Linked cluster expansion and 1/*d* expansions for classical spin systems

E. Halvorsen[1] and M. Bartkowiak[2]
[1]*Skoggt. 5, N-3183 Horten, Norway*
[2]*Solid State Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831-6030; Department of Physics and Astronomy, The University of Tennessee, Knoxville, Tennessee 37996-1200; and Institute of Physics, A. Mickiewicz University, ul. Umultowska 85, 61-614 Poznań, Poland*
(Received 25 October 1999; revised manuscript received 7 August 2000; published 11 December 2000)

We consider 1/*d* expansions for classical spin systems based on the vertex renormalized linked cluster expansion (LCE). The free multiplicities of the LCE graphs on a hypercubic lattice in an arbitrary dimension *d* are calculated using generating functions. The technique is applied to the Ising model and to a two-component classical lattice gas corresponding to an extended Hubbard model at half filling in the zero-bandwidth limit. We use a resummation of the LCE to generate 1/*d* expansions for the equation of state and for the critical temperature. The method, which is rather general and applicable to a wide range of models, proves convenient for calculating asymptotic power series expansions in 1/*d*. The vertex renormalized expansion is shown to break down at low temperature in higher order approximations, barring attempts to construct simple approximations that are both self-consistent and exact to some finite order in 1/*d*.

DOI: 10.1103/PhysRevB.63.014403 PACS number(s): 75.10.Hk, 02.30.Mv, 05.50.+q

I. INTRODUCTION

The molecular field approximation (MFA) for classical spin systems becomes exact in the limit of infinite coordination number *z* of the lattice. The first attempts to formulate an expansion in terms of the inverse powers of *z* for these systems were made more than 30 years ago.[1–3] A linked cluster expansion (LCE) based on an expansion of the partition function in terms of βJ, where β is the inverse temperature and *J* is the exchange, was developed. The limit of infinite *z* corresponds to the sum of all Cayley tree diagrams in the linked cluster expansion, and corrections were sought by classification of the remaining diagrams of the expansion in terms of higher powers of 1/*z*, complemented by various kinds of renormalizations to cure inconsistencies in the theories. The inconsistencies were later shown to be avoided, at least in principle, by constructing so-called Φ-derivable approximations,[4,5] such as for quantum many-body problems.[6] The key feature of this approach is that one constructs a functional Φ of the full propagator(s), from which all correlation functions and the grand canonical potential follow. The physical singularities are therefore guaranteed to appear for the same parameter values in all quantities.

The expansion in inverse powers of the lattice dimensionality *d* for the critical temperature of the spin-$\frac{1}{2}$ Ising model, as well as for other quantities, was successfully used by Fisher and Gaunt[7] for the case of hypercubic lattices, for which $z=2d$. They considered the high temperature series expansion, which was well known from investigations of the model in two and three dimensions, and carefully examined the *d* dependence of the weak lattice constants entering the expansion. They went to the fifth order in 1/*d* for the critical temperature and found a good agreement with the results of other methods. Later, this approach was applied to the general *n*-vector models by Gerber and Fischer.[8] They also investigated the spherical model (with $n\to\infty$), for which the critical point is exactly known in any dimension. This enabled them to prove rigorously that an asymptotic 1/*d* expansion exists, at least for this model, although it is not convergent. Remarkably, the critical temperature was found to be an analytic function of *d* in the interval $2<d<\infty$, which goes below the upper critical dimensionality. Therefore, even though a finite-order expansion in 1/*d* (as any other mean-field-type theory) cannot give correct critical indices due to its approximate treatment of long-range correlations, it does give information about nonuniversal parameters such as the critical temperature below the upper critical dimensionality.

The 1/*z* (or 1/*d*) criterion in the early attempts to rearrange the LCE had only a suggestive meaning.[5] In particular, the first order correction was taken to be the sum of all ring diagrams.[2] For the nearest neighbor interaction on a hypercubic lattice in *d* dimensions, the weight of a ring diagram with $2k$ bonds is $\mathcal{O}(d^{-k})$, as pointed out by Fishman and Vignale.[9] Therefore, if one takes the limit diagram by diagram, as it is done in the weak embedding expansion of Fisher and Gaunt,[7] only one ring diagram contributes to $\mathcal{O}(1/d)$ in the vertex renormalized LCE. This approach to the limit of infinite dimensions within the LCE was employed by Abe,[10] who simply took the vertex renormalized eight order expansion in βJ for the inverse susceptibility and restructured it into a 1/*d* expansion using Fisher and Gaunt's result as a guidance.

A great interest in the limit of infinite dimensions for correlated fermion systems has arisen within the last few years (see Ref. 11 for reviews). This followed the observations by Metzner and Vollhardt in their seminal paper[12] that for tight-binding fermions on a hypercubic lattice the appropriate scaling of the hopping matrix element, $t\sim d^{-1/2}$, has far reaching consequences. In general, the self-energy becomes site diagonal, and the nearest (or further) neighbor interactions reduce to the Hartree approximation in this limit.[13] Although a tremendous simplification of the problem is achieved, the problem of interacting fermions in infinite dimensions is still far more complicated than the MFA for classical spin models, and the calculation of 1/*d* corrections for correlated fermions is in general very diffi-

cult. In some special cases, however, this has been done. These include weak coupling treatments of correlated electron systems,[14] variational wave functions approach,[15] disordered electronic systems,[16] the spinless fermion model at half filling,[17] and the Falicov–Kimball model.[18] A common feature of some of these works is the use of the Φ potential as the starting point for the $1/d$ expansions. This is quite natural, because the limit of infinite dimensions itself can be considered a Φ-derivable approximation. Since the LCE with vertex renormalization for classical spin systems is quite analogous to propagator renormalized expansions for lattice fermions, it may be beneficial to use classical spin models as a testing ground for $1/d$ expansions based on resummation of graphs. Besides, since some quantum models have a classical spin or a lattice gas model as a limiting case, $1/d$ expansions for the classical models might be useful as benchmarks for other approximation schemes to the quantum models. Furthermore, perturbation expansions for correlated electron systems with the atomic limit as the unperturbed Hamiltonian are closely parallel to the LCE for classical spin systems.[19–21]

Expansions in $1/d$ (or $1/z$) have been considered recently by Georges and Yedidia[22] for the Ising model and by Fishman and co-workers[9,23] for the Ising and Heisenberg models. Georges and Yedidia make an expansion at fixed order parameter by introducing Lagrangian multipliers to enforce the constraint. Their expansion does not have a precise diagrammatic language, but they were able to associate shorthand graphs to the terms. These graphs reflect the rough structure of the expansion. In the works by Fishman and co-workers, mostly linear in $1/d$ corrections are considered, so that the results are independent of the actual structure of the lattice, except for the investigation of the random phase approximation (RPA) in Ref. 9, which goes to the second order. In both above approaches, the actual method is rather tightly bound to the problem. The usefulness of the LCE, which is a very general method, is acknowledged by the authors, but not exploited.

In this paper we present a systematic classification of the LCE diagrams for classical spin systems with respect to powers of $1/d$. The results are quite general at this level, because the details of the local part of the Hamiltonian is hidden in the vertices, i.e., semi-invariants. We restrict the considerations to interactions between nearest neighbor sites and between one kind of variables only. The latter is not a serious limitation, since a generalization to several variables effects only the algebraic level, and need not be reflected in the diagrammatic language. Generalizations to quantum spin models with nearest neighbor interaction should also be workable, but the additional complexity due to the time dependence may put serious practical limitations on how many orders in $1/d$ can be included, just as for correlated electron systems mentioned above.

In the following section we give a brief description of the LCE for classical spin models and of the vertex renormalization of the diagrammatic expansion. This serves to settle the notation and define the basic concepts of the rearrangement of the series in terms of the $1/d$ dependence. In Sec. III, we analyze the dimensional dependence of the free multiplicities, which are the lattice constants in the LCE, and take the form of polynomials in d. Our main result is to express the polynomial coefficients explicitly in terms of the free-multiplicities for the linear chain. In Sec. IV we discuss the $1/d$ expansion of the Φ potential for fixed semi-invariants, showing explicitly the series up to $\mathcal{O}(d^{-3})$. In Secs. V and VI we apply these results to two simple example systems: the spin-s Ising model, and a two component lattice gas corresponding to an extended Hubbard model at half filling with zero electron hopping between sites. An investigation of the phase diagram of the latter model in infinite dimensions for arbitrary filling was carried out by Micnas *et al.*,[24] showing a rich behavior. We restrict our treatment to pure power expansions in $1/d$ of the equation of state, which gives the critical temperature, and, for the lattice gas model, also the tricritical point. In these calculations we have benefited from using the MuPAD package.[25] The expansion of Φ can also be used as a starting point for Φ-derivable approximations which are correct to a given order in $1/d$, but necessarily include terms of all higher orders. This has already been done to the first order for spinless fermions.[17] These approximations, which we will simply call *self-consistent* $1/d$ *expansions* hereafter, are discussed for the classical spin systems in Sec. VII. We particularly emphasize higher order approximations, which are shown to break down for the ordered phase. In Sec. VIII, we summarize our results and present the main conclusions.

II. LINKED CLUSTER EXPANSION

Here we briefly describe the basic concepts of the LCE for classical spin systems. The emphasis is on the features important for development of a $1/d$ expansion in the following sections. The notation and terminology is mostly adapted from the review by Wortis,[5] and the readers can find a more complete account of the method there. We first discuss the bare expansion, then the renormalized LCE and Φ-derivable approximations are introduced.

We consider a physical system at temperature T described by Hamiltonian $\mathcal{H}$,

$$-\beta\mathcal{H}=\frac{1}{2}\sum_{\mathbf{i},\mathbf{j}} v(\mathbf{i},\mathbf{j})\sigma(\mathbf{i})\sigma(\mathbf{j})+\sum_{\mathbf{i}} h(\mathbf{i})\sigma(\mathbf{i}) + \sum_{\alpha,\mathbf{i}} p_\alpha(\mathbf{i})x_\alpha(\mathbf{i}), \tag{1}$$

where $\beta=1/(k_BT)$, and k_B is the Boltzmann constant. Here $-\beta$ is absorbed into the local fields $h(\mathbf{i})$ and $p_\alpha(\mathbf{i})$, which couple at site $\mathbf{i}$ to the commuting local variables $\sigma(\mathbf{i})$ and $x_\alpha(\mathbf{i})$, respectively, and into the interaction parameter $v(\mathbf{i},\mathbf{j})$, which couples the variables σ on sites $\mathbf{i}$ and $\mathbf{j}$. We have restricted our treatment to models with a nonlocal interaction between one type of variable σ, but generalization to interactions between several commuting variables is straightforward.[5] The form (1) is sufficiently general for our purpose, and is more general than a conventional spin model. The variables σ and x_α are not necessarily independent and can be built up from classical spinlike variables. Including

several types of local variables allows us to consider Ising-type models with single-site anisotropy, as well as more complicated classical lattice gas models such as that described in detail in Sec. VI.

The partition function is

$$Z = \mathrm{Tr}\exp(-\beta\mathcal{H}), \tag{2}$$

which in the noninteracting case ($v=0$) reduces to

$$Z_0 = \prod_{\mathbf{i}} \mathrm{tr}\exp\left[h(\mathbf{i})\sigma(\mathbf{i}) + \sum_{\alpha} p_{\alpha}(\mathbf{i})x_{\alpha}(\mathbf{i})\right]. \tag{3}$$

Here ''Tr'' denotes the sum over all configurations of the entire system, whereas ''tr'' denotes the sum over all configurations of the single-site subsystem. The logarithm of the partition function, $\mathcal{W}=\ln Z$, can be expanded in powers of the interaction v, and the coefficients can be expressed in terms of the bare semi-invariants $M_n^0(h)$, which are given by

$$M_0^0(h) = \ln \mathrm{tr}\exp\left(h\sigma + \sum_{\alpha} p_{\alpha}x_{\alpha}\right), \quad M_n^0(h) = \frac{\partial^n M_0^0}{\partial h^n}(h). \tag{4}$$

These are purely local quantities dependent on the fields $h = h(\mathbf{i})$ and $p_{\alpha} = p_{\alpha}(\mathbf{i})$ at site $\mathbf{i}$.

The diagrammatic expansion is then given by the linked cluster theorem which states that $\mathcal{W}$ is the sum of all topologically different unrooted connected graphs. The weight of a graph is calculated by assigning to the n-valent vertex $\mathbf{i}$ factor $M_n^0(h(\mathbf{i}))$, to each bond between sites $\mathbf{i}$ and $\mathbf{j}$ factor $v(\mathbf{i},\mathbf{j})$, and summing all the dummy indices of the vertices freely over the entire lattice. Finally, one must divide by the symmetry factor of the graph. The symmetry factor is the number of distinct ways in which the graph can be made isomorphic to itself.

It is often advantageous to do some kind of resummation in order to reduce the number of contributing graphs. This is also necessary to get symmetry-broken solutions with a finite number of graphs, and we will find it also convenient when generating the 1/d expansion. For the case of rooted graphs (i.e., for expectation values of local variables or for correlation functions), the vertex renormalized expansion is well defined by absorbing all kinds of decorations to the vertices of the 1-irreducible 1-skeletons into renormalized semi-invariants. The sums of decorations are described in terms of the self-fields G_n, where n is the valence of the external vertex of the decorations. The self-field G_n is the sum of all n-valent 1-insertions. Then we can define the renormalized semi-invariants by adding all kinds of decorations to the bare semi-invariants. This is formally expressed by

$$M_n(\mathbf{i}) = \exp\left(\sum_{l=1}^{\infty} G_l(\mathbf{i})\frac{\partial^l}{\partial\tilde{h}^l}\right) M_n^0(\tilde{h})\Big|_{\tilde{h}=h(\mathbf{i})}. \tag{5}$$

The self-fields themselves can be expressed in terms of the renormalized semi-invariants, so that their diagrammatic representations consist of 1-irreducible graphs only. Hence, the problem reduces to solving (5) for the M_n's.

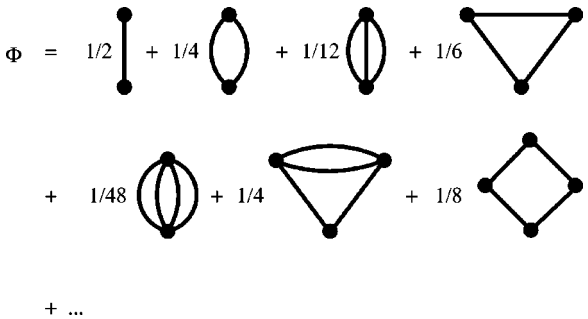

FIG. 1. First few diagrams of the Φ potential.

The logarithm of the partition function can also be expressed through a vertex renormalized expansion. It is given by

$$\mathcal{W} = \sum_{\mathbf{i}} M_0(\mathbf{i}) + \Phi - \sum_{\mathbf{i}} \sum_{n=1}^{\infty} G_n(\mathbf{i})M_n(\mathbf{i}), \tag{6}$$

where the functional Φ is the sum of all unrooted 1-irreducible graphs, as depicted in Fig. 1. The self-fields are then given by

$$G_n(\mathbf{i}) = \frac{\delta\Phi}{\delta M_n(\mathbf{i})}. \tag{7}$$

The general procedure to construct self-consistent and conserving approximations called Φ-derivable approximations is to choose a (finite or infinite) subset of graphs in the series in Fig. 1 as the approximate Φ, and use it to define the self-fields G_n by (7). These approximate G_n's are then put into (5), and the resulting nonlinear equations are solved for M_n's.

The simplest possible Φ-derivable approximation is to take only the first graph in Fig. 1. This is equivalent to the ordinary mean field theory for the classical spin systems, which becomes exact when $d\to\infty$. In the following sections we use the dimensional dependence of the graphs in the expansion for Φ to control the expansion around this limit, and to select the most important contributions to Φ. The dimensional dependence of the weight of a graph enters through the scaling of the parameters in the Hamiltonian with the dimension of the lattice, and through the free lattice sums for each vertex in the graphs. The scaling is necessary to render physical quantities (free energy per site, for instance) finite in the limit of infinite dimensions. For simple phases, the sum over lattice sites gives a multiplying factor called free multiplicity, which is simply the number of ways to embed the graph in the lattice. There are no restrictions on vertices occupying the same site.

In the following we restrict our treatment to models with nearest neighbor interaction on hypercubic lattices in d dimensions. Thus the triangular graph in Fig. 1 vanishes due to the topology of the lattice. The same applies to all other graphs containing closed loops with an odd number of nearest neighbor bonds. For the interaction between sites at $\mathbf{r}$ and $\mathbf{r}'$ we write

$$v(\mathbf{r},\mathbf{r}')=\frac{v}{2d}n(\mathbf{r}-\mathbf{r}'), \tag{8}$$

where

$$n(\mathbf{r})=\begin{cases}1 & \text{when } \mathbf{r} \text{ is a nearest neighbor distance,}\\ 0 & \text{otherwise,}\end{cases} \tag{9}$$

and $v(\mathbf{r},\mathbf{r}')\sim\mathcal{O}(1/d)$ is the necessary scaling when $d\to\infty$.[7]

III. FREE MULTIPLICITIES FOR HYPERCUBIC LATTICES

For hypercubic lattices, the free multiplicities of graphs can be expressed as polynomials in the dimension d only. The free multiplicities have previously been investigated in relation to the weak embedding lattice constants.[5,26] For simple approximations, it is also possible to calculate them by hand, or reduce the problem to simple momentum integrations, as was done in several other papers. However, to construct a $1/d$ expansion we need not only the free multiplicities of the graphs that we include in the expansion, but also estimates of those that we discard. This is necessary to make sure that no important contributions are lost. Here we analyze the graphs directly to find their dependence on the dimensionality of the hypercubic lattice. Starting from momentum integral representation we construct generating functions for the free multiplicities of large families of graphs.

Clearly, we only have to consider irreducible graphs, as the multiplicities of the reducible graphs are the products of their irreducible parts. A Cayley tree with n bonds, for example, has the free multiplicity $(2d)^n$. The 1-rooted and unrooted graphs have the same free multiplicity, because the free multiplicity of an unrooted graph is defined as the number of embeddings per lattice site. As an example, we first reconsider simple graphs: chains with fixed endpoints and rings. Then we move on to the discussion of more general topologies.

For a chain of n nearest neighbor bonds with endpoints fixed at sites $\mathbf{i}$ and $\mathbf{j}$, the number of embeddings $e_n(\mathbf{i}-\mathbf{j})$ is given by

$$e_n(\mathbf{i}-\mathbf{j})=\sum_{\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{n-1}} n(\mathbf{i}-\mathbf{r}_1)n(\mathbf{r}_1-\mathbf{r}_2)\cdots n(\mathbf{r}_{n-2}-\mathbf{r}_{n-1}) \times n(\mathbf{r}_{n-1}-\mathbf{j}), \tag{10}$$

where $n(\mathbf{r})$ is defined in (9). Let the site vectors have integer components (we set the lattice constant to unity). Then we have

$$e_n(\mathbf{r})=\frac{1}{(2\pi)^d}\int d^dk\,(n_{\mathbf{k}})^n\exp(i\mathbf{k}\cdot\mathbf{r})=\left.\frac{\partial^n}{\partial x^n}g_{\mathbf{r}}(x)\right|_{x=0}, \tag{11}$$

$$n_{\mathbf{k}}=\sum_{\mathbf{r}} n(\mathbf{r})\exp(-i\mathbf{k}\cdot\mathbf{r})=2\sum_{i=1}^{d}\cos(k_i), \tag{12}$$

$$g_{\mathbf{r}}(x)=\frac{1}{(2\pi)^d}\int d^dk\exp(xn_{\mathbf{k}}+i\mathbf{k}\cdot\mathbf{r})=\prod_{i=1}^{d} I_{|r_i|}(2x). \tag{13}$$

The ith component of $\mathbf{r}$ is r_i, and $I_\nu(x)$ is the modified Bessel function of the first kind and order ν (see Ref. 27). The integrals are over the first Brillouin zone. The generating function $g_{\mathbf{r}}(x)$ can be rewritten as

$$g_{\mathbf{r}}(x)=I_0(2x)^dD_{\mathbf{r}}(x),\quad D_{\mathbf{r}}(x)=\prod_{i=1}^{\infty}\frac{I_{|r_i|}(2x)}{I_0(2x)}. \tag{14}$$

The function $D_{\mathbf{r}}(x)$ does not depend on d for fixed $\mathbf{r}$ (by ''fixed'' we mean that the number of nonzero components and their values are fixed as d, and hence the total number of the components, is allowed to grow). In terms of $D_{\mathbf{r}}$, the final result for the multiplicity of the chain is

$$e_n(\mathbf{r})=\sum_{m=0}^{n}\binom{n}{m}\left(\frac{d^m}{dx^m}I_0(2x)^d\right)\frac{d^{n-m}}{dx^{n-m}}D_{\mathbf{r}}(x)\Bigg|_{x=0}. \tag{15}$$

From this general expression we can extract, for example, the leading contribution in d. It is given by the term with the largest possible m. We have

$$D_{\mathbf{r}}(x)=\frac{x^{\|\mathbf{r}\|}}{\prod_i |r_i|!}(1+\mathcal{O}(x^2)), \tag{16}$$

where $\|\mathbf{r}\|=\Sigma|r_i|$, so we must choose $m=n-\|\mathbf{r}\|$. The result is

$$e_n(\mathbf{r})=\frac{n!}{\left(\frac{n-\|\mathbf{r}\|}{2}\right)!\prod_i |r_i|!}d^{\frac{n-\|\mathbf{r}\|}{2}}(1+\mathcal{O}(d^{-1})) \tag{17}$$

when $n-\|\mathbf{r}\|$ is even and non-negative, and $e_n(\mathbf{r})=0$ otherwise.

To obtain the free multiplicity $r_0(2k)$ of a ring graph with $2k$ bonds, we just have to close the chain, i.e., we have to set $\mathbf{r}=0$ in Eq. (11):

$$r_0(2k)=e_{2k}(0)=\frac{(2k)!}{k!}\sum_{m=0}^{k}\frac{d!}{(d-m)!}\sum_{\prod_{i=1}^{k} b_i!(i!)^{2b_i}}\frac{k!}{}, \tag{18}$$

where the rightmost sum is over all non-negative integers b_i $(i=1,\ldots,k)$, such that

$$b_1+b_2+\cdots+b_k=m,\quad b_1+2b_2+\cdots+kb_k=k. \tag{19}$$

From (18), we find that the leading terms in d for the ring are

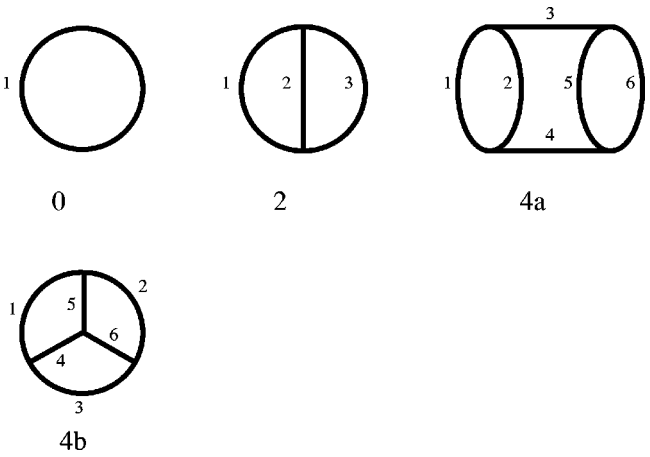

FIG. 2. Examples of generic graphs. The lines denote chains and their numbering corresponds to the variables in the generating function.

$$r_0(2k)=\frac{(2k)!}{k!}d^k\left[1-\frac{1}{4}k(k-1)d^{-1}+\frac{1}{288}k(k-1)(k-2)(9k+5)d^{-2}+\mathcal{O}(d^{-3})\right]. \tag{20}$$

The two simple examples above show that chains of various lengths are conveniently described as a whole by their generating functions. Moreover, graphs that differ only by the length of their chains are described by the same generating function and form a family. Therefore, we need to consider only the number of n-valent vertices ($n>2$) and the way in which they are connected. A family of graphs described by the same generating function can then be represented by a generic graph, such as the examples in Fig. 2. There, a line correspond to the generating function of a chain and all vertices except one should be summed freely over. These graphs correspond to the homeomorphically irreducible stars used in classification of graphs,[28] but we do not make any use of this fact, since we must allow for zero-length chains. Consequently, the scheme is also not a disjoint partition of 1-irreducible graphs. Each family generally includes reducible graphs, and may also include graphs of another family. However, the approach reduces the work considerably.

We denote the generating function for the free multiplicities of graphs in the family Γ in d dimensions by $g_\Gamma(d;\overline{x})$ where $\overline{x}=(x_1,x_2,\ldots,x_k)$ is a k-tuple corresponding to the variables for each of the k chains. The corresponding free multiplicity for a graph within this family is denoted by $r_\Gamma(\overline{n})$, where $\overline{n}=(n_1,n_2,\ldots,n_k)$ is the number of bonds in each chain.

If we consider any particular family Γ, we can immediately write down the generating function for the free multiplicities by using the integral representation in Eq. (13) for each of the chains. Summing over the site vectors for either of the vertices simply results in a ''momentum conservation'' at the vertices. Due to the special form of $n_{\mathbf{k}}$ for hypercubic lattices, the momentum integrals factor into products of multiple integrals. As a result, the generating function can be written as a power d of the one-dimensional generating function:

$$g_\Gamma(d;\overline{x})=g_\Gamma(1;\overline{x})^d. \tag{21}$$

For example, if we consider family 2 in Fig. 2, we get

$$r_2(\overline{n})=\left.\frac{\partial^{n_1+n_2+n_3}}{\partial x_1^{n_1}\,\partial x_2^{n_2}\,\partial x_3^{n_3}}g_2(1;\overline{x})^d\right|_{\overline{x}=\overline{0}}, \tag{22}$$

where

$$g_2(1;\overline{x})=\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}dk\int_{-\pi}^{\pi}dq\,\exp[2x_1\cos(k)+2x_2\cos(k+q)+2x_3\cos(q)] \tag{23}$$

and the leading d behavior (for $\delta=0,1$) is

$$r_2(2k_1+\delta,2k_2+\delta,2k_3+\delta)=2^\delta\frac{(2k_1+\delta)!}{k_1!}\frac{(2k_2+\delta)!}{k_2!}\frac{(2k_3+\delta)!}{k_3!}\times d^{k_1+k_2+k_3+\delta}(1+\mathcal{O}(d^{-1})). \tag{24}$$

The one-dimensional generating function can always be expressed as a multiple momentum integral, as in the above example. The integrand can be expanded to sufficiently high order in $x_1,x_2,\ldots,x_k$ and integrated term by term. This approach is quite feasible for simple graph families, using modern computer algebra packages. Alternatively, one can simply count the number of embeddings in the linear chain, which is a problem easy to code in most computer languages.

In the general case, we proceed by writing (21) as

$$g_\Gamma(d;\overline{x})=\sum_{p=0}^{\infty}\binom{d}{p}c_\Gamma(\overline{x})^p,\quad c_\Gamma(\overline{x})=g_\Gamma(1;\overline{x})-1, \tag{25}$$

then differentiating, and setting $\overline{x}=0$. Since there is always more than one path connecting any pair of vertices in the generic graph, each factor c_Γ must be differentiated at least twice to yield a nonzero contribution. Thus, we get nonzero contributions to the sum only for $p\leqslant[n/2]$, where $n=n_1+n_2+\cdots+n_k$ and $[\cdots]$ means integer part. Taking this into account, and writing out the binomial coefficient as a polynomial in d, we find that

$$r_\Gamma(\overline{n})=\sum_{m=0}^{[n/2]}d^m\sum_{p=m}^{[n/2]}\frac{S_p^{(m)}}{p!}\left.\frac{\partial^{n_1+n_2+\ldots+n_k}}{\partial x_1^{n_1}\,\partial x_2^{n_2}\cdots\partial x_k^{n_k}}c_\Gamma(\overline{x})^p\right|_{\overline{x}=0}, \tag{26}$$

where $S_p^{(m)}$ is the Stirling number of the first kind (see Ref. 27). This expression gives the free multiplicity directly as a polynomial in d. The coefficients are completely specified by the free multiplicities of the graphs within the same family in one dimension and with fewer or equal number of edges in

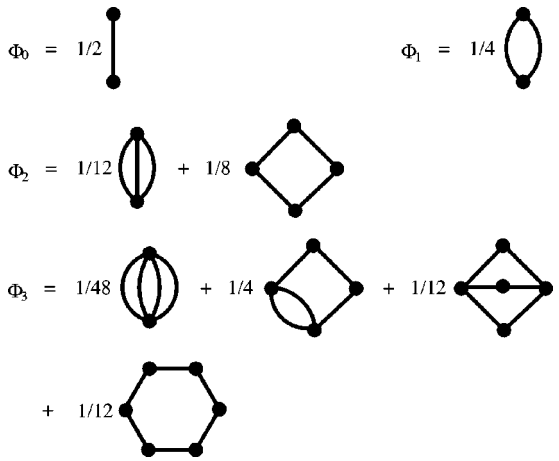

FIG. 3. The nth order in $1/d$ contributions Φ_n to Φ.

each chain. In practical calculations, the derivatives of c_Γ are found by expanding c_Γ and using polynomial algebra or, equivalently, direct convolution of the coefficients in the expansion. From this explicit calculation, it follows immediately that the free multiplicity of an arbitrary 1-irreducible graph with n nearest-neighbor bonds (except for $n=1$) is $\mathcal{O}(d^{[n/2]})$ or higher in $1/d$, in agreement with the results of previous works.[7,20]

IV. 1/*d* EXPANSION OF Φ

From the preceding section, we know how to calculate the free multiplicity of various irreducible graphs contributing to Φ. They are all in the form of polynomials in d. Furthermore, due to the scaling of the interaction, each bond carries a factor $\sim d^{-1}$. We can therefore easily find the d-dependence of the graphs in Fig. 1 (assuming a simple symmetry breaking, if any). The first graph has free multiplicity $2d$ and one interaction line, so it is $\mathcal{O}((1/d)^0)$. Likewise, the second, the third, and the fifth graphs are of order one, two, and three in $1/d$, respectively. The fourth and the sixth graphs, of course, vanish on the hypercubic lattice, whereas the seventh graph is $\mathcal{O}(1/d^2)$.

The 1-irreducible graphs with n bonds (except, again, $n=1$) are $\mathcal{O}(d^{[n/2]-n})$ or higher order in $1/d$. Therefore, one need only check graphs with up to, and including, $2m$ bonds in order to find all terms of order m or lower in $1/d$. In a vertex renormalized expansion we need then only consider a finite number of 1-irreducible graphs to be sure that all contributions to a given finite order in $1/d$ are included. We can therefore write the Φ potential as the sum

$$\Phi=\sum_{n=0}^{\infty}\Phi_n, \tag{27}$$

where

$$\Phi_n=\mathcal{O}(d^{-n}), \quad \text{when } d\to\infty. \tag{28}$$

Φ_n is the sum of a finite subset of 1-irreducible graphs from the expansion of Φ. The exact diagrammatic expressions for Φ_n for $n=0,\ldots,3$ are shown in Fig. 3. Note that these

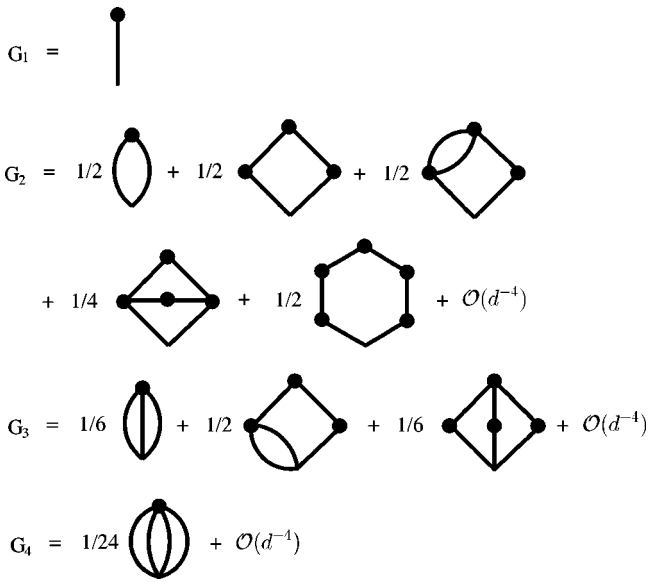

FIG. 4. Leading order in $1/d$ terms for the self-fields.

graphs are almost the same as the ''shorthand graphs'' of Ref. 22 for the free energy. The exceptions are the third graph from the left for Φ_3, which is absent in their expansion, and the single vertex which does not enter the expansion for Φ.

Using Eq. (7), we can also conveniently calculate the self-fields in a controlled way. The results are shown in Fig. 4. The leading contribution to G_n in high dimensions is from the graph with n bonds and two n-valent vertices (the clipped away vertex including), and its weight is $\sim d^{-(n-1)}$. To prove that all other terms are of higher order, we consider an arbitrary 1-irreducible graph D with at least one n-valent vertex V, total number of edges $m+n$, and weight W_D. Let $m>0$. If there are any multiple edges joining V and any other vertex in the remainder of the graph, these can be reduced to one edge without altering the free multiplicity of the graph. If there are in total $q\leqslant n-2$ such edges that are removed to obtain a graph D' with weight $W_{D'}$ and total number of edges $m+n'$ (where $n'=n-q$), then we have $W_D\sim d^{-q}W_{D'}$. Let V' be the vertex in D' corresponding to V in D. Any vertex connected to V' by a single edge must be joined to any other such vertex by a path composed of at least two edges and not visiting V' for the graph to be 1-irreducible and embeddable in a hypercubic lattice. Therefore, $m\geqslant n'$ and $W_{D'}$ is $\mathcal{O}(d^{-n'})$ or higher. Thus, we have that W_D is $\mathcal{O}(d^{-n})$ or higher, which is smaller by at least one order than the graph with n bonds and two n-valent vertices. In conclusion, we have

$$G_n=\frac{v^n}{n!}\left(\frac{1}{2d}\right)^{n-1}M_n+\mathcal{O}(d^{-n}). \tag{29}$$

V. THE ISING MODEL

In this section we construct $1/d$ expansion for the equation of states of the Ising model, using the approach described above. For the spin-s Ising model, the parameters in

TABLE I. Critical temperatures normalized by the $d=\infty$ (MFA) value.

d	s	Order of 1/d approximation			Best estimate (Refs. 28 and 29)
		1	2	3	
2	$\frac{1}{2}$	0.7500	0.6667	0.5990	0.5673
	1	0.8125	0.7363	0.6748	
	$\frac{3}{2}$	0.8300	0.7579	0.6991	
	∞	0.8500	0.7836	0.7289	
3	$\frac{1}{2}$	0.8333	0.7963	0.7762	0.7518
	1	0.8750	0.8411	0.8229	0.7989
	$\frac{3}{2}$	0.8867	0.8546	0.8372	0.8138
	∞	0.9000	0.8705	0.8543	0.8320

Eq. (1) are: $v(\mathbf{i},\mathbf{j})=\pm\beta Jn(\mathbf{i}-\mathbf{j})/2d$ for the ferromagnetic $(+)$ or antiferromagnetic $(-)$ model, and $h(\mathbf{i})=-\beta H(\mathbf{i})$, where $H(\mathbf{i})$ is the external magnetic field. The variables $\sigma(\mathbf{i})=S_z(\mathbf{i})/s$ are normalized spin operators. The above scaling of the parameters with s and d ensures well defined limits when either of the parameters tends to infinity. The zero-order bare semi-invariant for the model is

$$M_0^0(h)=\ln\frac{\sinh(h(2s+1)/(2s))}{\sinh(h/(2s))}. \tag{30}$$

We find the 1/d expansion for the renormalized semi-invariants of the ferromagnetic Ising model by solving Eq. (5) iteratively, using the self-fields in Fig. 4, and always truncating to the third order at each step of the iteration. Such an approach has also been used to generate high temperature series expansions.[5] The iteration is stopped when all semi-invariants in the expression for the full first semi-invariant M_1 are reduced to the mean-field semi-invariants, with the mean-field given by M_1 itself. M_1 is the magnetization, and the zero-field susceptibility χ for the paramagnetic phase is found by differentiating with respect to h, and setting h and M_1 to zero.

The critical temperature for the spin-s Ising model is a function of the spin and the lattice dimensionality, $T_c=T_c(d,s)$. Its 1/d expansion is easily found from the 1/d expansion of the zero-field susceptibility by inserting the ansatz

$$T_c(d,s)=T_c(\infty,s)\left(1+\frac{\tau_1(s)}{d}+\frac{\tau_2(s)}{d^2}+\frac{\tau_3(s)}{d^3}+\mathcal{O}(d^{-4})\right), \tag{31}$$

which gives

$$T_c(\infty,s)=\frac{J(s+1)}{3k_Bs}, \tag{32}$$

$$\tau_1(s)=-\frac{3}{10}\frac{2s^2+2s+1}{2s(s+1)}, \tag{33}$$

$$\tau_2(s)=-\frac{3}{1400}\frac{496s^4+992s^3+672s^2+176s-61}{2^2s^2(s+1)^2}, \tag{34}$$

$$\tau_3(s)=-\frac{3}{3500}\frac{4084s^6+12252s^5+13518s^4+6616s^3+719s^2-547s+108}{2^3s^3(s+1)^3}. \tag{35}$$

The leading term $T_c(\infty,s)$ is the well known MFA result, and it is not very sensitive to s. Also the coefficients $\tau_i(s)$ have a rather weak dependence on $s\in[\frac{1}{2},\infty]$. The limiting cases are

$$\tau_1(1/2)=-\tfrac{1}{2},\quad \tau_2(1/2)=-\tfrac{1}{3},\quad \tau_3(1/2)=-\tfrac{13}{24}, \tag{36}$$

and

$$\tau_1(\infty)=-\tfrac{3}{10},\quad \tau_2(\infty)=-\tfrac{93}{350},\quad \tau_3(\infty)=-\tfrac{3063}{7000}. \tag{37}$$

Of course, wherever applicable, the above results agree with those of previous works mentioned in the Introduction.

In order to illustrate the above results, in Table I, we

present explicit T_c values for $d=2$ and $d=3$ obtained in the first three orders in $1/d$, together with the exact result for $d=2$ and the best numerical estimates for $d=3$ coming from high-order high-temperature series expansion (HTSE).[28,29] It is seen that the subsequent corrections in $1/d$ expansion decrease rapidly and that the third-order results come very close to the T_c values obtained from the exact solution and from the HTSE.

VI. A TWO-COMPONENT LATTICE GAS

Exactly the same approach as above is applicable to the Hamiltonian

$$\mathcal{H}=\frac{W}{4d}\sum_{\langle \mathbf{ij}\rangle}(n_{\mathbf{i}\uparrow}+n_{\mathbf{i}\downarrow})(n_{\mathbf{j}\uparrow}+n_{\mathbf{j}\downarrow})+U\sum_{\mathbf{i}}n_{\mathbf{i}\uparrow}n_{\mathbf{i}\downarrow}-\mu\sum_{\mathbf{i}}(n_{\mathbf{i}\uparrow}+n_{\mathbf{i}\downarrow})-\sum_{\mathbf{i}}H_{\mathbf{i}}(n_{\mathbf{i}\uparrow}+n_{\mathbf{i}\downarrow})-\frac{1}{2}\sum_{\mathbf{i}}H^s_{\mathbf{i}}(n_{\mathbf{i}\uparrow}-n_{\mathbf{i}\downarrow}). \tag{38}$$

It describes a two-component classical lattice gas of, say, spin-up and spin-down electrons with the occupation operators $n_{\mathbf{i}\uparrow}$ and $n_{\mathbf{i}\downarrow}$, respectively, with the on-site interaction U, the nearest-neighbor interaction $W/2d$, the chemical potential μ, and site dependent fields $H_{\mathbf{i}}$ and $H^s_{\mathbf{i}}$. The fields are included here mainly for technical reasons. The model corresponds to an extended Hubbard model with zero electron hopping between sites. Here we limit our considerations to the half-filled lattice, i.e., with one particle per site, on average. In this case, due to the electron-hole symmetry of the system, $\mu=W+U/2$, and the extended Hubbard model (38) can be mapped to the Blume–Capel model with anisotropy constant $D=U/2+\ln(2)/\beta$ (Ref. 24).

The form (1) is obtained by defining the interacting variables $\sigma(\mathbf{i})=n_{\mathbf{i}\uparrow}+n_{\mathbf{i}\downarrow}-1$, which are coupled to the external field $h_{\mathbf{i}}=\beta H_{\mathbf{i}}$ and mutually by (8) with $v=\beta W$, and the additional local variables: $x_1(\mathbf{i})=\sigma(\mathbf{i})^2$, $x_2(\mathbf{i})=\frac{1}{2}(n_{\mathbf{i}\uparrow}-n_{\mathbf{i}\downarrow})$, $x_3(\mathbf{i})=x_2(\mathbf{i})^2$, and $x_4(\mathbf{i})=1$, which couple to the fields: $p_1(\mathbf{i})=-\beta U/4$, $p_2(\mathbf{i})=\beta H^s_{\mathbf{i}}$, $p_3(\mathbf{i})=\beta U$, and $p_4(\mathbf{i})=\beta(H_{\mathbf{i}}+\mu-W/2-U/4)$, respectively. We do not need the field coupling to the spin degrees of freedom here, so we set $p_2=0$ for the sake of simplicity.

The first order bare semi-invariant is then given by

$$M^0_1(h)=\frac{\sinh(h)}{\lambda+\cosh(h)},\quad \lambda=e^{\beta U/2}. \tag{39}$$

The system may order into a charge density wave with a simple A–B sublattice ordering on hypercubic lattices in high dimensions. We will therefore let the field $h(\mathbf{i})$ be a staggered field with value h on sublattice A, and $-h$ on sublattice B. The renormalized semi-invariants will then have spatial dependence only according to the sublattice, and we need not distinguish between sites on the same sublattice. We will therefore denote the renormalized semi-invariant $M_n(\mathbf{i})=M^s_n$ where $s=A$ or $s=B$, depending on whether $\mathbf{i}$ is in the A or B sublattice. The order parameter q is taken to be half the difference between the site occupation numbers on the two sublattices,

$$q=\tfrac{1}{2}(M^A_1-M^B_1). \tag{40}$$

In $d=\infty$ the charge-order equation of state can be written as

$$h=-vq+\frac{1}{2}\ln\left(\frac{1+q}{1-q}\,\frac{\sqrt{1+(\lambda^2-1)q^2}+\lambda q}{\sqrt{1+(\lambda^2-1)q^2}-\lambda q}\right), \tag{41}$$

which is valid for large enough temperatures and can be converted into a physical equation of state at all temperatures by a Maxwell construction. The above expression is analytic for small q and can be expanded as

$$h=(\lambda+1-v)q-\tfrac{1}{6}(\lambda+1)^2(\lambda-2)q^3+\tfrac{1}{40}(\lambda+1)^3(3\lambda^2-7\lambda+8)q^5. \tag{42}$$

From this, we can read off directly that there is a continuous zero-field phase transition at $v=1+\lambda$ when $\lambda<2$, and a first order zero-field transition for $\lambda>2$. This well known way of analyzing a continuous or weakly first order transition is also easily applicable to the $1/d$ expansion, which gives us an equation for M^s_1, and thus q, to a given order in $1/d$. This equation can then easily be solved for h as a power expansion in q and $1/d$. The linear in q term of the equation of state for large d reads

$$\begin{aligned}\chi^{-1}=&\frac{1}{r}-v+\frac{1}{2}\left(-\frac{1}{2}v^2+\frac{3}{2}rv^2\right)d^{-1}+\frac{1}{4}\left(-\frac{1}{6}v^3+rv^3-\frac{1}{8}rv^4-\frac{3}{2}r^2v^3+\frac{3}{8}r^2v^4+\frac{3}{4}r^3v^4\right)d^{-2}\\&+\frac{1}{8}\left(-\frac{1}{24}v^4+\frac{3}{4}rv^4-\frac{13}{8}r^2v^4-\frac{3}{4}r^3v^4-\frac{1}{12}r^2v^6+r^3v^5+\frac{1}{48}r^3v^6-3r^4v^5+\frac{5}{16}r^4v^6+\frac{15}{4}r^5v^6\right)d^{-3}+\mathcal{O}(d^{-4}),\end{aligned} \tag{43}$$

where

$$r=\frac{1}{\lambda+1}. \tag{44}$$

The higher-order in q terms are too long to be presented here. The tricritical point is given by the common zero of the first and the third order in q terms of the equation of state. The result is

$$U_{\rm tri}/W=K_\infty+\frac{1}{2}(1-K_\infty)d^{-1}+\frac{1}{2}(1-K_\infty)d^{-2}+\frac{11}{16}(1-K_\infty)d^{-3}+\mathcal{O}(d^{-4}), \tag{45}$$

$$k_B T_{\rm tri}/W = \frac{1}{3} - \frac{1}{6} d^{-1} - \frac{1}{6} d^{-2} - \frac{11}{48} d^{-3} + \mathcal{O}(d^{-4}), \quad (46)$$

where $K_\infty = 2\ln(2)/3$. The critical line $T_c = T_c(d,K)$ vs $K = U/W$ in the $T-U$ plane at zero staggered field in infinite dimensions is given by

$$k_B T_c(\infty,K)/W = r_0(K) = \frac{1}{\exp\left(\frac{K}{2r_0(K)}\right)+1}. \quad (47)$$

For general high dimensions, and $U < U_{\rm tri}$, we write

$$T_c(d,K) = T_c(\infty,K)\left(1 + \frac{\tau_1(K)}{d} + \frac{\tau_2(K)}{d^2} + \frac{\tau_3(K)}{d^3} + \mathcal{O}(d^{-4})\right), \quad (48)$$

where the coefficients are

$$\tau_1 = \frac{3r_0 - 1}{2(K - 2r_0 - Kr_0)}, \quad (49)$$

$$\tau_2 = (4Kr_0 - K^2 - r_0^2 - 3r_0^3 + 36r_0^4 - 10Kr_0^2 + 2K^2 r_0 - 30Kr_0^3 + 36Kr_0^4 + 11K^2 r_0^2 - 21K^2 r_0^3 + 9K^2 r_0^4) \times \frac{1}{12r_0(K - 2r_0 - Kr_0)^3}, \quad (50)$$

$$\tau_3 = (K^4 + 48r_0^4 - 280r_0^5 + 168r_0^6 + 1728r_0^7 - 108Kr_0^3 - 12K^3 r_0 + 812Kr_0^4 - 20K^4 r_0 - 1436Kr_0^5 - 2724Kr_0^6 + 3456Kr_0^7 + 56K^2 r_0^2 - 560K^2 r_0^3 + 172K^3 r_0^2 + 1464K^2 r_0^4 - 596K^3 r_0^3 + 81K^4 r_0^2 + 1272K^2 r_0^5 - 156K^3 r_0^4 + 4K^4 r_0^3 - 4824K^2 r_0^6 + 2344K^3 r_0^5 - 413K^4 r_0^4 + 2592K^2 r_0^7 - 2616K^3 r_0^6 + 692K^4 r_0^5 + 864K^3 r_0^7 - 453K^4 r_0^6 + 108K^4 r_0^7) \times \frac{1}{96r_0^2(K - 2r_0 - Kr_0)^5}. \quad (51)$$

This expansion is of little use near the tricritical point, since its location depends on the dimension of the lattice, but it is useful elsewhere. The critical line near the tricritical point can be found by using $U_{\rm tri} - U$ as a free parameter instead of U.

In order to illustrate the above results and compare them with those of the HTSE, in Fig. 5, we plot the critical lines and the tricritical points obtained from Eqs. (45)–(51) for the fixed finite value of $d=3$, i.e., for the case of the simple cubic lattice. It is seen that the subsequent corrections decrease rapidly up to the number of terms considered here. Moreover, the third order in 1/d result for the critical temperature T_c is in very good agreement with that from the sixth order of the HTSE.[30]

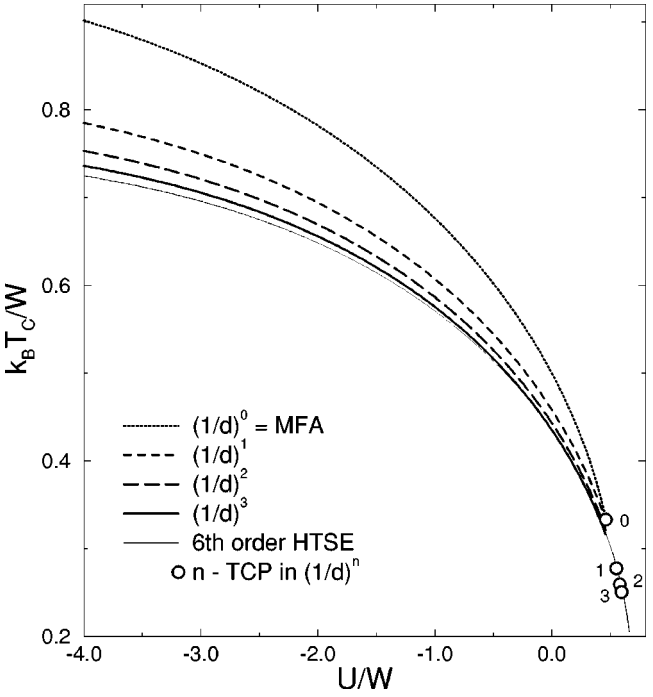

FIG. 5. Critical line and tricricritcal point (TCP) for the simple cubic lattice ($d=3$) up to $(1/d)^3$. The sixth-order HTSE result for T_c (Ref. 30) is shown for comparison.

VII. SELF-CONSISTENT 1/d EXPANSIONS

The possibility of performing self-consistent 1/d approximations, which then necessarily include infinite-order terms, deserves some comments. We will consider the ferromagnetic spin-1/2 Ising model as an example in the remainder of this section. The idea is to construct Φ-derivable approximations, choosing the diagrams for the approximate Φ according to the 1/d criterion. A crucial step in using this approach is to resum Eq. (5) to all orders in the nonvanishing self-fields. With Φ taken to be Φ_0 in Fig. 3, only G_1 is nonzero, and the series (5) is simply a Taylor series, which is trivial to resum. The result is the MFA. In this case, the resummation can even be avoided by expanding in the fluctuations around the mean field, such that all graphs with Cayley tree insertions vanish in all orders of the expansion.

Including the diagram Φ_1 in Fig. 3, i.e., taking the approximate Φ to be of the first order in 1/d, makes also G_2 nonvanishing. Actually, this self-consistent 1/d correction was considered in Ref. 31, although the author apparently was not aware of this way of looking at the approximation. The results are quite beautiful and reasonable for all values of the Hamiltonian parameters and in the whole range of the temperature, and give considerably better estimation for the critical temperature than the MFA. However, one can easily convince oneself that the series (5) is not convergent for arbitrary nonzero value of G_2. This is particularly clear from the resulting integral formulas for the renormalized semi-invariants,[4,5,31,32] which are manifestly nonanalytic functions of G_2 at $G_2=0$. The integral equation is however well defined for any $G_2 \geqslant 0$, which is the physically relevant region.

Following Ref. 5 the renormalized semi-invariants for the translationally invariant case can be written as

$$M_n(h) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \exp\left(ikh + \sum_{l=1}^{\infty} (ik)^l G_l \right) \hat{M}_n^0(k), \quad (52)$$

$$\hat{M}_n^0(k) = \int_{-\infty}^{\infty} dh\, M_n^0(h) e^{-ikh}. \quad (53)$$

The Fourier transforms of the bare semi-invariants for $n > 1$ are well defined, but the cases $n=0$ and $n=1$ must be treated with care to make mathematical sense. For the first-order bare semi-invariant, for example, we have

$$\hat{M}_1^0(k) = \mathrm{Pv} \frac{-i\pi}{\sinh(\pi k/2)}, \quad (54)$$

where Pv denotes the principal value, i.e., it must be interpreted in the sense of a distribution.

Bloch and Langer[4] have specially constructed an artificial model in which semi-invariants of order higher than a given order vanish, and consequently, there is only a finite number of nonvanishing self-fields. They have shown that in this case the form of the Dyson equation (5) implies a restricted domain of validity of the renormalized expansion in terms of the values of the renormalized semi-invariants. In our case, there are an infinite number of nonzero semi-invariants, but a finite number of nonzero self-fields that contribute in Eq. (52). We find that in some regions of the ordered phase, the values of higher-order renormalized semi-invariants become such that the integral in (52) is ill defined.

To see this, we first consider the highest nonvanishing self-field to be of even order $2n$. The integral in (52) will converge when $(-1)^n G_{2n} < 0$, but not for $(-1)^n G_{2n} > 0$. If $n=1$, as for the self-consistent $1/d$ approximation to the linear order, this problem does not arise, but if we consider higher-order self-consistent approximations, it might. An estimate, valid in high dimensions, can be given for the third-order in $1/d$ self-consistent approximation, for which the self-field graphs are shown in Fig. 4. In this case, $n=2$ and $G_4 = v^4 d^{-3} M_4/192$ is proportional to M_4. It is sufficient to consider the bare semi-invariant,

$$M_4^0 = -2(1-(M_1^0)^2)(1-3(M_1^0)^2), \quad (55)$$

and we see that M_4^0 becomes positive when the magnetization M_1^0 goes above $1/\sqrt{3}$. The same happens with the semi-invariant M_4 (and consequently, also G_4) renormalized by Cayley trees, because it is equal to the unrenormalized one with the argument shifted by the mean field. We have verified numerically that this is also the case for M_4 self-consistently renormalized within the third-order self-consistent $1/d$ approximation, as well as within a self-consistent approximation including all 1-irreducible graphs up to fourth order in v, inclusive in finite dimensions. The problem appears when the temperature is low enough or, equivalently, when the magnetization is large enough, just as one would expect from the above considerations. Thus, the appealing scheme of a self-consistent $1/d$ expansion actually breaks down at low temperature when carried beyond the first few orders. Even if one could analytically continue Eq. (52) to arbitrary values of G_4, one would still not avoid an unphysical singularity when M_4 crosses zero. The leading-order term of G_{2n} in high dimensions is proportional to, and depends only on M_{2n} [Eq. (29)], so that sign changes in the ordered phase occur also for self-fields of higher orders. The problems are therefore not specific to the order considered above as an example. If the highest nonvanishing self-field is of odd order, the integrand is controlled by the term arising from the self-field of one order lower.

Any additional correction to the highest nonvanishing self-field will be smaller than the leading term by at least a factor $1/d$, and, by considering sufficiently high dimensions, can be made small enough *not* to cure the problem. Therefore, if Eq. (52) is a correct resummation of the generally divergent series (5), the only possibility is to include all higher order self-fields in an approximate way. Since our goal was to make a self-consistent approximation that is correct to a given order in $1/d$, and the only reason for including self-fields of higher order is to regularize the integral (52) for all parameter values, it appears natural to use the leading order in $1/d$ for each of the remaining self-fields as a starting point. It remains to be seen if this is workable.

The breakdown of the renormalized expansion can also take place within other approximation schemes involving a finite number of self-field graphs when the dimensionality of the lattice is sufficiently high, because the self-fields may be dominated by the terms considered here.

It is quite plausible that this problem may arise also for other models, whenever the LCE using the atomic limit as the unperturbed Hamiltonian is applied. In particular, diagrammatic expansions for some quantum spin models or models of correlated fermions, in which the atomic states are used as the basis states (i.e., using the Hubbard operator formalism), have the graphical and algebraic structures of the classical spin systems considered here, and will therefore be subject to the same problems of higher-order renormalizations, at least in some limiting cases. Because the breakdown of the renormalized expansion is associated with the particular form of the Dyson equation, no conclusion can be drawn from this finding for perturbation expansions of correlated fermion models with the band part as the unperturbed Hamiltonian.

VIII. SUMMARY AND CONCLUSIONS

Within the framework of the LCE for classical spin systems with nearest neighbor interaction, we have considered power series expansions in $1/d$, as well as self-consistent $1/d$ expansions. Generating functions turned out to be particularly useful for analyzing the free multiplicities of the graphs for hypercubic lattices in arbitrary dimension d. They are uniquely given by the free multiplicities or generating functions for $d=1$, which can be relatively easily calculated. For the simple examples considered in this paper, the method is probably an overkill, but it is quite general, and its application is not limited to $1/d$ expansions for classical spin systems considered here.

We have presented a systematic classification of

1-irreducible graphs that contribute to the Φ potential for classical spin systems with respect to powers of $1/d$, showing explicitly the series up to $\mathcal{O}(d^{-3})$. These results have been applied to obtain the expansions in $1/d$ for the critical temperature of the spin-s Ising model, and a two-component lattice gas corresponding to the zero-bandwidth extended Hubbard model at half-filling. For the latter, we have also calculated the $1/d$ expansion for the tricritical point. To the best of our knowledge, these are new results, except for the zero-order (MFA) results, and the spin-1/2 Ising limits. The general expressions have been applied to the finite dimension $d=3$, i.e., for the simple cubic lattice. The results for T_c of the two-component lattice gas have been compared with those of the sixth-order high-temperature series expansion, showing an excellent agreement. The corrections to the critical temperatures of the two models considered here are in both cases negative, so it is clear that the inclusion of spatial correlations through $1/d$ corrections lower the critical temperature, as expected. The tricritical point of the two-component lattice gas tends towards lower temperature and stronger on-site repulsion, as the dimension is lowered. Since there are quantum models that have the classical systems considered here as limiting cases, the presented results should serve as a useful reference.

We have discussed the possibility of constructing self-consistent $1/d$ approximations within the renormalized LCE for classical spin systems, using spin-1/2 Ising model as an example. Except for the first few lowest orders, this approach was found to break down at low temperatures. The same applies to a self-consistent approximation including all 1-irreducible graphs up to fourth order in the interaction. The conclusion is that a truncation with a finite number of self-fields is insufficient, so that one must also include all higher order self-fields in some approximate way.

ACKNOWLEDGMENTS

E.H. wishes to thank Professor Jan Myrheim for helpful discussions. M.B. would like to thank Professor G. D. Mahan for his useful remarks and support. Research support is acknowledged from the University of Tennessee, from U.S. Department of Energy under Contract No. DE-AC05-00OR22725 with the Oak Ridge National Laboratory, managed by UT-Battelle, LLC, and from K.B.N. Poland, Project No. 2 P03B 037 17.

[1] R. Brout, Phys. Rev. **118**, 1009 (1960); **122**, 469 (1961).
[2] G. Horwitz and H. B. Callen, Phys. Rev. **124**, 1757 (1961).
[3] F. Englert, Phys. Rev. **129**, 567 (1963).
[4] C. Bloch and J. S. Langer, J. Math. Phys. **6**, 554 (1965).
[5] M. Wortis, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and S. Green (Academic, New York, 1974), Vol. 3.
[6] G. Baym, Phys. Rev. **127**, 1391 (1962).
[7] M. E. Fisher and D. S. Gaunt, Phys. Rev. **133**, A224 (1964).
[8] P. R. Gerber and M. E. Fisher, Phys. Rev. B **10**, 4697 (1974).
[9] R. S. Fishman and G. Vignale, Phys. Rev. B **44**, 658 (1991).
[10] R. Abe, Prog. Theor. Phys. **47**, 62 (1972).
[11] T. Pruschke, M. Jarrell, and J. K. Freericks, Adv. Phys. **44**, 187 (1995); A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
[12] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).
[13] E. Müller-Hartmann, Z. Phys. B: Condens. Matter **74**, 507 (1989).
[14] P. G. J. van Dongen, Phys. Rev. Lett. **67**, 757 (1992); H. Schweitzer and G. Czycholl, Solid State Commun. **74**, 735 (1990); Z. Phys. B: Condens. Matter **83**, 93 (1991).
[15] P. G. J. van Dongen, F. Gebhard, and D. Vollhardt, Z. Phys. B: Condens. Matter **76**, 199 (1989); F. Gebhard, Phys. Rev. B **41**, 9452 (1990).
[16] R. Vlaming and D. Vollhardt, Phys. Rev. B **45**, 4637 (1992); R. Strack and D. Vollhardt, *ibid.* **46**, 13 852 (1992).
[17] E. Halvorsen, G. S. Uhrig, and G. Czycholl, Z. Phys. B: Condens. Matter **94**, 291 (1994).
[18] A. Schiller and K. Ingersent, Phys. Rev. Lett. **75**, 113 (1995).
[19] Y. A. Izyumov and Y. N. Skryabin, *Statistical Mechanics of Magnetically Ordered Systems* (Consultants Bureau, New York and London, 1988).
[20] W. Metzner, Phys. Rev. B **43**, 8549 (1991).
[21] M. Bartkowiak and K. A. Chao, Phys. Rev. B **47**, 4193 (1993).
[22] A. Georges and J. S. Yedidia, J. Phys. A **24**, 2173 (1991).
[23] R. S. Fishman, Phys. Rev. B **41**, 4377 (1990); X. W. Jiang and R. S. Fishman, *ibid.* **47**, 8273 (1993).
[24] R. Micnas, S. Robaszkiewicz, and K. A. Chao, Phys. Rev. B **29**, 2784 (1984).
[25] The MuPAD Group (Benno Fuchssteiner *et al.*), *MuPAD User's Manual - MuPAD Version 1.2.2*, 1st ed. (Wiley, Chichester, New York, 1996).
[26] F. Lee and H. H. Chen, Phys. Rev. B **30**, 2724 (1984).
[27] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1972).
[28] C. Domb, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and S. Green (Academic, New York, 1974), Vol. 3.
[29] W. J. Camp and J. P. Van Dyke, Phys. Rev. B **11**, 2579 (1975).
[30] M. Bartkowiak, J. A. Henderson, J. Oitmaa, and P. E. de Brito, Phys. Rev. B **51**, 14 077 (1995).
[31] Z. Onyszkiewicz, Phys. Lett. **76A**, 411 (1980).
[32] Y. A. Izyumov, F. A. Kassan-Ogly, and Y. N. Skryabin, J. Phys. Colloq. **325**, C1, 86 (1971).