On the CAM Canonicality of the Cluster-Variation Approximations

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The cluster-variation method (CVM) proposed by Kikuchi is a general theory to give approximations, which are useful to discuss phase transitions qualitatively in many systems. Recently one of the present authors (M. S.) proposed the coherent-anomaly method (CAM). If we have a well-behaved series of approximations, which is called a *canonical series*, we can estimate critical exponents following the CAM. In this paper it is demonstrated by using the ferromagnetic Ising models that the CVM will provide a canonical series which shows coherent anomaly. Our result implies that combining the CVM with the CAM will give a powerful method to study phase transitions and critical phenomena.

§ 1. Introduction

The cluster-variation method (CVM) is a scheme to give approximate expressions for the free energy of infinite systems. It is based on the variational principle of free energy. We prepare a set of clusters of elements of the system and give a trial function of the free energy by using density matrices defined on these clusters. In this scheme, mean-fields acting on each cluster are expressed by a set of parameters $\{\lambda_i\}$ and they are regarded as variational parameters. We assume that the best approximation will be obtained when we choose the parameters $\{\lambda_i\}$ so that the trial free energy is reduced to its minimum. The CVM was formulated by Kikuchi[1] in 1951 for the Ising model and then it has been applied to a wide variety of systems[2] such as magnetic systems, liquid-gas systems, and solid solutions. It was reformulated by Morita[3)~5] to apply it to quantum spin systems and random systems.

The CVM has the following two merits. The first one is that it is easy to introduce external fields and to derive equations of state in this method. This enables us to give an approximate expression for an order parameter or response functions and to discuss phase transitions of the system. The second merit is that the CVM gives a systematic procedure to improve approximations. There each approximation is characterized by a set of prepared clusters, which are called *basic clusters*. It is expected that better approximation will follow from a set of larger clusters. As a matter of fact, Schlijper[6,7] proved for the Ising model that the approximate free energy obtained by the CVM converges monotonically to its exact value as larger clusters are included. Kikuchi also proved the convergence of the entropies obtained by the CVM to the exact one in some limit.[8]

In 1986, one of the present authors (M.S.)[9] proposed the coherent-anomaly method (CAM). It is a new general scheme to study phase transitions and critical phenom-

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ena. It studies the convergence rate of approximations. The property of a series of approximations which enables us to estimate the true values of critical exponents is called *canonicality* in the CAM.[9)]

The purpose of the present paper is to demonstrate that the CVM will provide a canonical series which shows coherent anomaly. This study was already reported briefly by the present authors and Fujiki in Refs. 10) and 11). Our result implies that combining the CVM and the CAM will give a powerful method to estimate critical exponents as well as critical temperatures of phase transitions.

§ 2. Kikuchi's approximation and its simplified versions

We consider the Ising model on the d-dimensional hyper-cubic lattice $\boldsymbol{Z}^d$. The Hamiltonian of this system is given by

$$\mathcal{H}=-J\sum_{\langle xy\rangle}S_xS_y-\mu_{\rm B}H\sum_x S_x\,,$$

where $\sum_{\langle xy\rangle}$ denotes the summation over all distinct nearest-neighbor pairs on the lattice. Here we assume that the exchange interaction is ferromagnetic, i.e. $J>0$. The parameter H is an external magnetic field and $\mu_{\rm B}$ denotes the Bohr magneton.

2.1. *Kikuchi's approximation*[1)]

Kikuchi's approximation is derived by the CVM from a set of three clusters given by

$$\Lambda_0=\{\{x\},\{x,x+e_i\},\{x,x+e_i,x+e_j,x+e_i+e_j\}\}\,, \tag{2·1}$$

where $\{e_i\}$'s are the unit vectors of $\boldsymbol{Z}^d$ and $i\neq j$. In other words, the basic clusters of Kikuchi's approximation are a singleton $\{x\}$, a doubleton of nearest-neighbors $\{x, x+e_i\}$, and a square $\{x, x+e_i, x+e_j, x+e_i+e_j\}$. Each cluster is considered as a part of the relevant infinite system and mean-fields from the outside of the cluster shall be acting on spins located on the cluster. The free energy for each cluster may be given as follows by introducing the mean-fields $\{\lambda_1, \lambda_2, \lambda_3\}$:

$$F(\{x\})=-k_{\rm B}T\log[{\rm Tr}\exp\beta(z\lambda_1+\mu_{\rm B}H)S_x]\,, \tag{2·2a}$$

$$\begin{aligned}F(\{x,x+e_i\})=-k_{\rm B}T\log[{\rm Tr}\exp\beta\{&(J+\nu_4\lambda_3)S_xS_{x+e_i}\\&+[(z-1)\lambda_1+\nu_4\lambda_2+\mu_{\rm B}H](S_x+S_{x+e_i})]\,,\end{aligned} \tag{2·2b}$$

$$\begin{aligned}&F(\{x,x+e_i,x+e_j,x+e_i+e_j\})\\&\quad=-k_{\rm B}T\log[{\rm Tr}\exp\beta\{[J+(\nu_4-1)\lambda_3](S_xS_{x+e_i}+S_{x+e_i}S_{x+e_i+e_j}\\&\qquad+S_{x+e_i+e_j}S_{x+e_j}+S_{x+e_j}S_x)\\&\qquad+[(z-2)\lambda_1+2(\nu_4-1)\lambda_2+\mu_{\rm B}H](S_x+S_{x+e_i}+S_{x+e_i+e_j}+S_{x+e_j})]\,,\end{aligned} \tag{2·2c}$$

where z is the number of nearest-neighbor sites ($z=2d$) and ν_4 is the number of squares which have a given bond as an edge ($\nu_4=2(d-1)$). Here λ_1 denotes a mean-field acting on a single spin from its neighboring spins, and λ_2 and λ_3 denote mean-fields acting on a single spin and on a product of a pair of nearest-neighbor spins, respectively, both from a square cluster of spins.

Because a cluster can be, in general, divided into its subclusters, the free energy of the cluster is regarded as a combination of contributions from its parts. Let A be a cluster in Λ_0 and B_i's are its subclusters included in the set Λ_0. Then

$$F(A)=\sum_{B_i\subseteq A} f(B_i)\,. \tag{2·3}$$

The explicit expressions of $F(A)$ are

$$\begin{aligned}
&F(\{x\})=f(\{x\})\,,\\
&F(\{x,\,x+e_i\})=f(\{x\})+f(\{x+e_i\})+f(\{x,\,x+e_i\})\\
&\qquad\qquad\qquad =2f(\{x\})+f(\{x,\,x+e_i\})\,,\\
&F(\{x,\,x+e_i,\,x+e_j,\,x+e_i+e_j\})\\
&\quad =4f(\{x\})+4f(\{x,\,x+e_i\})+f(\{x,\,x+e_i,\,x+e_j,\,x+e_i+e_j\})\,,
\end{aligned} \tag{2·4}$$

where we have used the translation invariance of the system. In other words, we extract a proper contribution $f(B_i)$ from each cluster B_i from (2·2) as follows,

$$f(\{x\})=F(\{x\})\,, \tag{2·5a}$$

$$f(\{x,\,x+e_i\})=F(\{x,\,x+e_i\})-2F(\{x\})\,, \tag{2·5b}$$

$$\begin{aligned}
f(\{x,\,x+e_i,\,x+e_j,\,x+e_i+e_j\})=&F(\{x,\,x+e_i,\,x+e_j,\,x+e_i+e_j\})\\
&-4F(\{x,\,x+e_i\})+4F(\{x\})\,.
\end{aligned} \tag{2·5c}$$

The free energy per spin is assumed to be expressed by using $\{f(B_i)\}$ as

$$f^{(\Lambda_0)}=\sum_{B_i\in\Lambda_0} n(B_i)f(B_i)\,. \tag{2·6}$$

Here $n(B_i)$'s are normalization factors to make $f^{(\Lambda_0)}$ be a value per spin. It is easy to find that

$$\begin{aligned}
&n(\{x\})=1\,,\\
&n(\{x,\,x+e_i\})=\frac{1}{2}z\,,\\
&n(\{x,\,x+e_i,\,x+e_j,\,x+e_i+e_j\})=\frac{1}{8}z\nu_4\,.
\end{aligned} \tag{2·7}$$

By (2·5) and (2·6), the trial function of Kikuchi's approximation is given explicitly by using (2·2) as

$$\begin{aligned}
f^{(\Lambda_0)}=&\left(1-z+\frac{1}{2}z\nu_4\right)F(\{x\})-\frac{1}{2}z(\nu_4-1)F(\{x,\,x+e_i\})\\
&+\frac{1}{8}z\nu_4F(\{x,\,x+e_i,\,x+e_j,\,x+e_i+e_j\})\,.
\end{aligned} \tag{2·8}$$

Then the mean-fields $\{\lambda_i\}$ are considered to be variational parameters and they are determined by the following simultaneous equations,

$$\frac{\delta}{\delta\lambda_1} f^{(\Lambda_0)}=0\,, \tag{2·9a}$$

$$\frac{\delta}{\delta\lambda_2} f^{(\Lambda_0)}=0\,, \tag{2·9b}$$

$$\frac{\delta}{\delta\lambda_3} f^{(\Lambda_0)}=0\,. \tag{2·9c}$$

2.2. *Simplified versions*

In the scheme of the CVM, Bethe's approximation can be viewed as a simplified version of Kikuchi's. In Bethe's approximation we introduce only one kind of mean-field λ_1 and impose a self-consistency condition between the one-spin cluster and the spin-pair cluster. It is obtained by eliminating the square $\{x, x+e_i, x+e_j, x+e_i+e_j\}$ from Λ_0 and considering variations only on a singleton and a doubleton, where $\lambda_2=\lambda_3=0$ and only one equation (2·9a) is solved. If we eliminate the doubleton $\{x, x+e_i\}$ from Λ_0 and consider a singleton and a square as basic clusters, we obtain another approximation by solving (2·9a) to determine λ_1 with $\lambda_2=\lambda_3=0$. This may be called a cactus-square approximation.[11]

Here we introduce a notation to classify approximations. The original Kikuchi approximation is formulated on a set Λ_0, which consists of a singleton, a doubleton and a square. We express this set Λ_0 simply by the notation (124). In Kikuchi's approximation we introduce three kinds of mean-fields (variational parameters) λ_1, λ_2 and λ_3. Remark that λ_1 and λ_2 act on a single spin, whereas λ_3 acts on a product of a pair of spins as shown in (2·2). Because the spin product (e.g. $S_x S_{x+e_i}$) is invariant under the total inversion of spins $\{S_y\}\to\{-S_y\}$ (i.e. Z_2-symmetric), the role played by λ_3 to determine the trial function $f^{(\Lambda_0)}$ is quite different from those by λ_1 and λ_2 as discussed by Minami, Nonomura and the present authors for the multi-effective-field theory.[12] We will call in this paper the mean-fields acting on a single spin or a product of an odd number of spins *odd mean-fields*, and call those acting on a product of an even number of spins *even mean-fields*. For example, we say that Kikuchi's approximation has two kinds of odd mean-fields (λ_1 and λ_2) and one kind of even mean-field (λ_3). Then we propose, for example, a notation [124; 2, 1] to express simply Kikuchi's approximation. Using this notation, Bethe's approximation and the cactus-square approximation are denoted by [12; 1, 0] and [14; 1, 0], respectively. In general, an approximation obtained by a set of clusters $\Lambda=\{B_1, B_2, \cdots, B_n\}$ with n_o kinds of odd mean-fields and n_e kinds of even mean-fields will be abbreviated to $[|B_1||B_2|\cdots|B_n|;\ n_o,\ n_e]$, where $|B_i|$ denotes a number of sites included in a set B_i.

In this paper we consider other two simplified versions of Kikuchi's approximation, which are denoted by [124; 2, 0] and [24; 1, 0]. The former was called Yvon's square approximation in Ref. 11). The latter can be viewed as an Ising spin version[13] of the first approximation found in the paper by Oguchi and Kitatani,[14] where they studied the quantum Heisenberg model by the CAM.

§ 3. Beyond Kikuchi's approximation

In this section we report some trial to improve Kikuchi's approximation, which was briefly reported in Ref. 11).

3.1. *Cube approximation*

We consider the Ising model on $\boldsymbol{Z}^d$, where $d \geq 3$ is assumed. Let C be the following cluster

$$C=\{x+le_i+me_j+ne_k|0\leq l,\, m,\, n\leq 1\}\,, \tag{3·1}$$

where $i\neq j$, $j\neq k$, $i\neq k$ and l, m and n are integers. That is, C is a cube consisting of eight sites. We add C to the previous set Λ_0,

$$\Lambda_C=\Lambda_0\cup C\,, \tag{3·2}$$

and we use Λ_C as a set of basic clusters as below.

The free energies for the singleton and the doubleton are the same as (2·2a) and (2·2b), respectively. However, (2·2c) should be replaced by the following free energy

$$\begin{aligned} &F(\{x,\, x+e_i,\, x+e_j,\, x+e_i+e_j\}) \\ &\quad=-k_B T\log[\mathrm{Tr}\exp\beta[J+(\nu_4-1)\lambda_3+\nu_8\lambda_5]S^{(2)}+\nu_8\lambda_6 S^{(2')}+\nu_8\lambda_8 S^{(4)} \\ &\qquad+[(z-2)\lambda_1+2(\nu_4-1)\lambda_2+\nu_8\lambda_4]S^{(1)}+\nu_8\lambda_7 S^{(3)}]\,, \end{aligned} \tag{3·3}$$

where

$$\begin{aligned} &S^{(1)}=S_x+S_{x+e_i}+S_{x+e_i+e_j}+S_{x+e_j}\,, \\ &S^{(2)}=S_xS_{x+e_i}+S_{x+e_i}S_{x+e_i+e_j}+S_{x+e_i+e_j}S_{x+e_j}+S_{x+e_j}S_x\,, \\ &S^{(2')}=S_xS_{x+e_i+e_j}+S_{x+e_i}S_{x+e_j}\,, \\ &S^{(3)}=S_xS_{x+e_i}S_{x+e_i+e_j}+S_{x+e_i}S_{x+e_i+e_j}S_{x+e_j}+S_{x+e_i+e_j}S_{x+e_j}S_x+S_{x+e_j}S_xS_{x+e_i}\,, \\ &S^{(4)}=S_xS_{x+e_i}S_{x+e_i+e_j}S_{x+e_j}\,, \end{aligned} \tag{3·4}$$

and

$$\nu_8=2(d-2)\,. \tag{3·5}$$

Here we have newly introduced three kinds of even mean-fields, λ_5, λ_6 and λ_8 and two kinds of odd ones, λ_4 and λ_7, which are acting from cubic clusters.

The cubic cluster C has six faces, each of which is a square. Let Ω_i denotes the i-th face and $h(\Omega_i)$ be a contribution from Ω_i ($i=1, 2, \cdots, 6$). The free energy of the cube C with mean-fields is given by

$$F(C)=-k_B T\log[\mathrm{Tr}\exp\beta\sum_{i=1}^{6}h(\Omega_i)]\,. \tag{3·6}$$

Assume that Ω_1 is a square $\{x,\, x+e_i,\, x+e_j,\, x+e_i+e_j\}$. Then we obtain

$$h(\Omega_1)=\frac{1}{2}[J+(\nu_4-2)\lambda_3+2(\nu_8-1)\lambda_5]S^{(2)}+(\nu_8-1)\lambda_6 S^{(2')}+(\nu_8-1)\lambda_8 S^{(4)}$$
$$+\frac{1}{3}[(z-3)\lambda_1+2(\nu_4-2)\lambda_2+3(\nu_8-1)\lambda_4]S^{(1)}+(\nu_8-1)\lambda_7 S^{(3)}, \tag{3·7}$$

where $S^{(i)}$'s are given by (3·4). The expressions for other $h(\Omega_i)$'s are obtained from (3·7) by appropriate transformations.

It is easy to find that

$$f(C)=F(C)-6F(\{x, x+e_i, x+e_j, x+e_i+e_j\})+12F(\{x, x+e_i\})-8F(\{x\}). \tag{3·8}$$

The free energy is assumed to be

$$f^{(\Lambda_C)}=\sum_{B_i\in\Lambda_C} n(B_i)f(B_i), \tag{3·9}$$

where $n(B_i)$'s are given by (2·7) and

$$n(C)=\frac{1}{48}z\nu_4\nu_8. \tag{3·10}$$

For $d=3$, for example, we obtain the following expression for (3·9) by using (2·5) and (3·8),

$$f^{(\Lambda_C)}=F(C)-3F(\{x, x+e_i, x+e_j, x+e_i+e_j\})+3F(\{x, x+e_i\})-F(\{x\}), \tag{3·11}$$

which corresponds to Eq. (1) in Ref. 11).

The mean-fields $\{\lambda_i\}$ are determined by the following eight simultaneous equations,

$$\frac{\delta}{\delta\lambda_i}f^{(\Lambda_C)}=0, \quad i=1, 2, \cdots, 8. \tag{3·12}$$

We called this approximation the cube approximation in Ref. 11). By using the notation introduced in § 2.2, it is denoted by [1248; 4, 4].

Two types of simplified versions of the cube approximation are considered;[11] a cactus-cube approximation denoted by [18; 1, 0] and Yvon's cube approximation denoted by [1248; 3, 0].

3.2. *Tanoji approximation*

In order to improve Kikuchi's approximation for the two-dimensional Ising model, we introduce another approximation, which was called the Tanoji approximation in Ref. 11). Let T_1 and T_2 be the following clusters,

$$T_1=\{x+ne_1+me_2|0\le n\le 1, 0\le m\le 2\}, \tag{3·13a}$$

$$T_2=\{x+ne_1+me_2|0\le n\le 2, 0\le m\le 2\}, \tag{3·13b}$$

where n and m are integers. The cluster T_1 is a set of six sites and T_2 consists of nine sites. We take the union of Λ_0 and $T_1 \cup T_2$ as a set of basic clusters;

$$\Lambda_T=\Lambda_0\cup T_1\cup T_2 . \qquad (3\cdot14)$$

The reason why we call this approximation the Tanoji approximation as in Ref. 11) is that the figure made of the nine sites of T_2 and the bonds connecting each nearest-neighbor pairs of sites seems to be a Chinese character which we Japanese call *Tanoji*.

In this approximation, we introduce 44 kinds of mean-fields.[11] Among them, 5 kinds of mean-fields act on a single spin as given by $S^{(1)}$, 11 kinds on products of spin pairs as $S^{(2)}$ or $S^{(2')}$, 13 kinds on three-spin products as $S^{(3)}$, 10 kinds on four-spin products as $S^{(4)}$, 4 kinds on five-spin products and one on six-spin products. The explicit expressions for $F(\{x, x+e_1, x+e_2, x+e_1+e_2\})$, $F(T_1)$ and $F(T_2)$ are rather lengthy. So we do not give them here. Only we remark that

$$f(T_1)=F(T_1)-2F(\{x, x+e_1, x+e_2, x+e_1+e_2\})+F(\{x, x+e_1\}) , \qquad (3\cdot15a)$$

$$f(T_2)=F(T_2)-4F(T_1)+4F(\{x, x+e_1, x+e_2, x+e_1+e_2\})-F(\{x\}) , \qquad (3\cdot15b)$$

and

$$f^{(\Lambda_T)}=\sum_{B_i\in\Lambda_T} n(B_i)f(B_i)$$

$$=f(\{x\})+2f(\{x, x+e_1\})+f(\{x, x+e_1, x+e_2, x+e_1+e_2\})+2f(T_1)+f(T_2) . \qquad (3\cdot16)$$

It should be remarked that if we substitute $\{F(B_i)\}$ for $\{f(B_i)\}$ in (3·16) by using (2·5) and (3·15), the terms $F(\{x, x+e_1\})$ and $F(\{x\})$ are canceled and we obtain

$$f^{(\Lambda_T)}=F(T_2)-2F(T_1)+F(\{x, x+e_1, x+e_2, x+e_1+e_2\}) , \qquad (3\cdot17)$$

which corresponds to Eq. (2) in Ref. 11). This approximation is abbreviated to [12469; 22, 22].

If we omit the contribution from T_1, we obtain a simplified version of the Tanoji approximation. In this case, $F(T_1)=f(T_1)=0$ and

$$F(T_2)=f(T_2)+4f(\{x, x+e_1, x+e_2, x+e_1+e_2\})+12f(\{x, x+e_1\})+9f(\{x\}) . \qquad (3\cdot18)$$

Then by (2·4) and (3·18), we find that the relation (3·15b) shall be changed to

$$f(T_2)=F(T_2)-4F(\{x, x+e_1, x+e_2, x+e_1+e_2\})+4F(\{x, x+e_1\})-F(\{x\}) . \qquad (3\cdot19)$$

By neglecting $f(T_1)$ in (3·16) and use (3·19) instead of (3·15b), we obtain

$$f^{(\Lambda_T\setminus T_1)}=F(T_2)-3F(\{x, x+e_1, x+e_2, x+e_1+e_2\})+2F(\{x, x+e_1\}) , \qquad (3\cdot20)$$

which corresponds to Eq. (3) in Ref. 11).

In its simplified versions, we take into account only 8 kinds of the odd mean-fields and 6 kinds of the even mean-fields among 44 kinds, which is denoted by [1249; 8, 6].

§ 4. Coherent anomalies of approximations

The magnetization of the system is obtained from the approximate free energy

$f^{(A)}$ by

$$m=\frac{\partial}{\partial(\beta H)}\left(-\frac{1}{k_B T}f^{(A)}\right). \tag{4·1}$$

In principle, we can determine the equation of state

$$m=m(T, H) \tag{4·2}$$

for each approximation by the CVM, though the explicit expression will be quite lengthy. Here we will discuss critical phenomena in the Ising models. In order to do it, the behavior of (4·2) only in the vicinity of the critical temperature T_c should be studied. Because the phase transition of the Ising model is of second order, we can assume that m is small near the critical temperature T_c in a weak external field $H \ll 1$. In this case, we can find that the equation of state (4·2) shows the same structure for any approximation given by the CVM as

$$a(T)m=b(T)m^3+c(T)H+o(m^3, H), \tag{4·3}$$

where $a(T)$, $b(T)$ and $c(T)$ are functions of the temperature. Then we find that $a(T)$ changes its sign at some temperature T_c in decreasing T, whereas the signs of $b(T)$ and $c(T)$ do not change at T_c in general.

From the above observation, the temperature T_c, defined by a zero of $a(T)$ can be regarded as an approximate critical temperature. In Tables I and II, we show the critical temperature of each approximation discussed in the previous sections for the two- and three-dimensional Ising models, respectively. It should be remarked that the approximation denoted by [124; 2, 1] is Kikuchi's approximation. The approximations [1249; 8, 6] and [12469; 22, 22] in two dimensions and [1248; 4, 4] in three dimensions have lower critical temperatures than Kikuchi's, which implies that they improve Kikuchi's approximation. It should be remarked that we can find the value of T_c of [1248; 4, 4] in the original paper by Kikuchi (see Eq. (D7.8) in Ref. 1)), where he called it the cubic-cell approximation.

Table I. CAM data of the approximations obtained by the CVM for the Ising model on the square lattice. There was a typographic error in Table I of Ref. 11). The correct value of the critical temperature in the Tanoji approximation is $k_B T_c/J=2.34630$ as shown below.

approximations	$k_B T_c/J$	$\bar{\chi}$
[12; 1, 0]	2.88539	0.5
[14; 1, 0]	2.77078	0.58541
[24; 1, 0]	2.70319	0.64869
[124; 2, 0]	2.62534	0.73799
[124; 2, 1]	2.42567	1.41697
[1249; 8, 6]	2.38643	1.73034
[12469; 22, 22]	2.34630	2.35463

Table II. CAM data of the approximations obtained by the CVM for the Ising model on the cubic lattice.

approximations	$k_B T_c/J$	$\bar{\chi}$
[12; 1, 0]	4.93261	0.25
[14; 1, 0]	4.89275	0.25811
[24; 1, 0]	4.86517	0.26402
[18; 1, 0]	4.83951	0.27078
[124; 2, 0]	4.76107	0.28880
[1248; 3, 0]	4.70604	0.30956
[124; 2, 1]	4.60973	0.4
[1248; 4, 4]	4.58099	0.41292

In any approximation obtained by the CVM, the magnetization m appears at T_c, with a critical exponent $\beta_0=1/2$ and the zero-field susceptibility χ_0 diverges there with a critical exponent $\gamma_0=1$, as derived from (4·3). In other words, critical exponents obtained by the CVM are classical ones (showing the same values as given by a simple mean-field approximation) and there is no improvement. The values of critical exponents are, however, different from their classical values if the dimensionality is less than the upper critical dimension d_u. It is shown by the renormalization-group argument that $d_u=4$ for the Ising model.

In 1986, one of the present authors (M. S.) generally discussed the convergence of approximations.[9] He concluded that when the true value of the critical exponent is different from the classical value, the critical coefficients of the classical singularities of approximations will diverge as the approximation converges to the exact one with raising the degree of approximations. As an example, we consider here the susceptibility χ_0. The critical coefficient $\bar{\chi}$ is defined by

$$\chi_0=\bar{\chi}\frac{T_c}{T-T_c}+O(1) \tag{4·4}$$

for $0<T-T_c\ll 1$. It can be calculated from $a(T)$ and $c(T)$ in (4·3). Let T_c^* be the exact value of the critical temperature and let

$$\delta=\frac{T_c-T_c^*}{T_c^*}\,. \tag{4·5}$$

As shown in Ref. 9), $\bar{\chi}$ should behave asymptotically as

$$\bar{\chi}\sim\delta^{-(\gamma-1)}\,, \tag{4·6}$$

as the approximation converges to the exact one. Because the convergence of approximations means $T_c\to T_c^*$ as raising the degree of approximations, $\bar{\chi}$ will show the asymptotic divergence (4·6). This phenomenon is called *the coherent anomaly*.[9]

In the coherent-anomaly method (CAM), the dependence of $\bar{\chi}$ on δ is essential and a series of approximations in which the relation (4·6) holds asymptotically for the limit $\delta\to 0$ is called a *CAM canonical series* or simply *a canonical series*.[9] If we find a method to derive a canonical series of approximations, we can estimate the true values of critical exponents following the CAM.[9),15)]

Tables I and II show $\bar{\chi}$ as well as T_c for the approximations given by the CVM. As expected, $\bar{\chi}$ becomes larger as T_c decreases. This implies that $\bar{\chi}$ will diverge if we can raise the degree of approximations infinitely. In order to examine the canonicality of the CVM, we plot these data on the $\log\delta$-$\log\bar{\chi}$ plane. The exact critical temperature for the square lattice is given by Onsager as

$$\begin{aligned}\frac{k_B T_c^*}{J}&=\{\tanh^{-1}(\sqrt{2}-1)\}^{-1}\\ &=2.269185\ldots\,.\end{aligned} \tag{4·7}$$

The most reliable value for the cubic lattice may be[16)~20)]

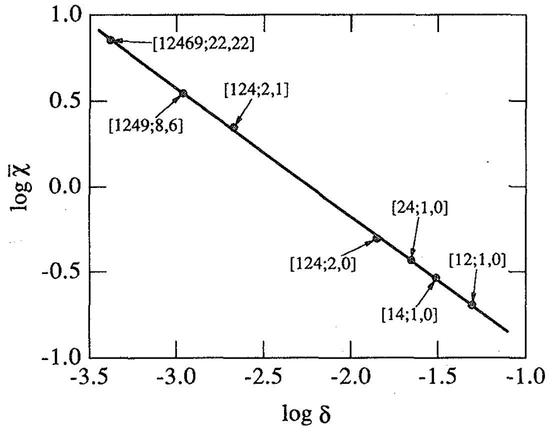

Fig. 1. The results for the square lattice are shown, where we have used the value given by (4·7). The line is obtained by the least-squares fitting and its slope is -0.74995.

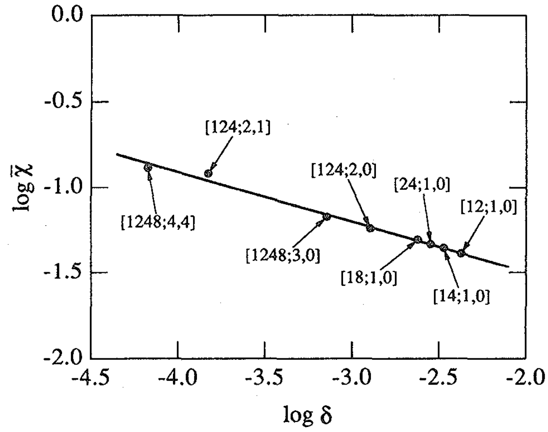

Fig. 2. The results for the cubic lattice are shown, where we have used the value given by (4·8). The line is obtained by the least-squares fitting and its slope is -0.2926.

$$\frac{k_B T_c^*}{J} = 4.5115\ldots. \tag{4·8}$$

Figures 1 and 2 are the results for the square lattice and the cubic lattice, respectively, where we have used the values given by (4·7) and (4·8). The lines in the figures are obtained by the least-squares fitting and the slope of them is given by 0.74995 for Fig. 1 and 0.2926 for Fig. 2. Because $\gamma = 7/4 = 1.75$ for the two-dimensional Ising model by the exact solutions $\alpha = 0$, $\beta = 1/8$ and the scaling relation $\alpha + 2\beta + \gamma = 2$, the slope in Fig. 1 should be 0.75 if the relation (4·6) is exact. For the three-dimensional Ising model, the reliable estimates[16)~20)] for γ are given between 1.24 and 1.25. Then the corresponding slope in Fig. 2 is $0.24 \sim 0.25$.

Figure 1 shows that the relation (4·6) holds quite well in the two-dimensional case. Of course, we cannot conclude the canonicality from a finite set of approximations, because it is defined as the asymptotic behavior of approximations. However, Fig. 1 suggests that the CVM will provide a canonical series in this case. How about the three-dimensional case? The plots in Fig. 2 are rather scattering and the slope is greater than the expected value. It is considered to come from the fact that the basic clusters for the approximations discussed here are rather small in the three-dimensional system. As a matter of fact, the basic clusters in Λ_0 are all two-dimensional, and if we use only three approximations which take into account the cubic cluster C as a basic cluster, the slope of the line obtained by the least-squares fitting is reduced to 0.2730. We expect that the slope will become the desired value, if we can include the approximations formulated by using a $3 \times 3 \times 3$ cluster as a basic cluster, because such a cluster may correspond to the Tanoji cluster T_2 in two dimensions.

§ 5. Concluding remarks

In the present paper we have given a brief review of Kikuchi's approximation and its simplified versions at first. Then we have reported our trial to improve them.

We calculated the critical temperatures T_c and the critical coefficients of the susceptibility $\bar{\chi}$ of the seven kinds and the eight kinds of approximations obtained by the CVM for the two- and the three-dimensional Ising models, respectively. The result of the two-dimensional system suggests that the approximations by the CVM may construct CAM canonical series. In three dimensions, the approximations discussed here are still in the low level, in comparison with those in two dimensions. However, we expect that the CVM will provide a canonical series also for the three-dimensional systems.

The CVM proposed by Kikuchi[1] is a systematic method to improve approximations for phase transitions. The monotonic convergence of approximate expressions of the free energy to the exact one was proved by Schlijper.[6),7)] However, the convergence of T_c to the exact value T_c^* is still an open problem, because the convergence of the magnetization has not yet been proved. The CAM canonicality is a property of the convergence *rate* of approximations. Then it may be hard to prove the canonicality of the CVM. However, as demonstrated in the present paper, the CVM will be a powerful method to study critical phenomena by combining it with the CAM, if it is confirmed that it provides a canonical series.

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References

1) R. Kikuchi, Phys. Rev. **81** (1951), 988.
2) For a review see D. M. Burley, in *Phase Transitions and Critical Phenomena*, ed. C. Domb and M. S. Green (Academic Press, London, 1972), vol. 2, p. 329.
3) T. Morita, J. Phys. Soc. Jpn. **12** (1957), 753, 1060.
4) T. Morita, J. Math. Phys. **13** (1972), 115.
5) T. Morita, J. Stat. Phys. **34** (1984), 319.
6) A. G. Schlijper, Phys. Rev. **B27** (1983), 6841.
7) A. G. Schlijper, J. Stat. Phys. **40** (1985), 1.
8) R. Kikuchi, CVM Entropy Algebra (preprint 1990).
9) M. Suzuki, J. Phys. Soc. Jpn. **55** (1986), 4205.
10) M. Katori and M. Suzuki, J. Phys. Soc. Jpn. **57** (1988), 3753.
11) S. Fujiki, M. Katori and M. Suzuki, J. Phys. Soc. Jpn. **59** (1990), 2681.
12) K. Minami, Y. Nonomura, M. Katori and M. Suzuki, Physica **A174** (1991), 479.
13) G. Tanaka and M. Kimura, Int. J. Mod. Phys. **B6** (1992), 2363.
14) T. Oguchi and H. Kitatani, J. Phys. Soc. Jpn. **57** (1988), 3973.
15) M. Suzuki, M. Katori and X. Hu, J. Phys. Soc. Jpn. **56** (1987), 3092.
16) G. S. Pawley, R. H. Swendsen, D. J. Wallace and K. G. Wilson, Phys. Rev. **B29** (1984), 4030
17) R. Pearson, Phys. Rep. **103** (1984), 185.
18) J. C. Le Guillou and J. Zinn-Justin, Phys. Rev. **B21** (1980), 3976; J. Phys. Lett. (Paris) **46** (1985), L137, and references cited therein.
19) R. B. Pearson, J. L. Richardson and D. Toussaint, Phys. Rev. **B31** (1985), 4472.
20) H. W. J. Blöte, A. Compagner, J. H. Croockewit, Y. T. J. C. Fonk, J. R. Heringa, A. Hoogland, T. S. Smit and A. L. Van Willigen, Physica **A161** (1989), 1.