Renormalized finite-cluster expansions

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There are many statistical systems in which degrees of freedom can be grouped according to their degree of correlation. We develop a cluster-expansion method for these systems based on selecting finite clusters of the most strongly interacting degrees of freedom. The starting point is Kubo's generalized cumulant formalism. We show how this expansion can be renormalized; that is, how the contributions of infinite classes of articulated finite clusters can be resummed. The elimination of articulated clusters from the renormalized expansion generates modified interactions in the finite clusters remaining in the expansion. When truncated at different orders, the final result is a hierarchy of mean-field approximations, which generally reproduce an increasing number of terms in exact series expansions for the system. High-order series-expansion coefficients can be obtained by perturbative renormalization of very large clusters, a convenient alternative to the complicated combinatorial analysis associated with standard expansion techniques for lattice models. We compare our work to previous finite-cluster techniques, such as the cluster-variation method of Kikuchi.

I. INTRODUCTION

Closed-form approximations for statistical systems, such as mean-field theories or cluster-variational techniques,[1,2] provide compact expressions that are useful over much of the phase diagram, but whose accuracy is difficult to ascertain. In contrast, it is possible to derive exact series-expansion coefficients and thus have precise error bounds,[3] but over a limited range of validity. In this paper we develop a cluster-expansion method that combines the precision of series expansions with the wide applicability of closed-form approximations. The algebraic structure is that of Kubo's generalized cumulant expansion.[4] Finite clusters of interacting particles (or, more generally, interacting degrees of freedom) are used to successively approximate the properties of the full system.

From each cluster added to the expansion, we extract the cumulant free energy, the piece that describes correlations involving *all* members of that cluster. It follows that cumulants become small as the cluster size approaches the correlation length, and that the cumulant vanishes when the members of a cluster can be broken into statistically independent subsets. The total free energy is approximated by a sum of finite-cluster cumulant free energies, and similar expansions are found for correlation functions. In Kubo's formulation, which we would term a bare expansion, particles within finite clusters interact as they do in the full system. Our crucial modification is to effectively sum the contributions of infinite classes of clusters by introducing renormalized interactions within the clusters remaining in the expansion. The renormalized potentials approximate the influence of the surrounding statistical system on a finite cluster. This is the physical basis behind the improved convergence of the renormalized expansion relative to the bare theory that we document herein.

Truncation of the cumulant expansion at any finite order yields a closed form approximation for the full system. The renormalized theory incorporates many aspects of self-consistency and variational optimization, and often provides useful information beyond the range of series expansions. At the same time we can precisely analyze the accuracy of the cumulant expansion and the enhancement of its convergence on renormalization. Developing each cluster free energy in a high- or low-temperature[5] series generally reproduces the exact series expansion of the full system to the level of the lowest-order cluster that is neglected. The first contributing cluster beyond the truncation is of higher order in the renormalized expansion, as compared to the bare expansion. Therefore the renormalized expansion reproduces more terms of the exact series expansion using the same number of clusters as the bare expansion.

Throughout this article we shall use terminology appropriate for an arbitrary n-state classical spin system on a lattice. This is only for the sake of concreteness and should not obscure the generality of our method. The spin variables may represent any discrete or continuous degree of freedom. For instance, finite-cluster methods have been used to describe solids by treating the displacements of atoms from the underlying lattice sites as continuous-spin variables.[6] The lattice gives us a convenient prescription for choosing clusters, but the cumulant formalism is not restricted to lattice systems. Clusters may be chosen from a topologically disordered system, from reciprocal-space modes, or by any other prescription that selects correlated degrees of freedom.

In other contexts a perturbation series for lattice systems has been resummed to obtain a renormalized expansion.[7] These treatments use free embedding diagrams, which are exemplified by Mayer-cluster functions,[8] instead of the finite clusters considered here. Indeed, the use of free embedding diagrams in previous work was motivated by the analogy to Mayer theory. Here we show that a finite-cluster series can be conveniently renormalized. Since finite clusters already represent an infinite-

order resummation of the free embedding expansion,[9] we expect more rapid convergence.

Finite-cluster methods have been considered many times in the past, but never exploiting the flexibility offered by Kubo's generalized cumulant formalism or from the viewpoint of a renormalized expansion. The most popular and successful finite-cluster method to date is Kikuchi's cluster-variational method (CVM).[10–12] The variety of problems that have been analyzed with the CVM shows the importance of these techniques.[2] The cumulant expansion developed in this paper provides a conceptual framework in which the CVM appears as one member of a hierarchy of closed-form approximations. The CVM is equivalent to a truncated cumulant expansion with maximum renormalization. As is shown in this paper, each further renormalization (corresponding to variational optimization in a CVM) entails greater algebraic complexity and introduces additional multiple-spin interactions in the cluster. For small clusters the version of the cumulant expansion equivalent to CVM often represents a desirable balance of accuracy and algebraic labor. When considering larger clusters, full renormalization becomes a formidable numerical task. However, the fully renormalized cluster expansion often does not reproduce correctly any additional terms in an exact series expansion than does a partially renormalized expansion (see Sec. VII). Thus the extra work of full renormalization may not always be justified or necessary.

Even when the renormalized cumulant expansion is equivalent to a CVM, the present viewpoint offers several conceptual advantages. The cumulant formalism is helpful in deciding which cluster should be added to an expansion to obtain a more accurate expression. As mentioned above, the accuracy of the cumulant approximation is readily determined. Also, the contribution of certain clusters is seen to vanish on renormalization, making their inclusion unnecessary. In some cases, the CVM equations, or, equivalently, equations for the fully renormalized interactions, have no solution. A standard example, discussed later in Sec. X, arises from the use of the "triangle" approximation for the Ising model on a fcc lattice.[10] From the CVM point of view, it has never been clear how to remedy this situation. In this work, we interpret this breakdown within the cumulant formalism and develop an alternative procedure. Finally, we illustrate how a theory including large clusters can be approached using the results of calculations confined to smaller clusters. This provides a way to proceed from relatively simple to more complicated and accurate calculations. High-order expressions for the free energy are obtained by incorporating the contributions of larger clusters through a perturbation analysis.

In an earlier paper, the renormalized finite-cluster method was developed by Shugard and Weeks[13] at the vertex level; that is, renormalization of one-body fields. Here we consider renormalization of arbitrary n-body interactions to further enhance convergence of the expansion. Much of our development is concerned with the general rules for constructing renormalized interactions and their physical interpretation. The basic cumulant formalism is described in the first several sections of this paper. In Sec. IV we introduce the Legendre transform that generates the renormalization, and physically interpret the structure of the renormalized potentials in the following section. We then pause from the formal development and in Sec. VI display some practical calculations for the Ising model.

In Sec. VII we illustrate how renormalization enhances convergence by examining the high-temperature expansion of bare and renormalized Ising model cumulants. Use of the high-temperature expansion allows us to quantify the ordering properties of the cumulant expansion. In Sec. VIII this ordering information is exploited in a scheme that yields high-order series-expansion coefficients with a minimum of algebraic or combinatorial labor. A critical comparison of our work with other approximation methods is given in Sec. IX. Finally, we consider cases where the cumulant expansion breaks down. In Sec. X we propose a scheme for optimization of the expansion when full renormalization is not possible. Calculation of the pair-correlation function is discussed in Sec. XI, and our conclusions are found in Sec. XII.

II. LATTICE MODELS

We consider a system of N interacting spins with total Hamiltonian (in units of $k_B T$)

$$H_{\mathbf{N}}(\mathbf{N}) = \sum_{\mathbf{j}\subseteq\mathbf{N}} h(\mathbf{j}) \ . \tag{1}$$

In principle, the above sum is over all possible clusters of spins in the macroscopic system, as indicated by the shorthand notation $\mathbf{j}\subseteq\mathbf{N}$. Throughout this paper, boldface letters denote clusters of spins from the N-member system. We follow the notation of Morita,[11] in which $\mathbf{i}\subseteq\mathbf{j}$ means that the cluster $\mathbf{i}$ is embedded in $\mathbf{j}$ or is equal to $\mathbf{j}$, while $\mathbf{i}\subset\mathbf{j}$ means that $\mathbf{i}$ is a subcluster of $\mathbf{j}$ but not equal to $\mathbf{j}$. The symbol $\mathbf{j}$ stands for both the particular *cluster* of spins and the *configuration* of the spins in that cluster. To avoid any ambiguity, the summation sign "$\sum_{\mathbf{j}}$" indicates a sum over clusters $\mathbf{j}$, while sums over configurations of spins are explicitly indicated with the trace symbol "$\mathrm{Tr}_{\mathbf{j}}$." In most cases of interest, only one-, two-, or three-body interactions contribute to $H_{\mathbf{N}}(\mathbf{N})$. There is no formal restriction against long-ranged or many-body interactions, although the complexity of the calculations increases accordingly. The piece of Hamiltonian $h(\mathbf{j})$ is a j-body interaction among a group of spins $\mathbf{j}$. In principle, $h(\mathbf{j})$ depends on the location of $\mathbf{j}$ within the lattice, although the Hamiltonians of most systems of interest generally have a high degree of translational symmetry. The decomposition of the Hamiltonian in Eq. (1) is somewhat arbitrary in that any interaction may be absorbed as part of a higher-body interaction, e.g., a one-body potential can be regarded as part of a two-body interaction. The cluster expansion is invariant to all such modifications as long as we include clusters as large as the highest-order piece of the Hamiltonian.

The partition function $Z_{\mathbf{N}}$ and free energy $W_{\mathbf{N}}$ (in units of $k_B T$) are given by

$$Z_{\mathbf{N}} = e^{-W_{\mathbf{N}}} = \mathrm{Tr}_{\mathbf{N}}\, e^{-H_{\mathbf{N}}(\mathbf{N})} \ . \tag{2}$$

By taking functional derivatives,[8] Z_N serves as a generating function for the j-body distribution function $\rho(\mathbf{j})$,

$$\rho(\mathbf{j})=\frac{\delta W_N}{\delta h(\mathbf{j})} , \tag{3}$$

where $\rho(\mathbf{j})$ is the probability of finding the particular cluster of spins in configuration $\mathbf{j}$. The distribution functions are normalized,

$$\operatorname{Tr}_{\mathbf{j}} \rho(\mathbf{j})=1 , \tag{4}$$

and lower-order densities are obtained from partial traces over higher-order distributions,

$$\rho(\mathbf{i})=\operatorname{Tr}_{\mathbf{j}-\mathbf{i}} \rho(\mathbf{j}) . \tag{5}$$

III. BARE CLUSTER EXPANSION

Kubo's generalized cumulant formalism[4] is the basis of our cluster expansion. The free energy of the full system W_N is written in terms of the corresponding quantity W_j for finite clusters $\mathbf{j}$,

$$Z_j=e^{-W_j}=\operatorname{Tr}_{\mathbf{j}} \exp\left[-\sum_{i\subseteq \mathbf{j}} h(\mathbf{i})\right] \quad \text{where } \mathbf{j}\subseteq \mathbf{N} . \tag{6}$$

Cluster functions $K_j^{(0)}$ are defined recursively in terms of the W_j,

$$K_1^{(0)}=W_1 , \tag{7}$$

$$K_2^{(0)}=W_2-\sum_{1\subset 2} K_1^{(0)} , \tag{8}$$

and, in general,

$$K_j^{(0)}=W_j-\sum_{i\subset j} K_i^{(0)} . \tag{9}$$

The cluster expansion converges to W_N since

$$W_N=\sum_{j\subseteq N} K_j^{(0)} \tag{10}$$

by construction. The $K_j^{(0)}$ defined in Eqs. (7)–(10) are functions of the "bare interactions" in (1) and called bare cluster functions to distinguish them from the renormalized cumulants [without the superscript "(0)"] defined in the following section.

Kubo[4] has shown that the cluster function $K_j^{(0)}$ vanishes if the spins within the cluster $\mathbf{j}$ can be divided into two statistically independent subsets. As a consequence, only *connected* clusters contribute to the expansion in (10). When there are no long-ranged correlations, we expect that $K_j^{(0)}$ for larger clusters will be small since they describe correlations involving *every* spin of the $\mathbf{j}$ cluster. The cluster functions rapidly decrease in magnitude when the size of the cluster approaches the correlation length of the system.

The cluster expansion (10) explicitly separates out the incremental contribution of each possible subcluster to the total free energy. There may be several different rules for choosing subclusters $\mathbf{j}$ from the N-membered lattice. As long as one method is followed consistently, the cumulant relations (7)–(10) remain valid, since the cumulants generated at one stage are subtracted from higher cumulants. The connected clusters in Eq. (10) could be defined as a set of vertices taken from the lattice plus some of the bonds (representing interactions between spins) connecting these vertices. In graph theory, this type of subcluster is termed a *weak embedding*.[14] Alternatively, only those subclusters containing *all* bonds present in the full lattice may be considered, giving the so-called *strong embeddings*.[14] When truncated at the same level, both approaches give the same result. The following discussion clarifies why different rules for generating clusters give the same result, and shows how to reduce the number of cluster functions that must be calculated.

Since practical calculations involve the evaluation of finite cluster free energies W_j in Eq. (6), it is useful to consider modified approaches that can reduce the number of clusters that must be dealt with explicitly. Here we show that there exists a simple rearrangement of the expansion (10), such that the free energy of only a subset of all possible clusters, termed *essential* clusters, need be calculated explicitly. (Later, in Sec. IV we further reduce the required number of clusters by appropriately modifying the cluster interactions.) This regrouping is possible because the contributions of the remaining *nonessential* clusters are first added to the total free-energy sum in (10), only to be subtracted out later when contributions from larger essential clusters, as calculated recursively in (9), are also taken into account.

More precisely, the set of all possible clusters in (10) can be divided into two classes, E (essential) and N (nonessential), with the following properties. Certain nonessential clusters $\mathbf{m}_i(\mathbf{j})$, $i=1,2,\ldots,$ can be associated with an essential cluster $\mathbf{j}$ if

$$\mathbf{m}_i(\mathbf{j})\subset \mathbf{j} , \tag{11}$$

and for *all* other essential clusters $\mathbf{k}$,

$$\mathbf{m}_i(\mathbf{j})\subset \mathbf{k} \text{ implies that } \mathbf{j}\subset \mathbf{k},\ \mathbf{k}\in E . \tag{12}$$

Thus each nonessential cluster $\mathbf{m}_i(\mathbf{j})$ is uniquely associated with the *smallest* essential cluster that contains it, since any other $\mathbf{k}$ which contains $\mathbf{m}_i(\mathbf{j})$ must also contain $\mathbf{j}$.

In the cumulant expansion (10) of W_N, all the $\mathbf{m}_i(\mathbf{j})$ and the associated $\mathbf{j}$ cluster can be grouped into an effective cumulant $\hat{K}_j^{(0)}$:

$$\begin{aligned} W_N &= \cdots+[K_{\mathbf{m}_1(\mathbf{j})}^{(0)}+K_{\mathbf{m}_2(\mathbf{j})}^{(0)}+\cdots+K_j^{(0)}]+\cdots \\ &\equiv \cdots+[\hat{K}_j^{(0)}]+\cdots . \end{aligned} \tag{13}$$

Since the cumulant expansion of all essential finite clusters can also be grouped into effective cumulants $\hat{K}_j^{(0)}$ by Eq. (12), the cumulants $K_{\mathbf{m}_i(\mathbf{j})}^{(0)}$ never need to be calculated separately from the $K_j^{(0)}$. Moreover, the $\hat{K}_j^{(0)}$ are automatically generated in place of the $K_j^{(0)}$ if *formally* the $K_{\mathbf{m}_i(\mathbf{j})}^{(0)}$ are treated as if they vanished. This is easily seen by considering the cluster expansion of the finite essential cluster $\mathbf{j}$:

$$K_j^{(0)}=W_j-K_{\mathbf{m}_1(\mathbf{j})}^{(0)}-K_{\mathbf{m}_2(\mathbf{j})}^{(0)}-\cdots-\sum_{\substack{\mathbf{n}\subset \mathbf{j}\\ [\mathbf{n}\neq\{\mathbf{m}_i(\mathbf{j})\}]}} K_n^{(0)} . \tag{14}$$

The nonessential cluster functions can be brought to the left-hand side of the above equation to generate $\hat{K}_{\mathbf{j}}^{(0)}$ as defined in (13), and we find

$$\hat{K}_{\mathbf{j}}^{(0)} = W_{\mathbf{j}} - \sum_{\substack{\mathbf{n}\subset\mathbf{j} \\ [\mathbf{n}\neq\{\mathbf{m}_i(\mathbf{j})\}]}} K_{\mathbf{n}}^{(0)} \ . \tag{15}$$

This is naturally accomplished in practical calculations by treating the $K_{\mathbf{m}_i(\mathbf{j})}^{(0)}$ as if they were zero. Indeed, note that the $K_{\mathbf{m}_i(\mathbf{j})}^{(0)}$ cancel when (14) is substituted into (13), leaving only $\hat{K}_{\mathbf{j}}^{(0)}$ as given by (15).

As an example, consider the two-dimensional square lattice. We can take E as the set of all *rectangular* clusters with all bonds connected, since any other cluster in (10) can be uniquely associated with the smallest rectangle containing it, and properties (11) and (12) are then satisfied. In particular, all (weak) embeddings that include a set of vertices but not all bonds connecting them, as well as all nonrectangular strong embeddings, are nonessential in this case. Examples of nonessential clusters associated with the essential 9-spin square cluster are given in Fig. 1.

The exact high- or low-temperature series[3,5] can be obtained by Taylor expansion of the bare cumulants in the approximate parameter. In the series-expansion literature, this is known as the finite-cluster method.[3] By regrouping the cumulant expansion, only a smaller number of essential cluster functions $\hat{K}_{\mathbf{j}}^{(0)}$ need to be Taylor-expanded. Usually the topology of a cluster (e.g., number of bonds, number of vertices, etc.) determines the leading contribution of a cluster to the series expansion. To avoid possible confusion, we emphasize that the leading-order contribution of the essential cluster function $\hat{K}_{\mathbf{j}}^{(0)}$ is the contribution from the lowest-order nonessential cluster associated with j. In Secs. VII and VIII we discuss how high-order series-expansion coefficients can be extracted from the renormalized cumulant expansion.

Throughout the rest of this paper we assume that all nonessential clusters have been eliminated from the cumulant expansion and only consider essential clusters. For conciseness we drop the special notation $\hat{K}_{\mathbf{j}}^{(0)}$ that indicates effective cumulants, and write $K_{\mathbf{j}}^{(0)}$ instead.

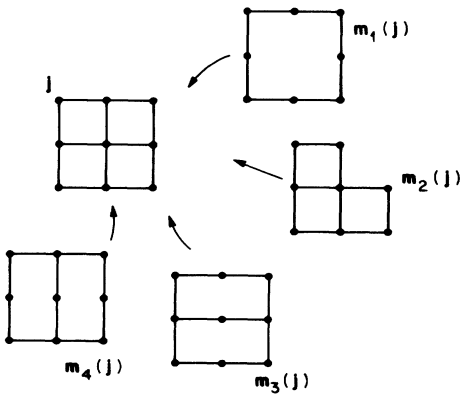


FIG. 1. The nine-vertex cluster j is an essential cluster from the square planar lattice. Also shown are several strong and weak embedded nonessential clusters $\mathbf{m}_1(\mathbf{j}),\mathbf{m}_2(\mathbf{j}),\ldots$ that are uniquely associated with j. The $\mathbf{m}_i(\mathbf{j})$ need not be explicitly considered if the cluster j is included in the cumulant expansion.

IV. RENORMALIZED EXPANSION

The free energy W_N is a function of the interaction potentials $h(\mathbf{j})$. Physically, the renormalized expansion tries to improve convergence by choosing new effective potentials in each finite cluster according to a well-defined prescription. This additional freedom allows more rapid convergence, and the prescription involves choosing modified interactions that bring about the *same* densities $\rho(\mathbf{j})$ in each finite cluster as those produced in the total system by the bare interactions. This is accomplished by a Legendre transformation from potentials to densities as independent variables.

The following transformation generates a free energy X_N that is a natural function of the densities:

$$X_N = W_N - \sum_{\mathbf{j}\in R} \mathrm{Tr}_{\mathbf{j}}\, \rho(\mathbf{j})h(\mathbf{j}) \ . \tag{16}$$

The Legendre transform is with respect to densities and potentials for clusters contained in the set R. The set of renormalized clusters R is a subset of all clusters contained in the N-member lattice. To illustrate, a few likely choices for R include all lattice points (1 clusters), all points and nearest-neighbor bonds (2 clusters), all rings of a certain size (e.g., a nearest-neighbor square in a square lattice) and their subclusters, etc. Factors governing the choice of R are discussed in detail below. The only restriction put on R is that all subclusters of any member of R are also contained in R, i.e., $\mathbf{j}\in R$ and $\mathbf{i}\subseteq\mathbf{j}$ imply $\mathbf{i}\in R$.

The free energy X_N is a natural function of the densities $\rho(\mathbf{j})$ for $\mathbf{j}\in R$, while remaining a function of the interaction potentials $h(\mathbf{j})$ for the complimentary set of clusters, $\mathbf{j}\notin R$. If we consider arbitrary variations of densities in the set R and the potentials that are dependent on them, we find, from (16) and (3),

$$\delta X_N = -\sum_{\mathbf{j}\in R} \mathrm{Tr}_{\mathbf{j}}\, \delta\rho(\mathbf{j})h(\mathbf{j}) \ . \tag{17}$$

Although other approaches are possible, it is simplest to constrain the density variations so that Eqs. (4) and (5) remain satisfied and further require

$$\frac{\delta X_N}{\delta\rho(\mathbf{j})} = -h(\mathbf{j}), \quad \mathbf{j}\in R \tag{18}$$

where $h(\mathbf{j})$ is the particular choice of the j-body interaction term given in (1). Derivatives with respect to interaction potentials $h(\mathbf{j})$, $\mathbf{j}\notin R$, generate densities, just as in (3),

$$\frac{\delta X_N}{\delta h(\mathbf{j})} = \rho(\mathbf{j}), \quad \mathbf{j}\notin R \ . \tag{19}$$

The free-energy function $\tilde{W}_N$, given by

$$\tilde{W}_N = X_N + \sum_{\mathbf{j}\in R} \mathrm{Tr}_{\mathbf{j}}\, \rho(\mathbf{j})h(\mathbf{j}) \tag{20}$$

and [except for $h(\mathbf{j})$ in the second term] regarded as a function of the densities $\rho(\mathbf{j})$, $\mathbf{j}\in R$, is easily seen to obey

the following variational principle,

$$\frac{\delta \tilde{W}_{\mathbf{N}}}{\delta \rho(\mathbf{j})}=0, \quad \mathbf{j}\in R \ . \tag{21}$$

The properties of $X_{\mathbf{N}}$ and $\tilde{W}_{\mathbf{N}}$ depend on the choice of R. We should perhaps label $X_{\mathbf{N}}$ and $\tilde{W}_{\mathbf{N}}$ with a superscript "R" to indicate that these quantities depend on which clusters are included in R, but this is not done to avoid cumbersome notation.

A cluster expansion for $X_{\mathbf{N}}$ or $\tilde{W}_{\mathbf{N}}$ can be generated by considering finite clusters whose densities (rather than interaction potentials) are equal to the macroscopic system values. The Legendre transform of the finite-cluster free energy defines natural functions $X_{\mathbf{j}}$ and $\tilde{W}_{\mathbf{j}}$ of cluster densities,

$$X_{\mathbf{j}}=W_{\mathbf{j}}-\sum_{\substack{\mathbf{i}\subseteq\mathbf{j}\\(\mathbf{i}\in R)}} \operatorname{Tr}_{\mathbf{i}} \rho(\mathbf{i})h(\mathbf{i}) \ , \tag{22}$$

$$\tilde{W}_{\mathbf{j}}=X_{\mathbf{j}}+\sum_{\substack{\mathbf{i}\subseteq\mathbf{j}\\(\mathbf{i}\in R)}} \operatorname{Tr}_{\mathbf{i}} \rho(\mathbf{i})h(\mathbf{i}) \ . \tag{23}$$

Comparing (22) and (23), we see that $\tilde{W}_{\mathbf{j}}$ is equal to the free energy of a $\mathbf{j}$ cluster with potentials chosen to reproduce the densities $\rho(\mathbf{i})$, $\mathbf{i}\in R$. It can be calculated directly from the partition function as in (6), provided the appropriate interactions are used. Cluster functions $K_{\mathbf{j}}$ and $\tilde{K}_{\mathbf{j}}$, also natural functions of density, are generated in the same recursive way as in the bare cumulant expansion:

$$X_{\mathbf{j}}=\sum_{\mathbf{i}\subseteq\mathbf{j}} K_{\mathbf{i}} \ , \tag{24}$$

$$\tilde{W}_{\mathbf{j}}=\sum_{\mathbf{i}\subseteq\mathbf{j}} \tilde{K}_{\mathbf{i}} \ , \tag{25}$$

$$K_{\mathbf{j}}=X_{\mathbf{j}}-\sum_{\mathbf{i}\subset\mathbf{j}} K_{\mathbf{i}} \ , \tag{26}$$

$$\tilde{K}_{\mathbf{j}}=\tilde{W}_{\mathbf{j}}-\sum_{\mathbf{i}\subset\mathbf{j}} \tilde{K}_{\mathbf{i}} \ . \tag{27}$$

Note that $K_{\mathbf{j}}=\tilde{K}_{\mathbf{j}}$ if $\mathbf{j}\notin R$ and the bare Hamiltonian does not contain $\mathbf{j}$-body or longer-ranged interactions. The sums in Eqs. (24)–(27) only include essential clusters. For $\mathbf{j}=\mathbf{N}$, these equations describe properties of the total system.

In each of the finite clusters contributing to $X_{\mathbf{N}}$ or $\tilde{W}_{\mathbf{N}}$, the densities $\rho(\mathbf{j})$, $\mathbf{j}\in R$, match and are equal to the distributions in the full N-member lattice, and we regard the $\rho(\mathbf{j})$, not the $h(\mathbf{j})$, as independent variables for all clusters in R. The finite-cluster interactions $h(\mathbf{j})$, $\mathbf{j}\in R$, consequently, depend on the densities and do not match the bare interactions of the full system; rather, they vary from cluster to cluster and within a cluster. In the discussion that immediately follows, the cumulant expansions of $X_{\mathbf{N}}$ or $\tilde{W}_{\mathbf{N}}$ are shown to contain far fewer nonzero cumulants than the expansion of $W_{\mathbf{N}}$, and the $K_{\mathbf{j}}$ and $\tilde{K}_{\mathbf{j}}$ are, in effect, sums of infinite classes of bare cluster functions. Therefore, we refer to the cluster expansion of $X_{\mathbf{N}}$ or $\tilde{W}_{\mathbf{N}}$ as a *renormalized cluster expansion,* and the potentials that are generated by the densities in Eq. (18) as *renormalized potentials.* They describe high-order effects from calculations involving only small clusters. In the following, we use a tilde to indicate renormalized potentials that are functions of cluster densities and add a subscript indicating the finite cluster where they are found. Thus $\tilde{h}_{\mathbf{k}}(\mathbf{j})$ denotes the renormalized j-body potential in cluster $\mathbf{k}$. When necessary to distinguish them, bare potentials are given a subscript $\mathbf{N}$ as a reminder that they are the potentials of the $\mathbf{N}$ cluster.

The desirable properties of the renormalized cluster expansion arise because the cluster functions for entire classes of *articulation clusters* vanish upon renormalization. A cluster $\mathbf{j}$ is said to contain $\mathbf{a}$ as an articulation subcluster if the removal of $\mathbf{a}$ causes $\mathbf{j}$ to fall apart into unconnected pieces. In the schematic drawing of Fig. 2, the removal of $\mathbf{a}$ leaves the disjoint subclusters $\mathbf{p}'$ and $\mathbf{q}'$. In the discussion below, we prove that $\tilde{K}_{\mathbf{j}}$ and $K_{\mathbf{j}}$ vanish if $\mathbf{a}\in R$ and there exist no terms in the bare Hamiltonian or clusters in R that involve spins from both $\mathbf{p}'$ and $\mathbf{q}'$. To prove this we consider four clusters and their associated cluster functions: the articulation subcluster $\mathbf{a}$, the cluster $\mathbf{p}$, which is the union of $\mathbf{a}$ with the fragment $\mathbf{p}'$, $\mathbf{p}=\mathbf{p}'\cup\mathbf{a}$, a similar cluster $\mathbf{q}$, $\mathbf{q}=\mathbf{q}'\cup\mathbf{a}$, and finally the whole cluster $\mathbf{j}=\mathbf{p}'\cup\mathbf{a}\cup\mathbf{q}'$.

The renormalized potentials are chosen to make the distribution $\rho(\mathbf{a})$ identical in each of the finite clusters $\mathbf{a}$, $\mathbf{p}$, $\mathbf{q}$, and $\mathbf{j}$, and in the macroscopic system. We assume that renormalized potentials can be found that produce matching distributions in the finite clusters $\mathbf{a}$, $\mathbf{p}$, and $\mathbf{q}$. Solving for these potentials generally involves nonlinear equations. In truncated expansions, the desired potentials usually, but may not always, exist. (See Sec. X.) To within an additive constant, the *total* renormalized interaction in the $\mathbf{a}$ cluster $\tilde{H}(\mathbf{a})\equiv\sum_{\mathbf{i}\subseteq\mathbf{a}}\tilde{h}_{\mathbf{a}}(\mathbf{i})$ is simply $-\ln\rho(\mathbf{a})$,

$$\rho(\mathbf{a})=\exp[\tilde{W}_{\mathbf{a}}-\tilde{H}(\mathbf{a})] \ , \tag{28}$$

where $\tilde{W}_{\mathbf{a}}$ is given by

$$e^{\tilde{W}_{\mathbf{a}}}=\operatorname{Tr}_{\mathbf{a}} e^{-\tilde{H}(\mathbf{a})} \ . \tag{29}$$

To remove any ambiguity, we specify the potential of a certain fiducial spin state be zero,

$$\tilde{H}(\mathbf{a}_0)=0 \ . \tag{30}$$

Next, consider the clusters $\mathbf{p}$ and $\mathbf{q}$. The quantities $\Delta\tilde{H}_{\mathbf{p}}(\mathbf{a})$ and $\Delta\tilde{H}_{\mathbf{q}}(\mathbf{a})$ are defined in terms of partial traces over the renormalized Hamiltonians of the $\mathbf{p}$ and $\mathbf{q}$ clusters, $\tilde{H}(\mathbf{p})$ and $\tilde{H}(\mathbf{q})$, respectively,

$$e^{-\Delta\tilde{H}_{\mathbf{p}}(\mathbf{a})-\Delta\tilde{H}^{0}_{\mathbf{p}}}=\operatorname{Tr}_{\mathbf{p}'}\exp[-\tilde{H}(\mathbf{p})] \ , \tag{31}$$

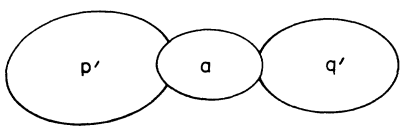


FIG. 2. Schematic drawing of an articulated cluster. Every path connecting a vertex in the $\mathbf{p}'$ subcluster to another in $\mathbf{q}'$ must pass through $\mathbf{a}$.

$$e^{-\Delta\tilde{H}_{\mathbf{q}}(\mathbf{a})-\Delta\tilde{H}^{0}_{\mathbf{q}}}=\operatorname{Tr}_{\mathbf{q}'}\exp[-\tilde{H}(\mathbf{q})]\ . \tag{32}$$

The constants $\Delta\tilde{H}^{0}_{\mathbf{p}}$ and $\Delta\tilde{H}^{0}_{\mathbf{q}}$ are fixed by requiring that $\Delta\tilde{H}_{\mathbf{p}}(\mathbf{a}_0)=\Delta\tilde{H}_{\mathbf{q}}(\mathbf{a}_0)=0$, as in (30). Since we have assumed that $\mathbf{a}\in R$, the **a**-body distribution in the **a**, **p**, and **q** clusters are required to match, and therefore

$$\tilde{H}(\mathbf{a})=\Delta\tilde{H}_{\mathbf{p}}(\mathbf{a})=\Delta\tilde{H}_{\mathbf{q}}(\mathbf{a})\ . \tag{33}$$

The crucial step in the proof follows from the fact that the renormalized potential for the **j** cluster can be constructed from the renormalized potentials of the smaller clusters, namely

$$\tilde{H}(\mathbf{j})=\tilde{H}(\mathbf{p})+\tilde{H}(\mathbf{q})-\tilde{H}(\mathbf{a})\ . \tag{34}$$

From Eqs. (31) and (32), the partial trace of $\exp[-\tilde{H}(\mathbf{j})]$ over $\mathbf{j}-\mathbf{a}=\mathbf{p}'+\mathbf{q}'$ is easily seen to yield an **a**-cluster distribution matching the distribution in the **p**, **q**, and **a** clusters. Also note that any other renormalized cluster **b** that is completely contained in **p** (or **q**) has the same distribution in the **j** cluster as in the **p** (or **q**) cluster. However, if **b** contains spins from **p**′, **a**, *and* **q**′, then this construction does not necessarily guarantee that the **b**-spin distribution in **j** and its subclusters agree.

The free energy of the **j** cluster is easily expressed in terms of $\tilde{W}_{\mathbf{a}}$, $\tilde{W}_{\mathbf{p}}$, and $\tilde{W}_{\mathbf{q}}$, where $\tilde{W}_{\mathbf{a}}$ is defined as in Eq. (29), and

$$e^{-\tilde{W}_{\mathbf{p}}}=\operatorname{Tr}_{\mathbf{p}}e^{-\tilde{H}(\mathbf{p})} \tag{35}$$

and

$$e^{-\tilde{W}_{\mathbf{q}}}=\operatorname{Tr}_{\mathbf{q}}e^{-\tilde{H}(\mathbf{q})}\ . \tag{36}$$

Comparing (31) and (32) with (35) and (36), we see that

$$\tilde{W}_{\mathbf{a}}+\Delta\tilde{H}^{0}_{\mathbf{p}}=\tilde{W}_{\mathbf{q}}\ , \tag{37}$$

$$\tilde{W}_{\mathbf{a}}+\Delta\tilde{H}^{0}_{\mathbf{q}}=\tilde{W}_{\mathbf{q}}\ . \tag{38}$$

Therefore,

$$e^{-\tilde{W}_{\mathbf{j}}}=\operatorname{Tr}_{\mathbf{j}}e^{-\tilde{H}(\mathbf{j})}=\operatorname{Tr}'_{\mathbf{p}}\operatorname{Tr}_{\mathbf{q}'}e^{-[\tilde{H}(\mathbf{p})+\tilde{H}(\mathbf{q})-\tilde{H}(\mathbf{a})]}$$
$$=\operatorname{Tr}_{\mathbf{p}}e^{-\tilde{H}(\mathbf{p})-\Delta\tilde{H}^{0}_{\mathbf{q}}}\ ,$$

and, with (38),

$$\tilde{W}_{\mathbf{j}}=\tilde{W}_{\mathbf{p}}+\tilde{W}_{\mathbf{q}}-\tilde{W}_{\mathbf{a}}\ . \tag{39}$$

This is the basic result of this section. The additivity of the free energies immediately implies that $\tilde{K}_{\mathbf{j}}=0$. Equation (39) shows that there are no terms in $\tilde{W}_{\mathbf{j}}$ mixing variables in cluster **p**′ with those in cluster **q**′. Hence cumulant contributions $\tilde{K}_{\mathbf{j}}$, which do mix interactions with *all* **j** spins, must vanish. This can be shown mathematically as follows. From Eq. (39) we know that $\tilde{W}_{\mathbf{j}}$ is a sum of cumulants of subclusters of either **p** or **q**. Hence

$$\tilde{K}_{\mathbf{j}}=\tilde{W}_{\mathbf{j}}-{\sum_{\mathbf{i}\subset\mathbf{j}}}'\tilde{K}_{\mathbf{i}}$$
$$=\tilde{W}_{\mathbf{j}}-\sum_{i\subseteq\mathbf{p}}\tilde{K}_{\mathbf{i}}-\sum_{\mathbf{i}\subseteq\mathbf{q}}\tilde{K}_{\mathbf{i}}+\sum_{\mathbf{i}\subseteq\mathbf{a}}\tilde{K}_{\mathbf{i}}=0\ , \tag{40}$$

where the prime in the first line in the above equation indicates that no clusters **n** such that $\mathbf{p}\subset\mathbf{n}\subseteq\mathbf{j}$ or $\mathbf{q}\subset\mathbf{n}\subseteq\mathbf{j}$ are included. Since $K_{\mathbf{j}}=\tilde{K}_{\mathbf{j}}$ for $\mathbf{j}\notin R$ [see discussion after Eq. (27)], it follows that the renormalization cluster expansions for the total free energies $\tilde{W}_{\mathbf{N}}$ and $X_{\mathbf{N}}$ analogous to (24) and (25) contain no articulated subclusters.

It is important to note that inclusion of high-order renormalization can actually *reintroduce* cumulants into the expansion that otherwise would vanish as articulated clusters. In the context of the proof presented above, it is clear that renormalization of **j**-body interactions introduces a term in $\tilde{H}(\mathbf{j})$ involving all spins of the **j** cluster. In such a case, the construction in (34) would be invalid. Similarly, $K_{\mathbf{j}}$ would not vanish if the bare Hamiltonian contained a term $h_{\mathbf{N}}(\mathbf{j})$ coupling all spins of **j**.

V. RENORMALIZED POTENTIALS AS INFLUENCE FUNCTIONS

The renormalized potentials describe the influence of the surrounding statistical system on a cluster. The cumulant expansion can be viewed as a series of approximations for this influence in which higher-order terms include correlations among successively larger surrounding clusters. These ideas are made precise in this section by examining the cluster expansion for the renormalized potentials.

Consider the renormalized interaction for a group of spins **j** within a cluster **k**. The *total* interaction among this group of spins in the cluster **k**, $\tilde{H}_{\mathbf{k}}(\mathbf{j})\equiv\sum_{\mathbf{i}\subseteq\mathbf{j}}\tilde{h}_{\mathbf{k}}(\mathbf{i})$, is separated into the bare potential $H_{\mathbf{N}}(\mathbf{j})$ plus a contribution $\Gamma_{\mathbf{k}}(\mathbf{j})$ from the renormalization

$$\tilde{H}_{\mathbf{k}}(\mathbf{j})=H_{\mathbf{N}}(\mathbf{j})+\Gamma_{\mathbf{k}}(\mathbf{j})\ . \tag{41}$$

[The contribution from renormalization to the total **k**-cluster potential is similarly $\Gamma_{\mathbf{k}}(\mathbf{k})$.] The cumulant expansion for $\Gamma_{\mathbf{k}}(\mathbf{j})$ is derived by expressing the difference between bare and renormalized potentials as a functional derivative of the Legendre-transformed free energies [see Eqs. (18) and (24)–(27)]. Since $\delta X_{\mathbf{k}}/\delta\rho(\mathbf{i})=-\tilde{h}_{\mathbf{k}}(\mathbf{i})$, we have

$$\Gamma_{\mathbf{k}}(\mathbf{j})=\sum_{\mathbf{i}\subseteq\mathbf{j}}\delta[X_{\mathbf{N}}-N_{\mathbf{k}}]/\delta\rho(\mathbf{i})$$
$$=\sum_{\substack{\mathbf{n}\\(\mathbf{n}\not\subseteq\mathbf{k})}}\sum_{\mathbf{i}\subseteq\mathbf{j}}c_{\mathbf{n}}(\mathbf{i})\ , \tag{42}$$

where

$$c_{\mathbf{n}}(\mathbf{i})\equiv\delta K_{\mathbf{n}}/\delta\rho(\mathbf{i}),\quad \mathbf{i}\subset\mathbf{n}\ . \tag{43}$$

Equation (42) shows how neighboring clusters, indicated by the variable **n**, renormalize the interactions among a group of spins **j** within a cluster **k**. The difference $X_{\mathbf{N}}-X_{\mathbf{k}}$ is equal to the sum of all cumulants $K_{\mathbf{n}}$ excluding those from clusters within or equal to **k**. Therefore the sum over **n** in (42) includes only those essential clusters that are partially or wholly *outside* **k** (and hence outside **j**) and that do not vanish after renormalization. Thus, $\mathbf{n}=\mathbf{j}$ is excluded in (42) and the theory only requires $c_{\mathbf{n}}(\mathbf{i})$ for which $\mathbf{i}\subset\mathbf{j}$ and not $\mathbf{i}=\mathbf{j}$. The sum on **n** is

further restricted to those clusters $\mathbf{n}$ that *overlap* $\mathbf{j}$ since the derivative $\delta K_{\mathbf{n}}/\delta\rho(\mathbf{i})$ with $\mathbf{i}\subseteq\mathbf{j}$ is nonzero only for such clusters.

The $c_{\mathbf{n}}(\mathbf{i})$ are the basic building blocks of the renormalized potential and the central objects in our analysis of the cluster expansion. They are a convenient decomposition of the total renormalized potential $\Gamma_{\mathbf{k}}(\mathbf{j})$ into one-body interactions $c_{\mathbf{n}}(\mathbf{1})$, two-body interactions $c_{\mathbf{n}}(\mathbf{2})$ beyond the $c_{\mathbf{n}}(\mathbf{1})$, and so on. In this section we show how the $c_{\mathbf{n}}(\mathbf{i})$ embody the influence of the cluster $\mathbf{n}$ on the spins in cluster $\mathbf{j}$.

In terms of the $c_{\mathbf{n}}(\mathbf{i})$, $\Gamma_{\mathbf{k}}(\mathbf{j})$ in (42) is given by

$$\Gamma_{\mathbf{k}}(\mathbf{j})=\sum_{\mathbf{j}\subset\mathbf{n}\not\subseteq\mathbf{k}}\sum_{\mathbf{i}\subseteq\mathbf{j}}c_{\mathbf{n}}(\mathbf{i}),\quad \mathbf{j}\in R\ . \tag{44}$$

The expansion (44) shows how a cluster potential is renormalized by its neighbors. As explained above, the sum over $\mathbf{n}$ only includes surrounding clusters that overlap $\mathbf{j}$ without actually being equal to or a subcluster of $\mathbf{k}$. Thus, the influence of spins that are far from $\mathbf{j}$ on $\Gamma_{\mathbf{k}}(\mathbf{j})$ is transmitted by clusters that simultaneously overlap both the far spins and the $\mathbf{j}$ cluster. Large clusters are required to connect distant spins to the cluster $\mathbf{j}$, and they can affect the potential $\Gamma_{\mathbf{k}}(\mathbf{j})$ only through high-order cumulants.

A concrete illustration of how the renormalized potential is built from the $c_{\mathbf{n}}(\mathbf{i})$ is provided in Fig. 3(a). There we consider a triangular cluster from a two-dimensional triangular lattice system. A few typical contributions to the renormalized potential from the many clusters that overlap the triangle are shown. If R contains no clusters larger than a triangle, then the hexagon is the smallest figure that contributes a three-body contribution to the triangle's renormalized potential, and therefore this interaction is of higher order than the one- and two-body parts of $\Gamma_3(\mathbf{3})$. In Fig. 3(b), the $c_{\mathbf{n}}(\mathbf{i})$ that form the renormalized potential of the hexagonal cluster are shown. Note that the outer bonds of the hexagon begin to be renormalized at the triangle level, while the inner bonds are renormalized only by overlapping hexagons and even higher-order figures. The inner bonds are more shielded from the surrounding system than the outer bonds, and therefore their renormalized potential, which describes the influence of the surrounding system, is of higher order. The ordering properties of the cumulant expansion are quantified in Sec. VII using the high-temperature expansion.

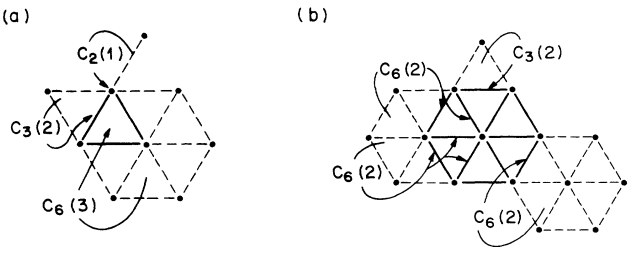


FIG. 3. The dashed figures represent some of the many clusters that renormalize interactions in the clusters drawn with solid lines. Each contribution to the renormalized potential arises from a function $c_{\mathbf{n}}(\mathbf{i})$, where $\mathbf{i}$ is a group of spins totally within the cluster being renormalized and $\mathbf{n}$ is a cluster that overlaps, but is not contained in, the renormalized cluster. In (a) a vertex potential of the triangular cluster is renormalized by an adjacent 2 cluster, a pair potential by a 3 cluster, and the three-body potential of the triangle by an overlapping hexagonal cluster. (b) shows how the pair bonds of a hexagonal cluster can be renormalized by triangular or hexagonal clusters.

The $c_{\mathbf{n}}(\mathbf{i})$ are the fundamental quantities used to describe the incremental addition of correlation with inclusion of larger clusters. So far, we have emphasized how surrounding spins influence a cluster via the $c_{\mathbf{n}}(\mathbf{i})$. Now, an alternative viewpoint is described in which the $c_{\mathbf{n}}(\mathbf{i})$ propagate correlations *within* a renormalized cluster. Besides gaining an additional physical interpretation of the $c_{\mathbf{n}}(\mathbf{i})$, the following also leads to the basic equations for calculation of the $c_{\mathbf{n}}(\mathbf{i})$.

Consider a scheme in which $\mathbf{j}$-cluster potentials are renormalized ($\mathbf{j}\in R$) and $\mathbf{k}$ is any cluster in the cumulant expansion that contains $\mathbf{j}$ as a subcluster. Since the densities must match, we have

$$\rho(\mathbf{j})=e^{\tilde{W}_{\mathbf{j}}}e^{-\tilde{H}(\mathbf{j})}=\operatorname*{Tr}_{\mathbf{k}-\mathbf{j}}e^{\tilde{W}_{\mathbf{k}}}e^{-\tilde{H}(\mathbf{k})},\quad \mathbf{j}\subset\mathbf{k}\ . \tag{45}$$

Equation (45) simply reflects the reduction of higher distribution functions to those of lower order as in (5); we obtain an equation for each $\mathbf{j}$-cluster potential that is renormalized and each higher-order cluster $\mathbf{k}$ in the expansion with $\mathbf{j}\subset\mathbf{k}$. Only a subset of these equations are independent: If $\mathbf{j}\subset\mathbf{k}\subset\mathbf{n}$ and we take Eq. (45) for reduction of $\rho(\mathbf{n})$ to $\rho(\mathbf{k})$, and $\rho(\mathbf{k})$ to $\rho(\mathbf{j})$ as independent equations, then the reduction of $\rho(\mathbf{n})$ to $\rho(\mathbf{j})$ follows from the previous equalities. Now, using (44), separate the full $\mathbf{k}$-cluster potential in (45) into the part unaffected by the trace, which involves only the $\mathbf{j}$ spins, plus the remainder,

$$\tilde{H}(\mathbf{k})=H_{\mathrm{N}}(\mathbf{j})+\sum_{(\mathbf{n}\not\subseteq\mathbf{k})}\sum_{\substack{\mathbf{i}\in R\\(\mathbf{i}\subseteq\mathbf{j})}}c_{\mathbf{n}}(\mathbf{i})$$
$$+[H_{\mathrm{N}}(\mathbf{k})-H_{\mathrm{N}}(\mathbf{j})]+\sum_{(\mathbf{n}\not\subseteq\mathbf{k})}\sum_{\substack{\mathbf{i}\in R\\(\mathbf{i}\subseteq\mathbf{k},\,\mathbf{i}\not\subseteq\mathbf{j})}}c_{\mathbf{n}}(\mathbf{i})\ . \tag{46}$$

The sums over clusters in the above equation may appear complicated, but they represent a geometrical construction that is quite simple. The variable $\mathbf{n}$ in Eq. (46) ranges over all clusters that overlap the cluster $\mathbf{k}$ but are not totally contained in $\mathbf{k}$. The variable $\mathbf{i}$ ranges over subclusters of $\mathbf{k}$. In the first line of (46), $\mathbf{i}$ ranges over those subclusters of $\mathbf{k}$ that are also subclusters of $\mathbf{j}$, as well as $\mathbf{j}$ itself. Similarly, let us rewrite $\tilde{H}(\mathbf{j})$ in the first equality in (45), using (44) with $\mathbf{k}=\mathbf{j}$, noting that the sum over $\mathbf{n}$ of all overlapping clusters $\mathbf{j}\subset\mathbf{n}$ in (44) can be broken into two parts: $\mathbf{j}\subset\mathbf{n}\subseteq\mathbf{k}$ and $\mathbf{j}\subset\mathbf{n}\not\subseteq\mathbf{k}$. The latter term cancels with the second term on the right-hand side in Eq. (46) when both these results are substituted into (45), and we obtain our basic result:

$$\sum_{(\mathbf{j}\subset\mathbf{n}\subseteq\mathbf{k})}\sum_{\substack{\mathbf{i}\in R\\\mathbf{i}\subseteq\mathbf{j}}}c_{\mathbf{n}}(\mathbf{i})=\tilde{W}_{\mathbf{j}}-\ln Q_{\mathbf{k}}(\mathbf{j})\ , \tag{47}$$

where

$$Q_k(\mathbf{j}) = e^{\bar{W}_k} \operatorname*{Tr}_{k-j} \exp\left[-\left\{ H_N(\mathbf{k}) - H_N(\mathbf{j}) + \sum_{\substack{n \\ n \not\subseteq k}} \sum_{\substack{i \in R \\ (i \subseteq k,\, i \not\subseteq j)}} c_n(\mathbf{i}) \right\} \right] . \quad (48)$$

The above equations are the fundamental nonlinear equations to be solved for the $c_n(\mathbf{i})$. Practical aspects of their solution are discussed in the following section. Within a normalization, $Q_k(\mathbf{j})$ is simply the **j**-body distribution obtained from the **k** cluster if both bare and renormalized **j**-body potential terms are removed from the total **k**-cluster interaction $\bar{H}(\mathbf{k})$. $Q_k(\mathbf{j})$ describes the influence of the rest of the **k** cluster on the **j** spins and is called an *influence* or *cavity distribution function.*

The $c_n(\mathbf{i})$ appearing on the left-hand side of Eq. (47) are for those **n** clusters that partially overlap the **j** spins. Since $c_n(\mathbf{i})$ for increasing **n** reflect higher-order correlations, Eq. (47) yields a picture of how correlations propagate within a cluster. Consider the pair of spins within a hexagonal cluster in a two-dimensional triangular lattice shown in Fig. 4(a). Then the $c_n(\mathbf{i})$ appearing on the left-hand side of Eq. (47) (assuming a uniform system for simplicity) are

$$\begin{aligned} &2c_2(\mathbf{1}_a)+2c_3(\mathbf{1}_a)+c_6(\mathbf{1}_a) \\ &+2c_2(\mathbf{1}_b)+c_3(\mathbf{1}_b)+c_6(\mathbf{1}_b) \\ &+c_3(\mathbf{2}_{ab})+c_6(\mathbf{2}_{ab}) \end{aligned} \quad (49)$$

when the pair $\mathbf{2}_{ab}$ is on the edge of the hexagon, and

$$\begin{aligned} &5c_2(\mathbf{1}_c)+6c_3(\mathbf{1}_c)+c_6(\mathbf{1}_c) \\ &+2c_2(\mathbf{1}_d)+2c_3(\mathbf{1}_d)+c_6(\mathbf{1}_d) \\ &+2c_3(\mathbf{2}_{cd})+c_6(\mathbf{2}_{cd}) \end{aligned} \quad (50)$$

when the pair $\mathbf{2}_{cd}$ occurs on an internal bond. The subscripts 2, 3, and 6 denote the pair, triangle, and hexagonal clusters, respectively. For convenience, let us focus only on the pair terms in (49) and (50), i.e., those that are functions of $\mathbf{2}_{ab}$ or $\mathbf{2}_{cd}$. For the external bond [Eq. (49)] we see that the influence of the rest of the cluster on $\mathbf{2}_{ab}$ is principally due to $c_3(\mathbf{2}_{ab})$, plus a high-order contribution from $\mathbf{c}_6(\mathbf{2}_{ab})$,

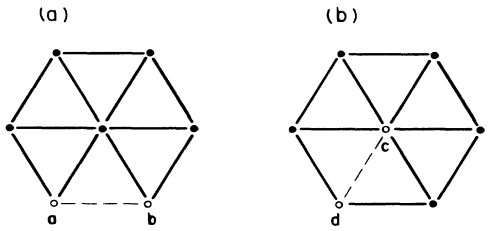
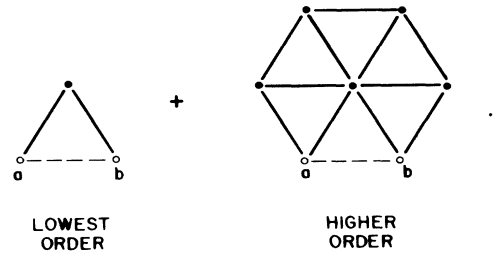
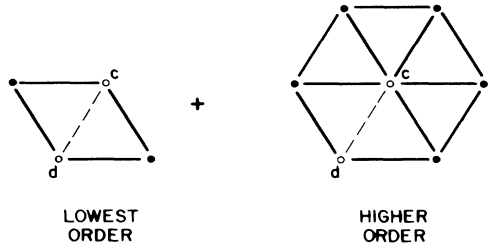


FIG. 4. External and internal pair bonds of a hexagonal cluster are shown in (a) and (b), respectively.



For the internal bond there are two triangular clusters that contribute to the lowest-order influence,



A physical picture emerges in which a bond in a hexagonal cluster feels to lowest order like a bond in a triangular cluster, and experiences the rest of the hexagonal cluster in higher order.

Within an articulated cluster, the two segments that become disjoint on removal of the articulation subcluster literally do not influence each other. That is, if the segments **p**′, **q**′, and **a** of the articulated cluster **j** are labeled as in Fig. 2, then $\ln Q_j(\mathbf{k})$, $\mathbf{k} \subseteq \mathbf{p}'$, contains only $c_n(\mathbf{i})$, where $\mathbf{n} \subseteq \mathbf{p}$, and similarly for the **q**′ segment.

VI. THE TRUNCATED CUMULANT EXPANSION

Practical calculations involve truncation of the cumulant expansion at some level. This generates a set of nonlinear equations for the renormalized interactions, whose solution is discussed in this section. Even though this section addresses how one sets up an actual calculation, it may also serve to clarify the abstract formalism presented in the preceding sections.

The Ising model is our example here. The bare Hamiltonian is a sum of one-body and nearest-neighbor pair interactions,

$$H_N = \sum_{1 \subset N} h(1) + \sum_{2 \subset N} h(2) , \quad (51)$$

where

$$h(1) = \frac{-B}{k_B T}\sigma , \quad (52)$$

$$h(2) = \frac{-J}{k_B T}\sigma\sigma' . \quad (53)$$

The spin variables σ take the values ± 1, and the sums in (51) are over N lattice points and $qN/2$ nearest-neighbor pairs.

There are many possible cumulant expansions for a given physical model, depending on the degree of renormalization and the level of truncation. Some remarks are given later on the strategy governing the choice of approximation. The set of clusters contained in the truncated

cluster expansion is called P. The set P contains the renormalized clusters R as a subset, and, like the set R, we require that any clusters that are subclusters of a member of P are also members of P.

It is not surprising that certain low-order cumulant expansions for spin models are equivalent to approximations derived by other, and sometimes more cumbersome, means. The choice of R equal to all one-spin clusters and P equal to one-spin and nearest-neighbor pairs is the well-known Bethe or pair approximation.[15] Extending the pair approximation so that P also includes the smallest closed-ring cluster of the lattice produces the method of Rushbrooke and Scoins.[9] The Kramers-Wannier expression[16] is obtained from that of Rushbrooke and Scoins by renormalizing nearest-neighbor pair as well as vertex interactions. All cluster-variational approximations[10–12] are generated by particular choices of the sets R and P, as discussed in Sec. IX. The cumulant formalism also generates other approximation schemes in addition to the family of cluster variational techniques.

Equations (47) and (48) constitute nonlinear equations that can be solved for the $c_n(\mathbf{i})$. We now illustrate the rules given in the preceding section for constructing the combinations of $c_n(\mathbf{i})$ found in the influence function $Q_k(\mathbf{j})$ of (47) and the renormalized potential in the exponential of (48). First, let us consider the pair approximation.[15] The only contribution to the renormalized vertex potential comes from $c_2(1)=\delta K_2/\delta\rho(1)$. [See Eq. (43).] The subscript 2 refers to a pair of nearest-neighbor spins and the argument 1 to the value of a single spin of the pair. In general, the $c_2(1)$ depend on the location of the 1 and 2 clusters in the lattice. For simplicity, we only consider homogeneous ferromagnetic phases of the Ising model here, so all the $c_2(1)$ are equivalent. Thus, Eqs. (47) and (48) for the pair approximation become

$$c_2(\sigma)=\tilde{W}_1-\tilde{W}_2-\ln\left[\operatorname*{Tr}_{\sigma'}\exp\left\{\frac{B}{k_BT}\sigma'+\frac{J}{k_BT}\sigma\sigma'-(q-1)c_2(\sigma')\right\}\right]. \tag{54}$$

The $c_2(\sigma)$ in (54) are determined to within an irrelevant constant because distributions only depend on the difference $c_2(\sigma=+1)-c_2(\sigma=-1)$. The constant for any j-body potential is fixed either by specifying one relation among the $c_n(\mathbf{j})$, perhaps adopting a particular spin state $\mathbf{j}_0$ as the zero of energy,

$$c_n(\mathbf{j}_0)=0 \quad \text{for all } \mathbf{n}\ , \tag{55}$$

or, as is customary for the Ising model,

$$\operatorname*{Tr}_{\mathbf{j}} c_n(\mathbf{j})=0\ . \tag{56}$$

The zero of energy is the only arbitrariness present in all vertex-renormalization theories (only one-body renormalized potentials), such as the pair approximation. In the Appendix we discuss the removal of additional irrelevant degrees of freedom for higher-body renormalization.

Equation (54) is sufficiently simple to permit analytic solution. For more sophisticated theories than the pair approximation, equations of this type are generally solved numerically. The natural iteration method of Kikuchi[17] is similar to application of the Picard scheme to (54): the nth guess for $c_2(\sigma)$ is inserted in the exponential of (54), and the trace and logarithm operation generates a refined estimate. We have found that in some cases Picard iteration can be numerically unstable. It is more convenient to resort to the nonlinear equation solving packages contained in most mathematical subroutine libraries. Note that explicit calculation of $\tilde{W}_1-\tilde{W}_2$ in (54) is not necessary; it is easier to simply determine the zero of energy according to (55) or (56).

A higher-order theory, equivalent to the Rushbrooke and Scoins approximation, results if we consider vertex renormalization with the cumulant expansion truncated after the smallest ring of the lattice.[13] Equations (47) and (48) yield the following nonlinear equations:

$$c_2(\sigma)=\tilde{W}_1-\tilde{W}_2-\ln\left[\operatorname*{Tr}_{\sigma'}\exp\left\{\frac{B}{k_BT}\sigma'+\frac{J}{k_BT}\sigma\sigma'-(q-1)c_2(\sigma')-pc_r(\sigma')\right\}\right], \tag{57}$$

$$2c_2(\sigma)+c_r(\sigma)=\tilde{W}_1-\tilde{W}_r-\ln\left\{\operatorname*{Tr}_{r-\sigma}\exp\left[\sum_{\substack{1'\subset r\\(1'\neq\sigma)}}\left\{\frac{B}{k_BT}\sigma'-(q-2)c_2(\sigma')-(p-1)c_r(\sigma')\right\}+\sum_{2\subset r}\frac{J}{k_BT}\sigma\sigma'\right]\right\}. \tag{58}$$

In the above equations $\mathbf{r}$ denotes the ring cluster, and p is the number of rings that intersect one vertex of the lattice. For example, $\mathbf{r}$ is a triangle for the plane triangular ($p=6$) and fcc ($p=24$) lattices, while $\mathbf{r}$ is always a square for a cubic lattice in d dimensions and $p=2d(d-1)$. In Eq. (58), σ' is the Ising spin variable associated with the cluster $1'$.

Comparison of (54) and (57) suggests an efficient numerical scheme when the expansion contains large clusters. In the present example, $c_r(\sigma)$ is of higher order than $c_2(\sigma)$. (This statement is made precise in terms of a high-temperature series expansion for the Ising model in the following section.) In fact, Eq. (57) reduces to (54) if $c_r(\sigma)$ vanishes. Therefore, one can solve (54) as a first approximation, and then use $c_2(\sigma)$ thereby obtained as a first guess for the renormalized potentials in both (57) and

(58). The same scheme can be used to proceed to the next vertex-renormalized approximation in which three nonlinear equations are solved. We have found this "bootstrap" scheme quite useful in practical calculations where one feeds an initial guess consisting of a large number of input parameters into a Picard iteration or nonlinear equation-solving routine. A good-quality initial guess is a great aid in obtaining the desired solution of the nonlinear equations.

There are two additional topics concerning practical calculations that we defer to the Appendix. First, the $c_{\mathbf{n}}(\mathbf{i})$ associated with a given truncation and degree of renormalization usually provide more free parameters than those necessary to uniquely determine the densities $\rho(\mathbf{j})$. In the Appendix we develop a systematic procedure that associates the proper number of free parameters with each $c_{\mathbf{n}}(\mathbf{i})$. Also, we discuss how the cumulant expansion can be transformed into a linear combination of finite-cluster free energies. Then the $\tilde{W}_{\mathbf{j}}$ can be used directly without ever calculating the cluster functions $\tilde{K}_{\mathbf{j}}$.

VII. ORDERING IN THE CUMULANT EXPANSION: THE ISING MODEL

The cluster expansion is now applied to the Ising model to provide a concrete illustration of the clustering property discussed in the preceding sections: cumulants associated with large clusters describe high-order correlations involving *all* the spins of the cluster. This principle, together with the sparseness of the renormalized expansion, often leads to rapid convergence of the cluster expansion. When the free energy of the Ising model is developed in a high- or low-temperature series expansion,[17] each term of the expansion represents correlation among a finite number of spins. Therefore the connection between cumulants of large clusters and high-order correlations can be made precise by determining how many terms of the exact high- or low-temperature series are reproduced at each level of the cluster expansion. The physical interpretation of the renormalized potentials is also reenforced by examining their high- or low-temperature series.

The high-temperature expansion for the zero-field Ising model is a power series in the parameter $w \equiv \tanh(J/k_B T)$.[1,18] [See Eqs. (51)–(53) for a definition of the Ising-model notation.] The free energy is written in the form

$$-\frac{W_N}{N} = \ln 2 + \frac{q}{2}\ln\cosh(J/k_B T) + \sum_l a_l w^l , \tag{59}$$

where the sum begins with l equal to the number of bonds in the smallest closed figure in the lattice, i.e., the size of the smallest ring cluster. In the following analysis, the accuracy of various truncated cumulant expansions are compared by determining how many coefficients a_l in (59) are reproduced exactly by the approximate expressions and by examining how much the remaining coefficients deviate from the a_l.

The bare cumulant expansion for the Ising model above T_c is a particular rearrangement of the infinite series (59). The first two terms of (59) are easily recognized as the cumulants of the 1 and 2 clusters in zero field:

$$K_1^{(0)} = -\ln 2 , \tag{60}$$

$$K_2^{(0)} = -\ln\cosh(J/k_B T) . \tag{61}$$

The rest of (59) is equal to a sum of higher cluster cumulants $K_{\mathbf{j}}^{(0)}$. The bare cumulants $K_{\mathbf{j}}^{(0)}$ have a high-temperature power series in w that begins with w^l, where l is the number of bonds in the cluster j, or the number of bonds in a weakly embedded cluster $\mathbf{m}(\mathbf{j})$ associated with $\mathbf{j}$. If the pair coupling J depended on the location of the bond in the lattice, then w^l would turn into a product of bond functions $w_{\alpha\beta}$ where every bond α—β in the cluster was represented.

In zero field, the high-temperature expansion is already trivially renormalized at the vertex level, since all one-body distributions are equal and satisfy $\rho(\sigma = \pm 1) = \frac{1}{2}$. Therefore as a simple application of the ideas presented in this work, we expect that vertex-articulated clusters, such as

do not appear in these expansions.[19] Indeed, this is a well-known property of the high-temperature series.[20] It is amusing to note that this reflects an elementary feature of the cumulant expansion, and that the properties of articulated clusters exploited in this special case generalize to nonzero field upon renormalization.

The series analysis illustrates how renormalization enhances the convergence properties of the cumulant expansion. We turn to a specific example, the Ising model on a plane triangular lattice. The free energy of this system has the exact series expansion,

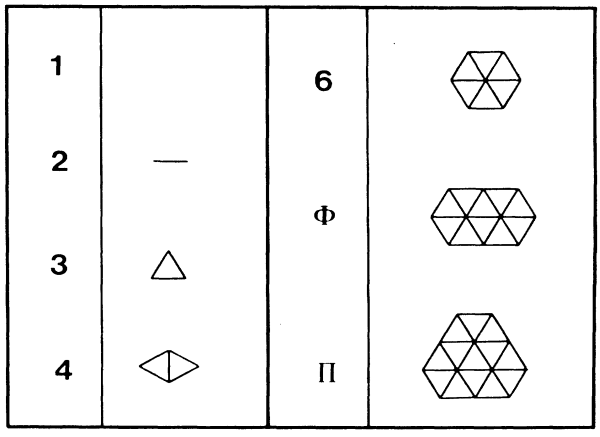


FIG. 5. Essential clusters from the two-dimensional triangular lattice.

$$\frac{-W_N}{N} = \ln 2 + 3\ln\cosh(J/k_BT) + 2w^3 + 3w^4 + 6w^5 + 11w^6 + 24w^7 + \tfrac{111}{2}w^8 + \tfrac{416}{3}w^9 + 363w^{10} + \cdots . \quad (62)$$

The first two bare cumulants, $K_1^{(0)}$ and $K_2^{(0)}$, are given in (60) and (61) above. The bare cumulants of the next few essential clusters are

$$-K_3^{(0)} = \ln(1+w^3) = w^3 - \tfrac{1}{2}w^6 + \tfrac{1}{3}w^9 - \tfrac{1}{4}w^{12} + \cdots ,$$
$$-K_4^{(0)} = \ln\left[\frac{1+2w^3+w^4}{(1+w^3)^2}\right] = w^4 - w^6 - w^7 - \tfrac{1}{2}w^8 + 2w^9 + 4w^{10} + 2w^{11} - \tfrac{19}{6}w^{12} + \cdots , \quad (63)$$
$$-K_5^{(0)} = \ln\left[\frac{(1+3w^3+2w^4+w^5+w^6)(1+w^3)}{(1+2w^3+w^4)^2}\right] = w^5 - 2w^7 - 4w^8 - w^9 + \tfrac{15}{2}w^{10} + 16w^{11} + 10w^{12} + \cdots ,$$

where **3**, **4**, and **5** represent clusters from the triangular lattice shown in Fig. 5. The bare cumulant expansion for a homogeneous plane triangular lattice is

$$\frac{W_N}{N} = K_1^{(0)} + 3K_2^{(0)} + 2K_3^{(0)} + 3K_4^{(0)} + 6K_5^{(0)} + \cdots . \quad (64)$$

Truncation of (64) after $K_3^{(0)}$ gives an estimate for the free energy correct to order w^3, after $K_4^{(0)}$ to order w^4, and $K_5^{(0)}$ to order w^5. This may be contrasted with the properties of the cumulant expansion with *renormalized* two-body potentials. Truncation of the cumulant expansion after K_3 with renormalized pair couplings produces the following expression for W_N,

$$-\frac{W_N}{N} - \ln 2 - 3\ln\cosh(J/k_BT) = \ln\left[\frac{2(1+w)(1-w)^3}{(2-w)}\right] = 2w^3 + 3w^4 + 6w^5 + 10w^6 + 18w^7 + \tfrac{65}{2}w^8 + \cdots , \quad (65)$$

which is correct through order w^5. Equation (65) is obtained by solving for the renormalized pair coupling that matches $\rho(2)$ in the **2** and **3** clusters. Also note that the coefficients of powers of w greater than 5 are much closer to the exact values than those of the bare cumulant expansion truncated after K_3, as can be seen by comparison of the series (65) to $K_3^{(0)}$ in (63). The disappearance of bond-articulated clusters because of pair renormalization explains both of these results. Since the cumulants for the bond-articulated clusters

etc. vanish after pair renormalization, the next contributing cluster is **6**, which is of order w^6. (Remember that the six-membered ring of outer bonds, whose cumulant is of order w^6, is associated with **6** as a nonessential cluster.) Pair renormalization causes the infinite class of bond-articulated cluster functions to vanish, effectively including them through the renormalized potentials. This explains the improvement in the coefficients of w^j, $j \geq 6$, on bond renormalization for the cluster expansion truncated at the pair level.

Truncation of the pair-renormalized expansion after K_6 leads to the free-energy expansion,

$$\frac{-W_N}{N} - \ln 2 - 3\ln\cosh(J/k_BT) = 2w^3 + 3w^4 + 6w^5 + 11w^6 + 24w^7 + \tfrac{105}{2}w^8 + \tfrac{338}{3}w^9 + 231w^{10} + \cdots , \quad (66)$$

which is exact through order w^7 and closely follows the exact expansion (62) for the next several terms. Again, the results can be explained by considering the lowest cluster without bond articulations omitted from the truncated expansion. In this case, it is the cumulant of the cluster Φ (see Fig. 5), which has subclusters of order w^8 associated with it (e.g., the ring of outer bonds). Even if the maximum degree of renormalization was applied to the theory truncated after the hexagon cluster, namely, renormalization of the 3-spin interactions, as in the CVM, the coefficient of w^8 in the high-temperature expansion would still differ from the exact value because the leading-order cumulant that is neglected, K_Φ, contributes at order w^8. Presumably, the coefficient of w^8 with 3-body renormalization lies somewhat closer to the exact value than the coefficient in the pair-renormalized theory shown in (66). Nevertheless, the effort of higher renormalization does not produce any more exact terms in the high-temperature series.

The functions $c_n(\mathbf{j})$ also have a series expansion that shows how larger clusters account for high-order correlations. The only nonzero $c_n(\mathbf{j})$ on pair renormalization for

the Ising model in zero field are the bond functions $c_n(2)=\delta K_n/\delta\rho(2)$. If we parametrize $c_n(\sigma,\sigma')$ as $c_{n,2}\sigma\sigma'$, we find $c_{n,2}$ by noting that

$$\frac{\delta K_n}{\delta\rho(2)}=\frac{\delta K_n}{\delta\langle\sigma\sigma'\rangle}\frac{\delta\langle\sigma\sigma'\rangle}{\delta\rho(\sigma,\sigma')}=\frac{\delta K_n}{\delta\langle\sigma\sigma'\rangle}\sigma\sigma' , \tag{67}$$

where $\langle\sigma\sigma'\rangle=\mathrm{Tr}_{\sigma\sigma'}[\sigma\sigma'\rho(\sigma,\sigma')]$, and hence $c_{n,2}=\delta K_n/\delta\langle\sigma\sigma'\rangle$. The high-temperature expansion of the nearest-neighbor spin-correlation function begins as $\langle\sigma\sigma'\rangle=w+O(w^2)$, so we reach the general conclusion that $c_{n,2}$ for the zero-field Ising model is of one lower order in w than K_n, since the operation of functional differentiation effectively removes one bond.

Just as the K_n are higher order in w as the cluster size increases, the renormalized potential functions $c_n(\mathbf{j})$ become higher order in the same way. This is verified for our example of the two-dimensional triangular Ising model. We consider a pair-renormalized cumulant expansion truncated after the hexagonal cluster. In the hexagonal cluster **6** (Fig. 5) the renormalized potential of the outer bonds are renormalized by $c_3(2)$ as well as several $c_6(2)$, while the inner bonds differ from their bare values only from the influence of several high-order $c_6(2)$. [See Fig. 3(b).] Thus the renormalized outer-bond coupling differs from the bare value of J/k_BT by

$$(w^2+2w^3+5w^4+13w^5+\tfrac{106}{3}w^6+94w^7+249w^8+\cdots)\sigma\sigma' , \tag{68}$$

while the corresponding value for the inner bond is

$$(2w^5+8w^6+20w^7+44w^8+\cdots)\sigma\sigma' . \tag{69}$$

Note that Eq. (68) is one order less than K_3, while Eq. (69) is one order less than K_6, consistent with the above discussion.

VIII. HIGH-ORDER FREE ENERGY FROM PERTURBATIVE RENORMALIZATION

At each level of approximation the free energy $\tilde{W}_N$ satisfies the variational condition (21) with respect to the densities $\rho(\mathbf{j})$, with $\mathbf{j}\in R$. The $c_n(\mathbf{j})$ may be regarded as parameters for a set of distribution functions that are normalized and in which higher densities reduce to lower ones [Eqs. (4) and (5)]. Thus, first variations of $\tilde{W}_N$ with respect to the $c_n(\mathbf{j})$ also vanish. Hence the free energy deviates by the *square* of any error in the renormalized potentials, due to, for instance, neglect of a higher-order $c_n(\mathbf{j})$. In this section we develop a perturbation scheme that exploits the variational properties of $\tilde{W}_N$. This method can be used to improve the accuracy of a closed-form approximation without solving for additional renormalized potentials. Also, it is a powerful technique for generating high-order series expansions with little algebra and far less combinatorial analysis than that found in most standard methods.[1,3]

The basic idea of the perturbation scheme is to use a set of $c_n(\mathbf{j})$ determined from a low-order theory to evaluate high-order cumulants. The error arising from the neglected higher-order $c_n(\mathbf{j})$ affects $\tilde{W}_N$ only at much higher order because of the variational principle. As demonstrated below, this allows determination of high-order series-expansion coefficients with a minimum of algebraic or combinatorial effort. In addition, this scheme is also the basis for the "bootstrap" procedure useful in numerical calculations described in Sec. VI. To illustrate the perturbation scheme, we again use the two-dimensional (2D) triangular Ising model and analyze the effect of neglecting the high-order contribution of $c_6(2)$ for the approximations considered in the preceding section.

When the pair-renormalized cluster expansion of the 2D triangular Ising model is truncated after the triangle cluster, the approximate free energy is given in Eq. (65). Above T_c, the only nonzero $c_n(\mathbf{j})$ is

$$c_3(2)=c_{3,2}\sigma\sigma' , \tag{70}$$

where

$$-c_{3,2}=-\tfrac{1}{4}\ln[e^{2J/k_BT}(2-e^{2J/k_BT})] \tag{71}$$

$$=w^2+2w^3+5w^4+12w^5+\tfrac{91}{3}w^6+78w^7+\cdots . \tag{72}$$

As expected from the preceding discussion, Eq. (72) deviates from (68) at order w^5 since this is the order at which corrections due to $c_6(2)$ appear in the latter. Now let us include the hexagon cluster in the expansion, but neglect $c_6(2)$ and evaluate $c_3(2)$ as given by the triangle approximation as in (70) and (71). We obtain a perturbative expression for the free energy that agrees with the fully renormalized-pair hexagon theory (66) through order w^9. This is a consequence of the variational principle: an error of order w^5 in the renormalized interactions causes a deviation of order w^{10} in the free energy.

The pair-renormalized hexagon level free energy of (66) differs from the exact free energy (62) at order w^8, not because we did not renormalize further, but because the cluster Φ (Fig. 5) was neglected in the expansion. Indeed, higher-body renormalization at the hexagon level as in the CVM would still not properly evaluate this cluster's contribution. To include this cluster using the perturbation scheme, we evaluate the partition function of Φ with *bare* inner bonds and outer bonds renormalized only by $c_3(2)$. Neglect of higher-order $c_n(\mathbf{j})$ does not affect the free energy until cumulants of order w^{10} or greater are considered. Including cumulants through K_Φ and renormalized interactions through $c_3(2)$ generates an approximation for $\tilde{W}_N$ which is exact through order w^8. The coefficient of w^9 is $\frac{410}{3}$ in this scheme, which differs slightly from the exact value $\frac{416}{3}$ because of a neglected weak embedding associated with cluster Π (Fig. 5). However, this coefficient is considerably more accurate than in the theory of Eq. (66), which, in fact, includes the higher renormalization produced by $c_6(2)$, but which is truncated at a lower level. Implementing full pair and higher-body renormalizations on the clusters Φ and Π would significantly increase the numerical effort without providing any more exact series coefficients.

In summary, through perturbative renormalization the exact series expansion until w^{10} can be obtained by only calculating $c_3(\mathbf{2})$ in the triangle approximation, an approximation that otherwise would only provide exact coefficients through order w^5. After determining $c_3(\mathbf{2})$ in a relatively minor calculation by matching the 2-body densities of the pair and triangle clusters, the only additional calculations needed are the evaluations of the partition functions of the higher clusters Φ and Π with fixed interactions. Since we neglect $c_6(\mathbf{2})$ and higher-order contributions in this example, the inner bonds of the higher clusters have bare interactions while the outer bonds are renormalized only by $c_3(\mathbf{2})$. Thus, to lower order the inner bonds are shielded from the surrounding lattice and are not renormalized. This perturbative scheme is equally valid below T_c, where we must also include one-body renormalized potentials to incorporate the broken symmetry. Series-expansion coefficients to high order can be obtained by Taylor expansion of the analytic expressions for the cluster free energies, as was done here. Commercially available programs for symbolic manipulation are particularly well suited to perform such power-series expansions.

IX. RELATION TO OTHER METHODS

The cumulant formalism generates a family of approximations organized according to the number of clusters retained in the expansion and the degree of renormalization. Specifically, the approximation is characterized by the size of the cluster sets P and R described previously. Many finite-cluster approaches developed in the past are equivalent to one of the myriad possible cumulant expansions. The cumulant formalism systematizes a large body of previous work and maps out hitherto unrealized flexibility. Moreover, many results that follow in a straightforward fashion from the preceding development were derived in the past with great difficulty or, in fact, were not derived but noted *a posteriori*. The relation between the cumulant expansion and free-embedding methods is discussed in an earlier paper by Shugard and Weeks.[13] We now turn our attention to the powerful class of cluster-variational methods developed by Kikuchi.[10–12]

The techniques presented in this paper are related to, but are more general than, Kikuchi's cluster-variational method (CVM).[10–12] When the set R is the largest possible subset of P (R can never be equal to P), then the renormalized cumulant expansion and CVM expression are equivalent. Morita[11] has provided a convenient formulation of Kikuchi's method in which an approximation to the functional

$$F[\rho(\mathbf{N})]=\operatorname{Tr}_{\mathbf{N}}\rho(\mathbf{N})[\ln\rho(\mathbf{N})+H_{\mathbf{N}}(\mathbf{N})] \tag{73}$$

is minimized with respect to density. The approximation consists of writing the N-body density as a sum of cluster functions $g(\mathbf{j})$,

$$\ln\rho(\mathbf{N})=\sum_{\mathbf{j}\subseteq\mathbf{N}}\ln g(\mathbf{j}) , \tag{74}$$

where the $g(\mathbf{j})$ are recursively defined,

$$\ln g(\mathbf{j})=\ln\rho(\mathbf{j})-\sum_{\mathbf{i}\subset\mathbf{j}}\ln g(\mathbf{i}) . \tag{75}$$

Equation (74) is truncated at some level and substituted in (73). The functional is then minimized with respect to the truncated density expression subject to the normalization and reducibility conditions for the densities given in Eqs. (4) and (5). The latter conditions are introduced by Morita using Lagrange undetermined multipliers, which turn out to be the finite-cluster free energies and the $c_n(\mathbf{i})$, respectively.

The cumulant expansion we have described is equivalent to including clusters $\mathbf{j}\in P$ in (74), but only minimizing densities $\rho(\mathbf{k})$, $\mathbf{k}\in R$. Those $g(\mathbf{j})$ for $\mathbf{j}\notin R$ are held proportional to the Boltzmann factor of the j-body bare potential,

$$g(\mathbf{j})\propto\exp[-h_{\mathbf{N}}(\mathbf{j})],\quad \mathbf{j}\notin R,\quad \mathbf{j}\in P \tag{76}$$

and are not optimized. As stated above, this becomes the cluster-variational method when R is the largest possible subset of P. Although this is not clear from the outset, the cluster-variational method always gives a superposition approximation for $\rho(\mathbf{j}_{\max})$,[17] i.e., $g(\mathbf{j}_{\max})=1$, where $\mathbf{j}_{\max}$ is the largest cluster included in (74). This corresponds to the requirement that R always be a subset of P.

For a given truncation of set P, the cluster-variational method is the cumulant expansion with the largest set R and hence will produce the lowest free energy. The effort of completely optimizing the densities is not always rewarded (see Sec. VII), and it is sometimes better to include more clusters in P without increasing R. For instance, in the high- or low-temperature limit including more clusters in P, and thereby gaining more correct terms in a series expansion, is always better than increasing R for smaller P unless the increased renormalization makes the higher-order clusters contributing to the series beyond P vanish. Moreover, optimizing many-body potentials or, equivalently, solving for many-body renormalized densities, quickly becomes a cumbersome numerical task for models with many spin states or with continuous symmetry. The cumulant formalism provides a way of systematically obtaining more accurate results without the complication of treating multidimensional functions. It must also be remembered that higher renormalizations may *reintroduce* lower-order clusters that vanished in a theory that was not fully renormalized (see Sec. IV).

The number of correct terms in a high- or low-temperature series expansion is straightforwardly determined from the cumulant expansion. This has been illustrated for the high-temperature coefficients of Ising model in Secs. VII and VIII. The corresponding analysis is more difficult using the standard formulation of the CVM, and the number of correct terms is generally reported *a posteriori*.[21] The notion that renormalization, or, equivalently, density optimization, makes the contribution of articulated clusters vanish has not been generally appreciated in the large body of work that makes use of finite-cluster approaches like the CVM.

X. CUMULANTS NEAR CRITICALITY AND WHEN RENORMALIZED POTENTIALS DO NOT EXIST

Convergence of the cumulant expansion hinges on the ability to safely neglect high-order, long-range correlations between spins. This fails near criticality, where renormalization-group methods are needed to cope with a diverging correlation length. Simple truncations of the cumulant expansion always give mean-field critical exponents. Without suitable modification (see Sec. XI), the truncated finite-cluster methods are also poorly suited to describe long-wavelength properties in other systems that, though noncritical, contain long-wavelength excitations. Examples are spin-wave excitations of the x-y model, long-wavelength properties of antiferromagnets on closed-packed lattices, and phonon excitations in crystals.

Despite these failings, cluster methods are frequently used to determine critical points. Even though the finite-correlation-length assumption breaks down at criticality, the phases on either side of the critical region can often be accurately described by the cumulant expansion. In some sense, the critical region is bracketed by the accurate mean-field-like description in neighboring areas of parameter space. Hence, the cluster expansion often yields surprisingly good estimates of critical temperatures, although scaling exponents near criticality are incorrect.

When a cumulant expansion is rapidly convergent, the magnitude of the higher terms decreases with cluster size. In contrast, the contribution of all cluster functions are of comparable magnitude near T_c and the expansion fails to converge after a few terms. It is not surprising that within some truncation schemes the equations for the renormalized potentials fail to have solutions in the critical region. This behavior is well known in the Ising model,[10,21] and similar behavior almost certainly can be found for other physical models. Since renormalization is equivalent to variational optimization of the free energy, this behavior shows that the approximate free energy of the truncated expansion is a nonconvex functional of densities in the critical region and variational optimization of the free energy is impossible. It has never been clear how to handle this failure within the cluster-variational method,[10–12] except to try a different truncation scheme.

Here we illustrate how the alternative conceptual framework of the renormalized cumulant expansion suggests a possible remedy when minimization of the free energy is impossible. The strategy behind renormalization is to make the cluster expansion as sparse as possible, and in this sense minimize the contribution of neglected clusters. When certain classes of articulated clusters cannot be completely eliminated, we demonstrate below that minimizing their contribution gives sensible results. This procedure is an alternative to, and is not equivalent to, free-energy minimization.

Equations (47) and (48) for the renormalized potentials are a consequence of holding all renormalized densities equal within the clusters included in the expansion. We have seen that enforcing this condition greatly enhances the convergence of the expansion by removing infinite classes of articulated cluster functions. When solutions to (47) and (48) do not exist, the density-potential functional relation for finite clusters is not invertible in the desired range of matching cluster densities *within the context of a particular truncated cumulant expansion.* That is, given a *truncated* set of the $c_{\mathbf{n}}(\mathbf{i})$ we are unable to match renormalized densities in all finite clusters. However, solutions may exist in other levels of approximation, sometimes alternating as more clusters are included,[21] and presumably they do exist in the complete expansion. Note that the finite-cluster $\tilde{W}_{\mathbf{j}}$ and their cumulants are always assumed to exist as functionals of densities. Indeed, we exploit their properties in the part of distribution-function space where a truncated set of corresponding $c_{\mathbf{n}}(\mathbf{i})$ cannot be found.

In the multidimensional space of finite-cluster distribution functions, articulated cumulants vanish along domains where the densities match among the finite clusters. Precisely which articulated clusters vanish, e.g., vertex-articulated, bond-articulated, etc., depends on which finite-cluster densities match, as explained in Sec. IV. Failure to find the desired set of renormalized potentials means that the region of density-function space parametrized by a truncated set of $c_{\mathbf{n}}(\mathbf{i})$ cannot intersect the line where the renormalized densities match. If the line of matching densities lies close enough so that a Taylor series of the cumulants about this line is valid, minimizing the density *mismatch* in the region parametrized by the $c_{\mathbf{n}}(\mathbf{i})$ minimizes the articulated cluster functions. Although the articulated cumulants are not completely removed, we have optimized the cluster expansion to make the neglected cumulants as small as possible.

This idea suggests the following equation, which replaces (47) and (48) when they cannot be solved:

$$\frac{\delta}{\delta c_{\mathbf{n}}(\mathbf{i})}\operatorname{Tr}_{\mathbf{j}}\left|e^{\tilde{W}_{\mathbf{j}}-\tilde{H}(\mathbf{j})}-\operatorname{Tr}_{\mathbf{k}-\mathbf{j}}e^{\tilde{W}_{\mathbf{k}}-\tilde{H}(\mathbf{k})}\right|^2=0\ ,\qquad \mathbf{i},\mathbf{j}\in R,\ \ \mathbf{k},\mathbf{n}\in P\ , \tag{77}$$

where $\tilde{H}(\mathbf{j})$ and $\tilde{H}(\mathbf{k})$ are the total (bare plus renormalized) interaction in the $\mathbf{j}$ and $\mathbf{k}$ clusters. Equation (77) reduces to (47) and (48) when the density mismatch can be made zero and, in general, minimizes the square of the density mismatch.

Consider a specific example, the Ising model on an fcc lattice for which the cumulant expansion with a renormalized pair interaction is truncated after the triangle cluster. In zero field and $T>T_c$, all the vertex functions $c_{\mathbf{n}}(\mathbf{1})$ are zero and we need to determine just one constant $c_{3,2}$, where $c_3(\mathbf{2})\equiv c_{3,2}\sigma\sigma'$ and 2 and 3 denote pair and triangular clusters. Let

$$z_0=\exp(J/k_BT)\ , \tag{78}$$

$$z=z_0\exp(-4c_{3,2})\ , \tag{79}$$

where $\ln z$ is the effective coupling constant if the 2-cluster Hamiltonian is written in an Ising-like form, and $\frac{1}{4}\ln(z_0z^3)=J/k_BT-3c_{3,2}$ is the analogous constant for the triangle cluster. Equations (47) and (48) reduce here to

$$1+z_0z^3-2z^2=0\ . \tag{80}$$

The physical root of the above equation, the one that smoothly goes to unity as $z_0 \to 1$ or $T \to \infty$, moves off the real axis when the bare coupling z_0 reaches $z_0' = \frac{4}{3}(\frac{2}{3})^{1/2} = 1.089\ldots$. Unfortunately, the triangle theory does not predict an ordering transition within the temperature range $1 < z_0 < z_0'$ where solutions with $\langle\sigma\rangle = 0$ can be found. Therefore there is a range of parameters where this approximation gives no physical result, and, in particular, no critical temperature is found. Aggarwal and Tanaka[21] have analytically continued these equations to complex temperature, but we do not see the physical justification of this procedure.

To continue the cluster expansion beyond z_0', we solve Eq. (77), which, for the Ising model, is equivalent to minimizing $|\langle\sigma\sigma'\rangle_3 - \langle\sigma\sigma'\rangle_2|$, the difference in spin-spin correlation functions between the triangle and pair clusters. It is easy to show that

$$\langle\sigma\sigma'\rangle_3 - \langle\sigma\sigma'\rangle_2 = \frac{2+2z_0z^3-4z^2}{3+z_0z^3+z_0z^5+3z^2} \tag{81}$$

has minimum magnitude when $z = (3/z_0)^{1/5}$. The free energy of the disordered phase as a function of J/k_BT is shown in Fig. 6. The curve for $z_0 < z_0'$, determined by Eq. (80), joins smoothly with the free-energy function for $z_0 > z_0'$, as found from solving (81) for the renormalized interaction. The two branches must join smoothly at z_0' because their slopes, given by $\langle\sigma\sigma'\rangle$, are equal at z_0'. (However, higher-order derivatives of the free energy do have a spurious discontinuity.) Note that above z_0' the nearest-neighbor spin-correlation function is different in the pair and triangle clusters. In general, $\langle\sigma\sigma'\rangle$ is obtained by differentiating the total cumulant free-energy sum with respect to J/k_BT as in Eq. (3), and here is given as a weighted sum,

$$\langle\sigma\sigma'\rangle = -3\langle\sigma\sigma'\rangle_2 + 4\langle\sigma\sigma'\rangle_3 , \tag{82}$$

above z_0'. A critical point is found on the branch above z_0' with critical temperature $k_BT_c/qJ = 0.8096$. The exact k_BT_c/qJ determined from series expansions is 0.8163,[18] while the Rushbrooke and Scoins approximation,[9] which also is truncated after the triangle cluster but includes no optimization of the pair potential ($z = z_0$), yields 0.8818.

The relative mismatch of the correlation functions,

$$\frac{\langle\sigma\sigma'\rangle_3 - \langle\sigma\sigma'\rangle_2}{\langle\sigma\sigma'\rangle} , \tag{83}$$

is quite small in the range between z_0' and the critical point. The mismatch (83) is zero at z_0' and is only 5.75×10^{-3} at $T = T_c$. Therefore, our conclusion that minimizing the mismatch is equivalent to minimizing the contribution of articulated clusters, which rests on the assumption that the mismatch is small, appears to be well justified in this case.

We emphasize that Eq. (77) is one example of several possible *ad hoc* procedures that allows some optimization of the cumulant expansion when fully renormalized potentials do not exist. While it illustrates the flexibility of the renormalized-cluster-expansion viewpoint, it does not overcome the inherent shortcomings of the truncated finite-cluster methods in describing phenomena involving long-range correlations.

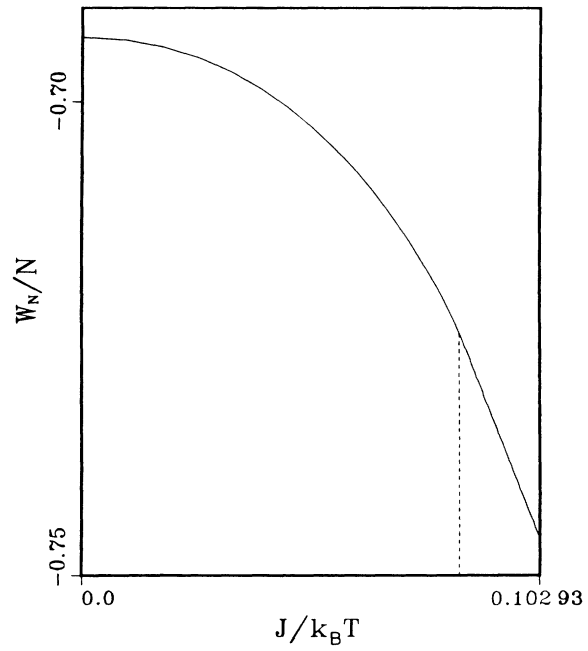


FIG. 6. Free energy per spin of the fcc Ising model above the critical temperature when the cumulant expansion is truncated after the triangle cluster. For J/k_BT less than 0.0849, it is possible to fully renormalize the cumulant series. Above this value, indicated by the dashed line, the pair-renormalization equations have no solutions. In the region between $J/k_BT = 0.0849$ and the critical point in this approximation, $J/k_BT = 0.102\,93$, we show results of the procedure described in the text, which is intermediate between vertex and pair renormalization.

XI. PAIR-CORRELATION FUNCTIONS

It is possible to directly compare the Fourier transform of pair-correlation functions with experimental x-ray or neutron-scattering data. This data can be readily extracted from the finite-cluster free-energy expression by exploiting the Legendre-transform relations given in Sec. IV. Essentially the same relations, though not explicitly using the Legendre transform, were obtained by Sanchez, who derived the pair-correlation function in the cluster-variational-method formalism.[22]

The pair-correlation function is generated by functional differentiation of W_N with respect to single-particle fields,

$$-\frac{\delta^2 W_N}{\delta h(1)\delta h(1')} = \rho(1,1') - \rho(1)\rho(1')$$

$$\equiv S_N(1,1') . \tag{84}$$

The density $\rho(1,1')$ is the joint probability of finding a spin at position $\mathbf{r}$ in state σ_r and another spin at $\mathbf{r}'$ in state $\sigma_{r'}$. Regarded as a matrix whose rows are labeled by $\mathbf{r}$ and σ_r and columns by $\mathbf{r}'$ and $\sigma_{r'}$, $S_N(1,1') = S_N(\mathbf{r},\sigma_r;\mathbf{r}',\sigma_{r'})$ is symmetric,

$$S_N(1,1') = -\frac{\delta\rho(1)}{\delta h(1')} = -\frac{\delta\rho(1')}{\delta h(1)} , \tag{85}$$

positive definite, and, for translationally invariant isotropic systems, a function of $\mathbf{r}$ and $\mathbf{r}'$ in the combination $|\mathbf{r}-\mathbf{r}'|$ only.

The matrix inverse $S_N^{-1}(1,1')$ of $S_N(1,1')$ is $-\delta h(1')/\delta\rho(1)$. From Eq. (18), it is easily seen that differentiation of the Legendre-transformed free energy X_N generates $S_N^{-1}(1,1')$,

$$S_N^{-1}(1,1') = \frac{\delta^2 X_N}{\delta\rho(1)\delta\rho(1')} . \tag{86}$$

X_N is a natural function of vertex densities $\rho(1)$ plus whatever densities are specified by the set R. When W_N or X_N is expressed in terms of finite-cluster free energies, it is more convenient to calculate $S_N^{-1}(1,1')$ rather than the correlation function itself. This is because the renormalized free energies are, in general, functions of all vertex potentials, while $\delta^2 X_j/\delta\rho(1)\delta\rho(1')$ vanishes unless both 1 and 1' are contained in $\mathbf{j}$. We now show that $S_N^{-1}(1,1')$ is a cumulant sum of inverse correlation functions in finite clusters.

The inverse correlation function within a finite cluster $\mathbf{j}$ is indicated with a subscript:

$$S_j^{-1}(1,1') = \frac{\delta^2 X_j}{\delta\rho(1)\delta\rho(1')} , \tag{87}$$

If we form cluster cumulants of the $S_j^{-1}(1,1')$ for a given spin pair 1 and 1',

$$\Delta S_j^{-1}(1,1') = S_j^{-1}(1,1') - \sum_{i\subset j} \Delta S_i^{-1}(1,1')$$

$$= \frac{\delta^2 K_j}{\delta\rho(1)\delta\rho(1')} , \tag{88}$$

from (24), then the inverse correlation function of the full system is simply

$$S_N^{-1}(1,1') = \sum_j \Delta S_j^{-1}(1,1') . \tag{89}$$

The $\Delta S_j^{-1}(1,1')$ are zero unless $1,1'\in\mathbf{j}$. When the sum in (89) is truncated at some finite order, $S_N^{-1}(1,1')$ vanishes beyond the range of the largest cluster in the expansion, but $S_N(1,1')$ itself decays smoothly with increasing distance between 1 and 1'. Thus the method can predict long-ranged correlations, even though only a few clusters are considered explicitly. In translationally invariant systems, the matrix inversions are performed by Fourier transformation.

XII. FINAL REMARKS

The starting point of the renormalized finite-cluster method developed in this work is an exact cluster expansion of the free energy. Finite-cluster methods have generally been approached from the point of view of variational optimization: one assumes a certain trial density and the free energy is then minimized with respect to the parameters of the trial function. The present work provides an alternative conceptual framework in which renormalization of the finite-cluster expansion replaces variational optimization. Each level of renormalization removes an infinite class of articulated clusters from the expansion and introduces effective fields corresponding to the articulation piece in the remaining clusters. Vertex renormalization eliminates vertex-articulated clusters and introduces vertex fields in all other clusters, nearest-neighbor pair renormalization does the same for pair articulated clusters and two-body fields, and so on. Approximation schemes are characterized by the degree of renormalization and the number of clusters retained in the renormalized expansion. The accuracy of a particular truncation of a renormalized expansion can be gauged by examination of the lowest-order nonvanishing cluster that is omitted. Simply knowing the number of vertices or bonds in the cluster is often sufficient to determine the leading order of the cumulant in terms of a high- or low-temperature expansion parameter, density, etc.

From the perspective given by the cluster-expansion method, it makes sense to balance the algebraic complexity of high-level renormalizations against the work of adding more clusters to the expansion. As explained above, the cost of high-level renormalization is not always rewarded by gaining more exact terms of a high- or low-temperature expansion. Full renormalization, equivalent to complete variational optimization, is a convenient and useful choice for small clusters and just a few possible spin states. There are cases where full renormalization is either not necessary or impractical. For instance, the equations for either renormalization or variational optimization become integral equations in systems with continuous degrees of freedom (e.g., vector spin models, solids described by displacements from perfect-lattice positions). Each higher level of renormalization adds more dimensions to the integral equation that must be solved, leading some workers to use Monte Carlo methods to cope with the large dimensionality.[6(c)] It may be more efficient in these cases to add more clusters without higher renormalization, thus allowing one to solve coupled integral equations rather than equations of higher dimensionality.

Finally, we comment on a future extension of this work. There are interesting physical systems that exhibit long-wavelength excitation, yet are tractable because these excitations are controlled by a quadratic Hamiltonian. Examples are spin-wave excitation in vector spin models or phonon modes in a solid. The flexibility of Kubo's notion of generalized cumulants enables us to generate an expansion using any definition of finite clusters, so long as the full statistical system is reproduced in the limit of large clusters. For a solid, we can choose clusters that include anharmonic interactions among members of the cluster, yet include the harmonic response of the full lattice. In effect, we consider a cluster expansion about a harmonic reference system, and the convergence of the expansion is enhanced by a novel method of generating finite clusters. More generally, we believe that a useful area for future research lies in the development of modified truncation schemes, which build in the exact long-wavelength properties of the system, while still maintaining the accurate description of short-wavelength properties afforded by the finite-cluster method.

APPENDIX: PRACTICAL CALCULATIONS

Here we consider two aspects of practical calculations using the cumulant expansion, determination of the number of independent variables and rewriting the cumulant sum directly in terms of finite-cluster free energies.

We develop a systematic procedure to determine the number of free parameters needed to describe higher-order renormalizations. Other procedures are conceivable, but the one suggested here is in accord with our physical notion of the role of higher cumulants since it associates the least number of free parameters with the many-body renormalized potentials. We first consider a specific example, the Ising model when vertices and bonds are renormalized. At the ring-expansion level, renormalization of nearest-neighbor bond-pair interactions requires determination of the functions $c_2(\sigma)$, $c_r(\sigma)$, and $c_r(\sigma,\sigma')$. As pointed out earlier, the vertex functions $c_2(\sigma)$ and $c_r(\sigma)$ really involve just one parameter since the zero of energy is arbitrary.

The pair function $c_r(\sigma,\sigma')$ for the Ising model also has just one free parameter. Of the four energy values for the states of a pair of Ising spins, one is an arbitrary zero of energy. Two more parameters are still arbitrary because the total renormalized potential is unchanged when vertex potentials for σ and σ' are added to $c_r(\sigma,\sigma')$ and subtracted with the right combinatorial factor from $c_2(\sigma)$, $c_2(\sigma')$, $c_r(\sigma)$, and $c_r(\sigma')$. The vertex and pair functions for the Ising model can be conveniently parametrized by taking the $c_i(\mathbf{1})$ to be an effective field times σ, and the $c_i(\mathbf{2})$ to be an effective coupling constant times $\sigma\sigma'$. By extension of our reasoning for the Ising model, vertex functions for an n-state spin model have $n-1$ free parameters and pair functions have $n^2-2(n-1)-1$ free parameters. The number of parameters associated with a j-body renormalized potential are determined recursively by subtracting from n^j-1 the number of parameters available in the lower-body potentials acting on the j spins.

Once renormalized potentials are determined by solution of Eqs. (47) and (48), the finite-cluster free energies $\tilde{W}_j$ are evaluated by a straightforward trace over the Boltzmann factor containing renormalized potentials. Instead of explicitly evaluating the cluster functions $\tilde{K}_j$, it is easier to invert the cumulant expansion and express $\tilde{W}_N$ as a linear sum of the $\tilde{W}_j$,

$$\tilde{W}_N=\sum_j \gamma_j \tilde{W}_j \ . \tag{A1}$$

The formal procedure for determining the constants γ_j, known as Moebius inversion, is lucidly explained by Domb in Ref. 18. It is usually quite simple to obtain the γ_j's by recursively expressing the $\tilde{K}_j$ as sums of the $\tilde{W}_j$. Perhaps even easier, a set of linear equations equivalent to Moebius inversion for the γ_j can be generated by sequentially writing (A1) in the limit that the system is composed of statistically independent **1** clusters, **2** clusters, etc. The combinatorial factors γ_j are independent of the cluster Hamiltonian, so they may be determined from considering these artificially decoupled systems. For instance, the γ_j for a cumulant expansion up to the ring level for a homogeneous lattice are determined by

$$\gamma_1+2\gamma_2+r\gamma_r=1 \ , \tag{A2}$$

$$\gamma_2+r\gamma_r=\frac{q}{2} \ , \tag{A3}$$

$$\gamma_r=\frac{p}{r} \ , \tag{A4}$$

where q and p are the number of bonds and rings incident on a vertex, respectively, r is the number of vertices or bonds in a ring cluster **r**, and $q/2$ and p/r are the number of bonds and rings, respectively, per vertex in the lattice. Equation (A2) is obtained by supposing that the system is composed of N independent spins. In this case $W_2=2W_1$, $W_r=rW_1$, etc., and (A2) is obtained by substitution of these results in (A1). Similarly, (A3) is obtained by imagining a system of statistically independent **2** clusters for which $W_1=0$, $W_r=rW_2$, and $W_N=\frac{1}{2}qW_2$. We finally obtain, for $\tilde{W}_N$,

$$\frac{\tilde{W}_N}{N}=(1+p-q)\tilde{W}_1+\left[\frac{q}{2}-p\right]\tilde{W}_2+\frac{p}{r}\tilde{W}_r \ , \tag{A5}$$

where the terms omitted from the truncated expansion above are the $\tilde{K}_j$ for **j** larger than the ring cluster **r**.

[1] C. Domb, Adv. Phys. **9**, 149 (1960).

[2] D. M. Burley, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1972), Vol. 2, Chap. 9.

[3] *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1974), Vol. 3.

[4] R. Kubo, J. Phys. Soc. Jpn. **17**, 1100 (1962).

[5] The cumulant expansion may not reproduce the exact low-temperature series for a phase of broken symmetry when the ground state is degenerate. In a future publication we will consider the construction of expansions with the proper low-temperature limit for some systems with degenerate ground states.

[6] (a) K. Honda, Prog. Theor. Phys. **52**, 385 (1974); **53**, 889, 1546 (1975); **55**, 1024 (1976); (b) J. A. Barker, J. Chem. Phys. **63**, 632 (1975); (c) B. Firey and N. W. Ashcroft, *ibid.* **82**, 2723 (1985); (d) F. H. Stillinger, Z. W. Salsburg, and R. L. Kornegay, *ibid.* **40**, 1564 (1964); Z. W. Salsburg, W. G. Rudd, and F. H. Stillinger, *ibid.* **47**, 4534 (1967); W. G. Rudd, Z. W. Salsburg, A. P. Yu, and F. H. Stillinger, *ibid.* **49**, 4857 (1968).

[7] M. Wortis, in *Phase Transitions and Critical Phenomena*, Ref. 2, Chap. 3.

[8] T. Morita and K. Hiroike, Prog. Theor. Phys. **23**, 385, 1003 (1961); G. Stell, in *The Equilibrium Theory of Classical Fluids*, edited by H. L. Frisch and J. L. Lebowitz (Benjamin, New York, 1964).

[9] G. S. Rushbrooke and H. I. Scoins, Proc. R. Soc. London, Ser. A **230**, 74 (1955).

[10]R. Kikuchi, Phys. Rev. **81**, 988 (1951); M. Kurata, R. Kikuchi, and T. Watari, J. Chem. Phys. **21**, 434 (1953).
[11]T. Morita, J. Phys. Soc. Jpn. **12**, 753, 1060 (1957); J. Math. Phys. **13**, 115 (1972); J. Stat. Phys. **34**, 319 (1984). See S. Katsura and R. Kikuchi [Physica **123A**, 595 (1984), and references contained therein] for a discussion of the relationship between the different approaches.
[12]J. M. Sanchez, F. Ducastelle, and D. Gratias, Physica **128A**, 334 (1984). See also J. M. Sanchez and J. L. Morán-López, Phys. Rev. B **32**, 3534 (1985).
[13]W. J. Shugard and J. D. Weeks, Phys. Rev. B **22**, 5245 (1980).
[14]C. Domb, in *Phase Transitions and Critical Phenomena,* Ref. 3, Chap. 1.
[15]H. A. Bethe, Proc. R. Soc. London, Ser. A **150**, 552 (1935).
[16]W. A. Kramers and G. H. Wannier, Phys. Rev. **60**, 252, 263 (1941).
[17]R. Kikuchi, J. Chem. Phys. **60**, 1071 (1974); **65**, 4545 (1976).
[18]C. Domb, in *Phase Transitions and Critical Phenomena,* Ref. 3, Chap. 6.
[19]The diagrams contributing to the expansion of the free energy in Eqs. (59) should not be confused with the familiar "high-temperature" clusters arising from the van der Waerden–type development of the Ising partition function (Refs. 1 and 18). The latter consists of all diagrams (including disconnected ones) where only an even number of bonds meet at a vertex.
[20]M. F. Sykes and D. L. Hunter, J. Phys. A **7**, 1589 (1974).
[21]S. K. Aggarwal and T. Tamaka, Phys. Rev. B **16**, 3963 (1977).
[22]J. M. Sanchez, Physica **111A**, 200 (1982).