Finally, we should like to calculate the lowest-order correction to the energy. We recall

$$p(y)=\exp\left\{n\left[S(y)-S\left(y-\frac{1}{n}\right)\right]\right\}$$

$$=\exp\left(\frac{\partial S}{\partial y}-\frac{1}{2n}\frac{\partial^2 S}{\partial y^2}+\cdots\right), \quad \text{(A.17)}$$

and

$$p\left(y+\frac{1}{n}\right)=\exp\left\{n\left[S\left(y+\frac{1}{n}\right)-S(y)\right]\right\}$$

$$=\exp\left(\frac{\partial S}{\partial y}+\frac{1}{2n}\frac{\partial^2 S}{\partial y^2}+\cdots\right).$$

Define

$$\exp\partial S/\partial y=\tilde{g}(y)\cong g(y), \quad \text{(A.18)}$$

and to order n^{-2},

$$\exp\left(\frac{1}{2n}\frac{\partial^2 S}{\partial y^2}\right)=\exp\left(\frac{1}{2n}\frac{\partial}{\partial y}\ln g(y)\right), \quad \text{(A.19)}$$

where $g(y)$ is given in Eqs. (A.15) and (A.16).

With these substitutions, the primitive equation becomes

$$\left(a\exp\left[\frac{1}{2n}\frac{\partial}{\partial y}\ln g(y)\right]\right)\tilde{g}^2(y)-2b\tilde{g}(y)$$

$$+\left(c\exp\left[\frac{1}{2n}\frac{\partial}{\partial y}\ln g(y)\right]\right)=0, \quad \text{(A.20)}$$

and if we note that both a and c are proportioned to the interaction v, we see that the interactions off the energy shell have been increased from a strength v to an effective strength

$$\tilde{v}\equiv v\exp\left[\frac{1}{2n}\frac{\partial}{\partial y}\ln g(y)\right]\approx v\left[1+\frac{1}{2n}\frac{\partial}{\partial y}\ln g(y)\right], \quad \text{(A.21)}$$

which is greater than v because, in the important region near y_0,

$$(d/dy)\ln g(y)>0, \quad y\approx y_0. \quad \text{(A.22)}$$

Consequently, the ground-state energy divided by the number of particles actually must increase as the volume is decreased (always at fixed density). For $n\gg 1$, this correction is quite negligible, and it always vanishes in the strong-coupling limit (in which $g(y)=1$, $\partial/\partial y[\ln g(y)]=0$). In the weak-coupling limit, or for the one-step model, this correction has the effect of slightly increasing the critical temperature for very small volume crystals.

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Some Cluster Size and Percolation Problems

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The problem of cluster size distribution and percolation on a regular lattice or graph of bonds and sites is reviewed and its applications to dilute ferromagnetism, polymer gelation, etc., briefly discussed. The cluster size and percolation problems are then solved exactly for Bethe lattices (infinite homogeneous Cayley trees) and for a wide class of pseudolattices derived by replacing the bonds and/or sites of a Bethe lattice by arbitrary finite subgraphs. Explicit expressions are given for the critical probability (density), for the mean cluster size, and for the density of infinite clusters. The nature of the critical anomalies is shown to be the same for all lattices discussed; in particular, the density of infinite clusters vanishes as $R(p)\approx C(p-p_c)$ $(p\geqslant p_c)$.

I. INTRODUCTION

RECENTLY Domb[1] has drawn attention to the problem of determining the distribution of cluster sizes for particles distributed in a medium in accordance with a statistical law. In the simplest case, the particles occupy at random the sites of a lattice (or, more generally, the vertices of a linear graph). Each site can accommodate one (and only one) particle and is occupied with a constant probability p. A group of particles which can be linked together by nearest-neighbor *bonds* from one occupied lattice site to an adjacent occupied site are said to form a *cluster*. The main theoretical task is to evaluate the mean cluster size and higher moments of the distribution as functions of the density (or concentration) of the particles, this being measured by the probability p.

[1] C. Domb, Conference on "Fluctuation phenomena and stochastic processes" at Birkbeck College, London, March 1959; Nature **184**, 509 (1959).

The problem has applications in various physical contexts, the distribution of grain size in sands and in photographic emulsions,[2] the behavior of dilute ferromagnets[3,4] and other diluted cooperative assemblies, the vulcanization of rubber and the formation of crosslinked polymer gels,[5] the clustering of impurities and defects in crystals, etc.

An alternative version of the problem is to consider the occupation of the *bonds* of a lattice (or linear graph). Each bond can be occupied with probability p; occupied bonds which meet at a lattice site are considered as linked together in a cluster. In this form, the cluster size problem is very closely related to the *percolation processes* introduced by Broadbent and Hammersley[6,7] and since discussed by Hammersley[8,9] and Harris.[10] In fact, if for "occupied" one reads "open" and for "unoccupied" reads "closed," a lattice with particles distributed on bonds becomes a *randomly dammed maze* such as considered by Broadbent and Hammersley. The flow of *fluid* through such a maze constitutes a percolation process and serves as a model for the diffusion of gas molecules through a porous solid, the spread of disease in an orchard, etc.[8] Interest centers on determining the subsequent distribution of fluid and the number of wetted "atoms" (i.e., sites). Clearly, a similar transposition can be made when sites rather than bonds are occupied. We shall refer to the two versions of the general problem as the *site problem* and the *bond problem*, respectively.

One of the interesting features of these problems is the existence of a *critical probability* p_c above which *unbounded clusters of infinite size* are formed in the lattice with a definite density. This phenomenon has significant physical implications. Thus, in a dilute ferromagnetic system, p_c represents the minimum concentration of ferromagnetic atoms necessary before long-range order can set in, and so marks the limit of the cooperative phase transition.[3,4] When $p=p_c$ the ferromagnetic Curie point occurs at zero temperature. When considering the gelation of polymers, p_c is proportional to the minimum number of crosslinks per molecule needed to ensure gel formation. The probability of a particle belonging to an infinite cluster then measures the gel fraction of polymer in relation to the sol fraction (finite clusters). For percolation processes, the formation of infinite clusters implies that the medium attains a finite (nonzero) permeabillty so that fluid will percolate indefinitely away from a source instead of being confined to the local neighborhood of the source. If the probability of cross infection in the spread of a disease exceeds the critical value, an epidemic occurs.

Bounds to the critical probability for various lattices have been obtained by Hammersley[7–9] and Harris,[10] but Domb has shown how p_c can be estimated directly from knowledge of the cluster size distributions.[1] For most physical applications, furthermore, it is useful to have more detailed information on the size distribution. In particular, the mean cluster size and the density of infinite clusters are expected to exhibit singularities at $p=p_c$ and consequently the behavior in the critical region is of considerable interest. Progress in the solution of these problems can be made by studying series expansions based on the enumeration of lattice configurations.[1] Unfortunately for the lattices of principal interest, the standard plane and three-dimensional lattices, it seems to be rather difficult to formulate a direct theoretical approach leading to solutions in closed form. Appreciable insight can be obtained, however, by examining pseudolattices such as the *Bethe lattices*[11] (i.e., infinite homogeneous Cayley trees) and, for example, the various (triangular) *cacti*[12] illustrated in Fig. 1.

As we show in this note, the cluster size problem can be solved exactly and in full detail for a wide class of pseudolattices of this general type. The relation between the behavior of these pseudolattices and that of the normal space lattices is quite closely analogous to that between the results of approximations like that of Bethe and of Rushbrooke and Scoins[11] and the consequences of the exact treatment of order-disorder phenomena on the corresponding lattices. Furthermore, the exact results for the Bethe lattices are useful in obtaining the series expansions for the normal lattices since only relatively few configurational corrections have to be made.[13] One might also hope, by examining the form of the exact solutions for various pseudolattices which allow only a limited number of closed configurations (subgraphs), to discover a general development analogous to that of Yvon for the order-disorder problem.[11] As yet, however, we have not been able to achieve this.

The theory for pseudolattices is developed in the remainder of this paper. The general approach via generating functions is outlined in Sec. II. In the following section, the generating functions for the Bethe lattices are derived. Some of these results have been obtained previously in the special context of polymer gelation by Flory,[5] and the theory is related to known results in the theory of branching processes (multiplicative or cascade processes).[14] In Sec. IV, the gener-

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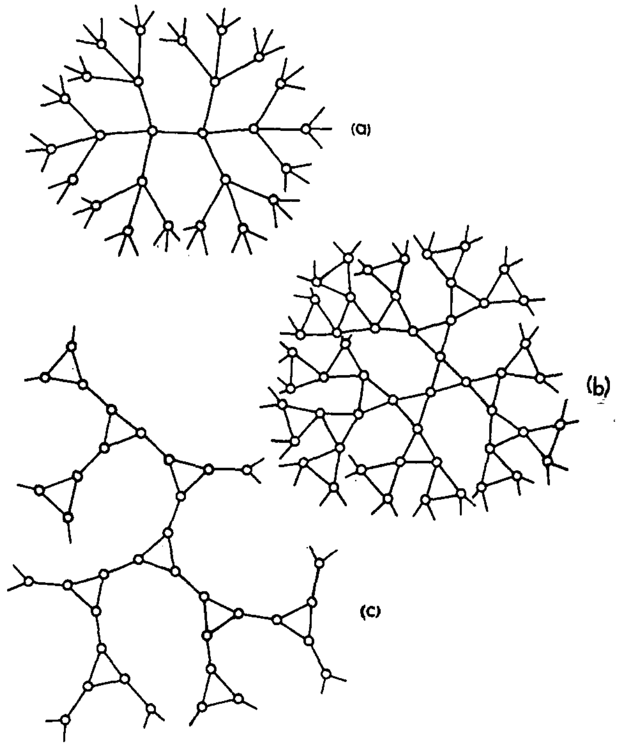

FIG. 1. Various simple pseudolattices: (a) Bethe lattice of coordination number $\sigma+1=4$, (b) simple (triangular) cactus of coordination number 4, (c) expanded cactus of coordination number 3.

ating functions are inverted to yield explicit formulas for the number of Cayley trees on a Bethe lattice and hence, for the other configurational coefficients. We then show how the generating functions can be modified to cover the "decoration" of each bond of a Bethe lattice by an arbitrary finite "bond-graph." In Sec. VI a similar procedure is carried through for the case where, in addition, the sites of a Bethe lattice (of coordination number $\sigma+1=3$) are also replaced by a specified "site-graph." This enables us, for example, to give explicit expressions for the mean cluster size and density of infinite clusters for the bond and site problems on the triangular cacti shown in Fig. 1. Other transformations and the possibility of generalizing the site decoration theory to $\sigma\geqslant 3$ are discussed in Secs. VII and VIII. The variation of the mean cluster size and other properties in the critical region are found to have the same analytic form for all lattices derived from the Bethe lattice, although the standard plane and three-dimensional lattices are expected to exhibit singularities of a different type.

II. GENERATING FUNCTIONS

Following Domb,[1] we approach the site problem on a general lattice by asking for the probability that a given site chosen at random is occupied by a particle belonging to a cluster of exactly s particles. For example, the probability of a given site belonging to a one cluster (isolated particle) is the probability that the chosen site is occupied times the probability that all the nearest-neighbor sites are unoccupied. For a lattice of coordination number $\sigma+1$, this is just $p_1=pq^{\sigma+1}$ where $q=1-p$. More generally, if a_{st} is the *number of distinct clusters of size s and perimeter t which contain the given lattice site* (the *perimeter* being the minimum number of unoccupied sites required to isolate the cluster), then the probability of a site belonging to such a cluster is

$$p_{st}=a_{st}p^sq^t. \tag{1}$$

Complete information on the cluster size distribution is thus contained in the generating function

$$A(x,y)=\sum_{s,t} a_{st}x^sy^t, \tag{2}$$

where the sum is over all possible clusters of finite size and perimeter that can occur on the lattice. In particular, the total probability that a site belongs to a finite cluster is

$$F(p)=A(p,q).$$

For small enough p, infinite clusters will be absent and $F(p)$ is merely the probability that the *a* site is occupied. Consequently, we obtain the basic identity

$$F(p)=A(p,q)\equiv p \quad \text{for } p<p_c. \tag{3}$$

On the other hand, for particle densities greater than the critical density, infinite clusters will spread through the lattice and the probability that a site belongs to an infinite cluster will be

$$R(p)=p-A(p,q). \tag{4}$$

The vanishing of $R(p)$ defines the critical probability p_c. The mean size density of clusters at a site is defined by

$$\langle s\rangle=\sum_{s,t} sp_{st}, \tag{5}$$

and so

$$\langle s\rangle=[x\partial A/\partial x]_{x=p,y=q}. \tag{6}$$

This relation holds for all p, but above p_c it represents the mean size of *finite* clusters only. Accordingly, it is convenient to normalize $\langle s\rangle$ by dividing by the probability $F(p)$ that a site belongs to a finite cluster. [Below p_c this is just equal to p, but above p_c one must use $A(p,q)$.] Thus,

$$S(p)=[x(\partial/\partial x)\ln A(x,y)]_{x=p,y=q}, \tag{7}$$

which for $p<p_c$ reduces simply to

$$S(p)=[\partial A/\partial x]_{x=p,y=q} \quad (p<p_c). \tag{8}$$

The mean cluster size will exhibit a sharp maximum at $p=p_c$ and this may be used to define the critical point. For all the pseudolattices which are soluble, the maximum in $S(p)$ is an infinite singularity and most probably this is generally true.

Higher moments of the cluster size distribution can be calculated by further differentiation of $A(x,y)$ with respect to x. Differentiation with respect to y yields moments of the perimeter distribution. Individual cluster contributions may be found by picking out the coefficients of the appropriate powers of x and y.

We remark parenthetically that $S(p)$ represents a "weight average" rather than a "number average," i.e., if there are n_s clusters of size s in the lattice, then $S(p)=\sum s(sn_s)/\sum sn_s$. For some purposes the number average size $S_0(p)=\sum sn_s/\sum n_s$ may be of interest. This can be calculated from $S_0(p)=[x(\partial/\partial x)\ln K(x,y)]$ with $x=p$ and $y=q$, where $K(x,y)$ is defined below. For pseudolattices it is found that $S_0(p)$ remains finite and continuous at $p=p_c$ but has a sharp peak as a result of a discontinuous change in the sign of the gradient.

For theoretical purposes, the configurational generating function

$$K(x,y)=\sum_{s,t}k_{st}x^sy^t \tag{9}$$

is more convenient than $A(x,y)$. This may be defined by

$$k_{st}=a_{st}/s \tag{10}$$

so that

$$A(x,y)=x(\partial/\partial x)K(x,y). \tag{11}$$

Alternatively, the coefficient k_{st} is defined as the number of cluster configurations of size s and perimeter t *per site* of the lattice. For a finite lattice of N sites, this is the total number of distinct clusters of a given type that can be placed on the lattice divided by the number of sites. In general, this will depend on N, but for any uniform d-dimensional lattice edge effects fall off relatively as $N^{-1/d}$, so that for large N, k_{st} becomes a *lattice constant*[11] independent of N. In a similar fashion, one may define the number of configurations per bond. If we indicate lattice constants with respect to sites by a superscript S and with respect to bonds by a superscript B, it is clear that

$$k^S=f^Sk^B, \tag{12}$$

where f^S is the number of bonds per site. Since $\sigma+1$ bonds radiate from each site and each bond is associated with two sites this is just $f^S=\frac{1}{2}(\sigma+1)$. Other transformation formulas may be written down in the same way.

The Bethe lattices and similar pseudolattices may be regarded as lattices of infinite dimension since in a finite Bethe lattice the relative number of sites in the edge is of order $1(\approx N^{-1/\infty})$. Consequently, the previous definition of a lattice constant breaks down. The definition may be extended in an unambiguous fashion, however, by introducing a convergence factor. If l is the least number of lattice steps from the origin to a characteristic point in an individual configuration, the factor $e^{-\beta l}$ is included in the sums for the total number of configurations and total number of sites (or bonds). These sums then define analytic functions of β, but after taking ratios to evaluate the lattice constant, β may be equated to zero. The lattice constants so defined have just the same transformation properties as on normal lattices.

The analysis of this section has been in terms of the site problem, but the only changes required for the bond problem is the use of lattice constants per bond rather than per site.

III. BETHE LATTICES

A. Bond Problem

Consider now the bond problem on the simple Bethe lattice of coordination number $\sigma+1$ as illustrated in Fig. 1(a). We observe that the perimeter of a cluster of s occupied bonds is given uniquely by

$$t=(\sigma-1)s+\sigma+1. \tag{13}$$

This follows by noting that the perimeter of a single bond is 2σ, and that whenever a new bond is added to a cluster, one bond of the original perimeter is lost but σ new unoccupied bonds must be added to form the new perimeter. It follows that the configurational generating function (9) is

$$K^B(x,y)=y^{\sigma+1}\sum_{s=0}^{\infty}b_sx^sy^{(\sigma-1)s}, \tag{14}$$

where $b_s=k_{s,(\sigma-1)s+\sigma+1}$ is the total number of s clusters (of bonds) per bond of the Bethe lattice. To simplify the analysis of the site problem, we have included a coefficient b_0 equal to the number of sites per bond. Its presence in (14) has no effect on the density of infinite clusters or on the other properties considered. The expression (14) may be rewritten in terms of the fundamental Bethe lattice generating function

$$B_\sigma(Z)=\sum_{s=0}^{\infty}b_sZ^s \tag{15}$$

as

$$K^B(x,y)=y^{\sigma+1}B_\sigma(Z), \tag{16}$$

where

$$Z(x,y)=xy^{\sigma-1}. \tag{17}$$

To calculate $B_\sigma(z)$ explicitly, we use the fundamental identity (3), namely,

$$F(p)=A(p,q)\equiv p \quad (p<p_c).$$

Now

$$A(x,y)=xy^{2\sigma}B_\sigma'(Z), \tag{18}$$

where the prime denotes differentiation with respect to Z. Thus, if

$$z=z(p)=Z(p,q)=p(1-p)^{\sigma-1}, \tag{19}$$

the generating function must satisfy

$$B_\sigma'[z(p)]=G(p)=(1-p)^{-2\sigma} \tag{20}$$

for small enough p. Now $B_\sigma(z)$ is a function only of z, but z is defined by (19) as a function of p for *all* p. To a given value of z, however, correspond *two* values of p, one of which tends to zero with z while the other tends to unity. Consequently, if we define $p^*(p)$ to be the root of the equation

$$p^*(1-p^*)^{\sigma-1}=p(1-p)^{\sigma-1}=z \tag{21}$$

which vanishes continuously with z (and hence as $p\rightarrow 0$ and as $p\rightarrow 1$), we may rewrite (20) as

$$G(p)=[1-p^*(p)]^{-2\sigma}. \tag{22}$$

In this form the result is thus valid for all p, and so the probability of a site belonging to a finite cluster is

$$F(p)=p(1-p)^{2\sigma}G(p)=p[(1-p)^{2\sigma}/(1-p^*)^{2\sigma}]. \tag{23}$$

Now z, as a function of p, attains a simple maximum at $p_m=1/\sigma$, which implies that the root of (22) which vanishes with z when $p\leq p_m$ is simply $p^*=p$. For $p>p_m$, however, z decreases again to zero so this root is no longer valid. Consequently, from (23) we have

$$\begin{aligned} F(p)&\equiv p \quad \text{for } p\leq 1/\sigma,\\ &\neq p \quad \text{for } p>1/\sigma. \end{aligned} \tag{24}$$

As explained in the previous section, this establishes that the critical probability is

$$p_c=1/\sigma. \tag{25}$$

The correctness of this result is easily verified by regarding the buildup of a cluster on the Bethe lattice as a branching or cascade process. If the cluster is to spread indefinitely, the expected number of occupied bonds leaving from one end of a given occupied bond must not be less than unity. Conversely, if the expected number exceeds unity an infinite cluster will be formed. Since the probability of traversing a bond is p and σ independent bonds proceed onwards from a given bond, the critical condition is $p_c\sigma=1$ in agreement with (25).

For the complete Bethe generating function, one derives from (20)–(22) the equation

$$dB\sigma/dZ=[1-X(Z)]^{-2\sigma}, \tag{26}$$

where $X(Z)=X(x,y)$ is the root of

$$X(1-X)^{\sigma-1}=Z=xy^{\sigma-1}, \tag{27}$$

which vanishes with Z. [Note that $X(p,q)=p^*(p)$.] This may be integrated to yield

$$B_\sigma(Z)=\frac{1}{\sigma+1}\frac{[2-(\sigma+1)X(Z)]}{[1-X(Z)]^{\sigma+1}}, \tag{28}$$

and with (16) this formally solves the problem.

From (23), the density of infinite clusters is

$$\begin{aligned} R(p)&=p\{1-[(1-p)/(1-p^*)]^{2\sigma}\}\\ &=p\{1-(p^*/p)^{[2\sigma/(\sigma-1)]}\}, \end{aligned} \tag{29}$$

while by differentiating (26) one finds for the mean cluster size

$$S(p)=(1+\sigma p^*)/(1-\sigma p^*). \tag{30}$$

As already noted, Eq. (21) for $p^*(p)$ shows that $p^*=p$ for $p\leq 1/\sigma$. At $p=p_c$ the gradient of $p^*(p)$ changes sign discontinuously, but the magnitude remains unchanged. Thereafter, $p^*(p)$ decreases monotonically and vanishes at $p=1$ as $(1-p)^{\sigma-1}$. Near p_c one has

$$p^*(p)\approx p_c-|p-p_c| \quad (p\simeq p_c), \tag{31}$$

so that the mean cluster size becomes hyperbolically infinite as

$$S(p)\approx 2/|1-(p/p_c)| \quad (p\simeq p_c), \tag{32}$$

and the density of infinite clusters vanishes linearly as

$$R(p)\approx[4\sigma/(\sigma-1)](p-p_c) \quad (p\rightarrow p_c+). \tag{33}$$

After removal of the root $p^*=p$, Eq. (21) is of degree $\sigma-1$ and so for the first few values of σ (i.e., small coordination numbers) it may be solved in closed form. One finds

(a) $\sigma=1$ (linear chain) $p_c=1$.

$$p^*(p)=p, \quad R(p)=0 \quad (\text{all } p), \tag{34a}$$

$$S(p)=(1+p)/(1-p), \tag{34b}$$

$$B_1(z)=1/(1-z). \tag{34c}$$

(b) $\sigma=2$, $p_c=\frac{1}{2}$,

$$p^*(p)=1-p \quad (p>\tfrac{1}{2}), \tag{35a}$$

$$R(p)=p-p^{-3}(1-p)^4 \quad (p>\tfrac{1}{2}), \tag{35b}$$

$$S(p)=1/|p-\tfrac{1}{2}|-1, \tag{35c}$$

$$B_2(z)=\tfrac{4}{3}\{[1+3(1-4z)^{\frac{1}{2}}]/[1+(1-4z)^{\frac{1}{2}}]^3\}. \tag{35d}$$

(c) $\sigma=3$, $p_c=\frac{1}{3}$,

$$p^*(p)=1-\tfrac{1}{2}p-[p(1-\tfrac{3}{4}p)]^{\frac{1}{2}} \quad (p>\tfrac{1}{3}), \tag{36b}$$

$$R(p)=p-p^{-2}[1-\tfrac{1}{2}p-p^{\frac{1}{2}}(1-\tfrac{3}{4}p)^{\frac{1}{2}}]^3 \quad (p>\tfrac{1}{3}). \tag{36c}$$

The typical behavior of the density of infinite clusters, etc., can be seen from Figs. 2 and 3 which refer to the Bethe lattice of coordination number four ($\sigma=3$).

B. Site Problem

To solve the site problem for the Bethe lattices, it is sufficient to note that the configurations involved are essentially identical with those required for the bond problem. In fact, a one-one correspondence can be set up which is described by

$$k^S{}_{s,t}=\tfrac{1}{2}(\sigma+1)k^B{}_{s-1,t}. \tag{37}$$

It follows immediately that the configurational generating function for the site problem is

$$K^S(x,y)=\tfrac{1}{2}(\sigma+1)xy^{\sigma+1}B_\sigma[Z(x,y)]. \tag{38}$$

The Bethe function $B_\sigma(Z)$ is defined as before by (28), (27), and (15) and, clearly, it determines the critical point and the nature of the critical singularities. These

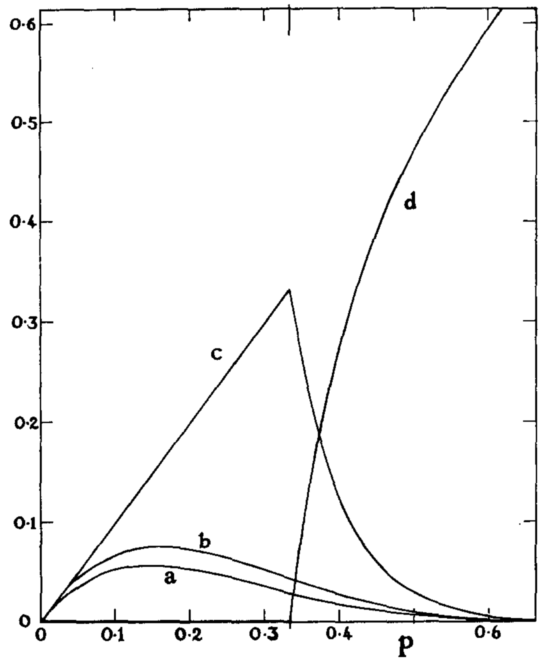

FIG. 2. Cluster distributions for the $\sigma=3$ Bethe lattice: (a) probability of a bond belonging to a cluster of one bond, (b) to a cluster of one or two bonds, (c) $F(p)$ the density of finite clusters, (d) $R(p)$ the density of infinite clusters. (Note the incomplete range of p.)

must, therefore, resemble those for the bond problem. Explicitly, the density of finite clusters is given by

$$F(p)=p^*(1-p)^2/(1-p^*)^2 \tag{39}$$

in place of (23), and the mean size by

$$S(p)=(1+p^*)/(1-\sigma p^*), \tag{40}$$

which exhibits directly the unchanged position of the critical point.

IV. CONFIGURATIONAL COEFFICIENTS

By the previous analysis, the coefficients in the expansions of the various generating functions for the Bethe lattices may all be expressed in terms of the coefficients $b_s(\sigma)$ defined in Eqs. (14) and (15). An explicit expression for these is most readily obtained from (26) which may be written

$$\sum_{s=1}^{\infty} sb_s(\sigma)z^{s-1}=[1-X(z)]^{-2\sigma}, \qquad X(1-X)^{\sigma-1}=z. \tag{41}$$

By Cauchy's theorem, one then has

$$sb_s(\sigma)=\frac{1}{2\pi i}\oint\frac{z^{-s}dz}{[1-X(z)]^{2\sigma}}, \tag{42}$$

where the contour of integration is a small closed loop encircling the origin. Near the origin, the analytic behavior of X is the same as z so that (42) may be transformed to an integral in the X plane, namely,

$$sb_s(\sigma)=\frac{1}{2\pi i}\oint\frac{(1-\sigma X)dX}{X^s(1-X)^{(s+1)(\sigma-1)+3}}. \tag{43}$$

This can be evaluated directly with the aid of the binomial theorem yielding

$$sb_s(\sigma)=\frac{2\sigma[(s+1)\sigma-1]!}{(s-1)![(s+1)\sigma-s+1]!}, \tag{44}$$

which expresses the total number of distinct Cayley trees of s branches passing through a specified bond of a Bethe lattice of coordination number $\sigma+1$.[15] From (44), one obtains for the number of trees *per bond*

$$b_s(\sigma)=\frac{2}{(s+1)(\sigma s+\sigma+1)}\binom{\sigma s+\sigma+1}{s}, \tag{45}$$

which remains valid for $s=0$.

V. BOND DECORATION

We consider now a class of lattices which can be derived from a Bethe lattice by replacing each bond by a replica of a given finite graph of sites and bonds, the *bond graph.* The simplest example of such a decorated

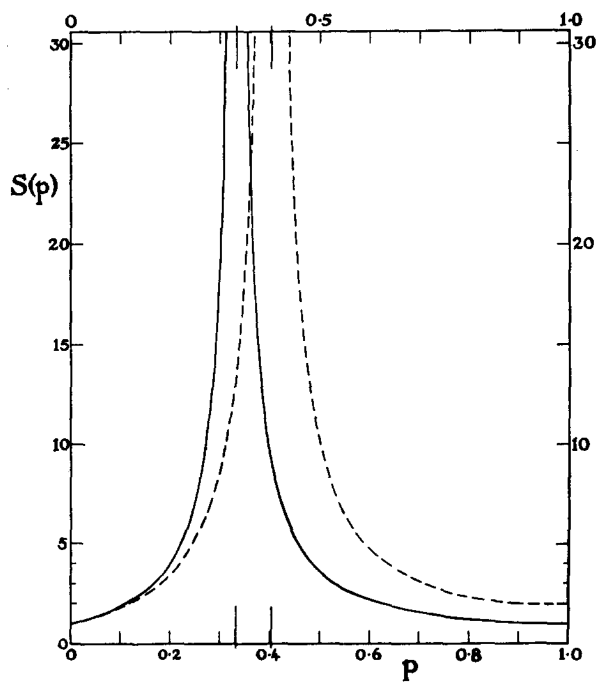

FIG. 3. Variation of $S(p)$ the mean cluster size density (for finite bond clusters): (a) for the $\sigma=3$ Bethe lattice (solid curve), (b) for the triangular cactus of same coordination number (broken curve).

[15] This expression for the number of Cayley trees on a Bethe lattice was originally conjectured by Dr. M. F. Sykes (private communication).

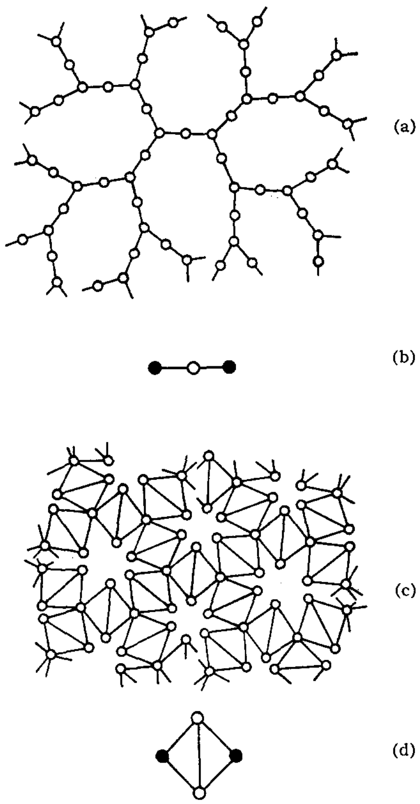

FIG. 4. Decorated Bethe lattices (a) and (c) derived from the $\sigma=2$ Bethe lattice by replacing bonds by the bond graphs (b) and (d).

lattice is that shown in Fig. 4(a) which represents a Bethe lattice of coordination number 3 with an extra site on each bond. The bond graph in this case is simply three sites connected by two bonds [Fig. 4(b)]. A more complicated example derived from the same Bethe lattice is shown in Fig. 4(c). Its bond graph is a square with one diagonal [Fig. 4(d)]. To simplify the general treatment, we will consider only bond graphs which are symmetric with regard to the two terminals or points of attachment [indicated in Figs. 4(b) and 4(d) by solid circles] and that the probability of occupation is the same for all bonds (or sites). Both these restrictions are quite easy to remove.

To construct the configurational generating function for a decorated lattice (from which all its properties may be deduced), we set up a one-many correspondence between configurations on the original (undecorated) Bethe lattice and those on the decorated lattice. Consider a specified bond graph in the decorated lattice, some bonds of which are connected in a cluster of occupied bonds (or sites). If it is possible to cross from one terminal of the bond graph to the other by a connected sequence of occupied bonds (or sites), then the bond graph is to be identified with the corresponding *occupied* bond on the original Bethe lattice. If, on the other hand, it is not possible to cross the bond graph (or it only contains unoccupied perimeter bonds or sites), then it should be identified with an *unoccupied* perimeter bond on the original lattice. On this basis, we define three bond generating functions, namely (for the bond problem),

$$c(x,y)=\sum_{s,t} c_{s,t}x^s y^t, \tag{46}$$

where $c_{s,t}$ is the number of distinct connected configurations of s occupied bonds and t perimeter bonds on the bond graph which join one terminal to the other;

$$d(x,y)=\sum_{s,t} d_{s,t}x^s y^t, \tag{47}$$

where $d_{s,t}$ is the number of distinct connected configurations of s occupied bonds and t perimeter bonds on the bond graph which are connected to one (specified) terminal but not to the other, including the case in which one terminal is joined only to unoccupied perimeter bonds;

$$e(x,y)=\sum_{s,t} e_{s,t}x^s y^t, \tag{48}$$

where $e_{s,t}$ is the number of distinct connected configurations of s occupied bonds and t perimeter bonds on the bond graphs which are not connected to *either* terminal.

By way of example, the bond generating functions for the two decorated lattices of Fig. 4 are

$$c(x,y)=x^2,\quad d(x,y)=xy+y,\quad e(x,y)=0, \tag{49}$$

and

$$\begin{aligned} c(x,y)&=x^5+5x^4y+8x^3y^2+2x^2y^3,\\ d(x,y)&=x^3y^2+3x^2y^3+2xy^3+y^2,\\ e(x,y)&=xy^4, \end{aligned} \tag{50}$$

respectively.

From the definition of $c(x,y)$, it follows that $c(p,q)$ is the probability of reaching one terminal of the bond graph starting from the other terminal. Conversely, $d(p,q)$ is the probability of failing to reach the other terminal from one terminal. Consequently, the identity

$$c(p,q)+d(p,q)\equiv 1 \tag{51}$$

is always valid and $c(p,q)$ is a monotonically increasing function of p.

The configurational generating function for the decorated lattice (indicated by a star) can now be derived by making the transformation $x\rightarrow x^*=c(x,y)$, $y\rightarrow y^*=d(x,y)$, and adding a correction for the clusters which do not span a bond graph. Thus, per bond of the decorated lattice,

$$K^{*B}(x,y)=g_B^{-1}K^B[c(x,y),d(x,y)]+g_B^{-1}e(x,y), \tag{52}$$

where g_B is the number of bonds in the bond graph. By (16), we have the explicit result

$$K^{*B}(x,y)=g_B^{-1}[d(x,y)]^{\sigma+1}B_\sigma[Z^*(x,y)]+g_B^{-1}e(x,y), \tag{53}$$

where

$$Z^*(x,y)=c(x,y)[d(x,y)]^{\sigma-1}. \tag{54}$$

These relations solve the bond problem for any bond-decorated Bethe lattice.

By (53), the critical singularities are determined entirely by the Bethe function $B_\sigma(Z^*)$. It is not immediately apparent, however, that the behavior in the critical region need resemble that for the original lattice. Nevertheless, it follows (51) that $Z^*(p,q)$ has a simple maximum as a function of p of magnitude $\sigma^{-\sigma}(\sigma-1)^{\sigma-1}$ which is exactly the value at which $B_\sigma(Z)$ becomes nonanalytic. Consequently, the critical point of a decorated lattice is determined by

$$c(p_c,q_c)=1/\sigma, \tag{55}$$

and the critical singularities of $R(p)$, $S(p)$, and other variables do have the same functional forms as those for the simple Bethe lattices [compare with Eqs. (32) and (33)]. In view of the probabilistic meaning of $c(p,q)$, the critical equation (55) can also be derived directly by viewing the formation of an infinite cluster as a branching process as in Sec. II.

The site problem on a bond-decorated lattice may be solved in a similar fashion by modifying the definitions of the bond generating functions $c(x,y)$, $d(x,y)$, and $e(x,y)$ so as to refer to sites of the bond graph in place of bonds. In the definition of $c(x,y)$ and $d(x,y)$, it must also be assumed that the first terminal site is already occupied but no factor x should be included for it. As an example, the bond functions for the site problem on the two lattices of Fig. 4 are

$$c(x,y)=x^2, \quad d(x,y)=xy+y, \quad e(x,y)=0, \tag{56}$$

and

$$\begin{aligned} c(x,y)&=x^3+2x^2y,\\ d(x,y)&=x^2y+2xy^2+y^2,\\ e(x,y)&=x^2y^2+2xy^3, \end{aligned} \tag{57}$$

respectively. Equation (51) remains valid in all cases.

The configurational generating function per site of the site-decorated lattice is then

$$K^{*S}(x,y)=\frac{\sigma+1}{(\sigma+1)g_S-2\sigma} \times\{x[d(x,y)]^{\sigma+1}B_\sigma[Z^*(x,y)]+e(x,y)\}, \tag{58}$$

where $Z^*(x,y)$ is defined by (54), and g_S is the number of sites of the bond graph (including the terminal sites). The nature of the critical singularities is unchanged and the critical probability is still determined by (55).

VI. SITE DECORATION

In this section, we endeavor to find generating functions for lattices derived from Bethe lattices by decorating the sites as well as the bonds. Each site of the underlying Bethe lattice will be replaced by a replica of a given *site graph* which we take to be symmetric under interchange of its $\sigma+1$ distinct terminals (points of attachment). Initially, we consider only the first nontrivial case in which the undecorated lattice is a Bethe lattice of coordination number three (i.e., $\sigma=2$). The simplest example of such a lattice is the infinite cactus illustrated in Fig. 1(b) in which the site graph is a triangle and the bond graph is merely a single site. The "expanded cactus" of Fig. 1(c) is obtained when the bond graph is left as a single bond. More generally, the triangles may be replaced by any finite symmetric three-terminal graph.

As before, we aim to solve the problem by setting up a many-one correspondence between configurations on the decorated lattice and those on the original Bethe lattice. In analogy with the three bond generating functions defined in (46)–(48), we thus introduce four site generating functions which, for the bond problem, are

$$t(x,y)=\textstyle\sum_{s,t} T_{st}x^sy^t, \tag{59}$$

where T_{st} is the number of distinct connected configurations of s occupied bonds and t unoccupied perimeter bonds on the site graph in which all three terminals are connected together;

$$u(x,y)=\textstyle\sum_{s,t} U_{st}x^sy^t, \tag{60}$$

where U_{st} is the number of configurations on the site graph in which the first terminal is connected to the second terminal but *not* to the third;

$$v(x,y)=\textstyle\sum_{s,t} V_{st}x^sy^t, \tag{61}$$

where V_{st} is the number of configurations in which the first terminal is connected to neither of the other two terminals (including the configuration of unoccupied perimeter bonds attached to the first terminal); and, finally,

$$w(x,y)=\textstyle\sum_{s,t} W_{st}x^sy^t, \tag{62}$$

where W_{st} is the number of configurations connected to none of the three terminals. For the triangular site graphs of Figs. 1(b) and 1(c), one has simply

$$t=x^3+3x^2y, \quad u=xy^2, \quad v=y^2, \quad w=0, \tag{63}$$

while for the relevant bond graphs

$$c=1, \quad d=0, \quad e=0, \tag{64a}$$

and

$$c=x, \quad d=y, \quad e=0, \tag{64b}$$

respectively.

By these definitions, $t(p,q)$ is the probability of being able to reach the second and third terminal from the first terminal, $u(p,q)$ is the probability that the second terminal only is accessible, and $v(p,q)$ is the probability that the site graph cannot be crossed at all. Consequently, in analogy with (51), the identity

$$t(p,q)+2u(p,q)+v(p,q)\equiv 1 \tag{65}$$

always holds.

In terms of these site generating functions, we may set up a correspondence with configurations on the undecorated Bethe lattice by identifying the decorated configurations included in $t(x,y)$ with a Bethe lattice at which three occupied bonds meet (a *triple point*), those included in $u(x,y)$ with a site at which only two occupied bonds meet (*double point*), and those in $v(x,y)$ with a site attached to only one occupied bond (*single point*). The problem may then be solved if we can determine the multivariable generating function

$$H(t,u,v',c)=\sum_{\lambda\mu\nu\gamma} h_{\lambda\mu\nu\gamma} t^\lambda u^\mu v'^\nu c^\gamma, \quad (66)$$

where t, u, v', and c are regarded simply as generating symbols and where $h_{\lambda\mu\nu\gamma}$ is the number of distinct cluster configurations per bond of a Bethe lattice of coordination number three with λ triple points, μ double points, ν single points, and a total of $\gamma+\nu$ occupied bonds (with γ nonnegative). In terms of this function, the configurational generating function per bond of the decorated lattice is given by

$$lK^{*B}(x,y)=H\{t(x,y),\, u(x,y),\, c(x,y)v(x,y)+d(x,y),\, c(x,y)\}$$
$$+c(x,y)[v(x,y)]^2+d(x,y)v(x,y)+e(x,y)+\tfrac{2}{3}w(x,y), \quad (67)$$

where l is the number of bonds of the decorated lattice per bond of the original lattice. If g_B is the number of bonds in the bond graph and j_B the number in the site graph, one has

$$l=g_B+\tfrac{2}{3}j_B. \quad (68)$$

The replacement of v' in (66) by $cv+d$ in (67) allows for the two possibilities: (a) the cluster on the decorated lattice extends across the bond graph leading to the single site graph and has perimeter bonds in the site graph, (b) the cluster on the decorated lattice does not reach across the bond graph so that its (local) perimeter lies entirely in the bond graph. The four end terms in (67) enumerate the small clusters which extend no further than across one bond graph.

To enumerate the cluster configurations $h_{\lambda\mu\nu\gamma}$ (on the $\sigma=2$ Bethe lattice), consider first those configurations with no triple points. These are just linear chains of bonds and double points, and their contribution to the generating function is simply ($\gamma\geqslant 0$)

$$v'\cdot 2uv'+v'\cdot 2uc\cdot 2uv'+v'(2uc)^2 2uv'+\cdots$$
$$=2uv'^2/(1-2uc). \quad (69)$$

The configurations containing triple points may be enumerated by setting up a many-one correspondence with the standard cluster configurations on the lattice. These latter are described by the configurational generating function

$$K^B(x,y)=y^3B_2(xy)=\tfrac{2}{3}y^3+xy^4+2x^2y^6+\cdots, \quad (70)$$

where the successive terms correspond to a single site with three unoccupied perimeter bonds, two sites connected by an occupied bond and four unoccupied perimeter bonds, three sites connected by two bonds, etc. *Each site* in one of these configurations may now be identified with a triple point of the $h_{\lambda\mu\nu\gamma}$ configurations. Each occupied bond x must then be identified with a linear chain of bonds and double points leading from one triple point to another, while each perimeter bond y corresponds to a linear chain leading from a triple point and terminating in a single point. The generating functions for these chains are

$$c+c\cdot 2uc+c(2uc)^2+\cdots=c/(1-2uc) \quad (71)$$

and

$$v'+2uc\cdot v'+(2uc)^2v'+\cdots=v'/(1-2uc), \quad (72)$$

respectively. By combining (69), (71), and (72) and remembering that each configuration has one more site than it has occupied bonds, we obtain

$$H(t,u,v',c)=tK^B[tc/(1-2uc),\, v'/(1-2uc)]$$
$$+2uv'^2/(1-2uc). \quad (73)$$

Consequently, by (67) and (70), the configurational generating function per bond for a site and bond decorated lattice is finally given in explicit terms by

$$lK^{*B}(x,y)=\frac{t(cv+d)^3}{(1-2uc)^3}B_2\left[\frac{tc(cv+d)}{(1-2uc)^2}\right]+\frac{2u(cv+d)^2}{1-2uc}$$
$$+v(cv+d)+e+w, \quad (74)$$

where c, d, e, t, u, v, and w are defined as functions of x and y by (46)–(48) and (59)–(62).

From this result, it follows as before that the critical point and singularities are determined only by the Bethe function. In view of the identities (51) and (65) which hold when $x=p$ and $y=q$, the argument of B_2 in (74) can be written

$$Z^*(p,q)=\left[\frac{tc}{1-2uc}\left(1-\frac{tc}{1-2uc}\right)\right]_{x=p,y=q},$$

and so exhibits a maximum as a function of p of magnitude $Z_m=\frac{1}{4}=z_c$. Consequently, the critical equation is

$$2u(p,q)c(p,q)+2t(p,q)c(p,q)=1, \quad (75)$$

and the analytic forms of the mean cluster size and other properties in the critical region are the same as for the original Bethe lattice.

The critical equation (75) can be derived directly from the branching process viewpoint by calculating the expected number of paths reaching from one terminal of a site graph through the following bonds to the nearer terminals of the next site graphs. By the probabilistic interpretation of c, u, and t, this is just the left-hand side of (75). (The first term comes from the two cases in which only one through route is open, while the second term represents the cases in which both further terminals are accessible.)

For the normal and expanded cacti of Fig. 1, one obtains with (63) and (64) the critical equations and critical points:

Triangular cactus (bond problem)

$$1-2p-2p^2+2p^3=0, \quad p_c=0.403032, \tag{76}$$

Expanded cactus (bond problem)

$$1-2p^2-2p^3+2p^4=0, \quad p_c=0.637278. \tag{77}$$

These critical probabilities should be compared with the results for the Bethe lattices of the same coordination number, namely, $(\sigma+1=4)$ $p_c=0.333333$ and $(\sigma+1=3)$ $p_c=0.500000$, respectively. As might be expected, the critical probability increases with the increasing connectivity of the lattice. (A similar phenomenon occurs in order-disorder lattice statistics where the increasing connectivity lowers the critical temperature below the Bethe approximation value.) We mention in passing the critical equation

$$1-2p-2p^2-2p^3+3p^4=0, \tag{78}$$

which may be derived for the simplest square Husimi tree[12] which also has coordination number $\sigma+1=4$. The corresponding critical point is

Square Husimi tree (bond problem)

$$p_c=0.353933, \tag{79}$$

which lies between the Bethe lattice and cactus results because of the low connectivity of a square compared with a triangle.

Explicit expressions for the mean cluster size, etc., may be derived by differentiating (74). As an example, we quote the results for the simple cactus (bond problem):

$$R(p)=p-\frac{2(1-p)^6(1+p-p^2)}{p^4(3-2p)^3} \quad (p\geqslant p_c) \tag{80}$$

$$S(p)=\frac{1+4p+2p^2-2p^3+p^5}{1-2p-2p^2+2p^3} \quad (p\leqslant p_c)$$

$$=\frac{4+10q+11q^2+14q^3-3q^4-20q^5+8q^6}{2(1+q-q^2)(1+2q)(1-4q^2+2q^3)} \quad (p\geqslant p_c). \tag{81}$$

The behavior of the cluster size is compared with that for the Bethe lattice of coordination in Fig. 3. As p tends to unity $S(p)$, the mean size of finite clusters on the cactus, approaches the value 2, whereas on the Bethe lattice $S(p)$ approaches 1. The reason for this difference arises from the existence on the cactus of two distinct clusters of minimum perimeter: the single bond and the triangle of three bonds. (Only the former, of course, occurs on the Bethe lattice.) In the limit $p\rightarrow 1$, these clusters dominate and appear equally frequently.

VII. BOND-TO-SITE TRANSFORMATION

The site problem on a Bethe lattice with decorated sites and bonds may be solved explicitly for the case $\sigma=2$ by modifying the definitions of the site generating functions (59)–(62) along the lines used to redefine the bond generating functions (see last two paragraphs of Sec. V). The argument then proceeds in parallel with that for the bond problem although the details differ slightly. The results will not be presented here, but it is worth noting that the site problem on the cacti of Figs. 1(b) and 1(c) can be solved immediately without further theoretical development.

To see this, consider a configuration of sites on the simple cactus of Fig. 1(b). Any such configuration can be put in direct one-one correspondence with a configuration of *bonds* on the underlying simple Bethe lattice of coordination number three. Each site on the cactus corresponds to the underlying bond on the Bethe lattice. Neighboring sites correspond to neighboring bonds. Consequently, the configurational generating function

$$xy^4+2x^2y^5+(14/3)x^3y^6+\cdots$$

per site or per bond, respectively, is the same for both problems. The critical probabilities are, therefore, identical as are all other properties.

Clearly this *bond-to-site* transformation can be applied to any suitably related pair of lattices. Thus, the expanded cactus of Fig. 1(c) can be derived from the decorated $(\sigma=2)$ Bethe lattice shown in Fig. 4(a) by identifying bonds on the decorated lattice with sites of the expanded cactus. Hence, the site problem on the expanded cactus is identical with the bond problem on the decorated Bethe lattice. By Eqs. (49) and (55), the critical probability for the two problems is $p_c=2^{-\frac{1}{2}}$.

In the same way, the bond problem on the plane honeycomb lattice, coordination number three, is isomorphic with the site problem on the plane kagomé lattice, coordination number four (reference 11, p. 187). At present, however, neither of these problems is soluble in closed form.

VIII. FURTHER GENERALIZATION

The multivariable generating function $H(t,u,v',c)$ defined in (66) enumerates on the $\sigma=2$ Bethe lattice configurations with a specified number of triple points, double points, single points, and bonds. Now, since the coordination number is 3, each triple point is associated with *no* unoccupied perimeter bonds, each double point is associated with *one* unoccupied bond, and each single point with *two* unoccupied bonds (and *one* occupied bond). Accordingly, if the substitutions $t=1$, $u=y$, $v'=xy^2$, and $c=x$ are made, the generating function $H(t,u,v',c)$ will merely classify cluster configurations by the total numbers of the internal bonds and of the perimeter bonds. But this is just what the configurational generating function for the simple problem does. In other words,

$$K^B(x,y)=H(1,y,xy^2,x)+\tfrac{2}{3}y^3+xy^4, \qquad (82)$$

where the last two terms account for the single site and single bond which are not included in H. If this expression is combined with (73), one obtains

$$H(t,u,v',c)=tH\left(1,\frac{v'}{1-2uc},\frac{tcv'^2}{(1-2uc)^3},\frac{tc}{1-2uc}\right)+\frac{2}{3}\frac{tv'^3}{(1-2uc)^3}+\frac{t^2cv'^4}{(1-2uc)^5}+\frac{2uv'^2}{(1-2uc)} \qquad (83)$$

and

$$K^B(x,y)=K^B\left(\frac{x}{1-2xy},\frac{xy^2}{1-2xy}\right)+\frac{2xy^4}{1-2xy}+\tfrac{2}{3}y^3. \qquad (84)$$

The first relation re-expresses $H(t,u,v',c)$ in a reduced form independent of its first argument. If we set $t=1$, (83) reduces to a functional equation for $H(1,u,v',c)$ which is equivalent to the functional relation (84) for $K^B(x,y)$. By Eq. (20), this may also be transformed into a functional equation for $B_2(z)$, namely,

$$B_2(z)=\frac{z^3}{(1-2z)^3}B_2\left[\frac{z^2}{(1-2z)^2}\right]+\frac{z}{1-2z}+\frac{2}{3}. \qquad (85)$$

This equation does not seem easy to solve directly in closed form although it defines $B_2(z)$ uniquely for small z as may be seen by assuming the power series expansion for $B_2(z)$ and determining successive coefficients by comparing like powers of z. It is easily verified, however, that the correct solution is provided by (35d).

When one attempts to generalize the foregoing approach to the site decoration of a Bethe lattice of coordination number 4, one is lead to introduce a generating function which enumerates configurations by number of quadruple points as well as by triple points, double points, etc. The terms in this generating function may be set in correspondence with configurations on the $\sigma=2$ and $\sigma=3$ Bethe lattices. The principle of the argument is the same as in Sec. VI, but is more involved and will not be presented. If s and t are the enumerating symbols for quadruple points and triple points, respectively, the result may be expressed most compactly by introducing the generating function $J_3(s,t;z)$ which reduces to $B_3(z)$ when $s=1$ and $t=1$. For this function we obtain in analogy to (83) the relation

$$J_3(s,t;z)=sz_1^4J_3(1,t^*;z^*)+z_0^3B_2(3tz_0^2)+z_0+\tfrac{1}{2}, \qquad (86)$$

where

$$\begin{aligned} z_0&=z/(1-3z),\\ z_1&=[1-(1-12tz_0^2)^{\frac{1}{2}}]/6tz_0,\\ z^*&=sz_0z_1^2/(1-6tz_0z_1),\\ t^*&=(t+sz_1)/sz_1. \end{aligned} \qquad (87)$$

When one sets $s=1$, the relation (86) reduces to a functional equation in *two* variables for $J_3(1,t;z)$. This equation may be solved in a double power series, but owing to its complexity, we have not been able to solve it in closed form. Consequently, it is not possible, for example, to give explicit expressions for the cluster size on such pseudolattices as the square Husimi tree.

Although we cannot give explicit formulas for all lattices derivable from the Bethe lattices by site and bond decorations, there seems no reason to doubt that the nature of the critical singularities will be the same in all cases. This seems to be connected with the infinite-dimensional and multiplicative properties of the Bethe lattices and their derivatives. By analogy with the behavior of other statistical lattice problems, such as the Ising model, one would expect the critical singularities to be sharper for the normal lattices in two and three dimensions than for the Bethe lattices. Thus, at $p=p_c$ the gradient dR/dp might well be infinite and the mean cluster size density might diverge as $|p-p_c|^{-\alpha}$ with α greater than unity. The sharpness would be expected to fall off with increasing dimension and approach the present results in the limit. Rigorous confirmation of these conjectures must await a comprehensive attack on the problem for the standard lattices, but some indication of their validity can be obtained from a numerical study of the initial terms of the configurational series.[13]

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