Six-state clock model on the square lattice: Fisher zero approach with Wang-Landau sampling

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We investigate the six-state clock model with nearest-neighbor interactions on the square lattice. We obtain the density of states of the finite systems up to $L=28$ using the Wang-Landau sampling. With the density of states and the Fisher zero approach, we successfully find two different critical temperatures 0.632(2) and 0.997(2) for the clock model. It seems that this study supports the recent results by [Lapilli *et al.* Phys. Rev. Lett. **96**, 140603 (2006)] that the transitions are not of Kosterlitz and Thouless type.

I. INTRODUCTION

The classical two-dimensional (2D) p-state clock model, a discrete version of the 2D *XY* model, has been investigated [1–15] since Kosterlitz and Thouless showed that the *XY* model has a type of critical behavior with essential singularities and topological ordering, so called, the Kosterlitz-Thouless (KT) phase transition [16,17]. The 2D p-state clock model for sufficiently large p has been also known to have a KT critical region at intermediate temperatures between the low-temperature (T_1) ferromagnetic phase and the high-temperature (T_2) paramagnetic phase [5,10,13–15]. However, contrary to the prior results a recent study [1] shows that for $p \leq 6$ the transition at T_2 is not a KT one and for all finite p not a KT transition at T_1, either.

In 1952, Yang and Lee proposed a mechanism for the occurrence of phase transitions in the thermodynamic limit [18,19]. Introducing an exponential variable, they treated the partition function as a polynomial equation. They suggest that the real axis crossing of the complex zero set of the polynomial is directly related to the phase transition in the thermodynamic limit. They illustrated their mechanism by solving exactly the lattice gas (ferromagnetic Ising model in a magnetic field) problem. Later on, this approach has been extended to treating other exponential variables such as the exponential term including temperature by Fisher and others along with computational developments [20].

Recent computational developments enabled researchers to get the exact or approximate density of states (DOS) of finite systems [21–30]. However, the extraction of the density of zeros for a finite and numerically accessible lattice had been considered very difficult. In recent years, there have been some attempts to overcome the difficulties [31]. Exact DOS can be obtained only for very finite systems like up to the linear size $L=9$ for the bipartite system on the two-dimensional triangular lattices with nearest-neighbor interactions [32]. However, approximate methods such as the Wang-Landau sampling [21,23–25] can obtain DOS of the quite large finite systems, for example, up to $L=36$ for the bipartite system on the two-dimensional triangular lattices with nearest-neighbor interactions [32].

In this Brief Reports, we investigate the six-state clock model with nearest \-neighbor interactions on the square lattice. We obtain the DOS of the finite systems up to $L=28$ using the Wang-Landau sampling. With the DOS and the Fisher zero approach, we analyze the phase transitions at T_1 and T_2. In addition, with conventional methods [33,34] we

analyze the transition temperatures also. In discussions and conclusions, we try to elucidate whether the transition types at both critical temperatures are of KT type or not.

II. MODEL AND TRANSITION TEMPERATURES WITH FISH ZERO APPROACH

The Hamiltonian of the six-state clock model without magnetic fields reads

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

where J is the exchange coupling constant, the summation over nearest-neighbor pairs on the square lattice and $\theta_i = 2\pi n_i/6$ with $n_i = 0, 1, \ldots, 5$. The Hamiltonian is invariant under the symmetries of the global spin rotation $U(1)$ and the global spin reflection Z_2. Therefore, on the square lattice without magnetic fields there is no difference between ferromagnets and antiferromagnets.

In Fig. 1, as an example we show energy DOS of the system size $L=20$. It is noted that the energy DOS is symmetric in energy, which indicates that there is no difference between ferromagnets and antiferromagnets. From DOS, we construct the high-degree polynomial for the Fisher zero set [20]. Typical zeros in the complex temperature plane are shown in Fig. 2(a). In the red (color online) circle, we can observe that there are two pairs of peaks toward the real axis. The two pairs of peaks [42] correspond to the two phase transition temperatures $T_1(L)$ and $T_2(L)$ for the finite system size $L=12$.

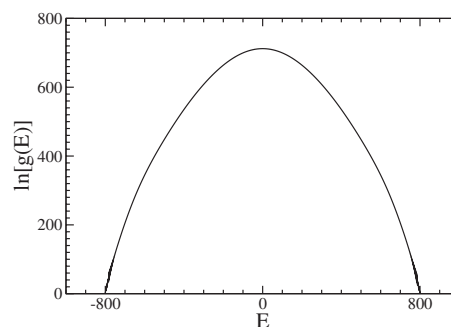There are shown in Fig. 2(b) the first Fisher zeros a_1 in the complex temperature plane for the system sizes

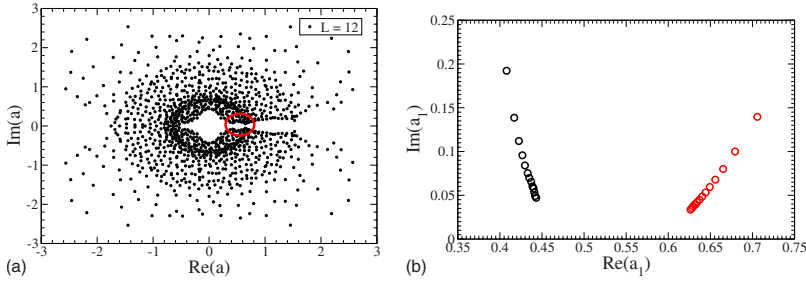FIG. 1. Energy DOS for the system size $L=20$. The energy is in units of J.

FIG. 2. (Color online) (a) Fisher zeros in the complex temperature plane of the six-state clock model for the system size $L=12$: $a=e^{-2\beta J}$. In the circle, we can observe that there are two pairs of peaks (first zeros) toward the real axis. (b) First Fisher zeros a_1 of the six-state clock model in the complex temperature plane for the system sizes $L=4-28$.
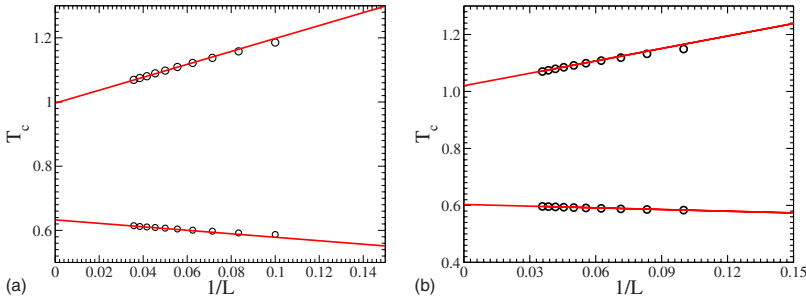

FIG. 3. (Color online) Plots of $T_c(1/L)$ of the six-state clock Ising model for $L=10-28$. $T_c(1/L)$ was obtained (a) from the Fisher zeros and (b) from the maximum positions of specific heat. (a) $T_1=0.632(2)$ and $T_2=0.997(2)$, (b) $T_1=0.6068(1)$ and $T_2=1.017(1)$ in the limit $L\rightarrow\infty$ were obtained from the finite-size scaling of $L=20-28$.
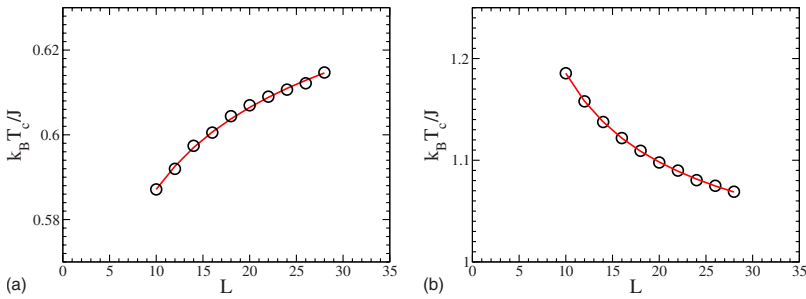

FIG. 4. (Color online) Low (right figure) and high (left figure) critical temperature $T_c(L)$ vs system size L from Fisher zeros using the KT form. We estimate the two KT temperatures as 0.74 and 0.88 from the finite-size scaling of $L=10-28$.
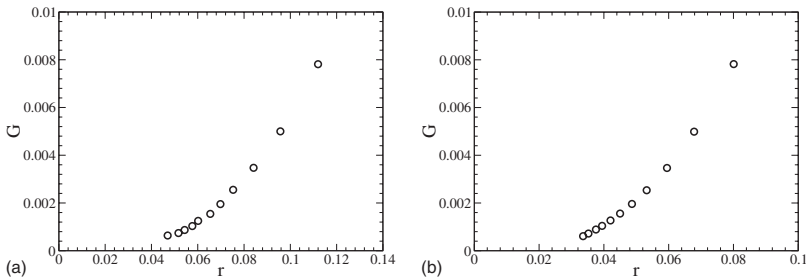

FIG. 5. Distribution of first Fisher zeros of low (right figure) and high (left figure) critical temperature for the system sizes $L=8-28$. Here, $G=1/(2L^2)$ and r is the imaginary part of the first Fisher zero a_1.
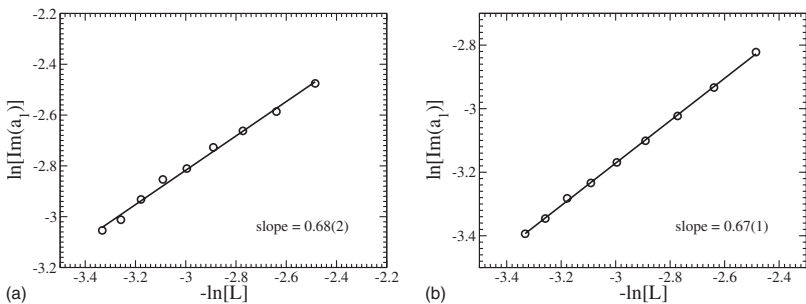

FIG. 6. Thermal scaling exponent of the low (right figure) and high (left figure) critical temperature for the system sizes $L=12-28$.
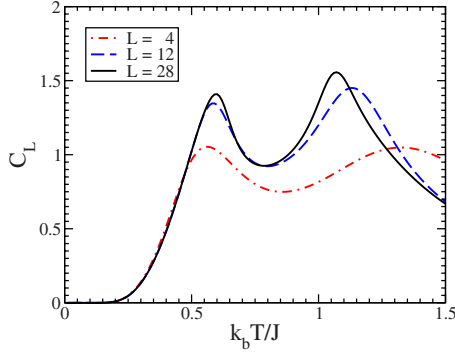
FIG. 7. (Color online) Specific heat with temperature for lattice sizes, $L=4$, 12, and 28.

$L=8-28$. It is found that the first zeros from the approximate density of states are reliable [31]. It was observed that the first Fisher zeros are not much affected by the different approximate DOS's. Also, it was noticed that the first Fisher zeros of the low-temperature phase transition is more sensitive to the approximate DOS than those of the upper one because the system is nearly ordered at the temperature [5]. The logarithm of approximate DOS, $\ln[g(E)]$, is believed to be correct in the first four or five leading digits from the comparison at the energy minimum and the next to the energy minimum.

Figure 3(a) shows the plots of $T_c(1/L)$ of the six-state clock Ising model for $L=10-28$. $T_c(1/L)$ was obtained from the Fisher zeros. $T_1=0.632(2)$ and $T_2=0.997(2)$ in the limit $L\rightarrow\infty$ were obtained from the finite-size scaling of $L=20-28$. Also, we make a finite-size scaling analysis based on the KT form [5]. According to the form, T_{KT} is given by

$$T_{KL}(L) = T_{KT} + \frac{c^2 T_{KT}}{(\ln bL)^2}. \quad (2)$$

In Fig. 4, we estimate the two KT temperatures using Eq. (2) as $T_1=0.74$ and $T_2=0.88$ from the finite-size scaling of Fisher zeros.

Janke and Kenna [31,35,36] presented a method to allow direct determination of the order and strength of phase transitions from the density of partition function zeros. Using the first Fisher zeros [35],

$$1/(2L^2) = \alpha_1 r^{\alpha_2} + \alpha_3, \quad (3)$$

where r is the imaginary part of the first Fisher zero a_1. The distribution of the first Fisher zeros are plotted in Fig. 5. For the low-temperature transition, we obtain $\alpha_2=2.78$ and $\alpha_3=$
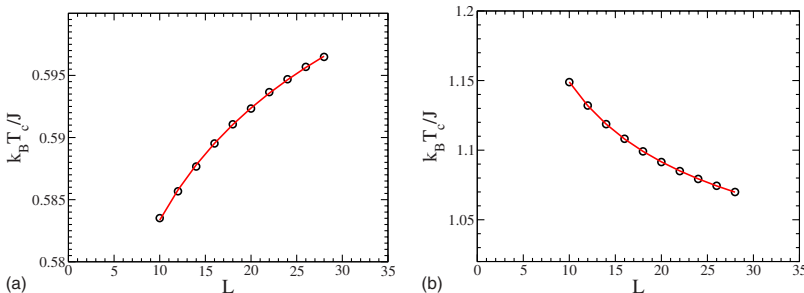
TABLE I. Transition temperatures for the 2D six-state clock model on the square lattice.

Researchers	T_1	T_2
Tobochnik [11]	0.6	1.3
Challa-Landau [10]	0.68(2)	0.92(1)
Yamagata-Ono [9]	0.68	0.90
Tomita-Okabe [5]	0.7014(11)	0.9008(6)
Our result from Fisher zeros ($L=10-28$, with KT form)	0.74	0.88
Our result from specific heat ($L=10-28$, with KT form)	0.79	0.86
Our result from Fisher zeros ($L=20-28$)	0.632(2)	0.997(2)
Our result from specific heat ($L=20-28$)	0.6068(1)	1.017(1)

-0.0002 and $\alpha_2=2.63$ and $\alpha_3=-0.0002$ for the upper temperature one. It seems that the values of α_2 and α_3 indicate the existence of a phase transition and that both transitions are not first order.

In addition, we obtain the thermal scaling exponents through the first Fisher zeros. Conventionally, the finite-size behavior of the specific-heat maximum has been used to get the critical scaling exponent $1/\nu$ and the Fisher zeros of the partition function is related to the finite-size behavior of the specific heat maximum ($y_t=1/\nu$ and see Eq. (4)) [34,37]. It is known that in the limit $L\rightarrow\infty$ the imaginary part $\text{Im}[a_1(L)]$ of the first zero behave following the finite-size scaling [38–41]

$$\text{Im}[a_1(L)] \sim L^{-y_t}. \quad (4)$$

From the above, we obtain the thermal scaling exponents of the low-temperatute and high-temperature phase transition $y_t=0.68(2)$ and $y_t=0.67(1)$, respectively (Fig. 6).

III. TRANSITION TEMPERATURES WITH CONVENTIONAL METHODS

The specific heat is calculated from the DOS

$$C_L(T) = \frac{1}{L^2 k_B T^2}[\langle E^2\rangle - \langle E\rangle^2], \quad (5)$$

and plotted in Fig. 7. We observe two peaks corresponding to the two phase transition temperatures, $T_1(L)$ and $T_2(L)$, of

FIG. 8. (Color online) Low (right figure) and high (left figure) critical temperature $T_c(L)$ vs system size L from specific heat maxima using the KT form. We estimate the two KT temperatures as 0.79 and 0.86 from the finite-size scaling of $L=10-28$.

the finite systems, $L=4$, 12 and 28. From the maximum positions of the specific heat, we obtain the critical temperatures, $T_1=0.632(2)$ and $T_2=0.997(2)$, in the limit $L\to\infty$ in Fig. 3(b), even though it is known [1] that the transitions do not occur at the peaks of C_L. Later, we will compare the results with the critical temperatures from the Fisher zero approach and discuss.

In Fig. 8, we estimate the two KT temperatures using Eq. (2) as $T_1=0.79$ and $T_2=0.86$ from the finite-size scaling of specific-heat maxima.

IV. DISCUSSIONS AND CONCLUSIONS

Table I shows all the transition temperatures of the previous research [5,9–11] and ours for the 2D six-state clock model on the square lattice. At first, it should be noted that all the previous results in the table were based on the assumption that the transitions are of KT type. As in Fig. 4, our results from Fisher zeros with KT form agree well with the previous results. Our results from Fisher zeros with a simple linear regression are not much different from the ones from specific-heat maxima with the simple linear regression. However, the critical temperatures based on the KT assumption are quite different from the estimated critical temperatures without any assumption. Recent work [1] shows that both the low-temperature transition and the high-temperature transition for the six-state clock model differ from KT. We find that this study supports the recent results by C. M. Lapilli *et al.* [1] that the transitions are not of KT type. It should be noted that our transition temperatures (approximately 0.6 and 1.0) agree well with the recent research results by C. M. Lapilli *et al.* when we assume that the transitions are not of KT type. Also, our results from specific heat agree quite well with the ones from Fisher zero approach. It should be mentioned that the thermal scaling exponents y_t support our conclusion too.

In this Brief Report, it is investigated the 2D six-state clock model with nearest-neighbor interactions on the square lattice. Using the Wang-Landau sampling, we obtain DOS of the finite systems up to $L=28$. With the DOS and the Fisher zero approach, we find two different critical temperatures (about 0.6 and 1.0) for the clock model when we assume that the transitions are not KT type. The partition function zero approach with approximate DOS from the Wang-Landau sampling is found to be very useful for locating the critical temperatures.

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