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

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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

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

where $\langle j,k \rangle$ runs over nearest neighbors, and $\theta_j$ 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 $\theta$ 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 CsMnI$_3$.

In two dimensions, the phase diagram of the $Z_n$ model is well understood in the framework of the renormalization group (RG). For $n \geq 5$, 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.

On three dimensional (3D) case, Blankschtein et al. 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

$$H = + \sum_{\langle j,k \rangle} \delta_{\sigma_j, \sigma_k},$$  \hspace{1cm} (2)

where $\sigma_j = 0, 1, 2$ and $\langle j, k \rangle$ runs over nearest neighbor pairs on a simple cubic lattice. The order parameter of this model is not evident. However, previous studies revealed that the low-temperature ordered phase, which is apparently not widely known in the related fields. It might be partly because their discussion was very brief and not quite clear. According to a suggestion in Ref. 3, 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.
which has the manifest $Z_6$ symmetry. In a recent detailed numerical study, Miyashita\cite{4} 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. 2.

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. 4 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 integer $n$ from the $n = 6$ case.

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

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

with the complex field $\Phi$ and its conjugate $\bar{\Phi}$. The $\lambda_n$-term is the lowest order term in $\Phi$ 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 $\lambda_n$, 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 $\lambda_n$ at the 3D XY fixed point. It may be estimated with the standard $\epsilon$-expansion method.

The lowest order result in $\epsilon$ can be easily obtained from the Operator Product Expansion (OPE) coefficients.\cite{3} As a result, we obtain the scaling dimension $y_n$ of $\lambda_n$ 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.\cite{3} 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 3-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 $\epsilon$ 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 following observation. For $n \geq 6$, $\lambda_n$ 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 $\lambda_6$ 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 groundstate 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)

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

where $\phi$ is the angular variable $\Phi \sim |\Phi|e^{i\phi}$. Namely, only the angular mode $\phi$ 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 $\int d^3x (\triangledown \theta)^2/2$.

Now let us consider effects of the symmetry breaking $\lambda_n$. The symmetry breaking term can be written as $-\lambda_n (\Phi^n + \Phi^{\ast n}) = -\lambda_n |\Phi|^4 \cos n \phi$. Using the rescaled field $\theta$, the total effective action at scale $l$ becomes

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

where the factor $K^3 \sim l^3$ comes from the scale transformation of the integration measure. In the thermodynamic limit, we should take $K \rightarrow \infty$ limit. Physically, it means that the $O(2)$ symmetry is spontaneously broken so that the angle is fixed to some value $\phi_0$ in a single infinite system. Then the Taylor expansion of the cosine in $\theta/\sqrt{K}$ becomes valid:

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

where

$$c_{2k} = (-1)^k \frac{n^{2k}}{(2k)!} \cos n \phi_0,$$
for a nonnegative integer \( k \). The five terms \( j = 1, \ldots, 5 \) are relevant perturbations. For any value of \( \phi_0 \), some of the coefficients \( c_j \) of these relevant terms are non-vanishing. 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 dimensions and independent of the microscopic model. Shortly speaking, the \( Z_n \) perturbation gives mass to the pseudo NG boson \( \theta \), 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 \( \lambda_n \) is eventually enhanced in the ordered phase below \( T_c \). It means that all region 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. For \( T \) slightly less than \( T_c \), the symmetry breaking perturbation \( \lambda_n \) 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 numerically measured an order parameter \( \Delta \) which corresponds to the effective barrier height. On the AFP model, Heilmann, Wang and Swendsen studied \( \langle \phi_0 \rangle \), which is the Fourier transform of the angle distribution density of average spins. The following consideration apply to 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 \( \lambda_n \) 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 \( \lambda_n \) is unchanged in this stage.

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

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

\[
\lambda_n \sim \text{const.}(T_c - T)^{\nu|y_n|},
\]

This also gives the effective value of the perturbation \( \lambda_n \) at the crossover from Stage (ii) to Stage (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 to \( L^2 \). Combining this with eq. (9), we conclude that the order parameter is a function of a single scaling variable:

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

where \( c \) is a constant. The function \( f \) is universal, but of course depends on the definition of \( \mathcal{O}_n \). 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 of the AFP model, they claimed the existence of the intermediate phase, in which
the order parameter $\langle \phi_6 \rangle$ is very small even for relatively large lattice (upto $L = 64$). However, we re-analyze their data to demonstrate the scaling relation (10), and hence the validity of the RG picture. In Fig. 2, we show the data taken from Fig. 3 of Ref. 1. 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 $x = cL^2(T_c - T)^{\nu |y_6|}$. 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

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

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. 3. On the other hand, the scaling function $f(x)$ for $\Delta$ in Ref. 4 is linear in $x$ by definition. He indeed found that $\Delta$ is scaled by $L^2$. However he did not discuss the temperature dependence. We have attempted to analyze the data in Figs. 6 and 7 in Ref. 3 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 are only small number of temperature points available in Ref. 3. 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 $\nu$ has been determined as $\nu \sim 0.67$ for the 3D XY universality class. 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 $\epsilon$-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 $\epsilon$-expansion. It would be interesting to carry out the calculation to higher orders in $\epsilon$, or to estimate $y_6$ by other means.

V. CONCLUSION AND DISCUSSIONS

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. 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 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. Firstly, 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 belong to the XY universality class. 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.

Secondly, as discussed in Ref. 3 the “bare” value of $\lambda_n$ (at a small length scale) may have opposite sign in some circumstances. Namely, the minima and maxima of the potential of $\phi$ are swapped. In such a case, the ordered phase may correspond to the Permutationally Symmetric Sublattice (PSS) phase proposed in Ref. 3 for the AFP model, or the Incompletely Ordered Phase (IOP) proposed in Ref. 3 for the 6CL model. In the vicinity of the critical point, the temperature dependence of the bare $\lambda_n$ is not essential because the leading dependence on the temperature is determined by the critical effect, as shown in eq. (11). However, it may be important in a wider temperature range. In particular, if the bare $\lambda_n$ changes sign at some temperature $T_L$ lower than $T_c$, we would have a transition 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. In fact, Blankschtein et al. argued it to exist in the STI model.
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1 Y. Ajiro, T. Inami and H. Kadowaki, J. Phys. Soc. Jpn. 59, 4142 (1990); H. Kadowaki, T. Ianni, Y. Ajiro and Y. Endoh, J. Phys. Soc. Jpn. 60, 1708 (1991).
2 D. Nelson, in Phase Transitions and Critical Phenomena, Vol. 7 ed. by C. Domb and J. L. Lebowitz, Academic Press, London. (1983).
3 D. Blankschtein, M. Ma, A. N. Berker, G. S. Grest and C. M. Soukoulis, Phys. Rev. B 29, 5250 (1984).
4 J. R. Banavar, G. G. Grest and D. Jasnow, Phys. Rev. B 25, 4639 (1982).
5 I. Ono, Prog. Theor. Phys. Suppl. 87, 102 (1986).
6 A. Rosengren and S. Lapinskas, Phys. Rev. Lett. 71, 165 (1993).
7 Y. Ueno, G. Sun and I. Ono, J. Phys. Soc. Jpn. 58, 1162 (1989).
8 J.-S. Wang, R. H. Swendsen and R. Kotecký, Phys. Rev. B 42, 2465 (1990).
9 Y. Okabe and M. Kikuchi, in Computational Physics as a New Frontier in Condensed Matter Research, ed. by H. Takayama et al., The Physical Society of Japan (1995).
10 M. Kolesik and M. Suzuki, Physica A 216, 469 (1995).
11 R. K. Heilmann, J.-S. Wang, R. H. Swendsen, Phys. Rev. B 53, 2210 (1996).
12 R. Kishi, Master thesis, Tokyo Institute of Technology (1999).
13 Y. Ueno and K. Mitsubo, Phys. Rev. B 43, 8654 (1991).
14 S. Miyashita, J. Phys. Soc. Jpn. 66, 3411 (1997).
15 J. Cardy, Scaling and Renormalization in Statistical Physics, Cambridge University Press (1996).
16 M. Kikuchi and Y. Okabe, unpublished.
17 The data were taken from the PostScript file in the e-print version of Ref. 11, cond-mat/9509140. The PostScript file contains useful “raw” data, thereby eliminating the errors in digitizing the figure (or the need to bother the authors asking for the old data.)
18 J. Zinn-Justin, Quantum Field Theory and Critical Phenomena (3rd ed.), Oxford University Press (1996).
19 M. L. Plumer and A. Mailhot, Phys. Rev. B 52, 1411 (1995).
20 B. D. Gaulin, A. Bunker and C. Kallin, Phys. Rev. B 52, 1415 (1995).
21 Y. Ueno and K. Kasono, Phys. Rev. B 48, 16471 (1993).
22 S. Lapinskas and A. Rosengren, Phys. Rev. Lett. 81, 1302 (1998).

FIG. 1. The RG flow diagram of the $Z_n$ models, projected onto the two-dimensional parameter space spanned by $u$ and $\lambda_n$. The $Z_n$ perturbation $\lambda_n$ 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 $\langle \phi_0 \rangle$ taken from Ref. 13. They are scaled by $x = c L^2 (T_c - T)^{|y_0|}$, for various system sizes and temperatures. The data are consistent with the scaling law (6) with the exponent $|y_0| = 4.8$. They also agree with the approximate scaling function $f(x) = I_1(x)/I_0(x)$, for $c = 0.025$. 

Scaling of the order parameter