Size dependence of coherent anomalies in self-consistent cluster approximations

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The behavior of coherent anomalies in Weiss-type and Bethe-type cluster approximations is studied. In the Weiss-type case, logarithmic corrections to the naive coherent-anomaly-method (CAM) scaling relation, which have been ignored in previous works, play an important role in the CAM analysis. A phenomenological theory of the Bethe-type approximation is proposed to show that a logarithmic correction term also exists in this approximation. The correction has, however, smaller influence on the CAM analysis in this case.

I. INTRODUCTION

Mean-field¹ and effective-field² theories have been used frequently to study cooperative phenomena. These theories include an essential feature of phase transitions, but they produce only classical critical exponents. We are now interested in estimating true critical exponents. Recently one of the present authors (M.S.) proposed the socalled coherent-anomaly-method (CAM) theory³⁻¹² in order to estimate nonclassical critical exponents based on systematic mean-field and effective-field approximations.

The formulation of Weiss-type cluster approximations is given in the following.^{5,7} The ferromagnetic Ising Hamiltonian on a *d*-dimensional lattice is considered here. A sphere cluster, Ω , with radius *r* is considered, and its boundary sites are denoted by $\partial\Omega$. The Weisstype mean-field Hamiltonian, H_{Weiss} , is given by

$$-\beta H_{\text{Weiss}} = KA + \frac{K}{J}hB + Kh_{\text{eff}}C , \qquad (1)$$

where

$$A = \sum_{\substack{i-j|=1\\i,j\in\Omega}} \sigma_i \sigma_j \quad (\text{energy of } \Omega) , \qquad (2)$$

$$B = \sum_{i \in \Omega} \sigma_i \quad (\text{magnetization of } \Omega) , \qquad (3)$$

and

$$C = \sum_{i \in \partial \Omega} w_i \sigma_i . \tag{4}$$

The parameter $\beta (= 1/k_{\rm B}T)$ denotes the inverse temperature and K denotes βJ . The quantity w_i in (4) denotes the number of free bonds at site *i*. The value of $h_{\rm eff}$ is determined by the self-consistency condition,

$$\langle \sigma_0 \rangle = h_{\rm eff} \ , \tag{5}$$

where $\langle \cdots \rangle$ on the left-hand side denotes the thermal expectation value under the Hamiltonian, (1), and σ_0 denotes the Ising spin at the center of the cluster, Ω .

The critical point is determined by the equation

$$a_{01} - 1 = 0 {,} {(6)}$$

where

$$a_{ij} = \frac{1}{i! j!} \left(\frac{\partial^{i+j} \langle \sigma_0 \rangle}{\partial h^i \partial h_{\text{eff}}^j} \right)_{h=h_{\text{eff}}=0} .$$
(7)

It has been observed and proved that the critical temperature obtained by (6) is always greater than the true one and converges to the true one when the cluster becomes large.⁴ The critical behavior of susceptibility, χ_{Weiss} , is given by^{3,4}

$$\chi_{\text{Weiss}} = -\frac{a_{10}}{bT_c^{\text{Weiss}}} \frac{T_c^{\text{Weiss}}}{T_c^{\text{Weiss}} - T} , \qquad (8)$$

where

$$b = \left(\frac{\partial(1-a_{01})}{\partial T}\right)_{T=T_c^{\text{Weiss}}, h=h_{\text{eff}}=0}$$
(9)

Therefore the critical behavior is always classical, that is, $\gamma=1$, irrespective of the cluster size, and it has been believed for long years before the discovery of the coherentanomaly-method (CAM) theory that this approximation is not useful to estimate the values of true critical exponents.

It has been, however, found by one of the present authors that the critical amplitudes of this approximation show anomalous behavior when the cluster size is increased and that their divergence has information on the true critical behavior.³ This divergence of critical amplitudes is called the "coherent anomaly," and the analysis of the true critical behavior using this coherent anomaly is called the "coherent-anomaly method," which is abbreviated as CAM.³ The scaling relation between the critical amplitude and the difference, δT_c , of the critical point and the true critical point, is assumed to hold, and it claims that the amplitude diverges with the exponent, which is equal to the difference of the true exponent and the classical exponent. For example, the critical amplitude of susceptibility, $\bar{\chi}_{Weiss}$, is supposed to diverge as

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TABLE I. The Monte Carlo estimation of Weiss-type cluster approximations cited from our previous paper (Ref. 7). Thirty-two different temperatures are simulated for each cluster. Sixteen temperatures of these 32 are near the Weiss critical point, which is estimated by short and coarse simulations. The rests are near the Bethe critical point. The cluster Ω is defined by $\{i \in \mathbb{Z}^d; |i| \leq r + 0.01\}$ for d-dimensional lattice. The value of d is 2 now.

	$T_{c}^{{ t Weiss}}$	$ar{\chi}$ Weiss	Monte Carlo steps
1	3.415732	0.321 861	Analytic
2	3.0931(14)	0.40409(33)	1.1×10^{7}
5	2.66305(62)	0.6627(12)	1.1×10^{7}
10	2.49624(23)	0.9413(16)	1.0×10^{8}
15	2.43268(17)	1.1670(23)	1.0×10^{8}
20	2.39844(19)	1.3578(42)	1.0×10^{8}
25	2.37663(17)	1.5305(72)	8.1×10^{7}
30	2.36165(17)	1.6957(80)	1.0×10^{8}
40	2.34166(20)	1.997(19)	1.0×10^{8}
50	2.329 39 (23)	2.250(27)	1.0×10^{7}

$$\bar{\chi}_{\text{Weiss}} \sim (T_c^{\text{Weiss}} - T_c^*)^{-\psi} , \quad \psi = \gamma - 1 , \qquad (10)$$

with respect to the most singular term, where \sim denotes the equality except the multiplication of a constant (and less significant terms, of course). The $\bar{\chi}_{\text{Weiss}}$ of (8) is

$$\bar{\chi}_{\text{Weiss}} = -\frac{a_{10}}{bT_c^{\text{Weiss}}} \ . \tag{11}$$

Katori and Suzuki⁵ studied the cluster Weiss approximation for the ferromagnetic Ising model on square and cubic lattices with several clusters. For the square lattice, the shape of their clusters is square or octagonal. The size of their maximum cluster is 13 in linear dimension and contains 145 sites. They calculated the critical points and critical amplitudes of susceptibility numerically by using the brick-laying transfer-matrix method and estimated the value of γ to be 1.622(8) first directly from the CAM scaling assumption, (10). They also estimated the value of γ as 1.8(1) using a modified trial function including a higher-order term. Although the expected value of γ is 1.75, this result was regarded as plausible because the deviation of γ from $\gamma=1.75$ seemed to be owing to the restricted size of the clusters. Thus a further study with larger clusters has been expected.

We have studied the Weiss-type approximations for larger clusters by the Monte Carlo method.⁷ Vector processors made large-scale and accurate Monte Carlo simulations possible.¹³⁻¹⁵ Our cluster shape is a sphere. The maximum radius of our clusters is 50 for the twodimensional lattice. The results of T_c^{Weiss} and $\bar{\chi}_{\text{Weiss}}$ are cited in Table I for further analyses of the present paper. The data of our clusters are listed in Table II. With the CAM scaling assumption (10) the estimated value of γ is, however, 1.66(1), which is not consistent with 1.75. This difficulty was also reported by Patrykiejew and Borowski.¹⁶ They pointed out that the value of ν is not estimated correctly¹⁶ from the fitting of $\delta T_c \sim L^{1/\nu}$. These results indicate that the naive CAM analysis of Weiss-type cluster approximations does not work successfully.

On the other hand, we proposed and studied the Bethetype cluster approximation, and it was found that the CAM scaling for magnetic susceptibility (10) seems to work successfully for it.⁷ This approximation is almost the same as the Weiss-type one except for the selfconsistency requirement. It uses the same Hamiltonian as (1). The self-consistency equation is

$$\langle \sigma_0 \rangle = \frac{1}{|\partial \Omega|} \langle D \rangle , \qquad (12)$$

where D is defined by

$$D = \sum_{i \in \partial \Omega} \sigma_i \quad \text{(boundary magnetization)} . \tag{13}$$

The critical point is determined by the equation

$$a_{01} - b_{01} = 0 , (14)$$

TABLE II. The features of the clusters used in our calculations of square lattice. In this table, n_{bond} and $n_{free \ bond}$ denote the numbers of bonds in the cluster and the number of free bonds from the boundary of the cluster, respectively. n_i (i=0, 1, 2, and 3) denote the numbers of sites that have *i* free bonds.

r	$ \Omega $	$ \partial \Omega $	$n_{ m bond}$	$n_{ m free\ bond}$	n_0	n_1	n_2	n_3
1	5	4	4	12	1	0	0	4
2	13	8	16	20	5	0	4	4
5	81	28	140	44	53	16	8	4
7	149	36	268	60	113	16	16	4
10	317	56	592	84	261	32	20	4
15	709	84	1356	124	625	48	32	4
20	1257	112	2432	164	1145	64	44	4
25	1961	140	3820	204	1821	80	56	4
30	2821	168	5520	244	2653	96	68	4
40	5025	224	9888	324	4801	128	92	4
50	7861	280	15520	404	7581	156	124	0

TABLE III. The results for Bethe-type cluster approximations, cited from our previous paper (Ref. 7). The data of Monte Carlo steps are the same as Table I.

r	T_c^{Bethe}	$ ilde{\chi}$ Bethe
1	2.885 42	0.500 0
2	2.6989(17)	0.65001(38)
5	2.46258(89)	1.1531(25)
10	2.38235(20)	1.7138(26)
15	2.35158(14)	2.1692(39)
20	2.33486(12)	2.5689(52)
25	2.32405(13)	2.9193(63)
30	2.316914(85)	3.2348(91)
40	2.30714(19)	3.837(24)
50	2.301 01(16)	4.369(27)

where a_{ij} has the same form as (7) and

$$b_{ij} = \frac{1}{i! \, j!} \frac{1}{|\partial\Omega|} \left(\frac{\partial^{i+j} \langle D \rangle}{\partial h^i \, \partial h^j_{\text{eff}}} \right)_{h=h_{\text{eff}}=0} \,. \tag{15}$$

The critical amplitude of magnetic susceptibility is

$$\bar{\chi}_{\text{Bethe}} = -\frac{a_{01}b_{10} - a_{10}b_{01}}{wT_c^{\text{Bethe}}} , \qquad (16)$$

where w is

$$w = \left(\frac{\partial(a_{01} - b_{01})}{\partial T}\right)_{T = T_c^{\text{Bethe}}, h = h_{eff} = 0}$$
(17)

The Monte Carlo method is used to solve the approximation for the clusters whose radius are 2-50. The results thus obtained are also cited in Table III. The estimated value of γ based on the simple CAM scaling (10) is 1.745(3).

Now there remains a problem concerning the relation between the critical temperatures and critical amplitudes of Weiss- and Bethe-type approximations in order to estimate correctly the true critical point and the true critical exponents. The purpose of this paper is to clarify this relation.

In the next section, a phenomenological theory for the Weiss-type approximation is studied. This phenomenology is already proposed by Suzuki *et al.*⁴ We have confirmed this theory based on our Monte Carlo data. This theory produces a logarithmic correction in CAM scaling, which has been ignored in the previous study, but we will point out that this correction is important in CAM analysis. In Sec. III, the phenomenological theory for Bethetype approximation is proposed. The three-dimensional Ising model is analyzed based on these theories in Sec. IV. The critical amplitudes of other quantities are studies in the Sec. V. Section VI contains the summary and discussion.

II. WEISS-TYPE CASE

The Weiss-type cluster approximation is studied in this section. We study two problems. The first one is the relation between the cluster size r and the difference δT_c

of the critical point of cluster approximation T_c and the true critical point T_c^* . The second problem is the relation between the cluster size r and the critical amplitude of susceptibility $\bar{\chi}_{\text{Weiss}}$. To answer them, we study phenomenologically how the factors in expressions (6) and (11) behave following Suzuki *et al.*⁴

A. r dependence of T_c^{Weiss}

The explicit form of a_{01} is obtained from (7). It is

$$a_{01} = K \langle \sigma_0 C \rangle_0 = K \sum_{i \in \partial \Omega} w_i \langle \sigma_0 \sigma_i \rangle_0 , \qquad (18)$$

where $\langle \cdots \rangle_0$ denotes the thermal expectation value under the Hamiltonian (1) with $h_{\text{eff}} = 0$. In other words, it is the expectation value on a free boundary cluster. Near and above the true critical point, the correlation function $\langle \sigma_0 \sigma_i \rangle$ may be written as

$$\langle \sigma_0 \sigma_i \rangle \simeq \frac{C_i}{r^{d-2+\eta_{cs}}} \exp(-r/\xi) ,$$
 (19)

where C_i is a constant that may depend on site *i* in a nonsingular form. The form of the exponent, $d - 2 + \eta_{cs}$, follows the convention. Then the dependence of a_{01} on the cluster size and temperature is written as

$$a_{01} \simeq N r^{\omega} \exp(-r/\xi) , \qquad (20)$$

where $\omega = 1 - \eta_{cs}$. If the temperature lies in the region where the cluster size is large enough compared with the correlation length of an infinitely large lattice ξ_0 , the above ξ seems to diverge with the same exponent as that of ξ_0 . The Weiss critical point lies in such a region as is observed in the relation (23).

Therefore we can replace ξ by $a(T - T_c^*)^{-\nu}$, and the expression of a_{01} is rewritten as

$$a_{01} \simeq N r^{\omega} \exp[-r(T - T_c^*)^{\nu}/a]$$
 (21)

near the Weiss critical point. We have confirmed by using the scaling plot of a_{01} the above-mentioned argument. In the square lattice case, the Monte Carlo estimations of a_{01} near the Weiss critical point of each cluster for $r = 2 \sim 50$ are used. The values of $\ln(a_{01}r^{-\omega})$ are plotted versus $r(T - T_c^*)^{\nu}$. The exact value of ν , namely 1, is used. The plots are given in Fig. 1. These figures support expression (21). The value of the exponent ω is estimated to be roughly 0.30. Therefore the value of the exponent, η_{cs} , may be 0.70.

From (6) and (21), the critical point is obtained as^4

$$\delta T_c \equiv T_c - T_c^* = a^{1/\nu} \left(\frac{\ln N + \omega \ln r}{r} \right)^{1/\nu}$$
$$\equiv \left(\frac{a_1 + a_2 \ln r}{r} \right)^{1/\nu} , \qquad (22)$$

where a_1 and a_2 are constants. It is concluded that T_c converges to T_c^* when the cluster is large. The leading singularity of this δT_c is not $(1/r)^{1/\nu}$ but $(\ln r/r)^{1/\nu}$. The







FIG. 1. The scaling plot of the summation of center-to-boundary correlations a_{01} of the two-dimensional clusters. The Monte Carlo estimations of a_{01} of the clusters whose sizes are r=2-50 are used for the plot. For every cluster, the estimations at 32 temperatures that are near the Weiss or Bethe critical point of each cluster are used. The value of ν in (21) is 1. The three figures, (a), (b), and (c) correspond to $\omega=0.2$, 0.3, and 0.4, respectively. The results of r=2 and 5 have large deviations. This plot supports the phenomenological description (21), and the value of ω is about 0.30.

ratio of the cluster radius to the correlation length of the infinite lattice at the Weiss critical point is

$$\frac{r}{\xi} \sim \ln r \ . \tag{23}$$

This ratio diverges to infinity when the cluster size is increased in the Weiss-type approximations. Thus the cluster has to be large enough for expression (19) of the correlation function to be correct.

The results in Table I are fitted by the function (22) to estimate the critical exponent ν and to test the validity of this theory. The value of the true critical point, $T_c^* = 2.269185...$, is used for the fitting. The obtained estimations are listed in Table IV. These results are consistent with the true value $\nu=1$. The logarithmic term in (22) is crucial for the correct estimation of the value of ν . Without this term, an incorrect estimation¹⁶ is obtained.

B. Critical amplitude of χ_{Weiss}

The expression of a_{10} and the derivative of a_{01} are necessary to get the behavior of $\bar{\chi}_{Weiss}$ given in (11). The factor a_{01} has already been studied, and we can use (21). Its temperature derivative b is

$$b \sim \frac{\partial a_{01}}{\partial T} \sim r(\delta T_c)^{\nu-1}$$
 (24)

The quantity a_{10} is obtained from (7) as

$$a_{10} = \frac{K}{J} \langle \sigma_0 B \rangle_0 = \frac{K}{J} \sum_{i \in \Omega} \langle \sigma_0 \sigma_i \rangle_0 .$$
 (25)

This a_{10} will behave as

$$a_{10} = M(\delta T_c)^{-\gamma} , \qquad (26)$$

because the cluster is larger than the correlation length of the infinite lattice at T_c^{Weiss} as is shown in (23).

Thus, from (11), the asymptotic behavior of $\bar{\chi}_{Weiss}$ is given by⁴

$$\bar{\chi}_{\text{Weiss}} \sim \frac{1}{r(\delta T_c)^{\nu}} \frac{1}{(\delta T_c)^{\gamma-1}} .$$
(27)

From the $r - \delta T_c$ relation (22), this is expressed using only r as

$$\bar{\chi}_{\text{Weiss}} \simeq \frac{r^{\mu}}{(a_1 + a_2 \ln r)^{\mu + 1}} ,$$
 (28)

where μ denotes $(\gamma - 1)/\nu$. On the other hand, if this $\bar{\chi}_{\text{Weiss}}$ is expressed using only δT_c , it has essentially singular behavior because there is the $\ln r$ term in (22). Therefore, for the Weiss-type approximation, r is the better parameter to analyze the critical exponent than δT_c . The factor $r(\delta T_c)^{\nu}$ of Eq. (27) is the logarithmic correction for the CAM scaling assumption (10) because of the relation (23). The existence of this correction may be harmful to the estimation of the critical exponent because this log correction is difficult to distinguish from the power-law behavior for the clusters whose sizes are presently tractable. This correction term is responsible for the previously estimated value⁷ of γ , 1.66, based only on the power-law behavior (10). The correction term is plotted in Fig. 2 using the results in Table I. If the powerlaw form is fitted to these corrections, the estimation is $(\delta T_c)^{-0.09}$, which coincides with the observed deviation, 1.75-1.66=0.09. Therefore we can conclude that this correction term is responsible to the deviation observed

TABLE IV. The estimated values of ν from the relation between r and T_c^{Weiss} . Function (22) is fitted for the results in Table I. The exact value of ν is 1.



FIG. 2. The observed logarithmic corrections for $\bar{\chi}$ weiss by Monte Carlo analysis. For this purpose, the values of $1/(\bar{\chi}_{\text{Weiss}}\delta T_c^{0.75})$ are plotted in (a) vs the values of $r\delta T_c$ from the results in Table I. The values of $\ln(1/\bar{\chi}_{\text{Weiss}}\delta T_c^{0.75})$ are plotted in (b) vs the values of $\ln \delta T_c$. The solid line shows the function, $2.87(\delta T_c)^{-0.094}$. This plot indicates that these logarithmic corrections are difficult to distinguish from the power-law behavior.

TABLE V. The estimated values of μ from the fitting of (28) to the results in Table I are listed. The expected value of $\mu = (\gamma - 1)/\nu$ is 0.75.

Used region of r	ν	γ =	Used region of r	μ	
$5 \sim 50$	1.027(9)		$5 \sim 50$	0.76(2)	
$10 \sim 50$	1.02(2)		$10 \sim 50$	0.74(6)	

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in the simple CAM analysis.

The function (28) is fitted for the results in Table I. The estimations are given in Table V. These results are consistent with the expected value of $\mu = (\gamma - 1)/\nu =$ 0.75. The value of γ is obtained from the estimated values of μ and ν . The errors of statistical estimations in the present paper indicate one standard deviation.

III. BETHE-TYPE CASE

The Bethe-type cluster approximation is studied in this section. A phenomenological theory is proposed. It is necessary to describe the behavior of the summation of boundary-to-boundary correlations.

A. r dependence of T_c^{Bethe}

The expression of b_{01} is calculated from (15) as

$$b_{01} = \frac{K}{|\partial\Omega|} \langle DC \rangle_0 = \frac{1}{|\partial\Omega|} \sum_{i \in \partial\Omega} \sum_{j \in \partial\Omega} w_i \langle \sigma_i \sigma_j \rangle .$$
(29)

Therefore, if the cluster is large enough, this is rewritten as

$$b_{01} \sim \sum_{j \in \partial \Omega} \langle \sigma_i \sigma_j \rangle_0 , \qquad (30)$$

where σ_i is any (but the typical) boundary spin. If the cluster radius r is much larger than the correlation length ξ , the correlation function $\langle \sigma_i \sigma_j \rangle_0$ will be approximated as

$$\langle \sigma_i \sigma_j \rangle_0 \sim \frac{1}{|i-j|^{d-2+\eta_{ss}}} \exp(-|i-j|/\xi_s) , \qquad (31)$$

where ξ_s is the correlation length of boundary-toboundary correlation function and is smaller than the bulk correlation length ξ . If the cluster size is infinitely large, this ξ_s diverges at T_c^* , and its critical exponent is denoted by ν_s . The b_{01} is estimated from (31) to be

$$b_{01} \sim \sum_{j \in \partial \Omega} \frac{\exp(-|i-j|/\xi_s)}{|i-j|^{d-2+\eta_{ss}}} \sim \xi_s^{\omega'} .$$
(32)

Therefore b_{01} is written as

$$b_{01} = N'(\delta T)^{-\omega'\nu} , (33)$$

where the exponent ω' may be different from $(1-\eta_{ss})\nu_s/\nu$ because some unnegligible correction may appear from the integration over the surface. The condition that the ratio r/ξ be large is satisfied, which is shown in the following.

This behavior (33) is confirmed by the Monte Carlo results for a two-dimensional lattice. The values of b_{01} near the Bethe critical point of each cluster are plotted in Fig. 3. The power-law dependence is clearly observed. The value of ω' is roughly estimated to be 0.20.

With (20) and (33), the equation that determines the critical point, (14), reduces to

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FIG. 3. Plot of the values of $\ln b_{01}$ of two-dimensional clusters. The Monte Carlo estimations near the Bethe critical point of each cluster are shown. The cluster sizes are the same as those in Fig. 1. The power-law dependence (33) is clearly observed.

$$r^{\omega} \exp[-r(\delta T_c)^{\nu}/a] = \frac{N'}{N} (\delta T_c)^{-\omega'\nu} . \qquad (34)$$

This is transformed using the variable, $x = r/\xi = r(\delta T_c)^{\nu}/a$, as

$$x^{\omega'} \mathrm{e}^{-x} = \frac{N'}{N} a^{\omega'} r^{\omega' - \omega} .$$
(35)

The exponent, $\omega' - \omega$, on the right-hand side is nonpositive, and the rhs converges to 0 when the cluster size becomes large because the sum of boundary-toboundary correlations is smaller than the sum of centerto-boundary correlation and their exponent will be different. This is correct in two dimensions where the values of ω and ω' are estimated to be 0.30 and 0.20, respectively. Therefore this equation has two solutions as shown in Fig. 4. One is near x=0, and it has power-law dependence on r. This is a fictitious solution because the susceptibility diverges to negative. Furthermore, the phenomenological description, (20) and (33), is not correct when the parameter $x = r/\xi$ becomes zero. The other solution logarithmically diverges to infinity if r becomes large. This solution determines the Bethe-type critical point. It behaves as $x \sim \ln r + O(\ln \ln r)$, which is the same form as the Weiss approximation, (23), as far as the leading term is concerned. In this case, however, more subtle correction terms appear. The δT_c and r depend singularly on each other. Then the estimation of ν based on this relation is difficult.



FIG. 4. The shape of the graphs of Eq. (35). There are two solutions, F and T, for large cluster, because the exponent in the rhs of Eq. (35) is negative. The solution F is fictitious and not physical. The solution T determines the critical point of the Bethe-type cluster approximation.

B. Critical amplitude of χ_{Bethe}

The critical amplitude of susceptibility, (16), is

$$\bar{\chi}_{\text{Bethe}} = \frac{b_{01}(a_{10} - b_{10})}{wT_{e}^{\text{Bethe}}} .$$
 (36)

The factor b_{10} is calculated using (15) to be

$$b_{10} = \frac{K}{J|\partial\Omega|} \langle DB \rangle_0 . \tag{37}$$

This is the summation of the boundary-to-bulk correlations, and it is smaller than the summation of the centerto-bulk correlations. The center-to-bulk summation a_{10} diverges as $\delta T_c^{-\gamma}$. Therefore $a_{10} - b_{10}$ diverges as $\delta T_c^{-\gamma}$. The behavior of $\bar{\chi}_{\text{Bethe}}$ is derived from (17), (20), (25), and (33) as

$$\bar{\chi}_{\text{Bethe}} = \frac{a_2}{r(\delta T_c)^{\nu} + a_1} \frac{1}{(\delta T_c)^{\gamma - 1}} , \qquad (38)$$

where a_1 and a_2 are constants. The correction term to the ordinary naive CAM scaling, $r(\delta T_c)^{\nu} + a_1$, appears again, and this correction is not simply logarithmic as is observed from (35) in this case. This correction term is plotted in Fig. 5 for the results in Table III. When this correction is fitted with a power-law function for these corrections, we get a function $(\delta T_c)^{-0.01}$. This order of deviation is consistent with the result⁷ of the naive CAM analysis, 1.745(3).

The influence of the correction terms on the estimation of the value of γ in the Bethe-type case is smaller than in the Weiss-type case. This is explained qualitatively from our phenomenology. The correction term comes from the size dependence of $r(\delta T_c)^{\nu}$ or $x = r/\xi$.

TABLE VI. The estimated values of ν and γ from the fitting of (38) to the results in Table III.

Used region of r	ν	γ	
$5 \sim 50$	0.6(5)	1.75(1)	
$10 \sim 50$	0.5(3)	1.75(1)	



FIG. 5. The corrections for the CAM scaling, (10), of Bethe-type cluster approximations plotted in the same manner as Fig. 2. The results in Table III are used. The solid line in (b) shows the function $2.91(\delta T_c)^{-0.012}$. When only the power-law behaviors are assumed, these correction terms are regarded as $\delta T_c^{-0.01}$. Therefore the deviations of exponent is 0.01, although it was 0.09 in Weiss-type case.

TABLE VII. The critical points and critical amplitudes of Weiss-type cluster approximations for cubic lattice.

r	T_{c}^{Weiss}	$ar{oldsymbol{\chi}}$ Weiss	Monte Carlo steps
1	5.44678	0.193942	analytic
2	5.07427(69)	0.23055(13)	1.0×10^{8}
5	4.721 18(73)	0.30240(91)	1.0×10^{8}
10	4.602 68 (52)	0.3713(29)	1.0×10^{8}
12	4.58407(53)	0.3895(36)	1.0×10^{8}
15	4.56604(26)	0.4203(54)	4.0×10^{8}
20	4.548 41 (3 7)	0.4461(69)	5.0×10^{7}

The Weiss-type solution, x_{Weiss} , behaves like $\omega \ln r$. On the other hand, the Bethe-type solution, x_{Bethe} behaves like $(\omega - \omega')[\ln r + O(\ln \ln r)]$. Therefore the influence of the correction term is expected to be smaller in the Bethe-type than in the Weiss-type. If the values of ω and ω' are equal, there exists no such correction term, as was discussed in the case of the confluent transfer-matrix method¹¹ in the generalized cactus trees. The situation is, however, different in our Bethe-type approximation.

Function (38) is fitted for the results in Table III, and the estimations of ν and γ are given in the Table VI. The estimation of γ works correctly. The estimation of ν is, however, not good, and it is accompanied by a large error, which is understood from the fact that ν appears as the logarithmic corrections in (38).

IV. ANALYSIS OF THE THREE-DIMENSIONAL FERROMAGNETIC ISING MODEL

The Weiss- and Bethe-type cluster approximations for a cubic lattice have been also studied by the Monte Carlo method.⁷ For the clusters, r=15 and 20, further simulations were tried and the results have been given in Tables VII and IX. The results for r = 15 of the Weiss- and Bethe-type approximations and for r=20 of the Bethetype approximation are improved, and other results are cited from our previous paper.⁷ The data for the used clusters are listed in Table VIII. These results are analyzed on the basis of the present phenomenological theory. Function (21) is fitted for the r and T_c^{Weiss} in Table VII. The estimated values of T_c^* and ν are 4.508(2) and 0.64(3), respectively, from r=2 to 21. Function (28) is fitted for r and $\bar{\chi}_{\text{Weiss}}$ in Table VII. The used cluster size r is 2–20, and the estimated value of μ is 0.30(1). The value of γ is estimated from these estimations of ν and $\mu [=(\gamma - 1)/\nu]$ as 1.19(2).

The results for Bethe-type in Table IX are fitted by the function (38) and the estimated values of T_c^* and γ are listed in Table X. The logarithmic correction for the CAM scaling is expected to be small for the threedimensional Bethe-type approximation as is analyzed in the last section. Thus the power-law function (10) is fitted for the results in Table IX. The estimated values of T_c^* and γ are listed in Table XI.

The precise estimations of the critical point and exponents of the three-dimensional Ising model have been made. Although there are small deviations depending on the estimation methods, the values of T_c^* , γ , and ν are 4.5116(1),^{17,18} 1.24, and 0.63,^{19,20} respectively. The critical temperature is estimated correctly from our data by the present theory. The present estimations of γ have some deviations. These deviations may originate in the smallness of clusters. The maximum size of three-dimensional clusters is smaller than half of that of two-dimensional clusters in linear dimension in this study.

V. OTHER QUANTITIES

We have discussed only the critical behavior of susceptibility in the second and third sections. These arguments can be generalized to other quantities.

As is understood easily, the singular behavior of self-consistent approximations originates in the selfconsistency equation, which determines the critical point:

$$F(T_c, r) = 0$$
 . (39)

This equation is linearized near the critical point T_c as

$$F(T,r) = f(r)(T - T_c)$$
, (40)

where

TABLE VIII. The features of the clusters used in our calculations of cubic lattice. The notations are the same as those of Table II.

r	Ω	$ \partial \Omega $	nbond	$n_{ m free}$ bond	n_0	n_1	n_2	n_3	n_4	n_5
1	7	6	6	30	1	0	0	0	0	6
2	33	26	60	78	7	0	12	8	0	6
5	515	222	1302	486	293	72	72	48	24	6
7	1419	446	3 810	894	973	144	168	128	0	6
10	4169	978	11556	1902	3191	384	300	264	24	6
12	7153	1 410	20 136	2646	5743	576	444	384	0	6
15	14147	2262	40 314	4254	11885	1008	552	672	24	6
20	33401	4 0 2 6	96 432	7542	29375	1728	1116	1152	24	6

TABLE IX. The critical points and critical amplitudes of Bethe-type approximations for cubic lattice. The numbers of Monte Carlo steps are the same as those in Table VII except for r=20 whose number of Monte Carlo steps is increased up to 1.0×10^8 .

r	T_c^{Bethe}	$ar{\chi}_{ ext{Bethe}}$
1	4.932 6070	0.25
2	4.7473(17)	0.29720(39)
5	4.599 89(75)	0.3891(11)
10	4.551 78(4 3)	0.479.8(26)
12	4.543 43(47)	0.5003(40)
15	4.535 97(24)	0.5392(33)
20	4.529 23(35)	0.5895(92)

$$f(r) = \frac{\partial F(T, r)}{\partial T} \bigg|_{T=T_e} .$$
(41)

Consider any quantities, A, whose true and classical critical exponents are ζ and ζ_{cl} , respectively. The classical singularity comes from the factor F(T,r). Thus the classical critical coefficient \overline{A} of A may be expressed in the form

$$\bar{A} = \hat{A}f(r)^{\zeta_{c1}} . \tag{42}$$

The coefficient \hat{A} show a coherent anomaly corresponding to the true critical behavior of A. The $f(r)^{\zeta_{cl}}$ reduces the true critical divergence of \hat{A} by $(T_c - T_c^*)^{\zeta_{cl}}$ and a singular form of f(r) introduces the correction term to naive CAM scaling in some cluster approximations discussed in this paper.

For the Weiss-type approximation, from (21) or (22), it is expressed as

$$\bar{A} \simeq (\delta T_c)^{\zeta} [(\delta T_c)^{-1} r (\delta T_c)^{\nu}]^{\zeta_{cl}} = \frac{(a_1 + a_2 \ln r)^{\mu + \zeta_{cl}}}{r^{\mu}}$$
(43)

where $\mu = (\zeta - \zeta_{\rm cl})/\nu$.

For the Bethe-type approximation, from (35), it is expressed as

$$\bar{A} \simeq A_2 (\delta T_c)^{\zeta - \zeta_{cl}} [r(\delta T_c)^{\nu} + a_1]^{\zeta_{cl}} .$$
(44)

If the values of ζ and ζ_{cl} are $-\gamma$ and -1, respectively, expressions (43) and (44) reduce to (28) and (38), respectively. The expressions for the coherent anomalies of spontaneous magnetizations are obtained when the values of ζ and ζ_{cl} are β and $\frac{1}{2}$, respectively.

VI. SUMMARY AND DISCUSSION

The nature of the Weiss- and Bethe-type cluster approximations has been studied phenomenologically in the

TABLE X. The estimated values of T_c^* and γ from the fitting of (38) to the results in Table IX.

Used region of r	T_c^*	γ	
$2 \sim 20$	4.509(1)	1.267(2)	
$5 \sim 20$	4.506(1)	1.286(1)	

TABLE XI. The estimated values of T_c^* and γ from the fitting of the naive CAM scaling (10) to the results in Table IX.

Used region of r	T_c^*	γ	
$2 \sim 20$	4.507(2)	1.28(1)	
$5 \sim 20$	4.508(5)	1.27(3)	

present paper. Their critical temperatures give the upper bound of the true one and converge to the true value when the cluster is infinitely large. For the Weiss-type approximation, the leading terms are given in (22). The values of ν and T_c^* can be estimated correctly with this expression. On the other hand, the correction is a complicated and subtle essentially singular form in the Bethe case as is observed in (34) or (35). It is difficult to obtain a good estimation of ν from the relation between r and T_c .

The critical amplitude of magnetic susceptibility, $\bar{\chi}$, diverges as the cluster size is increased. The exponent of this divergence in terms of δT_c is $\gamma - 1$ as is generally insisted on in the CAM theory,³ but it is accompanied with correction terms. For the Weiss-type case,⁴ the correction has practically appreciable influence on the estimations of the critical point and exponent. The $\bar{\chi}_{\text{Weiss}}$ is compactly expressed as a function of cluster size r, but an essentially singular expression is necessary if we express it only using δT_c . For the Bethe-type case, the correction to the CAM scaling is small for the present range of cluster size. Therefore the CAM scaling works successfully without considering this correction. When the cluster is large, the use of relation (38) produces correct estimations of T_c^* and γ , although the estimation of ν is difficult. These theories have been applied to the results of the three-dimensional Ising ferromagnet to obtain the estimation of T_c^* and γ , which are consistent with the estimations based on other methods.

There have been proposed cluster-type effective theories for many models, for example, the spin glass, quantum spin systems¹⁰ and percolation.²¹ The present argument can be extended to these approximations easily and appropriate expressions for critical point and coherent anomalies are obtained.

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- ¹P. Weiss, J. Phys. Radium 4, 661 (1907).
- ²H. A. Bethe, Proc. R. Soc. London, Ser. A 150, 552 (1935).
- ³M. Suzuki, J. Phys. Soc. Jpn. **55**, 4205 (1986); see also *Qauntum Field Theory*, edited by F. Mancini (Elsevier Science, New York, 1986), p. 505; M. Suzuki, Phys. Lett. A **116**, 375 (1986).
- ⁴M. Suzuki, M. Katori, and X. Hu, J. Phys. Soc. Jpn. 56, 3092 (1987).
- ⁵M. Katori and M. Suzuki, J. Phys. Soc. Jpn. 56, 3113 (1987).
- ⁶J. L. Monroe, Phys. Lett. A **131**, 427 (1988).
- ⁷N. Ito and M. Suzuki, in *Proceedings of Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, edited by D. P. Landau (Springer-Verlag, Heidelberg, 1990). Detailed references on CAM are given in this paper.
- ⁸X. Hu, M. Katori, and M. Suzuki, J. Phys. Soc. Jpn. 56, 3865 (1987).
- ⁹X. Hu and M. Suzuki, J. Phys. Soc. Jpn. 57, 791 (1988).

- ¹⁰M. Suzuki, J. Phys. Soc. Jpn. 57, 2310 (1988).
- ¹¹M. Suzuki, J. Phys. Soc. Jpn. 58, 3642 (1989).
- ¹²M. Suzuki, J. Stat. Phys. 53, 483 (1988).
- ¹³N. Ito and Y. Kanada, Supercomputer 5(3), 31 (1988).
- ¹⁴N. Ito and Y. Kanada, Supercomputer 7(1), 29 (1990).
- ¹⁵N. Ito and Y. Kanada, Proceedings of Supercomputing '90, New York, 1990, IEEE Computer Society, Los Alamos, 1990.
- ¹⁶A. Patrykiejew and P. Borowski, Phys. Rev. B **42**, 4670 (1990).
- ¹⁷G. S. Pawley, R. H. Swendsen, D. J. Wallace, and K. G. Wilson, Phys. Rev. B 29, 4030 (1984).
- ¹⁸M. N. Barber, P. B. Pearson, D. Toussaint, and J. L. Richardson, Phys. Rev. B **32**, 1720 (1985).
- ¹⁹D. S. Gaunt and M. F. Sykes, J. Phys. A 12, L25 (1979).
- ²⁰J. Zinn-Justin, J. Phys. (Paris) 40, 969 (1979).
- ²¹X. Hu and M. Suzuki, in Space-Time Organization in Macromolecular Fluids, edited by F. Tanaka, M. Doi, and T. Ohta (Springer-Verlag, Berlin, 1989), p. 188.