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Super-Effective-Field Theory and Coherent-Anomaly Method in Cooperative Phenomena

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Conceptual arguments on the coherent-anomaly method (CAM) and on the super-effective-field theory are presented to explain the basic ideas of these theories. Some possible applications are also suggested.

KEY WORDS: Coherent-anomaly method; CAM; super-effective-field theory; critical phenomena; mean-field approximation; power-series CAM; continued-fraction CAM; Padé approximants CAM; correlation-identity-decoupling CAM.

1. INTRODUCTION

I learned from Prof. N. van Kampen a great deal of fundamental physics and ways of thinking including criticism during my stay in Utrecht from 1970 to 1971. In particular, I have been influenced greatly concerning the importance of fluctuation in nonequilibrium systems.(1–5) Fluctuations are important in the formation of macroscopic order from the unstable point, as I clarified in scaling theory.(6–8) In van Kampen's Ω-expansion,(1) Gaussian fluctuations are mainly taken into account as corrections to the deterministic path of the relevant system. Nonlinear fluctuations play an essential role in critical phenomena. Larger fluctuations give greater contributions to the fractional singularities of physical quantities near the critical point. Such a situation can be treated in ordinary phase transitions rather well by Wilson's renormalization group (RG) method(9) through recursion formulas. Each approximate RG gives an approximate set of fractional values of critical exponents. It is not clear whether such an approximate series of RG converges. In fact, it is an asymptotic expansion in many situations, such as the ε-expansion.

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On the other hand, the mean-field or effective-field approximations have been used very frequently as a starting point of theories of phase transitions. No fluctuation is included in the Weiss mean-field theory.[10] Bethe[11] took fluctuations into account to study phase transitions. His method is a cluster effective-field theory. Any physical quantity x may be separated into the following two parts:

$$x = y + \Delta x \tag{1}$$

as in van Kampen's Ω-expansion, where y denotes the average $\langle x \rangle$ and Δx the remaining fluctuating part, namely $\langle \Delta x \rangle = 0$. In order to study the fluctuation $\langle (\Delta x)^2 \rangle$ correctly, we have to take into account as many configurations as possible, because it expresses the deviation of possible configuration of x from the average $\langle x \rangle$. For this purpose, it is very convenient to consider clusters and to investigate all the configurations of the relevant cluster in a statistical mechanical way. Larger fluctuations can be included in larger clusters systematically. This leads to Fisher's finite-size scaling law.[12,13] This scaling law is closely related to the Fisher–Kadanoff scaling law[14,15] on the correlation function $C(R)$,

$$C(R) \simeq \frac{A}{R^{d-2+\eta}} e^{-\kappa R} \tag{2}$$

for an infinite system, but the former is more microscopic and fundamental in the sense that the latter can be derived from the former as the limit of infinite cluster size L. That is, this is a crossover phenomenon from a finite analytic expression to a singular behavior (2). It should be noted here that this crossover phenomenon occurs for a fairly large value of the cluster size L, as is well known.[14,15]

Now there arises the question whether it is possible to find a new scheme to make use of a crossover from a classical singular behavior to a fractional one which occurs for a rather small value of the cluster size L. This question has been answered[16] affirmatively by the theory of the coherent-anomaly method[16–32] (the CAM theory). This is based on the observation[16] of the occurrence of a very effective crossover from classical to fractional behaviors in generalized cluster-mean-field approximations. It is quite remarkable that nonclassical exponents can be estimated even from the combination[16] of the Weiss and Bethe approximations, and more precisely by combining[24] these two approximations with the Kramers–Wannier–Kikuchi approximation.[33,34] That is, even the analysis of very small clusters can predict rather reasonable fractional critical exponents. This shows that the convergence of the CAM is extremely rapid, as is seen more explicitly from many other applications[17–32] of the CAM theory.

From this new point of view, to construct mean-field-type approximations is quite substantial even to study nonclassical critical behaviors. Then is it possible to find a mean-field approximation for any kind of phase transition? This is answered affirmatively by introducing the super-effective-field theory.[35,36]

2. BASIC IDEA OF THE SUPER-EFFECTIVE-FIELD THEORY

The basic idea of this new theory is to introduce a generalized effective field, which is independent of decoupled interactions used in the ordinary mean-field approximations. Consider an arbitrary finite cluster whose Hamiltonian is written as $\mathscr{H}_{\text{cl}}$. Here I introduce a super-effective field Λ_k conjugate to a possible local order parameter Q_k at the site k as

$$\tilde{\mathscr{H}} = \mathscr{H}_{\text{cl}} - \sum_{k \in \partial\Omega} \Lambda_k \tilde{Q}_k \tag{3}$$

where $\tilde{Q}_k = \varepsilon_{0k} Q_k$ and ε_{ij} denotes the "modular factor" to take into account the (hidden) symmetry of the system. The local operator Q_k is defined by the sum of products of some local operators, whose support is assumed to be D_k. The symbol $\partial\Omega$ denotes the boundary region of the cluster Ω, say $\partial\Omega = D_1 + D_2 + \cdots + D_z$, as shown in Fig. 1. The super-effective-fields are determined by the self-consistency condition that

$$\langle Q_0 \rangle = \langle \tilde{Q}_k \rangle \qquad \text{for all } k \tag{4}$$

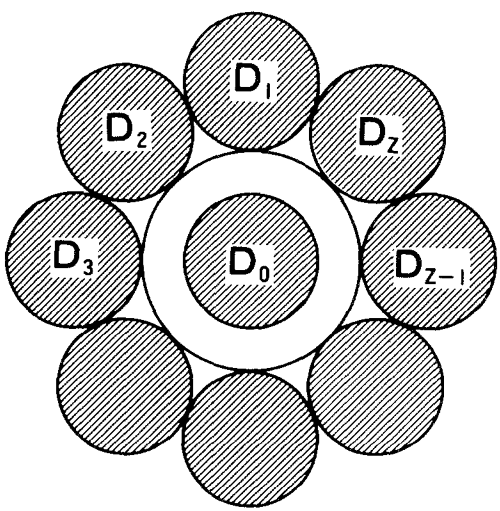

Fig. 1. A super-effective-field cluster[35,36] in which each domain D_j is the support of the local order parameter Q_j.

As far as the linear terms in $\{\Lambda_k\}$ are concerned, equations (4) are expressed in terms of Kubo's canonical correlation functions $\langle Q_j; Q_k\rangle_{\rm cl}$ defined by

$$\langle Q_j; Q_k\rangle = \frac{1}{\beta}\int_0^\beta \langle Q_j Q_k(i\hbar\lambda)\rangle \, d\lambda \tag{5}$$

where $\langle \cdots \rangle_{\rm cl}$ is the average for the cluster Hamiltonian $\mathscr{H}_{\rm cl}$ and

$$Q_k(z) = e^{iz\mathscr{H}_{\rm cl}/\hbar} Q_k e^{-iz\mathscr{H}_{\rm cl}/\hbar} \tag{6}$$

Thus, using the canonical correlation functions (5), we can obtain the critical point T_c for the phase transition characterized by the possible order parameter $Q = \sum_j Q_j$.

Furthermore, whether this choice of possible order parameters is correct or not can be checked by applying the CAM to a systematic series of super-effective-field approximations and by studying the coherent anomaly.

This super-effective-field theory has already been applied[35,36] to chiral phase transitions[37–42] and spin glasses.[43–53]

At a glance, the above super-effective-field theory looks like a simple extension of the ordinary effective-field theory of phase transitions to more complicated cases such as topological orders. It is, however, much more profound in the sense that the relevant long-range order can be formed through the super-effective-field term virtually introduced in (3) and that this virtual term is not directly related to the original Hamiltonian but it expresses a hidden symmetry of the system. One might consider, instead, an effective Hamiltonian of the form

$$\mathscr{H}_{\rm eff} = -J_{\rm eff} \sum_{\langle ij\rangle} Q_i Q_j \tag{7}$$

where the effective interaction strength $J_{\rm eff}$ is estimated perturbationally from the original Hamiltonian, but this is a weak coupling theory and quite phenomenological. It is not useful to estimate the real critical point of the original system correctly. On the other hand, the present super-effective-field theory is a strong coupling theory and consequently it is very powerful in investigating the real phase transition of the relevant system, although calculations in this scheme are rather complicated, as is seen from some explicit applications[36] to topological phase transitions.

3. BASIC SCHEME OF THE COHERENT-ANOMALY METHOD (CAM)

As briefly discussed in the Introduction, the basic idea of the CAM is to note the coherent anomaly that the critical coefficients of the classical singularities of the relevant response functions become anomalously large (or small) as the degree of approximation increases.[16] These coherent anomalies yield the true critical singularities of the relevant physical quantities. Thus, systematic cluster mean-field approximations are extremely useful even from the modern viewpoint of critical phenomena.

Therefore the basic procedure of the coherent-anomaly method is to construct systematically self-consistent mean-field approximations for each phenomenon and to extract a common feature inherent among them by making an analytic continuation of the degree of approximation. It is quite remarkable that such a common feature on intrinsic critical singularities appears in the coefficients of the classical singularities obtained in the generalized systematic mean-field (or effective-field) approximations. Until the CAM theory was proposed, no one had paid attention to the amplitude of the classical singularity, for it had been believed to be irrelevant to the true criticality.

In order to explain how the true criticality is estimated from these coherent anomalies, I discuss here a simple example of the magnetic susceptibility $\chi_0(T)$ of ferromagnets, which is expected to show the following fractional singularity:

$$\chi_0(T) \sim \frac{1}{(T - T_c^*)^\gamma} \tag{8}$$

near the true critical point T_c^* with the fractional critical exponent γ. As is well known, even generalized mean-field approximations yield the Curie–Weiss law

$$\chi_0(T) \simeq \frac{\bar{\chi}(T_c)}{\varepsilon}; \qquad \varepsilon = \frac{T - T_c}{T_c} \tag{9}$$

near each mean-field critical point T_c. However, the mean-field critical coefficient $\bar{\chi}(T_c)$ becomes anomalously large[16–22] as the degree of approximation increases, namely

$$\bar{\chi}(T_c) \to \infty \qquad \text{as} \quad T_c \to T_c^* \tag{10}$$

Thus, we may assume[16–22] that

$$\bar{\chi}(T_c) \simeq \frac{f_\chi}{(T_c - T_c^*)^\psi} \sim \delta(T_c)^{-\psi} \tag{11}$$

near $T_c = T_c^*$, namely, for $\delta(T_c) \equiv (T_c - T_c^*)/T_c^* \ll 1$. This coherent-anomaly exponent ψ can be easily estimated from mean-field critical data on $\bar{\chi}(T_c)$ as a function of T_c obtained in cluster-mean-field approximations[16–22] or obtained by high-temperature expansions.[26,27]

More explicitly, we can estimate ψ through the formula

$$\psi = \log\left(\frac{\bar{\chi}(T_c^{(1)})}{\bar{\chi}(T_c^{(2)})}\right) \Big/ \log\left(\frac{\delta T_c^{(2)}}{\delta T_c^{(1)}}\right) \tag{12}$$

when the true critical point T_c^* is known. Here I have used the notation

$$\delta T_c^{(j)} = T_c^{(j)} - T_c^* \tag{13}$$

When the true critical point T_c^* is unknown, we need at least three mean-field-type approximations to estimate the three parameters T_c^*, ψ, and f_χ. When more than three approximations are obtained, the least squares fitting can be used to estimate the above three parameters. The nonclassical critical exponent γ can be estimated through the coherent-anomaly relation[16,17]

$$\gamma = 1 + \psi \tag{14}$$

This relation is derived in three different ways,[16,17] through (1) the finite-degree-of-approximation scaling, (2) the envelope theory, and (3) the scaling law. Thus, the intrinsic critical fluctuation can be studied through the CAM. If we specify a series of cluster-mean-field approximations, the critical point T_c and the critical coefficient $\bar{\chi}(T_c)$ can be obtained in any accuracy. In this sense, the CAM supplies a very precise procedure to study the criticality, which corresponds to a precise experimental measurement.

The above procedure can be extended to any other physical quantities.

4. PERTURBATIONAL EXPANSIONS, CLUSTER-MEAN-FIELD APPROXIMATIONS, AND CAM THEORY

Up to now, the most typical method to study the criticality has been to perform the high-temperature expansions, namely perturbational expansions, and to apply the Padé approximation or the ratio method to these perturbational expansions. These classical methods are, however, only very primitive extrapolation schemes.

Here I give another interpretation of the high-temperature expansions, namely, one can construct generalized mean-field approximations by comparing the perturbational expansions of them with the original high-temperature expansions.

For example, the susceptibility $\chi_0(T)$ is generally expanded as

$$\chi_0(T) = (N\mu_B^2/k_B T)(1 + zJ/k_B T + \cdots) \tag{15}$$

where z denotes the number of nearest neighbors and J is the interaction strength of the system. The above high-temperature expansion may be interpreted as the expansion of the following Weiss approximation of $\chi_0(T)$:

$$\chi_0^{(W)}(T) = \frac{N\mu_B^2}{k_B T} \cdot \frac{1}{1 - zJ/k_B T} \simeq \frac{\mu_B^2}{J} \frac{1}{z} \frac{1}{\varepsilon} \tag{16}$$

where $\varepsilon = (T - T_c)/T_c$ and $T_c = zJ/k_B$.

If we take into account the next term in (15), it depends on the off-diagonal elements of the Hamiltonian. For the Ising model described by

$$\mathscr{H} = -J \sum_{\langle ij \rangle} S_i S_j; \qquad S_j = \pm 1 \tag{17}$$

the susceptibility $\chi_0(T)$ is expanded as

$$\chi_0(T) = \frac{N\mu_B^2}{k_B T} [1 + zx + z(z-1) x^2 + \cdots] \tag{18}$$

where $x = \tanh(J/k_B T)$. Then it may be interpreted as the expansion of the following well-known Bethe approximation of $\chi_0^{(B)}(T)$,

$$\chi_0^{(B)}(T) = \frac{N\mu_B^2}{k_B T} \frac{1+x}{1-(z-1)x} \simeq \frac{N\mu_B^2}{J} \frac{1}{z-2} \frac{1}{\varepsilon} \tag{19}$$

These interpretations are particularly useful from the viewpoint of the CAM. In fact, even the critical coefficients of these simple approximations show the coherent anomaly, namely the critical coefficient $1/(z-2)$ in the Bethe approximation is much larger than the critical coefficient $1/z$ in the Weiss approximation; the critical point $T_c^{(B)}$ defined by

$$k_B T_c^{(B)} = 2J \Big/ \log\left(\frac{z}{z-2}\right) \tag{20}$$

is lower than that of the Weiss approximation, $T_c^{(W)} = zJ/k_B$. This is nothing but the coherent anomaly.

This suggests the following power-series CAM theory.

5. POWER-SERIES CAM THEORY

When the relevant physical quantity $Q(x)$ is given as a power series

$$Q(x) = a_0 + a_1 x + a_2 x^2 + \cdots \tag{21}$$

we make an expansion of the inverse of $Q(x)$ in the form

$$F(x) = 1/Q(x) = b_0 + b_1 x + b_2 x^2 + \cdots \tag{22}$$

The coefficients $\{b_k\}$ can be easily obtained from $\{a_k\}$, and consequently the zeros of the nth approximation $F_n(x) = b_0 + b_1 x + \cdots + b_n x^n$ can also be obtained. Thus, we have

$$F_n(x) \simeq \bar{F}(x_c)\varepsilon; \qquad \varepsilon = (x_c - x)/x_c \tag{23}$$

where $F_n(x_c) = 0$. This critical coefficient $\bar{F}(x_c)$ shows a coherent anomaly of the form

$$\bar{F}(x_c) \sim (x_c^* - x_c)^{\psi} \tag{24}$$

near the true critical point x_c^*. Then the original physical quantity $Q(x)$ shows the following fractional singularity[26]:

$$Q(x) \sim 1/(x_c^* - x)^{\varphi}; \qquad \varphi = 1 + \psi \tag{25}$$

For example, consider the high-temperature expansion of the susceptibility in the two-dimensional Ising model[16]:

$$\chi_0(T) = \frac{N\mu_B^2}{k_B T}(1 + 4x + 12x^2 + 36x^3 + 100x^4 + 276x^5 + 740x^6 + 1972x^7 + 5172x^8 + 13{,}492x^9 + 34{,}876x^{10} + 89{,}764x^{11} + \cdots) \tag{26}$$

where $x = \tanh(J/k_B T)$, and J denotes the strength of the Ising interaction. It is easily shown that

$$(b_1, b_2, ..., b_{21}, ...) = (-4, 4, -4, 12, -20, 44, -84, 188, -372, 788, -1604, 3444, -7204, 15660, -33316, 72908, -156596, 344500, -746308, 1651868, -3607236, ...) \tag{27}$$

The inverse functions shows a remarkable coherent anomaly (Fig. 2). It is shown more explicitly in Fig. 3.[6] From the slope in Fig. 3, we obtain $\psi \simeq 0.753$ (or 0.748), and consequently $\gamma \simeq 1.753$ (or 1.748), which agrees very well with the exact value $\gamma = 1.75$.

Many other applications of this power-series CAM theory will be reported elsewhere.[32]

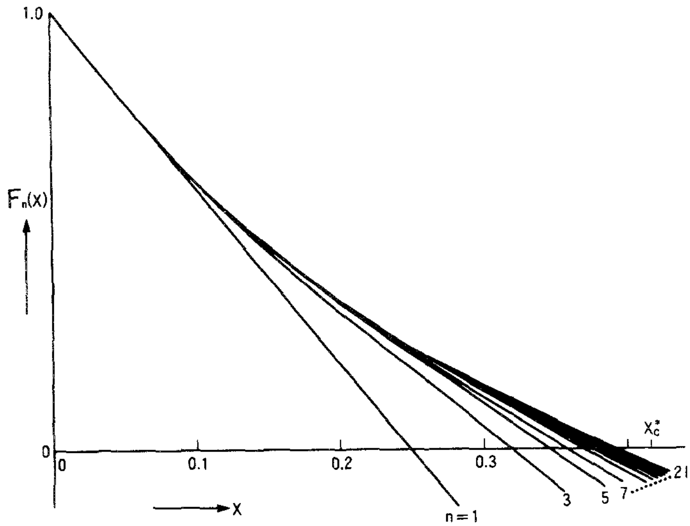

Fig. 2. A systematic change of the inverse of the susceptibility $\chi_0(T)$ for the two-dimensional Ising model.

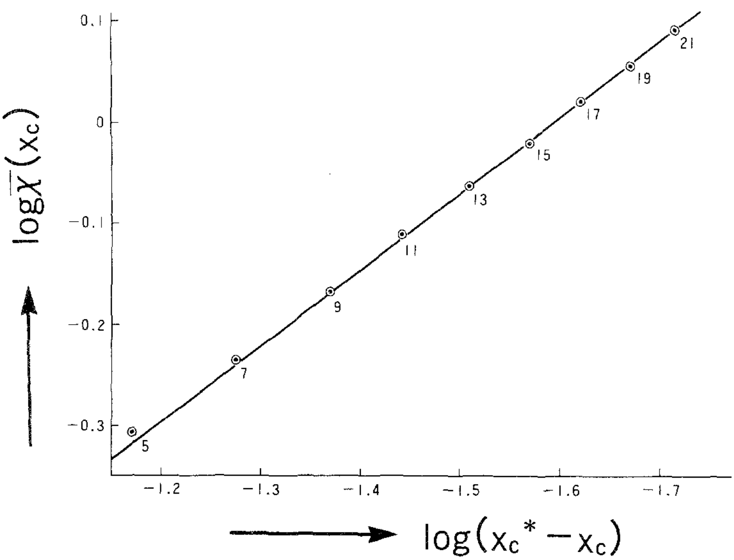

Fig. 3. Coherent anomaly of the susceptibility in the two-dimensional Ising model on the square lattice.[26] The straight line corresponds to $\psi = 0.75$.

6. CONTINUED-FRACTION CAM THEORY

Continued-fraction expansions may be more efficient[27] than power-series expansions in applying the CAM theory.

For example, the susceptibility $\chi_0(T)$ of the two-dimensional Ising model is expanded in the following continued fraction:

$$\chi_0(x) = \cfrac{N\mu_B^2/k_B T}{1 - \cfrac{4x}{1 + \cfrac{x}{1 - \cfrac{2x^2}{1 - \cfrac{2x^4}{1 + \cfrac{0.5x^2}{1 + 9.5x^2} \ddots}}}}} \tag{28}$$

with $x = \tanh(J/k_B T)$. It looks irregular, but we can find an interesting result by applying the CAM theory to the above expression (28), as shown[27] in Fig. 4. It should be noted that the degree of approximation does not necessarily increase monotonically, but all the critical coefficients lie on the straight line, namely, they show a coherent anomaly. This is a

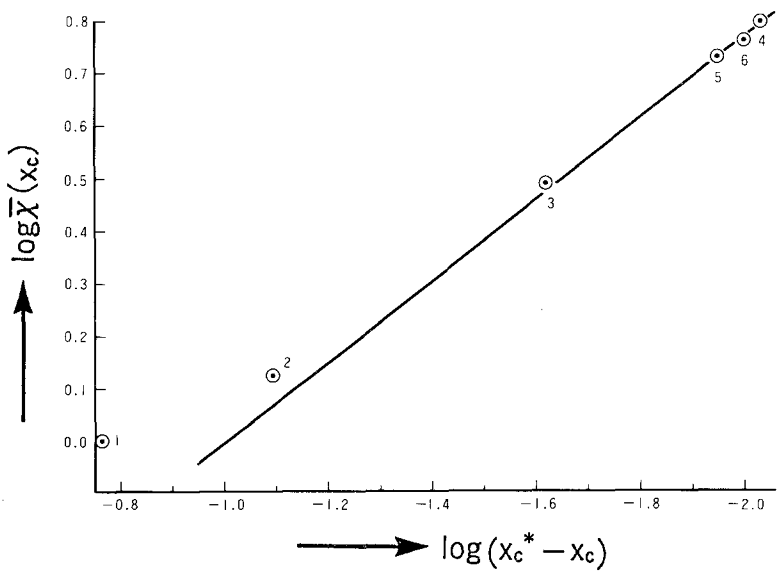

Fig. 4. Coherent anomaly of the susceptibility of the two-dimensional Ising model based on the continued-fraction expansion.[27] The straight line corresponds to $\psi = 3/4$.

large merit of this continued-fraction-expansion CAM theory compared with other methods, such as the Padé approximation method.

Some applications to other systems will be presented elsewhere.[27,32]

7. PADÉ APPROXIMANTS CAM THEORY

The power-series and continued-fraction CAM theories are easily extended to the Padé approximants of the form

$$P_{m,n}(x) = \frac{c_0 + c_1 x + \cdots + c_m x^m}{d_0 + d_1 x + \cdots + d_n x^n} \tag{29}$$

The coefficients $\{c_j\}$ and $\{d_j\}$ are determined from the power series (21). The approximant $P_{0,n}$ corresponds to the inverse $F(x)$ of $Q(x)$. Thus, the Padé approximant (29) is an extension of (22). Similarly to (23), we may have

$$P_{m,n}(x) \simeq \frac{x_c}{x_c - x} \bar{P}_{m,n}(x_c) \tag{30}$$

for appropriate series of the integers m and n, where $x = x_{m,n}$ satisfying $1/P_{m,n}(x_{m,n}) = 0$. The critical coefficient $\bar{P}_{m,n}(x_c)$ may take the following singularity:

$$\bar{P}_{m,n}(x_c) \simeq \frac{f[m,n]}{(x_c^* - x_c)^{\psi}} \tag{31}$$

with a coherent-anomaly exponent ψ. The coefficient $f[m,n]$ might depend on the choice of the series (m,n). The critical exponent φ is given by (25), just as before. As is already known,[54] it is possible to study critical exponents by using only the Padé approximation, namely by applying Padé approximants to the derivative of the logarithm of $Q(x)$ and by estimating the coefficient of their poles. It is, however, expected that the present method may be more efficient than the original Padé method because the zeros of the denominators of such Padé approximants scatter according to the choice of m and n.

On the other hand, according to the CAM, we introduce the degree of approximation by using such zeros and consequently it is possible to arrange the critical coefficients or residues of Padé approximants according to this newly introduced degree of approximation, namely $\delta(x_c) = (x_c - x_c^*)/x_c^*$. This new scheme gives a very rapidly convergent estimate of criticality, as will be explicitly applied to many systems elsewhere.[32]

8. CORRELATION-IDENTITY-DECOUPLING CAM THEORY IN CLASSICAL SYSTEMS

Correlation functions are very fundamental physical quantities in statistical physics and useful even in the CAM theory. In particular, the following general correlation identity[55,56] is very useful:

$$\langle fg \rangle = \langle f \langle g \rangle' \rangle \tag{32}$$

in commutable classical systems. Here f and g are arbitrary classical functions which do not contain common variables, and $\langle g \rangle'$ is the canonical average of g over the partial Hamiltonian $\mathscr{H}_g$, which is connected to the variables contained in g, namely

$$\langle g \rangle' = \mathrm{Tr}\, g e^{-\beta \mathscr{H}_g} / \mathrm{Tr}\, e^{-\beta \mathscr{H}_g} \tag{33}$$

where $\mathscr{H} = \mathscr{H}' + \mathscr{H}_g$ and $\mathscr{H}'$ does not contain the variables in g. The proof of (32) is very simple, as follows.[56] Quite analogously to the arguments in ref. 55, we have

$$\begin{aligned} \langle fg \rangle Z &= \mathrm{Tr}\, fg e^{-\beta \mathscr{H}} = \mathrm{Tr}'\, e^{-\beta \mathscr{H}'} f\, \mathrm{Tr}_g\, g e^{-\beta \mathscr{H}_g} \\ &= \mathrm{Tr}' [e^{-\beta \mathscr{H}'} f\, \mathrm{Tr}_g\, e^{-\beta \mathscr{H}_g} (\mathrm{Tr}_g\, g e^{-\beta \mathscr{H}_g} / \mathrm{Tr}_g\, e^{-\beta \mathscr{H}_g})] \\ &= \mathrm{Tr}'\, \mathrm{Tr}_g\, e^{-\beta \mathscr{H}'} e^{-\beta \mathscr{H}_g} (f \langle g \rangle') \end{aligned} \tag{34}$$

with $Z = \mathrm{Tr}\exp(-\beta \mathscr{H})$. This yields the general correlation identity (32).

For example, in the Ising model,

$$\mathscr{H} = -\sum_{i,k} J_{ik} S_i S_k - \mu_B H \sum_j S_j \tag{35}$$

with $S_j = \pm 1$, we have the following identity:

$$\langle f(S_j)\, S_k \rangle = \left\langle f(S_j) \tanh \beta \left(\sum_i J_{ik} S_k + \mu_B H \right) \right\rangle \tag{36}$$

for an arbitrary function $f(S_j)$. This is the so-called Callen identity.[57] If we put $f(S_j) = 1$, then we obtain

$$\langle S_k \rangle = \left\langle \tanh \left(\beta J \sum_{k=1}^{z} S_k + \beta \mu_B H \right) \right\rangle \tag{37}$$

for $J_{ik} = J$, where z denotes the number of nearest neighbors. By decoupling the right-hand side into $\tanh(z\beta J \langle S_k \rangle + \beta \mu_B H)$, we arrive at the mean-field equation of state

$$m = \tanh(z\beta J m + \beta \mu_B H)$$

for $m = \langle S_k \rangle$. This yields the Weiss mean-field critical point $T_c^{(W)} = zJ/k_B$ and the Curie–Weiss law (16).

If we decouple higher-order correlation identities, then we obtain better approximations. Thus, we can derive, in principle, a systematic series of mean-field-like approximations. This scheme may be called the "correlation-identity-decoupling CAM theory." It will be applied explicitly elsewhere.

9. GREEN'S FUNCTION DECOUPLING CAM THEORY IN QUANTUM SYSTEMS

The idea of the correlation-identity-decoupling CAM theory is easily extended to quantum systems in which the Green's functions are useful. As is well known, there exists a hierarchy of Green's functions in quantum many-body systems and systematic decoupling of them may make it possible to apply the CAM. This scheme will be applied to frustrated quantum spin systems and fermion systems.

10. SUMMARY AND DISCUSSION

The combination of the present super-effective-field theory and the coherent-anomaly method will give a unified theory of phase transitions. They can be applied even to exotic phase transitions such as chiral orders and spin glasses. The basic idea of the CAM theory will be extended to the Ginzburg–Landau–Wilson Hamiltonian, in which the Feynman diagram technique is useful. This suggests a new scheme of Feynman-diagram-expansion CAM theory. The super-effective-field theory may also be applied to the gas–liquid transition and the Alder transition.[58]

An application of the present super-effective-field CAM theory will also be applied to the lattice gauge theory, as will be reported elsewhere.

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