01 \geq T \geq 0.93$ to Eq. (2) with appropriately chosen $\tau(\varepsilon)$ (see Fig. 6) and λ.

initial relaxation time which is about 100 MCS, it decays like in a power law up to a finite time τ, then a crossover occurs and it changes to decay exponentially. The time scale τ is called the relaxation time depending on the temperature. Therefore, it is natural to expect the scaling form [18] for the PM regime;

$$m(t,\varepsilon) = \tau(\varepsilon)^{-\lambda}\overline{m}(t/\tau(\varepsilon)) \quad \left(\varepsilon \equiv \frac{|T-T_{\mathrm{KT}}|}{T_{\mathrm{KT}}}\right), \tag{2}$$

where λ is the dynamic exponent. We use this scaling form to estimate T_{KT} precisely from the NER function. This method is similar to that used in low-dimensional quantum systems [29,30], in which the correlation function and resulting correlation length are used instead of the relaxation function and the relaxation time. First, we estimate $\tau(\varepsilon)$ at each temperature using the scaling form (2). We plot $\tau^\lambda m$ as a function of t/τ in the double-log scale with independent scaling parameters λ and τ. In this fitting, it is somehow easy to decide the best fitting parameters, since changing the parameter τ causes just the parallel translation of curve. Precisely speaking, since λ is a constant independent of temperature, we first fix λ, and estimate τ at each temperature. It is repeated for several values of λ. The best value of λ is determined by minimizing the total amount of fitting residual. The result with $\lambda = 0.068(6)$ is shown in Fig. 2. The estimated τ are plotted in Fig. 3.

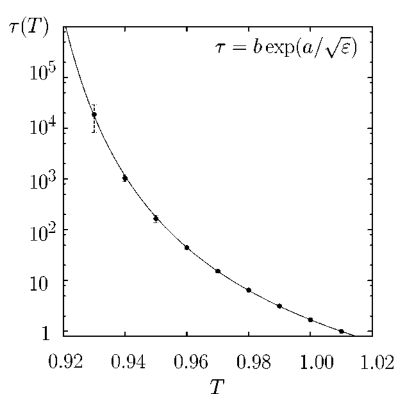

FIG. 6. Relaxation times $\tau(\varepsilon)$ in a unit of τ at $T = 1.01$. The curve fitted to Eq. (3) with $T_{\mathrm{KT}} = 0.899$ is shown.

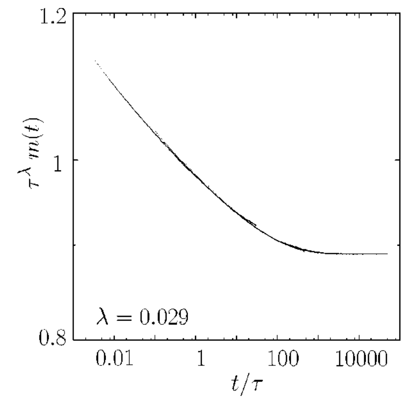

FIG. 7. Scaling plot of magnetization curves for all the temperatures in $0.68 \geq T \geq 0.60$ to Eq. (2) with appropriately chosen $\tau(\varepsilon)$ (see Fig. 8) and λ.

C. Estimation of T_{KT}

Next, we estimate T_{KT} from the estimated $\tau(\varepsilon)$. As T approaches T_{KT}, the correlation length diverges exponentially as $\xi \sim \exp(a'/\sqrt{\varepsilon})$ [1,2]. We expect that the relaxation time diverges in the same way;

$$\tau(\varepsilon) = b\,\exp(a/\sqrt{\varepsilon}), \tag{3}$$

instead of power-law divergence in standard second-order transitions. It is reasonable if one assumes the relation $\tau \sim \xi^z$ with a definite value of z. Using the χ^2 fitting with parameters a, b, and T_{KT}, we obtain the best fitting as shown in Fig. 3 with $T_{\mathrm{KT}} = 0.894(4)$. The result is summarized in Table I together with those obtained so far. The transition temperature is estimated with high accuracy and is consistent to those obtained by the EMCS. Assuming the dynamic scaling hypothesis, the exponent λ is related to other standard exponents as

$$\lambda = \eta/2z. \tag{4}$$

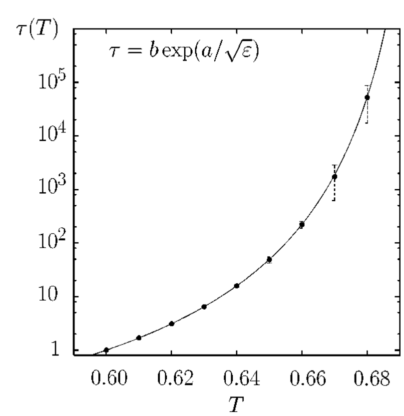

FIG. 8. Relaxation times $\tau(\varepsilon)$ in a unit of τ at $T = 0.60$. The curve fitted to Eq. (3) with $T_{\mathrm{KT}} = 0.704$ is shown.

TABLE II. Transition temperatures and exponents for the six-state clock model.

Ref.	T_{KT2}	η	λ	T_{KT1}	η	λ
[26]	0.6	0.10		1.3		
[27]	0.68(2)	0.100(2)		0.92(1)	0.275(25)	
[28]	0.75	0.15		0.90	0.26	
[28]	0.7014(11)	0.113(3)		0.9008(6)	0.243(4)	
Result	0.704(5)		0.029(3)	0.899(5)		0.067(6)

If one assumes the KT's prediction, $\eta=1/4$, this reveals the estimation for the dynamical exponent $z=1.84(17)$.

III. SIX-STATE CLOCK MODEL

The same analysis is applied to the six-state clock model, which is a discrete-state version of the XY model. In the q-state clock model in two dimensions with $q\geqslant 5$, it is pointed out that there exist successive phase transitions of PM-KT-FM phases [25] at $T=T_{KT1}$ and $T=T_{KT2}<T_{KT1}$. To analyze both transitions, we calculate the relaxation of magnetization in $1.01\geqslant T\geqslant 0.60$. The results are plotted in Fig. 4. For the higher transition point $T=T_{KT1}$, the scaling plot of the data in $1.01\geqslant T\geqslant 0.93$ fitted to Eq. (2) with $\lambda=0.067(6)$ is shown in Fig. 5. The estimated relaxation times are plotted in Fig. 6. The χ^2 fitting to Eq. (3) is also shown with $T_{KT1}=0.899(5)$.

It is noted that the scaling relation [Eq. (2)] can be applied to the FM-KT transition point as well as to the PM-KT one. Thus, we analyze the lower transition point at $T=T_{KT2}$. The scaling plot of the data in $0.68\geqslant T\geqslant 0.60$ fitted to Eq. (2) with $\lambda=0.029(3)$ is shown in Fig. 7. The estimated relaxation times are plotted in Fig. 8. The χ^2 fitting to Eq. (3) is also shown with $T_{KT2}=0.704(5)$. The results are summarized in Table II. The transition temperatures are also estimated with high accuracy and are consistent with those obtained by the EMCS. If one assumes the expected values $\eta=1/4$ at $T=T_{KT1}$ and $\eta=1/9$ at $T=T_{KT2}$ [25] with Eq. (4), it is provided that the estimations for the dynamical exponent are $z=1.87(18)$ and $1.92(22)$, respectively.

IV. REMARKS

We propose a nonequilibrium relaxation analysis of the KT transition. The scaling relations [Eqs. (2) and (3)] are used. It provides a systematic procedure for accurate estimations of the transition temperature and exponent. One can analyze very large sizes even in slowly relaxing systems since the equilibration is not necessary. We apply the method to the FM XY model and six-state clock model and obtain the transition temperatures and dynamical exponents in Tables I and II, which are consistent with those obtained so far. It is remarkable that the simulated size 1001×1000 is much larger than those calculated in equilibrium simulations. This method is simple and it can be applied to various kinds of models which show the KT-like behavior.

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[30] K. Nomura and K. Okamoto, J. Phys. A **27**, 5773 (1994).
[31] The total amount of calculation time consists of equilibration and averaging, and it is proportional to the equilibration time, since, usually, the averaging time is taken several times the equilibration one. The equilibration from a fixed nonequilibrium state is achieved when the spin correlation grows up to the scale of the equilibrium correlation length or the system size. In the critical regime, since the correlation length becomes larger than simulated sizes, the equilibration time becomes longer as the system size is larger. Therefore, available sizes of system are reduced in slowly relaxing systems.