Ordered phase and scaling in Z_n models and the three-state antiferromagnetic Potts model in three dimensions

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Based on a renormalization-group picture of Z_n symmetric models in three dimensions, we derive a scaling law for the Z_n order parameter in the ordered phase. An existing Monte Carlo calculation on the three-state antiferromagnetic Potts model, which has the effective Z_6 symmetry, is shown to be consistent with the proposed scaling law. It strongly supports the renormalization-group picture that there is a single massive ordered phase, although an apparently rotationally symmetric region in the intermediate temperature was observed numerically.

I. INTRODUCTION

The symmetry and the dimensionality are important factors to determine the universality class of critical phenomena. The $O(2)$ symmetry is the simplest among the continuous symmetry, and statistical models with the $O(2)$ symmetry has been studied intensively. A natural question then would be the effect of the symmetry breaking from the continuous $O(2)$ to the discrete Z_n. A simple spin model with Z_n symmetry is the n-state clock model with a Hamiltonian

$$H=-\sum_{\langle j,k\rangle}\cos(\theta_j-\theta_k), \tag{1}$$

where $\langle j,k\rangle$ runs over nearest neighbors and θ_j takes integral multiples of $2\pi/n$. The standard *XY* model with $O(2)$ symmetry is defined by the Hamiltonian of the same form; the only difference is that θ takes continuous values.

The Z_n symmetry is fundamentally different from $O(2)$ because of its discrete nature. On the other hand, for large n, it is natural to expect the Z_n symmetry to have similar effects to that of the $O(2)$ symmetry. Understanding these two apparently contradictory aspects is an interesting problem. Besides the theoretical motivation, there are some possible experimental realizations of the effective Z_n symmetry. For example, the stacked triangular antiferromagnetic Ising (STI) model with effective Z_6 symmetry may correspond to materials such as[1] $CsMnI_3$.

In two dimensions, the phase diagram of the Z_n model is well understood[2] in the framework of the renormalization group (RG). For $n\geqslant 5$, there is an intermediate phase between the low-temperature ordered phase with the spontaneously broken Z_n symmetry and the high-temperature disordered phase. The intermediate phase is $O(2)$ symmetric and corresponds to the low-temperature phase of the *XY* model.

In the three-dimensional (3D) case, Blankschtein *et al.*[3] in 1984 proposed an RG picture of the Z_6 models, to discuss the STI model. They suggested that the transition between the ordered and disordered phases belongs to the (3D) *XY* universality class, and that the ordered phase reflects the symmetry breaking to Z_6 in a large enough system. It means that there is no finite region of rotationally symmetric phase which is similar to the ordered phase of the *XY* model. Unfortunately, their paper is apparently not widely known in the related fields. It might be partly because their discussion was very brief and not quite clear.

In fact, there has been a long-standing controversy on the the three-state antiferromagnetic Potts (AFP) model on a simple cubic lattice, defined by the Hamiltonian

$$H=+\sum_{\langle j,k\rangle}\delta_{\sigma_j\sigma_k}, \tag{2}$$

where $\sigma_j=0,1,2$ and $\langle j,k\rangle$ runs over nearest-neighbor pairs on a simple cubic lattice. Due to the frustration, the order parameter of this model is not evident. However, previous studies revealed that the low-temperature ordered phase, which is called as BSS phase, corresponds to a spontaneous breaking of the Z_6 symmetry.[4] Thus the effective symmetry of this model may be regarded[5] as Z_6, although it is not apparent in the model. It is now widely accepted that there is a phase transition with critical exponents characterized by the 3D *XY* universality class,[8–12] at temperature $T_c\sim 1.23$ (we set the Boltzmann constant $k_B=1$.) On the other hand, according to numerical calculations, there appears to be an intermediate phase below T_c and above the low-temperature phase. While there have been various proposals[5–7] for the intermediate region, most reliable numerical results at present indicate that the intermediate region appears to be a rotationally symmetric phase which is similar to the ordered phase of the 3D *XY* model.[10–12] However, the ''transition'' between the intermediate region and the low-temperature phase is not well understood. According to the suggestion in Ref. 3, the intermediate ''phase'' would be rather a crossover to the low-temperature massive phase.

On the other hand, there has been a claim of an intermediate phase[13] also in the six-state clock (6CL) model, which has the manifest Z_6 symmetry. In a recent detailed numerical study, Miyashita[14] found that the intermediate region appears to have a rotationally symmetric character, as found in the AFP model. However, through a careful examination of the system size dependence, he concluded that it is just a crossover to the massive low-temperature phase, and that the rotationally symmetric *XY* phase does not exist in the thermodynamic limit. His conclusion is consistent with the suggestion in Ref. 3.

In this article, based on the RG picture, we derive a scaling law of an order parameter which measures the effect of symmetry breaking from $O(2)$ to Z_n. We demonstrate that the Monte Carlo results on the AFP model in Ref. 11 is consistent with the scaling law, supporting the RG picture with a single phase transition.

II. RENORMALIZATION-GROUP PICTURE

Since the discussion of the RG picture in Ref. 3 was rather brief, it would be worthwhile to present the RG picture here, with some clarifications and more details. We also make a straightforward extension to general integer n from the $n=6$ case.

A generic Z_n symmetric model may be mapped, in the long-distance limit, to the following Φ^4-type field theory with the Euclidean action

$$S=\int d^3x[|\partial_\mu\Phi|^2+u|\Phi|^2+g|\Phi|^4-\lambda_n(\Phi^n+\bar{\Phi}^n)] \quad (3)$$

with the complex field Φ and its conjugate $\bar{\Phi}$. The λ_n term is the lowest-order term in Φ which breaks the symmetry from $O(2)$ to Z_n. The phase transition corresponds to the vanishing of (the renormalized value of) the parameter u. The temperature T in the Z_n statistical system roughly corresponds to u as $u\sim T-T_c$ where T_c is the critical temperature.

In the absence of the symmetry breaking λ_n, the transition belongs to the so-called 3D *XY* universality class. Its stability under the symmetry breaking to Z_n is determined by the scaling dimension of λ_n at the 3D *XY* fixed point. It may be estimated with the standard ϵ-expansion method.

The lowest-order result in ϵ can be easily obtained from the operator product expansion (OPE) coefficients.[15] As a result, we obtain the scaling dimension y_n of λ_n in $4-\epsilon$ dimensions as

$$y_n=4-n+\epsilon\left(\frac{n}{2}-1-\frac{n(n-1)}{10}\right)+O(\epsilon^2). \quad (4)$$

y_n is defined so that the effective strength of the perturbation $\lambda_n(l)$ at scale l is proportional to l^{y_n} near the *XY* fixed point. The case $n=4$ is actually the special case $N=2$ of the ''cubic anisotropy'' on the 3D $O(N)$ fixed point.[15] Extrapolating the $O(\epsilon)$ result to 3D ($\epsilon=1$), we see that the Z_n perturbation is irrelevant at the 3D *XY* fixed point for $n\geq n_c$. The threshold n_c is estimated to be 4 in $O(\epsilon)$ In fact, $n=2$ and $n=3$ corresponds to the 3D Ising and three-state (ferromagnetic) Potts model, which do not belong to *XY* universality class. Thus n_c is expected to be at least 4. This is consistent with the above result from $O(\epsilon)$. However, extrapolating the lowest-order result in ϵ to 3D ($\epsilon=1$) is not quite reliable; the true value of n_c might be larger than 4. On the other hand, we can make the following observation. For $n\geq 6$, λ_n is marginal or irrelevant at the 3D Gaussian fixed point ($g=0$). Thus it is natural to expect them to be irrelevant at the more stable 3D *XY* fixed point, namely $n_c\leq 6$. In fact, the numerical observation of the 3D *XY* universality class in 6CL and AFP model strongly suggests that λ_6 is irrelevant at the *XY* fixed point and hence $n_c\leq 6$. In the following, we restrict the discussion to the irrelevant case $n\geq n_c$.

For the $O(2)$ symmetric case $\lambda_n=0$, low-temperature phase $u<0$ is renormalized to the low-temperature fixed point. It describes the massless Nambu-Goldstone (NG) modes on the ground state with the spontaneously broken $O(2)$ symmetry. Let us call the low-temperature fixed point as NG fixed point. In terms of the field theory, it is described by the $O(2)$ sigma model (free massless boson field)

$$S=\int d^3x\frac{K}{2}(\partial_\mu\phi)^2, \quad (5)$$

where ϕ is the angular variable $\Phi\sim|\Phi|e^{i\phi}$. Namely, only the angular mode ϕ remains gapless as a NG boson. In three dimensions, the coupling constant K renormalizes proportional to the scale l, and goes to infinity in the low-energy limit. The coupling constant may be absorbed by using the rescaled field $\theta=\sqrt{K}(\phi-\phi_0)$ so that the action is always written as $\int d^3x(\partial_\mu\theta)^2/2$.

Now let us consider effects of the symmetry breaking λ_n. The symmetry breaking term can be written as $-\lambda_n(\Phi^n+\bar{\Phi}^n)=-\lambda_n|\Phi|^n\cos n\phi$. Using the rescaled field θ, the total effective action at scale l becomes

$$S=\int d^3x\frac{1}{2}(\partial_\mu\theta)^2-\lambda_nK^3\int d^3x\cos\left[n\left(\phi_0+\frac{\theta}{\sqrt{K}}\right)\right], \quad (6)$$

where the factor $K^3\sim l^3$ comes from the scale transformation of the integration measure. In the thermodynamic limit, we should take $K\to\infty$ limit. Physically, it means that the $O(2)$ symmetry is spontaneously broken so that the angle is fixed to some value ϕ_0 in a single infinite system. Then the Taylor expansion of the cosine in $\theta/\sqrt{K}$ becomes valid:

$$K^3\cos\left[n\left(\phi_0+\frac{\theta}{\sqrt{K}}\right)\right]=\sum_{j=0}^{\infty}c_jK^{3-j/2}\theta^j, \quad (7)$$

where

$$c_{2k}=(-1)^k\frac{n^{2k}}{(2k)!}\cos n\phi_0,$$

$$c_{2k+1}=-(-1)^k\frac{n^{2k+1}}{(2k+1)!}\sin n\phi_0 \quad (8)$$

for a nonnegative integer k. The five terms $j=1,\ldots 5$ are relevant perturbations. For any value of ϕ_0, some of the coefficients c_j of these relevant terms are nonvanishing. We therefore conclude that, unlike the 2D case, the Z_n perturbation is always relevant for any value of n at the NG fixed point. We emphasize that this conclusion is universal in three

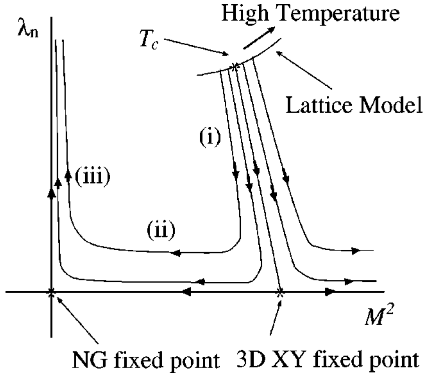

FIG. 1. The RG flow diagram of the Z_n models, projected onto the two-dimensional parameter space spanned by u and λ_n. The Z_n perturbation λ_n is irrelevant at the 3D *XY* fixed point, but is relevant at the NG fixed point. For T slightly less than T_c, the RG flow is divided into the three stages (i), (ii), and (iii).

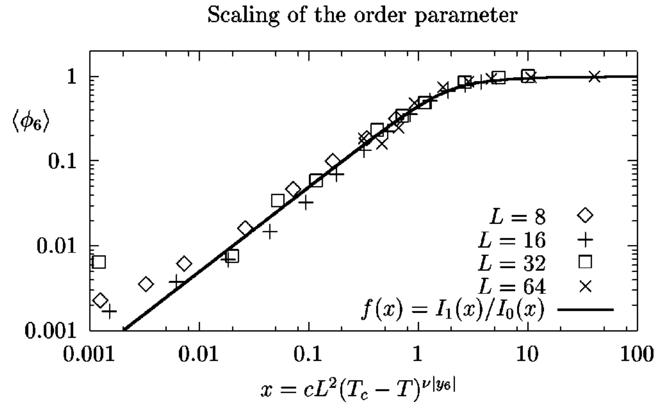

FIG. 2. The order parameter $\langle \phi_6 \rangle$ taken from Ref. 11. They are scaled by $x = cL^2(T_c - T)^{\nu|y_6|}$, for various system sizes and temperatures. The data are consistent with the scaling law (10) with the exponent $\nu|y_6| = 4.8$. They also agree with the approximate scaling function $f(x) = I_1(x)/I_0(x)$, for $c = 0.025$.

dimensions and independent of the microscopic model. Shortly speaking, the Z_n perturbation gives mass to the pseudo-NG boson θ, which would be massless NG boson in the absence of the perturbation. In contrast, in two dimensions the coupling constant K of the free boson field theory is dimensionless, and the above argument does not apply. It is related to the absence of a spontaneous breaking of a continuous symmetry.

We now have a global picture of the RG flow as shown in Fig. 1. The phase transition between the ordered phase and the disordered phase is governed by the *XY* fixed point. This means that the critical exponents are identical to those of the *XY* model. This is consistent with the numerical results. In the disordered phase above T_c, there will be no essential effect of the Z_n perturbation. However, the nature of the ordered phase is more interesting. The Z_n perturbation λ_n is eventually enhanced in the ordered phase below T_c. It means that all regions below T_c belong to the massive phase with the spontaneously broken Z_n symmetry. There is no rotationally symmetric intermediate phase, unlike the 2D case. Only a precisely $O(2)$ symmetric model with $\lambda_n = 0$ is renormalized to the NG fixed point below T_c, corresponding to the rotationally symmetric low-temperature phase.

An interesting aspect of the RG flow diagram is that the Z_n perturbation is irrelevant at the 3D *XY* fixed point but is relevant at the low-temperature NG fixed point. This could be related to a nontrivial system size dependence found in a Monte Carlo renormalization-group calculation.[16] For T slightly less than T_c, the symmetry breaking perturbation λ_n is renormalized to a small value by the RG flow, and remains small until the RG flow reaches near the NG fixed point. It means that the mass of the pseudo-NG bosons is suppressed by the fluctuation effect. At a finite scale (for example, in a finite-size system), the ordered phase near T_c is very similar to the low-temperature phase of the *XY* model. This naturally explains the numerical observation of the apparently rotationally symmetric ‘‘phase’’ in 6CL or the AFP model. For larger n, the mass is more suppressed, and the low-temperature side of the transition appears to be $O(2)$ symmetric until the system size becomes very large. However, for any finite n, the low-temperature side of the transition $T < T_c$ is not truly massless nor $O(2)$ symmetric in the thermodynamic limit, as already pointed out.

III. SCALING LAW IN THE ORDERED PHASE

Based on the RG picture, we derive a scaling law on an order parameter $\mathcal{O}_n$ which characterizes the symmetry breaking from the $O(2)$ to Z_n symmetry. There are various possible definitions of $\mathcal{O}_n$. On the 6CL model, Miyashita[14] numerically measured an order parameter Δ which corresponds to the effective barrier height. On the AFP model, Heilmann, Wang, and Swendsen[11] studied $\langle \phi_6 \rangle$, which is the Fourier transform of the angle distribution density of average spins. The following consideration applies to the both cases.

For large enough L and T slightly lower than T_c we divide the RG flow to three stages, as shown in Fig. 2:

(i) The RG flow near the 3D *XY* fixed point. The symmetry breaking λ_n is irrelevant, and is renormalized proportional to $l^{-|y_n|}$ at length scale l.

(ii) The RG flow from the neighborhood of the 3D *XY* fixed point to the NG fixed point. For simplicity, we assume that the symmetry breaking λ_n is unchanged in this stage.

(iii) The RG flow near the NG fixed point. λ_n is relevant, giving a mass to the NG boson.

The length scale l_c, at which the crossover from stages (i) to (ii) occurs, is given by $l_c \sim \text{const}(T_c - T)^{-\nu}$, where ν is the correlation length exponent of the 3D *XY* universality class. Thus, at the crossover,

$$\lambda_n \sim \text{const}(T_c - T)^{\nu|y_n|}. \tag{9}$$

This also gives the effective value of the perturbation λ_n at the crossover from stages (ii) to (iii).

In the presence of the Z_n perturbation, the spin configuration would be dominated by the ordered regions which are separated by domain walls in a large system. The free energy costed by the domain walls is proportional to their area, which scales as L^2 for the system size L. Therefore the effective ‘‘barrier height’’ is proportional[14] to L^2. Combining this with Eq. (9), we conclude that the order parameter is a function of a single scaling variable

$$\mathcal{O}_n = f(cL^2(T_c - T)^{\nu|y_n|}), \tag{10}$$

where c is a constant. The function f is universal, but of course depends on the definition of the $\mathcal{O}_n$. While the scaling by L^2 was used in Ref. 14, we find that the temperature dependence of the order parameter is also governed by a scaling. Interestingly, the exponent $\nu|y_n|$ is completely determined by the 3D *XY* fixed point.

IV. COMPARISON WITH THE NUMERICAL RESULTS

In the numerical study[11] of the AFP model, the authors claimed the existence of the intermediate phase, in which the order parameter $\langle \phi_6 \rangle$ is very small even for relatively large lattice (up to $L = 64$). However, we reanalyze their data to demonstrate the scaling relation (10), and hence the validity of the RG picture. In Fig. 2, we show the data taken[17] from Fig. 3 of Ref. 11. We chose $\nu|y_6| = 4.8$ to give the best scaling. The data for various temperature and various system sizes fall remarkably into a single curve as a function of the scaling variable $x = cL^2(T_c - T)^{\nu|y_n|}$. This supports the proposed scaling relation (10). Furthermore, if we approximate the effective potential by $-x\cos 6\phi$, the scaling function is given by

$$f(x) = \frac{\int d\phi \cos(6\phi) e^{x\cos(6\phi)}}{\int d\phi e^{x\cos(6\phi)}} = \frac{I_1(x)}{I_0(x)}, \tag{11}$$

where I_n is the modified Bessel function. Choosing $c = 0.025$, the scaled data agree with this simple function rather well. We note that the data appear to deviate from the scaling law for small x. This may be due to the insufficient system size L or the relatively large statistical error.

We emphasize that the present scaling relation is a strong evidence of the single phase transition at the temperature T_c. In contrast, the scaling of the ''spontaneous magnetization'' $\rho = |\Phi| \propto (T_c - T)^\beta$ does not distinguish our picture and the ''intermediate phase'' scenario of Ref. 11.

On the other hand, the scaling function $f(x)$ for Δ in Ref. 14 is linear in x by definition. The author indeed found that Δ is scaled by L^2. However, he did not discuss the temperature depedence. We have attempted to analyze the data in Figs. 6 and 7 in Ref. 14, to find that they are roughly consistent with our scaling law (10) with the exponent $\nu|y_6| \sim 4$. The estimate is difficult because there is only small number of temperature points available in Ref. 14. According to our picture, the exponent $\nu|y_6|$ is a universal quantity determined by the 3D *XY* universality class. Considering the available data, the above results on AFP and 6CL models are consistent with the universality hypothesis, although not conclusive. It would be interesting to obtain more numerical data on these models to check our scaling law (10).

The exponent ν has been determined as $\nu \sim 0.67$ for the 3D *XY* universality class.[18] Combining with the above estimates of $\nu|y_6|$, $|y_6|$ is estimated as about 6. Unfortunately, the irrelevant eigenvalue y_6 has not been much discussed in the literature. The lowest-order result (4) in the ϵ expansion gives $|y_6| = 3$, which is not quite consistent with the numerical estimate. However, it is perhaps not surprising to obtain an inaccurate result in the lowest order of the ϵ expansion. It would be interesting to carry out the calculation to higher orders in ϵ, or to estimate y_6 by other means.

V. DISCUSSIONS AND CONCLUSION

In this article, we clarified a RG picture of phase structure of 3D Z_n symmetric models, which was introduced earlier by Blankschtein *et al.*[3] There is no finite region of intermediate phase with a (spontaneously broken) $O(2)$ symmetry, but only a crossover to a massive phase where the discreteness of Z_n is relevant. Based on the RG picture, we have derived a scaling law of the order parameter in the 3D Z_n models. The existing Monte Carlo data[11] on the AFP model, which was used to claim the intermediate phase, was shown to be consistent with the scaling law. Thus we conclude that the RG picture is valid on the AFP model, and there is only one transition at $T_c \sim 1.23$ with the 3D *XY* universality class.

We would like to make a few final remarks. First, we note that the RG argument used in the present article does not contradict to the transition of other than *XY* universality class, because only the local stability of the *XY* fixed point was discussed. It is possible that a lattice model with Z_n symmetry is renormalized to another (unknown) RG fixed point. Actually, it appears somewhat controversial whether the transition of the STI model belongs to the *XY* universality class.[19,20] On the other hand, the available numerical results strongly supports that the 6CL and AFP models at the critical temperature are renormalized into the *XY* fixed point. Once the transition is known to be *XY* universality class, the RG picture and the scaling law discussed in this article should apply to the ordered phase, for the temperature slightly below the critical point.

Second, as discussed in Ref. 3, the ''bare'' value of λ_n (at a small length scale) may have opposite sign in some circumstances. Namely, the minima and maxima of the potential of ϕ are swapped. In such a case, the ordered phase may correspond to the permutationally symmetric sublattice (PSS) phase proposed in Ref. 6 for the AFP model, or the incompletely ordered phase (IOP) proposed in Ref. 13 for the 6CL model. In the vicinity of the critical point, the temperature dependence of the bare λ_n is not essential because the leading dependence on the temperature is determined by the critical effect, as shown in Eq. (10). However, it may be important in a wider temperature range. In particular, if the bare λ_n changes sign at some temperature T_L lower than T_c, we would have a transition[3] at T_L. Such a transition would be controlled by the NG fixed point. The existing numerical data indicates that there is no such phase transition in the standard AFP model on the simple cubic lattice or in the standard 6CL model. However, such a transition may be possible in some modified models.[21,22] In fact, Blankschtein *et al.*[3] argued it to exist in the STI model.

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