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Recursive Enumeration of Clusters in General Dimension on Hypercubic Lattices

Abstract

A recursive method for enumerating clusters on a hypercubic lattice in d spatial dimensions is presented from which the weak embedding constants are determined as polynomials in d . A tabulation for all clusters having no free ends is available for $n_b \leq 15$, where n_b is the number of bonds. As illustrated here and elsewhere, this tabulation can be used to generate many series expansions. A novel method of checking the enumeration with an algebraic calculation is presented.

Disciplines

Physics

Comments

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Recursive enumeration of clusters in general dimension on hypercubic lattices

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A recursive method for enumerating clusters on a hypercubic lattice in d spatial dimensions is presented from which the weak embedding constants are determined as polynomials in d . A tabulation for all clusters having no free ends is available for $n_b \leq 15$, where n_b is the number of bonds. As illustrated here and elsewhere, this tabulation can be used to generate many series expansions. A novel method of checking the enumeration with an algebraic calculation is presented.

I. INTRODUCTION

Series expansions have been used for about half a century to calculate thermodynamic quantities.^{1,2} While most of the first works involved high-temperature expansions,² this method can be and has been applied to study other problems, such as percolation,³ via low-density (or high-density) expansions. As is well known, the principal difficulty in this program is the enumeration of terms or diagrams involved in such an expansion. The methods used so far² become hard to implement as dimension increases, since the number of diagrams (or clusters, in percolation problems) increases rapidly with dimension. With the advent of the renormalization group⁴ (RG) interest has developed to treat systems in high spatial dimension d , and also in noninteger d , in order to study the dependence of the critical exponents throughout the range $d < d_c$, where their values depart from those of mean-field theory. Renormalization group calculations,⁴ or the Ginsburg criterion,⁵ indicate that for the Ising model $d_c = 4$, for percolation^{6,7} and for the spin glass⁸ $d_c = 6$, and for lattice animals⁹ $d_c = 8$. In order to test these predictions and the dependence of the exponents on $\epsilon = d_c - d$, it is necessary to have expansions¹⁰⁻¹³ in which the enumeration of diagrams is carried out as a polynomial function of d which can then assume noninteger values. Even in lower dimension the use of continuous d is of value, as witness the current discussion^{14,15} of the exact value of the lower critical dimension of the Ising-spin glass which is estimated to be about 2.6.

The present paper presents a description of such an enumeration of bond clusters which has been used¹⁶⁻¹⁹ and is being extended to treat a wide class of statistical problems. For classical problems, an enumeration of bond clusters having no free ends is sufficient²⁰ for the construction of low-density series and one can thereby get much longer series.²¹ A tabulation of the necessary cluster weights (or weak embedding constants as they are usually known) for clusters with less than 16 bonds for hypercubic lattices of d dimensions is deposited with the Physics Auxiliary Publication Service of the American Institute of Physics.²² Although the continuation of critical properties to noninteger d is not unique, the weights as polynomials in d do implement the same analytic con-

tinuation²³ as used in the Wilsonian version⁴ of the RG and therefore are suitable for comparison with ϵ -expansion results.

Briefly, this paper is organized as follows. In Sec. II we describe the recursive method we have used to obtain the weak embedding constants as polynomials in d . In Sec. III we present a novel method of checking such a calculation, viz., using the weak embedding constants we evaluate a nontrivial quantity which we also calculate using straightforward algebraic manipulations. Section IV contains some observations on our results.

II. RECURSION RELATIONS FOR CLUSTER WEIGHTS

In this section we describe the recursion relations for the weak embedding constants which we used to generate various low-density expansions. For this purpose we start with some definitions.

We consider clusters on a d -dimensional hypercubic lattice of N_{tot} sites, although our technique may be extended to treat, say, a d -dimensional hypertetrahedral lattice (e.g., triangular for $d=2$, face-centered cubic for $d=3$, etc.). A cluster G on such a lattice is a connected set of bonds, each bond being a connection between nearest-neighboring sites. To each cluster G , with $n_s(G)$ sites, there corresponds an $n_s(G) \times n_s(G)$ incidence matrix $M(G)$, such that $M_{ij} = 1$ if sites i and j are connected by a bond of G and $M_{ij} = 0$ otherwise. Two clusters G and G' are topologically equivalent (TE) if either (a) $M(G) = M(G')$ or (b) it is possible to relabel the sites within G' so that the resulting $M(G')$, denoted $M'(G')$, is identical to $M(G)$. Thus, for example, all self-avoiding chains of length l are TE to one another. We now wish to consider the number of clusters which can be placed on the lattice which are TE to a given cluster G . In the limit when the lattice becomes large in all dimensions, the number of clusters TE to G is asymptotically $N_{\text{tot}} W(G)$. Thus $W(G)$ is the number of ways per site of forming a cluster TE to G and is often referred to as the weak embedding constant of G . As we shall see in a moment, if G consists of $n_b(G)$ bonds, $W(G)$ is a polynomial of degree of most $n_b(G)$ in d . We seek to construct a tabulation of the $W(G)$ for all topologically inequivalent (TI)

clusters with $n_b(G) \leq n_0$, where n_0 is as large as possible. At present we have $n_0 = 13$.

In essence, our approach utilizes a simple recursive scheme. Suppose we know $W(G)$ for $n_b(G) \leq n$ and we wish to get the $W(G)$'s for $n_b(G) = n + 1$. Consider an arbitrary cluster G with $n_b(G) = n$ bonds and $n_s(G)$ sites and imagine adding a bond to site i to form a new diagram with $n + 1$ bonds and either $n_s(G) + 1$ sites or $n_s(G)$ sites. The recursion relation describing this process of adding a bond to G at site i is

$$g_i(G)[2d - z_i(G)]W(G) = h(i; G; G_i^+)W(G_i^+) + \sum_j' h(i; G; G_{ij})W(G_{ij}), \quad (1)$$

$i = 1, 2, \dots, m(G)$

where the symbols are as follows: $z_i(G)$ is the number of bonds of G which intersect site i and $g_i(G)$ is the number of sites in G (including i itself) which are TE to i . Two sites i and j are TE if it is possible to renumber the sites of G , with j renumbered as i to obtain a new G (denoted G') such that $M(G) = M(G')$. Thus the left-hand side of Eq. (1) gives the number of clusters per site which are formed by adding bonds to clusters TE to G at sites TE to site i . There is one such equation for each set of TE sites, so that $m(G)$ is the number of TI sites in G . [For simplicity, we assume the diagram is relabeled, if necessary, so that the set of TI sites in G is $1, 2, \dots, m(G)$]. Since adding a bond gives rise to a multiplicative factor $2d - z_i(G)$, one sees that $W(G)$ is a polynomial in d of degree at most $n_b(G)$. For families of lattices where the coordination number z is a nonlinear function of d , this would not be true. (However, universality with respect to lattice structure indicates that the critical exponents depend not on z , but rather on the value of d .) In the addition process of Eq. (1) we may obtain either a new diagram G_i^+ with $n + 1$ sites or a new diagram G_{ij} in which a bond is added between pre-existing sites i and j , and in (1) the prime indicates that j is summed over values such that only TI clusters G_{ij} appear. The coefficients h on the right-hand side of Eq. (1) are the appropriate fractional parentage coefficients for this process. They tell how many directed bonds $i' \rightarrow j'$ in G_i^+ or G_{ij} are TE to the added bond $i \rightarrow j$.

For example, if G is the cluster of Fig. 1, then G_1^+ , G_{14} , and G_{16} are the clusters shown in Figs. 2(a), 2(b), and 2(c), respectively, and for site 1 Eq. (1) is

$$2(2d - 1)W(G) = 2W(G_1^+) + 2W(G_{14}) + 12W(G_{16}). \quad (2a)$$

Likewise, if bonds are added to sites 2 and 3, the clusters of Figs. 2(d)–2(g) are obtained, and the respective versions of Eq. (1) are

$$2(2d - 2)W(G) = 2W(G_2^+) + 2W(G_{25}), \quad (2b)$$

$$2(2d - 2)W(G) = W(G_3^+) + 2W(G_{14}), \quad (2c)$$

where we noted that G_{36} and G_{14} are TE. Since sites 1, 2, and 3 are, respectively, TE to sites 6, 5, and 4, there are $m(G) = 3$ recursion relations for the diagram of Fig. 1. The values of the $W(G)$'s appearing in Eqs. (2) are given in Appendix A.

FIG. 1. A parent cluster G .

Note that for special clusters, like polygons [viz., Fig. 2(c)], it is possible for the directed bond $i \rightarrow j$ to be TE to the directed bond $j \rightarrow i$. It is obviously necessary to construct algorithms for determining when two sites, two directed bonds, and two diagrams are TE to one another.

Since the computer codes needed to implement Eq. (1) are clearly rather complicated, it is desirable to have various checks of their correctness. First, we give some rather trivial checks. For this purpose we note that Eq. (1) is of the form

$$g_i(G)[2d - z_i(G)]W(G) = \sum_{j: n_s(G_j) = n_s(G) + 1} b_{ij}W(G_j) + \sum_{j: n_s(G_j) = n_s(G)} c_{ij}W(G_j). \quad (3)$$

The coefficients in Eq. (3) satisfy certain sum rules. For instance, for any G we have

$$\sum_{i=1}^{m(G)} g_i(G) = n_s(G). \quad (4)$$

FIG. 2. Clusters which result from adding a bond to the parent cluster shown in Fig. 1: (a) G_1^+ , (b) G_{14} , (c) G_{16} , (d) G_2^+ , (e) G_{25} , (f) G_3^+ , and (g) $G_{36} = G_{14}$.

FIG. 3. A cluster which contains two cutting bonds (4,5) and (8,9), and two free ends (4,11) and (9,10).

Also, the number of ways not to add bonds depends on the number of bonds of G :

$$\sum_{i=1}^{m(G)} g_i(G) z_i(G) = 2n_b(G). \quad (5)$$

Furthermore, the number of ways a given G can appear on the right-hand side of Eq. (3) can be determined from its structure. To see this, classify bonds into three types: free ends, cutting bonds, and others. Free ends are bonds which intersect a site with $z_i = 1$ (e.g., 4-11 and 9-10 in Fig. 3), and can be an added bond in only one way, in which case n_s is increased by unity. Therefore

$$\sum_i b_{ij} = n_f(G_j), \quad (6a)$$

where $n_f(G)$ is the number of free ends of G . Cutting bonds are such that their removal causes the cluster to separate into two disjoint subclusters of bonds (e.g., 4-5 and 8-9 in Fig. 3) and they can never be an added bond. All other bonds (i,j) can be added in two ways, either from site i to site j or from site j to site i . A graph G has $n_b(G) - n_c(G) - n_f(G)$ of these, where $n_c(G)$ is the number of cutting bonds in G . Then

$$\sum_i c_{ij} = 2[n_b(G_j) - n_f(G_j) - n_c(G_j)]. \quad (6b)$$

Note that in one stage of iteration in adding bonds to all clusters having n bonds, we obtain a list of TI clusters having $n+1$ bonds. It is essential that all clusters with $n+1$ bonds in this list actually be TI. That is, consider the cluster of Fig. 2(e). It can be obtained not only from the cluster of Fig. 1, but also from those of Figs. 4(a)-4(c)

FIG. 4. Possible parents for the cluster of Fig. 2(e).

by adding a suitable bond. However, the various realizations of Fig. 2(e) so obtained will in general be numbered differently. If no precautions are taken, our list of new clusters will contain two (or more) realizations of a new cluster such as that of Fig. 2(e). If we fail to recognize that two newly generated realizations are actually, TE, we will not satisfy Eq. (6). In fact, in such a case the left-hand side of this equation will be too small. The above sum rules (4)-(6) test for the most obvious misclassification of clusters. We will return later to other checks.

Having constructed and checked the recursion relations for adding bonds to clusters of n bonds, it remains to solve them for the weights of clusters with $n+1$ bonds. First we explicitly count the $W(G)$'s for diagrams with no free ends (NFE). The set of NFE diagrams is relatively small and also their enumeration is rapidly done because of their compactness. For instance, of the 2500 TI clusters with up to 11 bonds only 33 are NFE clusters. Direct enumeration of clusters with free ends becomes rapidly unfeasible as their size increases, and for them the recursion relations are indispensable. All clusters with at least one free end will appear at some stage as a G_i^+ in Eq. (1). Thus we solve Eq. (1) by writing

$$W(G_i^+) = h(i; G; G_i^+)^{-1} \left\{ g_i(G) [2d - z_i(G)] W(G) - \sum_j' h(i; G; G_{ij}) W(G_{ij}) \right\}. \quad (7)$$

Any G_{ij} appearing on the right-hand side of this equation is either an NFE cluster (whose weight was explicitly calculated) or is a cluster which was previously determined by solving an earlier version of Eq. (7). For this to be true, it is necessary that we consider G_i^+ in Eq. (7) in increasing order of $n_s(G_i^+)$, so that a cluster with at least one free end appears on the left-hand side of Eq. (7) before it appears on the right-hand side. An NFE cluster can never be a G_i^+ and therefore its weight had to be obtained elsewhere. At this stage of the calculation we have a redundancy check because a given cluster G will occur on the left-hand side of as many equations (7) as it has TI free ends. In each case we check that all such solutions for a given $W(G_i^+)$ are identical.

It is clearly not practical to give an explicit list of all our results. Instead, we have deposited with the Physics Auxiliary Publication Service of the American Institute of Physics a listing of all NFE clusters with less than 16 bonds together with their weak embedding constants.²² Using this listing and solving the set of Eqs. (7), one can construct a list of all clusters G with up to a given number of bonds with their weights $W(G)$. In order to construct a low-concentration series for some quantity χ , one should calculate

$$\chi(p) = \sum_G \chi(G) W(G) n_s(G) p^{n_b(G)} (1-p)^{n_p(G)}, \quad (8)$$

where $n_p(G)$ is the number of perimeter bonds of G and $\chi(G)$ is the desired quantity evaluated for the cluster G . To get the percolation susceptibility, for example, one takes $\chi(G) = n_s(G)$. In the case of averages of two-point

correlations, f_{ij} , one takes $\chi(G) = n_s(G)^{-1} \sum_{ij \in G} f_{ij}$ in order to evaluate $\chi(p) = \sum_i [f_{ij}]_p$, where $[]_p$ denotes a configurational average.

In order to avoid keeping track of the number of perimeter bonds in all TE clusters, one uses the cumulant quantity, defined recursively by

$$\chi_c(G) = \chi(G) - \sum_{\gamma \subseteq G} \chi_c(\gamma), \quad (9)$$

where the sum is over all subclusters γ of G , with $\gamma = G$ excluded. Then the series in Eq. (8) reduces to

$$\chi(p) = \sum_G \chi_c(G) n_s(G) W(G) p^{n_b(G)}. \quad (10)$$

As was shown in Ref. 20, one can use only the subset of NFE clusters to construct series for classical quantities. The complete enumeration can be carried out to higher order for NFE clusters than for all clusters, since the NFE clusters form a small subset of all clusters. At the present stage we have the weights of all NFE clusters with up to 15 bonds and extension of this list even further is planned.

In this way one can construct several series, such as those for the susceptibilities for percolation, lattice animals, an Ising-spin glass, resistor networks, etc. The construction of such series using only NFE clusters is illustrated in Ref. 20 for the Ising model, lattice animals, and localization. We will give elsewhere details of the procedures for the other problems mentioned above. The procedure using only NFE clusters is also used in Sec. III to construct an additional check of our tabulations.

III. $\chi^{(3)}$ CHECK

The checks mentioned above are only self-consistency checks. In particular, if we had calculated the weights of some of the NFE clusters incorrectly, none of the checks discussed above could reveal that fact. What we need is an absolute, or external, check. Comparing with other independently calculated published series is an external check, subject, of course, to availability and to the correct-

ness of such work. Also, most of the series available involve only a small subset of the whole list of clusters. Since the correctness of the data, having done the above checks, depends on the correctness of the NFE data, we have devised a test wherein we use the NFE clusters to evaluate a quantity which can also be calculated algebraically without reference to clusters.

For this purpose, consider the following third-order correlation function for Gaussian random walks:

$$\chi_{ij}^{(3)} = \frac{1}{2} \text{Tr}(x_i^3 x_j^3 e^{-H(x)}) / \text{Tr}(e^{-H(x)}), \quad (11)$$

where

$$H(x) = \frac{1}{2} \sum_i x_i^2 - \frac{1}{2} K \sum_{i,j} \gamma_{ij} x_i x_j, \quad (12)$$

where $\gamma_{ij} = 1$ if sites i and j are nearest neighbors (on an undiluted d -dimensional hypercubic lattice) and is zero otherwise, and Tr indicates integration over all x 's from $-\infty$ to $+\infty$. We will evaluate $\chi^{(3)} \equiv \sum_j \chi_{ij}^{(3)}$ first algebraically, then by using NFE clusters.

A. Algebraic evaluation of $\chi^{(3)}$

Since $e^{-H(x)}$ is a Gaussian, we can write

$$\chi_{ij}^{(3)} = \frac{1}{2} (9G_{ii}G_{jj}G_{ij} + 6G_{ij}^3), \quad (13)$$

where

$$G_{ij} = \text{Tr}(e^{-H(x)} x_i x_j) / \text{Tr}(e^{-H(x)}) \quad (14)$$

is the usual lattice Green's function. We may interpret the two terms in $\chi_{ij}^{(3)}$ as follows. In the first term $G_{ii} = G(0)$ is the generating function for the number of returns of a random walk to the origin and G_{ij} is that for random walks between sites i and j . The second term in $\chi_{ij}^{(3)}$ is the generating function for three simultaneous random walks between sites i and j . Contributions of the two types corresponding to the two terms in Eq. (13) are shown in Fig. 5. The $\chi^{(3)}$ check to order K^n will depend upon all clusters G such that all bonds of

FIG. 5. Schematic representation of the two terms in Eq. (13).

FIG. 6. A cluster with 15 bonds for which all bonds cannot be covered as in Fig. 15 by walks with a total of 15 or less steps. Such a covering requires three walks with a combined total of at least 16 steps.

G can be covered by diagrams of the type of Fig. 5 having a total of n or less steps. To order K^{15} we do not check all clusters with 15 or less bonds. For instance, the cluster shown in Fig. 6 only affects the diagrammatic

evaluation in order K^{16} even though it has 15 bonds.

Returning to Eq. (14), we see that if r_{ij} has components $(n_1, n_2, \dots, n_d)$ in units of the lattice constant, then G_{ij} can be written as

$$G(n_1, n_2, \dots, n_d) = \left[\frac{1}{2\pi} \right]^d \int_{-\pi}^{+\pi} dq_1 \int_{-\pi}^{+\pi} dq_2 \cdots \int_{-\pi}^{+\pi} dq_d \frac{e^{i(n_1 q_1 + n_2 q_2 + \cdots + n_d q_d)}}{1 - 2K(\cos q_1 + \cos q_2 + \cdots + \cos q_d)} \quad (15a)$$

$$= \int_0^\infty e^{-\lambda} \prod_{k=1}^d \left[\frac{1}{2\pi} \int_{-\pi}^{+\pi} dq_k e^{in_k q_k + 2K\lambda \cos q_k} \right] d\lambda. \quad (15b)$$

The factor in large parentheses is a modified Bessel function for which a well-known power series in K exists.²⁴ The G 's we need below will, by Eq. (15b), be expressible as a power series in K whose coefficients are polynomials in d . Also $\sum_j G_{ij} = (1 - 2Kd)^{-1}$. Thus

$$\chi^{(3)} = \frac{9}{2} G(0)^2 (1 - 2dK)^{-1} + 3S, \quad (16)$$

where S is a sum of G 's which correct to order K^{15} is

$$\begin{aligned} S = & [G(0)]^3 + 2d \{ [G(1)]^3 + [G(2)]^3 + [G(3)]^3 + [G(4)]^3 + [G(5)]^3 \} \\ & + 2d(d-1) \{ 2[G(4,1)]^3 + 2[G(3,2)]^3 + 2[G(3,1)]^3 + [G(2,2)]^3 + 2[G(2,1)]^3 + [G(1,1)]^3 \} \\ & + 4d(d-1)(d-2) \{ [G(3,1,1)]^3 + [G(2,2,1)]^3 + [G(2,1,1)]^3 + \frac{1}{3}[G(1,1,1)]^3 \} \\ & + \frac{4}{3}d(d-1)(d-2)(d-3) \{ 4[G(2,1,1,1)]^3 + [G(1,1,1,1)]^3 \} + \frac{4}{15}d(d-1)(d-2)(d-3)(d-4)[G(1,1,1,1,1)]^3, \end{aligned} \quad (17)$$

where the arguments of G not given are zero: $G(n) \equiv G(n, 0, 0, \dots, 0)$, $G(n, m) \equiv G(n, m, 0, 0, \dots, 0)$, etc. In this way $\chi^{(3)}$ can be expressed as a power series in K and d :

$$\chi^{(3)} = \frac{1}{4} \sum_{m=0}^{\infty} K^m \sum_{l=0}^m \alpha_{ml} d^l, \quad (18)$$

and the coefficients α_{ml} are given in Table I for $m \leq 15$.

B. Graphical evaluation of $\chi^{(3)}$

To obtain the graphical expansion of $\chi^{(3)}$ in its most convenient form, we found it convenient to introduce replicas:

$$\chi^{(3)} = \frac{1}{2n} \sum_j \sum_{\alpha=1}^n \langle x_{0\alpha}^3 x_{j\alpha}^3 \rangle_\alpha, \quad (19)$$

where $\langle \rangle_\alpha$ denotes an average with respect to weight

$$\exp \left[- \sum_\alpha H(x_\alpha) \right].$$

Although Eq. (19) is valid for any n (replication has no effect on the calculation), we let $n \rightarrow 0$ to simplify some of our analysis. We write

$$\chi^{(3)} = \frac{1}{2N_{\text{tot}}} \lim_{n \rightarrow 0} \left[\frac{1}{n} \frac{\partial^2 \ln Z(\lambda)}{\partial \lambda^2} \right]_{\lambda=0}, \quad (20)$$

where

$$Z(\lambda) = \text{Tr} \exp \left[-\frac{1}{2} \sum_{i,\alpha} x_{i\alpha}^2 + \frac{1}{2} K \sum_{i,j,\alpha} \gamma_{ij} x_{i\alpha} x_{j\alpha} + \lambda \sum_{i,\alpha} x_{i\alpha}^3 \right] \quad (21a)$$

$$\begin{aligned} &= \text{Tr} \left\{ \prod_i \left[\rho_i^z \exp \left[-\frac{1}{2} \sum_{\alpha} x_{i\alpha}^2 + \lambda \sum_{\alpha} x_{i\alpha}^3 \right] \right] \right. \\ &\quad \left. \times \prod_{\langle ij \rangle} \left[\rho_i^{-1} \rho_j^{-1} \exp \left[K \sum_{\alpha} x_{i\alpha} x_{j\alpha} \right] \right] \right\}, \end{aligned} \quad (21b)$$

where $z = 2d$, $\langle ij \rangle$ indicates that the product is over pairs of nearest-neighboring sites, and ρ_i is an arbitrary function of the $x_{i\alpha}$'s for $\alpha = 1$ to n . We write this as

$$Z(\lambda) = \text{Tr} \left[\prod_i e^{-h_i^{(0)}} \prod_{\langle ij \rangle} (f_{ij} / \rho_i \rho_j) \right] \quad (22)$$

and develop $Z(\lambda)$ as an expansion in $(\rho_i^{-1} \rho_j^{-1} f_{ij} - 1)$:

$$Z(\lambda) = \text{Tr} \left[\prod_i e^{-h_i^{(0)}} \prod_{\langle ij \rangle} [1 + (\rho_i^{-1} \rho_j^{-1} f_{ij} - 1)] \right]. \quad (23)$$

In this expansion we associate a factor $\rho_i^{-1} \rho_j^{-1} f_{ij} - 1$ with an occupied bond. Then the product over $\langle ij \rangle$ gives rise to 2^{N_B} terms, each corresponding to a graph Γ , where N_B is the number of bonds in the lattice. Thus

$$Z(\lambda) = [z_0(\lambda)]^{N_{\text{tot}}} + \sum_{\Gamma} \delta Z(\lambda; \Gamma), \quad (24)$$

where

$$z_0(\lambda) = \text{Tr}_i e^{-h_i^{(0)}}, \quad (25a)$$

$$\delta Z(\lambda; \Gamma) = \text{Tr} \prod_i e^{-h_i^{(0)}} \prod_{\langle ij \rangle \text{ occ}} (\rho_i^{-1} \rho_j^{-1} f_{ij} - 1), \quad (25b)$$

where Tr_i indicates a trace over only $x_{i\alpha}$'s for site i and the product in Eq. (25b) is over occupied bonds of Γ . If Γ consists of k disjoint clusters of bonds, $\delta Z(\lambda; \Gamma) \sim n^k$. Since we need only terms of order n as $n \rightarrow 0$, we may restrict the sum over Γ to a sum over TI clusters G :

$$Z(\lambda) = [z_0(\lambda)]^{N_{\text{tot}}} + N_{\text{tot}} \sum_G W(G) \delta Z(\lambda; G). \quad (26)$$

Thus to order n

$$\frac{1}{N_{\text{tot}}} \ln Z(\lambda) = \ln z_0(\lambda) + \sum_G' W(G) \delta Z(\lambda; G) / z_0(\lambda)^{N_{\text{tot}}}. \quad (27)$$

We now choose ρ_i so that $Z(\lambda; G)$ vanishes if G has one or more free ends. The condition for this is²⁰

$$\rho(\{x_{i\alpha}\}) = \frac{\text{Tr}_j e^{-h_j^{(0)}} [\rho(\{x_{j\alpha}\})]^\sigma f_{ij}}{\text{Tr}_j e^{-h_j^{(0)}} [\rho(\{x_{j\alpha}\})]^z}, \quad (28)$$

where $\sigma = z - 1 = 2d - 1$. For $\lambda = 0$, this equation is solved exactly by $\rho = \rho_0(\{x_{i\alpha}\})$ with

$$\rho_0(\{x_{i\alpha}\}) = [(E - z\Delta)/(E - \sigma\Delta)]^{n/4} \exp(\frac{1}{2}\Delta[x^2]), \quad (29)$$

TABLE I. The coefficients α_{lm} in Eq. (18).

l, m	α_{lm}	l, m	α_{lm}	l, m	α_{lm}
0,0	30	1,1	36	2,1	144
2,2	72	3,1	24	3,2	144
3,3	144	4,1	-432	4,2	1080
4,3	288	4,4	288	5,1	-216
5,2	0	5,3	1008	5,4	576
5,5	576	6,1	5592	6,2	-14 064
6,3	10 464	6,4	2016	6,5	1152
6,6	1152	7,1	3528	7,2	-3312
7,3	-6912	7,4	8640	7,5	4032
7,6	2304	7,7	2304	8,1	-159 984
8,2	419 544	8,3	-391 968	8,4	128 736
8,5	17 280	8,6	8064	8,7	4608
8,8	4608	9,1	-95 448	9,2	108 576
9,3	136 656	9,4	-253 440	9,5	88 128
9,6	34 560	9,7	16 128	9,8	9216
9,9	9216	10,1	8 017 128	10,2	-22 116 672
10,3	23 233 248	10,4	-112 83 552	10,5	1 981 440
10,6	176 256	10,7	69 120	10,8	32 256
10,9	18 432	10,10	18 432	11,1	4 244 472
11,2	-4 576 896	11,3	-7 236 000	11,4	14 045 760
11,5	-7 886 016	11,6	1 039 104	11,7	352 512
11,8	138 240	11,9	64 512	11,10	36 864
11,11	36 864	12,1	-616 436 136	12,2	1 787 709 648
12,3	-2 051 820 000	12,4	1 192 561 632	12,5	-352 303 488
12,6	37 626 624	12,7	2 078 208	12,8	705 024
12,9	276 480	12,10	129 024	12,11	73 728
12,12	73 728	13,1	-303 843 960	13,2	309 919 248
13,3	631 069 056	13,4	-1 260 399 744	13,5	851 739 840
13,6	-247 703 040	13,7	13 764 096	13,8	4 156 416
13,9	1 410 048	13,10	552 960	13,11	258 048
13,12	147 456	13,13	147 456	14,1	67 041 085 320
14,2	-203 434 791 552	14,3	250 911 765 792	14,4	-164 443 114 368
14,5	61 117 656 192	14,6	-12 097 987 200	14,7	867 571 200
14,8	27 528 192	14,9	8 312 832	14,10	2 820 096
14,11	1 105 920	14,12	516 096	14,13	294 912
14,14	294 912	15,1	32 551 601 112	15,2	-34 595 738 400
15,3	-71 549 190 624	15,4	155 209 441 152	15,5	-119 829 125 376
15,6	46 196 538 624	15,7	-8 258 699 520	15,8	199 019 520
15,9	55 056 384	15,10	16 625 664	15,11	5 640 192
15,12	2 211 840	15,13	10 322 192	15,14	589 824
15,15	589 824				

where here and in Eq. (32) below $[x^n] \equiv \sum_a x_a^n$ and

$$\Delta = (2\sigma)^{-1} [1 - (1 - 4\sigma K^2)^{1/2}] . \quad (30)$$

In order to use Eq. (20) we evaluate ρ in powers of λ up to order λ^2 as

$$\rho_i(\{x_{i\alpha}\}) = \rho_0(\{x_{i\alpha}\}) [1 + \lambda \phi_1(\{x_{i\alpha}\}) + \lambda^2 \phi_2(\{x_{i\alpha}\})] , \quad (31)$$

where

$$\phi_1(\{x_{i\alpha}\}) = a[x] + b[x^3] , \quad (32a)$$

$$\begin{aligned} \phi_2(\{x_{i\alpha}\}) = & nc + d[x^2] + e[x^4] + f[x]^2 \\ & + g[x][x^3] + h[x^3]^2 , \end{aligned} \quad (32b)$$

where the coefficients $a-h$ are given in Appendix B. With this choice of ρ , the sum in Eq. (27) is restricted to TI NFE clusters and the first term, $\ln z_0(\lambda)$, gives the exact result for the Cayley tree of coordination number σ (since the Cayley tree supports no NFE clusters). This scheme based on NFE clusters has been previously applied to several problems.²⁰

In principle we could evaluate Eq. (27) as it stands up to order K^{15} by carrying the sum over G to include all NFE clusters with less than 16 bonds. In the remainder of this section we discuss the simplification of this equation using a cumulant expansion. For this purpose we write Eq. (27) as

$$\frac{1}{N_{\text{tot}}} \ln Z(\lambda) - \ln z_0(\lambda) = \sum_G' W(G) \left[(-1)^{n_B(G)} + \sum_{\gamma \subseteq G} (-1)^{n_B(G) - n_B(\gamma)} \text{Tr}_{i:i \in \gamma} \left[\prod_{i \in \gamma} [z_0(\lambda)]^{-1} e^{-h_i^{(0)}} \right] \prod_{\langle ij \rangle} (\rho_i^{-1} \rho_j^{-1} f_{ij}) \right] , \quad (33a)$$

where γ is summed over the $2^{n_B(G)} - 1$ subdiagrams formed by either including or not including every bond of G . Diagrams γ need not be connected, $\gamma = G$ is included in the sum, but the diagram with no bonds is not. An alternative form of Eq. (33a) is

$$\begin{aligned} \frac{1}{N_{\text{tot}}} \ln Z(\lambda) - \ln z_0(\lambda) \\ = \sum_G W(G) \sum_{\gamma \subseteq G} (-1)^{n_B(G) - n_B(\gamma)} Y(\gamma) , \end{aligned} \quad (33b)$$

where

$$Y(\gamma) = \text{Tr}_{i:i \in \gamma} e^{-h_i^{(0)}} \left[-1 + \prod_{\langle ij \rangle \in \gamma} \rho_i^{-1} \rho_j^{-1} f_{ij} \right] \prod_i [z_0(\lambda)]^{-1} . \quad (34)$$

But the alternating series in Eq. (33b) is a definition of the cumulant of $Y(G)$ denoted $[Y(G)]_c$:

$$[Y(G)]_c = \sum_{\gamma \subseteq G} (-1)^{n_B(G) - n_B(\gamma)} Y(\gamma) , \quad (35)$$

which we may calculate recursively as

$$[Y(G)]_c = Y(G) - \sum_{\gamma \subset G} [Y(\gamma)]_c , \quad (36)$$

where now $\gamma = G$ is not allowed in the sum. Only connected NFE clusters have nonzero values of $[Y(G)]_c$. Thus

$$\frac{1}{N_{\text{tot}}} \ln Z(\lambda) - \ln z_0(\lambda) = \sum_G W(G) [Y(G)]_c , \quad (37)$$

and $Y(G)$ is

$$\begin{aligned} Y(G) = & \text{Tr}_{i:i \in G} \prod_{i \in \gamma} \left[\exp \left[-\frac{1}{2} \sum_{\alpha} x_{i\alpha}^2 + \lambda \sum_{\alpha} x_{i\alpha}^3 \right] \rho_i^{z - z_i(G)} \right] \\ & \times \prod_{\langle ij \rangle} \exp \left[K \sum_{\alpha} x_{i\alpha} x_{j\alpha} \right] \\ & - \left[\text{Tr}_j \exp \left[-\frac{1}{2} \sum_{\alpha} x_{j\alpha}^2 + \lambda \sum_{\alpha} x_{j\alpha}^3 \right] \rho_j^z \right]^{n_s(G)} , \end{aligned} \quad (38)$$

where $z_i(G)$ is the number of sites which are connected by occupied bonds of G to site i . Because the list of NFE clusters is very short, the use of Eq. (36) presents little difficulty.

Then Eq. (20) becomes

$$\chi^{(3)} = \lim_{n \rightarrow 0} \left[\frac{1}{2n} \frac{\partial^2 \ln z_0(\lambda)}{\partial \lambda^2} + \frac{1}{2n} \sum_G' W(G) \frac{\partial^2 [Y(G)]_c}{\partial \lambda^2} \right] , \quad (39)$$

and the first term on the right-hand side of Eq. (39) is $\chi_{\text{CT}}^{(3)}$, the exact solution for $\chi^{(3)}$ on the Cayley tree given explicitly in Appendix C. The second term is evaluated by expanding the form in Eq. (38) in powers of λ , using the results of Appendix A for the coefficients in Eq. (32). Then the evaluation of Eq. (39) up to order K^{15} reproduced the result given in Table I obtained algebraically. Thus we are quite confident that our weights for the NFE clusters for up to 15 bonds is correct and complete. Up to order 13 bonds we have also checked that the total number of lattice animals as calculated using only NFE clusters agrees with the result of counting all clusters. Thus we have rather comprehensive checks that our tabulation of diagram weights for continuous d are in fact correct.

IV. DISCUSSION

For high dimensions, say $d \geq 3$, the method we have outlined seems to be an appropriate one for obtaining series for quantities which depend on the topology, but not on the detailed shape, of clusters. In particular, when dealing with a series having no simplifying features, the method is quite powerful. Also if one wants series for noninteger dimension, the above method is clearly useful. In cases where free ends can be eliminated, one can use the much shorter tabulation of no-free-end clusters attached. Typically, a free end elimination is convenient for nonquantum problems and is carried out as in Sec. III or elsewhere.²⁰ Diffusion statistics are to some extent reducible to resistance correlations²⁵ which in turn can be ex-

pressed in terms of no-free-end clusters.²⁶ In addition, it should be noted that one can extend this technique to treat higher-order susceptibilities as well. For the percolation problem these series can be used¹⁶ to obtain the gap exponent $\Delta = \beta + \gamma$, and thereby get a series estimate for β , as well as universal amplitude ratios.

In contrast, quantities which are position dependent cannot be treated in the manner of this paper, although we are currently studying how the necessary more general enumeration might be done using more powerful computers. (The work was done mainly on the VAX 750 at the University of Pennsylvania.) Knowing the total number of occurrences of a cluster would be an essential check on calculations for the correlation length which rely on a complete enumeration of all possible shapes of cluster G contributing to $W(G)$.

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APPENDIX A: THE WEAK EMBEDDING CONSTANTS OF THE DIAGRAMS APPEARING IN EQ. (2)

The weak embedding constants of the diagrams appearing in Eq. (2) are the following:

$$W(G) = 16d^5 - 32d^4 + 16d^3 + 6d^2 - 5d ,$$

$$W(G_1^+) = 32d^6 - 80d^5 + 56d^4 + 10d^2 - 17d ,$$

$$W(G_{14}) = 8d^4 - 20d^3 + 16d^2 - 4d ,$$

$$W(G_{16}) = \frac{1}{3}(8d^3 - 21d^2 + 13d) ,$$

$$W(G_2^+) = 32d^6 - 96d^5 + 88d^4 + 4d^3 - 46d^2 + 18d ,$$

$$W(G_{25}) = 8d^4 - 24d^3 + 24d^2 - 8d ,$$

$$W(G_3^+) = 64d^6 - 192d^5 + 176d^4 - 76d^2 + 28d .$$

APPENDIX B: THE COEFFICIENTS $a-h$

Here we give formulas for the coefficients $a-h$ appearing in Eq. (32) for the solution for ρ_i up to order h^2 . These results are obtained by inserting the expansions of Eqs. (31) and (32) into Eq. (28) and equating coefficients of like terms. We define

$$E_x = 1 - x\Delta ,$$

$$D_n = 1 - \sigma(K/E_\sigma)^n .$$

Then

$$a = 3KE_\sigma^{-2}D_1^{-1}D_3^{-1} ,$$

$$b = K^3E_\sigma^{-3}D_3^{-1} ,$$

$$\begin{aligned} c = & \frac{15}{4}E_\sigma^{-3}D_3^{-2} + \frac{9}{2}\sigma KE_\sigma^{-4}D_1^{-1}D_3^{-2} + \frac{9}{4}\sigma^2 K^2E_\sigma^{-5}D_1^{-2}D_3^{-2} + \frac{27}{4}\sigma K^4E_\sigma^{-7}D_3^{-2}D_4^{-1} + 9\sigma K^2E_\sigma^{-5}D_3^{-2}D_2^{-1} \\ & + \frac{9}{2}\sigma^2 K^3E_\sigma^{-6}D_3^{-2}D_1^{-1}D_2^{-1} + \frac{27}{2}\sigma^2 K^6E_\sigma^{-9}D_3^{-2}D_4^{-1}D_2^{-1} - \frac{15}{4}(1 + K^3E_\sigma^{-3})^2E_z^{-3}D_3^{-2} \\ & - \frac{9}{2}zK(1 + K^3E_\sigma^{-3})E_z^{-2}E_\sigma^{-2}D_1^{-1}D_3^{-2} \\ & - \frac{9}{4}z^2K^2E_z^{-1}E_\sigma^{-4}D_1^{-2}D_3^{-2} - \frac{27}{4}zK^4E_z^{-2}E_\sigma^{-5}D_3^{-2}D_4^{-1} - 9zK^2E_z^{-1}E_\sigma^{-4}D_3^{-2}D_2^{-1} - \frac{9}{2}z\sigma K^3E_z^{-1}E_\sigma^{-5}D_3^{-2}D_1^{-1}D_2^{-1} \\ & - \frac{27}{2}z\sigma K^6E_z^{-1}E_\sigma^{-8}D_3^{-2}D_4^{-1}D_2^{-1} , \end{aligned}$$

$$d = 27\sigma K^6E_\sigma^{-8}D_2^{-1}D_3^{-2}D_4^{-1} + 18K^2E_\sigma^{-4}D_2^{-1}D_3^{-2} + 9\sigma K^3E_\sigma^{-5}D_1^{-1}D_2^{-1}D_3^{-2} ,$$

$$e = \frac{9}{2}K^4E_\sigma^{-5}D_3^{-2}D_4^{-1} ,$$

$$f = \frac{9}{2}K^2E_\sigma^{-4}D_1^{-2}D_3^{-2} ,$$

$$g = 3K^4E_\sigma^{-5}D_1^{-1}D_3^{-2} ,$$

$$h = \frac{1}{2}K^6E_\sigma^{-6}D_3^{-2} .$$

APPENDIX C: CAYLEY-TREE RESULT

The exact result for $\chi_{CT}^{(3)}$ for a Cayley tree of coordination number $\sigma + 1 = 2d$ is

$$\chi_{CT}^{(3)} = \frac{1}{2E_\sigma^3} \left[\frac{9(1+q)}{(1-q^2)^3(1-\sigma q)} + \frac{6(1+q^3)}{(1-q^2)^3(1-\sigma q^3)} \right] ,$$

where $q = K/E_\sigma$.

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