Incompletely ordered phase in the three-dimensional six-state clock model: Evidence for an absence of ordered phases of XY character

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By employing our interfacial method, which uses Monte Carlo simulations, we show in various ways that the three-dimensional six-state clock model has an incompletely ordered phase (IOP) due to entropy gains where two nearest clock-spin states are dominant with equal weight. Our obtained results strongly imply its equivalence with the three-state antiferromagnetic Potts model, confirming the absence of ordered phases of XY character and the existence of a different universality class for the upper phase transition of the IOP. The disordered flat phase recently found in the restricted solid-on-solid model is pointed out to be an IOP.

Two-dimensional (2D) clock models have been intensively studied so far,[1] but there are few studies on 3D ones. One seems to expect that high-state clock models undergo a phase transition from a disordered state to an intermediate state which shows the same critical behavior as expected in the XY model, like the 2D models with the state number larger than four.[1] However, there are no grounds for this. Besides the above question, recent studies on related models such as antiferromagnetic (AF) Potts models have also stimulated our interest in the 3D six-state clock (6CL) model with the following questions. Is it equivalent to the three-state AF Potts (3AFP) model with ferromagnetic next-nearest neighbor interactions in three dimensions in the same way as it holds in two dimensions?[2] If the answer is yes, then does it undergo a phase transition belonging to a distinct universality class as Ueno *et al.*[3] argued or a phase transition of the XY universality class as Banaver *et al.*[4] and Wang, Swendson, and Kotecký[5] argued in the 3AFP model?

Recently, we studied the 3D q-state AF Potts models by developing an interfacial approach by use of Monte Carlo (MC) simulation.[3] The MC interfacial approach has been found to have various advantages in studying properties of ordered phases as well as critical behaviors. In fact we obtained that each of these Potts models with $q=3-5$ undergoes a second-order phase transition while the $q=6$ model does not. Further we got strong suggestions that the $q=3$ and 4 models are in different universality classes; the $q=5$ model is also suggested to be in some distinct universality class, which is only a suggestion. Our results are contrary to the theoretical results obtained by Banavar *et al.*[4] who argue that equivalence between the q-state AF Potts model and the $n(=q-1)$ vector model. Very recently, Wang, Swendson and Kotecký studied the 3AFP model[5] and obtained critical exponents ν and γ which are close to the corresponding values of the $n=2$ vector model obtained by Le Guillou and Zinn-Justin.[6]

The present model is also attractive according to the suggestion from the studies in the 2D case[7] that it is closely related to the 3D stacked triangular AF Ising model with ferromagnetic next-nearest-neighbor interactions. We also studied the latter 2D model, as well as the 3D model by our interfacial method.[8] Our results clearly revealed the existence of the Kosterlitz-Thouless phase transition in two dimensions as expected, whereas in three dimensions they are contrary to the phase transition of the XY universality class. Therefore it is our main purpose to solve these problems by studying, with our interfacial method, the 6CL model with Hamiltonian

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

where $J(>0)$ is the nearest-neighbor (NN) coupling constant and $\theta_i=\pi n_i/3$ and $n_i=0,1,\ldots,5$.

Let us briefly introduce our method.[3] The *total* interfacial free energy under boundary conditions (BC) α and β is given as the excess total free energy between the systems with an interface and without interface,

$$\Delta F_{\alpha\beta}(T,L)=F_{\alpha\beta}(T,L)-F_{\alpha\alpha}(T,L)\ . \tag{2}$$

Here, our lattice has L stacked triangular planes besides the top and bottom boundary planes on which the spins are fixed according to BC, α or β. Each triangular plane is $L\times L$ in size along two different lattice axes and is under the periodic BC's. Then the stiffness exponent which plays a central role in the present study is defined by

$$\Delta F_{\alpha\beta}(T,L)\sim AL^{a_{\alpha\beta}(T)}\ . \tag{3}$$

This is the asymptotic form for $L\to\infty$ below the critical point T_c, where $a_{\alpha\beta}(T)$ becomes a constant ($a_0>0$) and this a_0 represents a measure of magnetic stiffness of the ordered phase. For $L<\infty$, owing to the finite-size effect $a(T)$ depends on T and L in the region of $L<\xi$, where ξ is the correlation length, as seen from finite-size scaling $\Delta F(T,L)=f(tL^{1/\nu})$, where $t=(T-T_c)/T_c$ and $\xi\sim|t|^{-\nu}$; $f(x)\sim x^{a_0\nu}$ for $|x|\gg 1(T<T_c)$ and f_0+f_1x for $|x|\ll 1$. However, since

$$(\partial a/\partial L)/|\partial a/\partial t|=|t|/\nu L\ll 1$$

in the critical region, the L dependence of $a(T)$ is almost negligible in the situation of usual simulations. T_c is given by $a(T_c)=0$.

In the case of two successive phase transitions with critical points T_1 and $T_2(T_1>T_2)$ as seen in the stacked triangular Ising antiferromganet[8] one has two stiffness exponents a_1 and a_2 for two ordered phases. Naturally $a_1<a_2$. Then finite-size scaling yields $\Delta F_{\alpha\beta}(T,L)=f_1(t_1L^{1/\nu_1})$ and $\Delta F_{\gamma\delta}(T,L)=L^{a_1}f_2(t_2L^{1/\nu_2})$ with appropriate BC's $\alpha\beta$ and $\gamma\delta$, respectively, for the critical regions at t_1 and T_2.

It is worth noting that our interfacial method has the excellent advantage (which has been found in this occasion) that the error of $\Delta F(T)$ is much smaller than that of each of the excess energy and entropy $\Delta E(T)$, $\Delta S(T)$, i.e.,

$$|\delta F(T)| \ll |\delta E(T)|, |\delta S(T)| .$$

In order to calculate $\Delta F(T)$ at $T<T_c$, suppose one performs MC simulations from some high-temperature $T_0(>T_c)$ down to T at intervals of ΔT to get a series of $\Delta E(T_i)$ with $i=0,1,..,n$, where $T_n=T$. Since T_0 is chosen so that $\Delta F(T_0)=0$, $\Delta S(T_0)=\Delta E(T_0)/T_0$. Then $\Delta S(T)$ is given in a simple way by

$$\Delta S(T)=\Delta S(T_0)+\sum_{i=1}^{n}[\Delta E(T_i)-\Delta E(T_{i-1})]/T_{i-1} .$$

Eventually $\delta S(T)$ becomes the same order of magnitude as $\delta E(T)$, whereas $\delta F(T)$ is reduced to $10^{-1}\sim 10^{-2}$ of δE depending on $n(T)$,

$$|\delta F(T)|<(T_0-T)/T\overline{|\delta E|}/\sqrt{n(T)} ,$$

where $\overline{|\delta E|}$ is the average of errors. This large reduction led to the results obtained previously with remarkably high accuracy, despite relatively small sizes and short simulation time.[3]

In order to consider the relations between 3D 6CL and 3AFP models, it is useful to make a cell transformation for the Potts model described by

$$\mathcal{H}_{PT}=J_1\sum\delta(\sigma_i,\sigma_j)-J_2\sum\delta(\sigma_i,\sigma_j) ,$$

where $J_1(>J_2>0)$ and J_2 are NN and next-nearest-neighbor (NNN) interactions, respectively, and σ_i takes 1, 2, and 3. We take a cubic lattice instead of the hexagonal one; otherwise one has another model with different symmetry from the 6CL one. Let us consider cells spins each of which consists of spins in a cubic of size $2\times2\times2$. Each cell has six antiferromagnetic ground states $\hat{0}\equiv(1,2)$, $\hat{1}\equiv(1,3)$, $\hat{2}\equiv(2,3)$, $\hat{3}\equiv(2,1)$, $\hat{4}\equiv(3,1)$, $\hat{5}\equiv(3,2)$, where (a,b) is the state in which Potts states a and b occupy two sublattices. In terms of cell spins $\hat{\sigma}_X$ which are assumed to take only these six states, one gets interactions $V(\hat{\sigma}_X,\hat{\sigma}_Y)$ with

$$V(\hat{0},\hat{0})<V(\hat{0},\hat{1})=V(\hat{0},\hat{5})<V(\hat{0},\hat{2})=V(\hat{0},\hat{4})<V(\hat{0},\hat{3})$$

for the NN's which have the same Z_6 symmetry as the 6CL model in Eq. (1).

Let us assume that this picture is still valid for the 3AFP model with $J_2=0$, as previously studied,[3-5] though $V(\hat{0},\hat{0})=V(\hat{0},\hat{1})=V(\hat{0},\hat{5})=0$. The ordered phase found in it has an incomplete order such that states 2 and 3 occupy one sublattice at random while state 1 occupies the other sublattice dominantly which we shall represent (1,2|3). This incompletely ordered phase (IOP) is nothing but a mixed state of (completely) ordered states $\hat{0}=(1,2)$ and $\hat{1}=(1,3)$ which are nearest. Then one can expect, in the 6CL model, such an IOP as state 0|1 where clock states 0 and 1 are dominant with equal weight. This phase is also expected to have the same nonintegral stiffness exponent $a\simeq1.25$ as obtained in the 3AFP model.[3]

Now we apply our method to the 6CL model. We impose three different BC's: with one boundary fixed in state 0, the other is fixed in 1, 2, and 3, respectively, i.e., $\alpha\beta=01$, 02, 03. If there appears an ordered phase of XY character its stiffness exponent should be 1 irrespective of these BC's, $a_{01}=a_{02}=a_{03}=1$. On the other hand, if the IOP exists then $a_{01}<0$ and a_{02}, $a_{03}>0$ are required for the existence of state 0|1. We have performed MC simulations using a standard single-spin-flip Metropolis algorithm for the systems of size $L=12$, 16, 18, 21, 24 with $5\sim20\times10^3$ MC steps/spin at each measuring temperature of interval $\Delta T=0.1$ (in the unit of $J=1$); the thermal average was done after discarding the initial data of 30%.

When comparing ΔF_{01} with ΔF_{02} and ΔF_{03} on their T dependence we have found distinct differences between $T\simeq2.0$ and 3.0 though ΔF_{02} and ΔF_{03} show the same behavior. It is more clearly seen in th T dependence of the stiffness exponent in Fig 1. The curves for BC's 02 and 03 behave very similarly making a step at intermediate temperatures and vanishing at the same critical point $T_I\simeq3.03$. On the other hand, the curve for BC 01 decreases monotonously with T rising and vanishes at another critical point $T_M\simeq2.73$. It is remarkable that $a_{03}(T)\simeq1.25$ at $2.4\lesssim T\lesssim2.8$, in agreement with the result for the 3AFP model ($a\simeq1.25$). We have made another calculation with different random numbers and obtained almost the same results as in Fig. 1, with $T_I\simeq3.03$, $T_M\simeq2.71$ and $a_{03}\simeq1.23$ at $2.4\lesssim T\lesssim2.9$ except

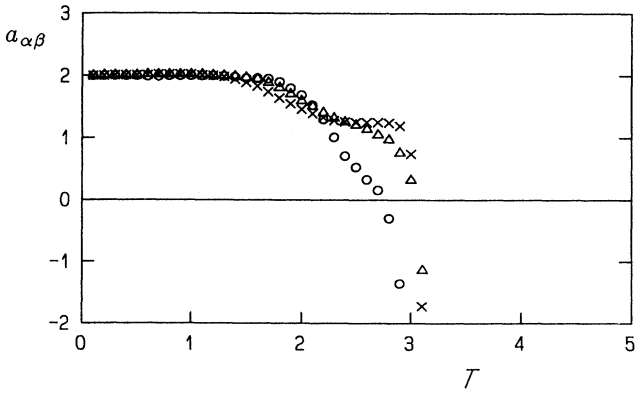

FIG. 1. Stiffness exponent vs temperature for the systems with BC's 01 (○), 02 (△), and 03 (×).

that the data of a_0 at $2.1<T<2.7$ describe a little concave curve contrary to those in Fig. 1. These results clearly deny the existence of the ordered phase of XY character and strongly support the existence of the same IOP as found in the 3AFP model, suggesting the equivalence of both models.

Let us closely consider the IOP which has $a_{01}<0$ and a_{02}, $a_{03}>0$. $a_{01}<0$ means there is no interface tension between domains which are in NN states; strictly speaking the free energy for a domain wall decreases as the domain gets larger in size. However, there is interface tension between domains in the states more distant than the nearest neighbors. Thus one gets a state distribution function for the IOP, where two NN states are dominant as given in Fig. 2. These are in contrast to the properties of the low-temperature phase (LTP) where only one state is dominant and $a_{01}=a_{02}=a_{03}=d-1$. These characteristics are also confirmed in the interface profiles of each state for the system of $L=24$ with BC 02 as shown in Fig. 3. These profiles were taken instantaneously to avoid the ambiguity that comes from the displacement of the interface as a whole. Nevertheless, one can consider that they are almost in thermal equilibrium because the values of the profiles at each point are the ones averaged over 24×24 lattice points. At $T=2.1$ the profiles of states 0, 1, and 2 cross with each other with a gentle slope, indicating diffuse interfaces. At $T=2.8$ where the IOP exists, there are distinct regions where states 0 and 1, 1 and 2 coexist with equal weight, whereas states 0 and 2 still repel each other. This can be simply explained by considering the differences in the energy levels of the NN interactions: the difference between states 0 and 2 is three times larger than the one between 0 and 1. Thus in the IOP thermal fluctuation can get over the lowest-energy barrier but is repelled by the other energy barriers.

In order to see the correlation among spin states in the IOP we have also calculated the susceptibilities X_{01} and X_{15}, where

$$X_{\alpha\beta}=N^{-1}\sum_{ij}[\langle\delta(\sigma_i,\alpha)\delta(\sigma_j,\beta)\rangle - \langle\delta(\sigma_i,\alpha)\rangle\langle\delta(\sigma_j,\beta)\rangle] .$$

BC 00 was imposed because with the periodic BC fluctuation had been too large to get definite results in the IOP region. With very small absolute values X_{01} is negative and positive at low and high temperatures, respectively, while it fluctuates weak without regular size dependence between $T\simeq2.4$ and 3.0. In contrast X_{15} is very large with the negative sign and strongly size dependent between $T\simeq2.4$ and 3.0. These results are all consistent with the properties and the picture of the IOP given above.

In order to ensure the equivalence of both the 6CL and 3AFP models, we have estimated critical exponent ν for the IOP transition applying finite-size scaling for $\Delta F_{03}(T)$ at $2.6<T<T_I$, and obtained $\nu=0.57\pm0.03$. This value is very close to 0.58 ± 0.01 for the 3AFP model[3] and 0.57 ± 0.03 for the 3D stacked triangular AF Ising model (which has an IOP with $a_1\simeq1.25$),[8] but obviously far

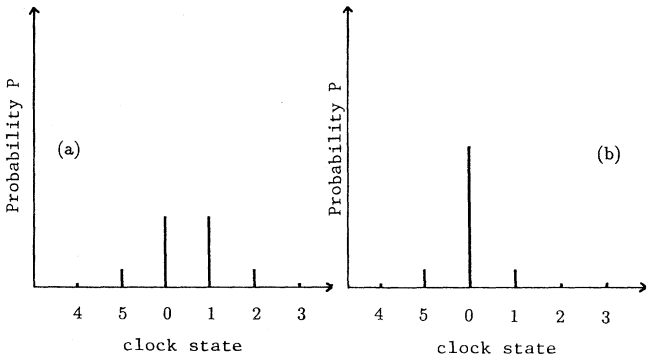

FIG. 2. State distribution functions (probability P vs clock state) expected for the IOP (a) and LTP (b).

from 0.669 for the XY model.[6] All the results obtained here strongly imply the equivalence of both models. Further, no wonder that the IOP transition is in a distinct universality class[3] because the IOP is a different type of order.

It is of considerable interest to consider other phase transition from the IOP to the LTP. It is remarkable to observe that this has an extremely large critical region ranging roughly from T_M to $T\simeq1.2$, where a becomes 2, i.e., $1>T/T_M>0.44$. This extreme width can be explained by observing in Fig. 2 that the symmetry of the LTP is not a subgroup of the IOP and *vice versa*. There-

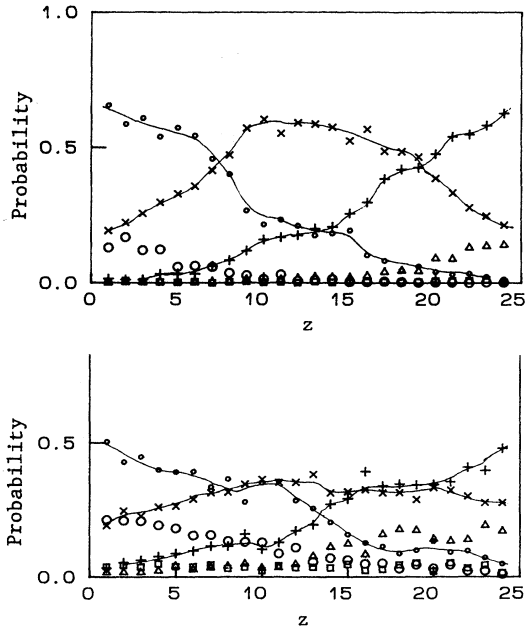

FIG. 3. Interface profiles along the triangular plane axis z for the system of $L=24$ with BC 02 at $T=2.1$ (upper) and 2.8 (lower) where the symbols represent the clock states: 0 (∘), 1 (×), 2 (+), 3 (△), 4 (□), 5 (○). Thin curves are guides to the eye.

fore, this transition cannot finish in an infinitesimal change of the state. In other words, there is a large temperature region where both the phases coexist. This is a new type of second-order phase transition which does not undergo the usual symmetry change considered by Landau.[9]

It was already shown that the phase transitions in the 3D AF Potts models of $q=3$, 4, and 5 with $J_2=0$ are completely due to entropy gains.[3] They exhibit characteristic T dependence of ΔS starting $\Delta S<0$ at $T=0$ and making a sharp peak at some temperature near T_c. We have also obtained in the 6CL model with BC 03 the same behavior above $T\simeq 2.4$ except that $\Delta S>0$. As already suggested the IOP is maintained by the entropy gained within the region of phase space limited by the second lowest energy barrier, or the entropy for partitioning the system into domains in a pair of NN states. Thus the present study has clarified that entropy-gained phase transitions can occur even in other models than those which have frustrations[10,8] or highly degenerate ground states.[3]

There exist other kinds of IOP's in the four- and five-state AFP models which have $a_1\simeq 1.85$ and 0.66, respectively.[3] Further, the IOP found here looks very similar to the disordered flat (DOF) phase found recently in the restricted-solid-on-solid model for the roughening of crystal surfaces.[11] It is a surface consisting dominantly of two nearest heights with the average height of a half-integer which is stabilized by entropy and NNN interactions. The height distribution functions for the rough, DOF and flat phases correspond well to the state distribution functions for the disordered phase, the IOP, and the LTP of the 6CL model, respectively (see Fig. 2). Therefore, the DOF phase itself is an IOP. It is as well equivalent[11] to the valence-bond-solid phase in quantum spin chains.[12] In the 3D general 6CL model, since it includes the ferromagnetic six-state Potts model[13] that undergoes a first-order transition, the IOP region is expected to shrink to the first-order transition surface. This is quite reasonable in view of the role entropy plays in the temperature-driven first-order transition. In this way, entropy plays a crucial role in IOP's and entropy-gained phase transitions, and they seem to exist much more than expected but unexplored.

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