impurity effects; the above values of q and P must thus be considered as upper limits. A small "nuclear" term found in the specific heat of ytterbium[5] was attributed to impurities since the crystal structure of this metal is cubic and quadrupole interactions with the crystalline field are thus identically zero.

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Ising Model and Self-Avoiding Walks on Hypercubical Lattices and "High-Density" Expansions

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The high-temperature expansions of the partition function Z and susceptibility χ of the Ising model and the number of self-avoiding walks c_n and polygons p_n are obtained exactly up to the eleventh order (in "bonds" or "steps") for the general d-dimensional simple hypercubical lattices. Exact expansions of $\ln Z$ and χ in powers of $1/q$ where $q=2d$, and $1/\sigma$ where $\sigma=2d-1$, for $T>T_0$ are derived up to the fifth order. The zero-order terms are the Bragg–Williams and Bethe approximations, respectively. The Ising critical point is found to have the expansion

$$\theta_c=kT_c/2dJ=1-q^{-1}-1\tfrac{1}{3}q^{-2}-4\tfrac{1}{3}q^{-3}-21\frac{34}{45}q^{-4}-133\frac{14}{15}q^{-5}-\cdots,$$

while for self-avoiding walks

$$\mu=\lim_{n\to\infty}|c_n|^{1/n}=\sigma[1-\sigma^{-2}-2\sigma^{-3}-11\sigma^{-4}-62\sigma^{-5}-\cdots].$$

Numerical extrapolation yields accurate estimates for θ_c and μ when $d=2$ to 6 and indicates that χ diverges as $(T-T_c)^{-[1+\delta(d)]}$ where

$$3/\delta(d)\simeq 4,\,12,\,32\pm1,\,80\pm2,\,188\pm12,\cdots\quad(d=2,3\cdots),$$

and that $c_n\approx An^{\alpha}\mu^n$ $(n\to\infty)$ with

$$1/\alpha(d)\simeq 3,\,6,\,14\pm0.3,\,32\pm1.5,\,72\pm7,\cdots.$$

1. INTRODUCTION

An interesting conclusion that has emerged from the study of phase transitions in lattice systems is that the nature of the singularities characterizing the transition point are chiefly dependent on the dimensionality of the lattice. Thus, one-dimensional systems (with finite ranged forces) show no transitions, while all two-dimensional Ising models (at least those with nearest-neighbor interactions) have logarithmically divergent specific heats at T_c.[1–3] More strikingly, it has been shown that the ferromagnetic susceptibility of the Ising model diverges at the critical point as

$$\chi(T)\approx C/(T-T_c)^{1+\delta}, \qquad (1.1)$$

where $\delta=\frac{3}{4}$ in two dimensions[4] and $\delta=\frac{1}{4}$ in three dimensions.[5–8] Approximate theories of the mean-field type always predict $\delta=0$.[3] Intuitive considerations, however, do suggest that $\delta(d)$ should decrease with dimension and approach this mean-field value as $d\to\infty$. This line of thought is supported by the recent development[9–11] of schemes for expanding the partition functions of interacting systems in inverse powers of a 'coordination parameter' z which is probably best regarded as a measure of the range of the interaction.[12,13]

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[3] C. Domb, Advan. Phys. **9**, Nos. 34 and 35 (1960). This is an important review of work on the Ising model.
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[5] C. Domb and M. F. Sykes, Proc. Roy. Soc. (London) **A240**, 214 (1957).
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[7] G. A. Baker, Jr., Phys. Rev. **124**, 768 (1961).
[8] For the Heisenberg model in three dimensions, the index δ is apparently $\frac{1}{3}$, see C. Domb and M. F. Sykes, Phys. Rev. **128**, 168 (1962).
[9] R. Brout, Phys. Rev. **118**, 1009 (1960); *ibid.* **122**, 469 (1961).
[10] G. Horwitz and H. B. Callen, Phys. Rev. **124**, 1757 (1961).
[11] R. B. Stinchcombe, G. Horwitz, F. Englert, and R. Brout, Phys. Rev. **130**, 155 (1963).
[12] G. A. Baker, Jr., Phys. Rev. **126**, 2071 (1962); *ibid.* **130**, 1406 (1963).
[13] A. F. J. Siegert (to be published) and in *Statistical Physics*, 1962 Brandeis Lectures (W. A. Benjamin, Inc., New York, 1963).

In these 'high-density' expansion methods the leading term is the mean-field (Bragg-Williams) approximation. Higher order terms, however, become increasingly singular and it is fair to say that the validity and significance of this approach are not yet quite clear.

A problem closely related to lattice statistics is that of the number, c_n, and other properties of self-avoiding walks on lattices.[14] Such walks are also of interest in their own right as a model of polymer molecules with 'excluded-volume' and as a simple non-Markoffian process.[15] It has been proved[16] that the limit

$$\mu = \lim_{n\to\infty} |c_n|^{1/n} \tag{1.2}$$

exists but its exact value is not known for any nontrivial lattice. Numerical extrapolations, however, yield estimates for μ (which is the analog of the critical point) and indicate that

$$c_n \approx A n^{\alpha} \mu^n \quad (n \to \infty), \tag{1.3}$$

where the index α [which is analogous to δ in (1.1)] has the value $\frac{1}{3}$ for all simple two-dimensional lattices and the value $\frac{1}{6}$ in three dimensions.[6,14,15,17] Heuristic arguments again suggest that $\alpha(d)$ decreases to zero (the Markoffian value) as $d \to \infty$.

To elucidate the general problem of dependence on dimensionality and coordination number, it seemed worthwhile to investigate the Ising model and self-avoiding walks for lattices of dimensionality higher than three. The results of such a study are presented in this paper. Of course the behavior of model physical systems in four or more space-like dimensions is not directly relevant to comparison with experiment! We can hope, however, to gain theoretical insight into the general mechanism and nature of phase transitions. Indeed for the general d-dimensional simple hypercubical lattices which we have studied ($d=2$ corresponds to the plane-square lattice, $d=3$ to the simple cubic lattice) it proves possible to expand the Ising partition function and susceptibility above T_c in inverse powers of d, the coefficients being closed expressions in T. Similar expansions may also be derived for the generating functions for self-avoiding polygons and walks. More surprisingly one may also obtain $(1/d)$ expansions for the critical temperature itself and for the walk limit μ. [These are given explicitly in Eqs. (5.18) and (5.28) to (5.30) below.] The zeroth order terms in these $(1/d)$-expansions are found to correspond to the Bragg-Williams approximation. On the other hand, if the expansions are made in the variable $(1/\sigma)$ where $\sigma=2d-1$, the leading terms correspond to the Bethe approximation.

To obtain these expansions we have calculated the number of self-avoiding walks $c_n(d)$ for all d and for $n=1$ to 11, and the first eleven high-temperature expansion coefficients of the Ising susceptibility for all d (and corresponding terms for the partition function). Extrapolation of the numerical values of these coefficients in the now standard ways[6,7,15,18] yields accurate values of μ and of the critical points for d up to six. Corresponding estimates for the indices $\alpha(d)$ and $\delta(d)$ may then also be obtained. These indices are found to approach zero rapidly—apparently exponentially fast—as d increases. (Unfortunately they do not seem to obey any obvious simple formula!) The behavior of the specific heats at the transition and the probability of a self-avoiding return to the origin can also be estimated.

The arrangement of the paper is as follows. In Sec. 2 the notation and formulation of the problems are summarized. The way in which the number of dimensions enter is described in Sec. 3, while the detailed enumeration problem is discussed in Sec. 4. Expressions valid for all d are given and numerical values are tabulated for $d=2$ to 6. In Sec. 5 these results are used to derive the expansions in $(1/d)$ and $(1/\sigma)$. The numerical extrapolations are described in Sec. 6 where estimates of the critical points, indices etc. are tabulated. Finally, the results are discussed briefly in Sec. 7.

2. NOTATION AND FORMULATION

We consider a d-dimensional simple hypercubical lattice whose sites are given by the points $\mathbf{r}=(r_1,r_2,\cdots r_d)$ where the integer coordinates r_j take all possible combinations of positive or negative values. (For a finite toroidal lattice of $N=L^d$ sites the r_i are identified modulo L.) Each site has

$$q=2d \tag{2.1}$$

nearest-neighbor sites corresponding to the d Cartesian axes of the lattice. The parameter q is thus the coordination number but, since we are considering only one class of lattices, it is tied to the dimensionality.[19] It is convenient to define

$$\sigma = q-1 = 2d-1. \tag{2.2}$$

Self-Avoiding Walks

Let $c_n=c_n(d)$ denote the number of distinct n-step walks starting at the origin and consisting only of nearest-neighbor steps which never visit the same lattice point twice and let $u_n=u_n(d)$ be the corresponding number of returns to the origin, i.e., self-avoiding

[14] M. E. Fisher and M. F. Sykes, Phys. Rev. **114**, 45 (1959).
[15] M. E. Fisher and B. J. Hiley, J. Chem. Phys. **34**, 1253 (1961).
[16] J. M. Hammersley, Proc. Cambridge Phil. Soc. **53**, 642 (1957).
[17] M. F. Sykes, J. Chem. Phys. **39**, 410 (1963).
[18] J. W. Essam and M. E. Fisher, J. Chem. Phys. **38**, 802 (1963).
[19] It would clearly be desirable to investigate a wider class of d-dimensional lattices. A number of families of such lattices are known, see: E. S. Barnes, Acta Arithmetica **5**, 57 (1958), E. S. Barnes and G. E. Wall, J. Australian Math. Soc. **1**, 47 (1959–60). In the first instance, however, it seems reasonable to consider only the simple hypercubical lattices which at least for low d are probably not seriously atypical.

walks which close on the last step thus forming a polygon. The number of distinct polygons per site of a large lattice[20] is then given by

$$p_n = u_n/2n. \tag{2.3}$$

In the present case, of course, $p_n \equiv u_n \equiv 0$, if n is odd. To the leading order c_n and u_n behave asymptotically as μ^n where the limit

$$\mu = \mu(d) = \lim_{n\to\infty} |c_n|^{1/n} \tag{2.4}$$

is known to exist[16] and be equal to[21] $\lim |u_{2m}|^{1/2m}$ $(m \to \infty)$ for d finite. It is sometimes convenient to regard c_n (and similarly u_n and p_n) as the expansion coefficients of the generating function

$$C(z) = 1 + \sum_{n=1}^{\infty} c_n z^n. \tag{2.5}$$

The asymptotic behavior of c_n is then determined by the singularities of $C(z)$ nearest to the origin. By (2.4) the dominant singularity is on the real positive axis at

$$z = z_c = 1/\mu. \tag{2.6}$$

Ising Model

We consider the Ising model for spin $\frac{1}{2}$ with nearest-neighbor interactions only, specified by the Hamiltonian

$$\mathcal{H} = -J \sum_{(ij)} s_i s_j - mH \sum_i s_i, \tag{2.7}$$

where $s_i = \pm 1$, m is the magnetic moment per spin and H the magnetic field. The second sum runs over all N lattice sites and the first sum runs over all nearest-neighbor pairs. To effect a fair comparison between different lattices the interaction energy per spin in the lowest energy state should be constant. This condition can be met by normalizing the 'exchange' energy J according to

$$J = J(d) = J_0/q = J_0/2d, \tag{2.8}$$

and holding J_0 fixed. The corresponding dimensionless temperature variable is then

$$\theta = kT/qJ = kT/J_0. \tag{2.9}$$

The partition function and susceptibility per spin in zero field ($H=0$) may be expanded at high temperatures most conveniently in terms of the variable

$$v = \tanh(J/kT) = \tanh(1/q\theta). \tag{2.10}$$

The expansions are

$$\ln Z(T) = \lim_{N\to\infty} \frac{1}{N} \ln Z_N(T)$$

$$= \ln 2 + \tfrac{1}{2} q \ln \cosh(J/kT) + \sum_{n=3}^{\infty} g_n v^n \tag{2.11}$$

and

$$\chi(T) = (m^2/kT)[1 + \sum_{n=1}^{\infty} a_n v^n], \tag{2.12}$$

where, as is well known,[3] g_n and a_n are the number of distinct graphs of n lines per site of the lattice[22] constructed according to the rules:

(a) the lines of the graph lie on the nearest-neighbor bonds of the lattice and no more than one line may lie on any bond;

(b) for the partition function each vertex of a graph must be even, i.e., the join of an even number of lines;

(c) for the susceptibility there must be one odd vertex at the origin and one at some (any) other site. All other vertices must be even.

The graphs contributing to g_n thus consist of a polygon or a number of separated polygons or polygons touching at vertices but with no common bonds. Similarly, the contributions to a_n come from a chain of bonds connecting the origin to the second odd vertex (this chain forming a self-avoiding walk of n or less steps) together with separated or touching polygons.

In zero field, ferromagnetic lattices ($J>0$) in two or more dimensions undergo a phase transition at the critical temperature T_c. (It might be remarked that this has only been proved rigorously for certain two-dimensional lattices!) The transition point may be defined (for a ferromagnet) by the divergence of the susceptibility to $+\infty$ and hence by the divergence of the series (2.12) i.e.,[23]

$$\omega = \omega(d) = \lim_{n\to\infty} |a_n|^{1/n} \tag{2.13}$$

$$= 1/v_c = 1/\tanh(1/q\theta_c),$$

so that

$$\theta_c = 1/d \ln[(\omega+1)/(\omega-1)]. \tag{2.14}$$

Correspondingly, the asymptotic behavior of the coefficients a_n determines the nature of the singularity in $\chi(T)$ at T_c. In two dimensions it is known rigorously[1,3] that

$$\omega(2) = 1+\sqrt{2}, \quad \theta_c(2) = 0.567296\cdots. \tag{2.15}$$

[20] Consider the total number of distinct n-sided polygons that can be traced out on a toroidal lattice of $N=L^d$ sites when $L>n$. If this number is $P_n(L)$ then $p_n = P_n(L)/L^d$, which is independent of L for $L>n$ since no polygon can loop the torus. Each distinct polygon can be traced in two directions starting from any one of its n vertices and so corresponds to $2n$ of the u_n self-avoiding returns to a fixed point.

[21] J. M. Hammersley, Proc. Cambridge Phil. Soc. 57, 516 (1961).

[22] The phrase 'per site of the lattice' implies that the total number of distinct graphs on a torus of N sites is expressed as a polynomial in N (which is always possible if the torus is sufficiently large that it cannot be looped by connected components of the graph considered) and that only the coefficient of N is retained. If the graph is connected this is the only nonzero coefficient but disconnected graphs yield higher powers.

[23] Strictly we should have here 'lim sup' rather than 'lim' but the expansion coefficients are found to be sufficiently regular that the two limits agree.

3. ENUMERATION IN d DIMENSIONS

The general problem of enumerating the number of self-avoiding walks and polygons and of calculating the expansion coefficients g_n and a_n has previously been considered in detail for two- and three-dimensional lattices.[3,14,24,25] It depends finally on the calculation of the values of the *lattice constants*[3,24] of the necessary nonreducible graphs of n or fewer lines. (The *lattice constant* of a particular connected graph is the number of distinct ways it can be embedded in the lattice per site of the lattice.[20,22])

The new feature of the present problem is that the dimensionality is larger than three and we wish to obtain results valid for *arbitrary d*. Fortunately, in the case of the simple hypercubical lattices this difficulty can be overcome as follows. Consider a self-avoiding walk of n steps. If $d>n$ the walk can extend at most into a subspace of n dimensions (each step being directed into a new dimension i.e., parallel to a new lattice axis). Some of the walks, however, will extend only into $l=n-1,\ n-2,\ \cdots 3,\ 2$, or 1 dimensions. Suppose $c_{n,l}$ is the number of n step (self-avoiding) walks in l dimensions which extend into the full l-dimensional space. The number of distinct ways such a walk could be embedded in a hypercubical lattice of higher dimension d is given by the binomial coefficient $\binom{d}{l}$ since this is just the number of ways of choosing a set of l dimensions from the total number d. Thus, the number of walks in d dimensions that extend into an l-dimensional subspace but not into one of the higher dimension is $c_{nl}\binom{d}{l}$. Summing over all the distinct possibilities $l=1,\ 2,\ \cdots d$ yields

$$c_n(d)=\sum_{l=1}^{n} c_{nl}\binom{d}{l}. \tag{3.1}$$

The calculation of $c_n(d)$ for all d is thus reduced to the evaluation of the n integral coefficients $c_{n1},\ c_{n2},\ \cdots c_{nn}$. Conversely, if the values of $c_n(d)$ are known for $d=1,\ 2,\ \cdots n$, the Eqs. (3.1) can be solved successively to yield the c_{nl} and, hence, $c_n(d)$ for $d>n$.

By setting $d=\frac{1}{2}(\sigma+1)$ or $d=\frac{1}{2}q$ and expanding the binomial coefficients one may alternatively express $c_n(d)$ as a polynomial in σ or q of degree n, namely,

$$c_n(d)=\sum_{t=0}^{n} C^{\sigma}{}_{nt}\sigma^t=\sum_{t=1}^{n} C^{q}{}_{nt}q^t. \tag{3.2}$$

The lower limit in the second sum is $t=1$ (rather than $t=0$) since each binomial coefficient has a factor $d=\frac{1}{2}q$ so that $C^{q}{}_{n0}$ must vanish. In general, however, $C^{\sigma}{}_{n0}$ will not vanish.

The above arguments may obviously be generalized to the case of graphs with closed loops. Thus, a closed walk of $2m$ steps can extend at most into m dimensions since for each step along a given axis there must be a complementary step parallel to the same axis but of opposite sense. Consequently, we have

$$u_{2m}(d)=\sum_{l=2}^{m} u_{2m,l}\binom{d}{l}, \tag{3.3}$$

where $u_{2m,l}$ is the number of closed walks of $2m$ steps in l dimensions which extend into all l dimensions. The lower limit is $l=2$ since there are clearly no closed self-avoiding walks in one dimension. As before one also has

$$u_{2m}(d)=\sum_{t=0}^{m} U^{\sigma}{}_{2m,t}\sigma^t=\sum_{t=1}^{m} U^{q}{}_{2m,t}q^t \tag{3.4}$$

and similar expressions for the number of polygons $p_{2m}(d)$.

As a simple example consider p_4, the number of squares per site of the lattice. To describe a square from one of its corners we need (a) to choose the lattice site on which the corner resides, (b) to choose two orthogonal directions for the sides of the square which can be done in $\binom{d}{2}$ ways, and (c) select one of the 2×2 possible senses along the chosen axes. Since each square has four identical corners from which it might be described we conclude that

$$p_4=\tfrac{1}{4}\times2\times2\binom{d}{2}=\binom{d}{2}. \tag{3.5}$$

This result could have been found directly on the basis of the previous arguments, however, by observing that the number of self-avoiding returns of 4 steps on the plane-square lattice is simply $u_4(2)=8$ so that $p_4(2)=p_{4,2}=\frac{1}{8}u_4(2)=1$ from which (3.5) follows by the analog of (3.3).

Similar arguments clearly apply to graphs like the simple 'figure eight' [see Fig. 1(a)]

$$p_{n,x}=(r,s)_8,\quad r+s=n \tag{3.6}$$

and to more closely connected graphs of n lines which

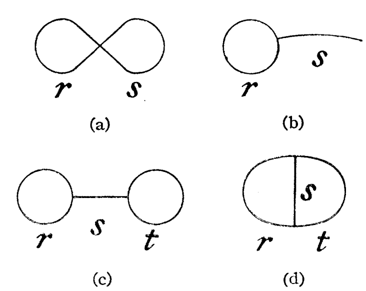

FIG. 1. Connected graphs (a) simple figure eight; (b) tadpole; (c) dumbbell; (d) star figure eight.

[24] C. Domb and M. F. Sykes, Phil. Mag. 2, 733 (1957); C. Domb and M. E. Fisher, Proc. Cambridge Phil. Soc. 54, 48 (1958).

[25] M. F. Sykes, J. Math. Phys. 2, 52 (1961).

can fill out fewer than $\frac{1}{2}n$ dimensions. For example, the number of cubes (3-cubes) in d dimensions is simply

$$p_{12,\text{cube}}=\binom{d}{3}. \tag{3.7}$$

On the other hand, the lattice constants for more open graphs like the 'tadpole' [see Fig. 1(b)]

$$p_{n,x}=(r,s)_T, \quad r+s=n \tag{3.8}$$

and the 'dumbbell' [see Fig. 1(c)]

$$p_{n,x}=(r,s,t)_D, \quad r+s+t=n \tag{3.9}$$

can be expressed in the forms (3.1) or (3.3) but with upper limits $n-\frac{1}{2}r$ and $n-\frac{1}{2}(r+t)$, respectively, $(r, t=4, 6, 8,\cdots)$. For the important irreducible 'star figure eights' [see Fig. 1(d)]

$$p_{n,x}=(r,s,t)_S, \quad r+s+t=n \tag{3.10}$$

the corresponding upper limits are only $\frac{1}{2}(r+s+t-1)=\frac{1}{2}n-\frac{1}{2}$ if all r, s, t are odd, or $\frac{1}{2}(r+s+t-2)=\frac{1}{2}n-1$ if r, s, t are even. (These are the only possibilities on the simple cubical lattices since $r+s$, $s+t$ and $t+r$ must clearly be even integers greater than 3.)

Since the high-temperature expansion (2.11) for the Ising partition function involves only combinations of polygons, the same arguments show that the general coefficient $g_{2m}(d)$ may also be written in the forms (3.3) and (3.4), i.e., with upper limit m. Similarly, the susceptibility expansion coefficients $a_n(d)$, since they involve the open chain (or walk) of n steps, as well as closed configurations can be expressed as in (3.1) or as in (3.2) i.e., as a polynomial in σ or q of degree n. The possibility of expanding the partition function and the susceptibility in powers of $(1/\sigma)$ and $(1/q)$ stem directly from this conclusion.

4. CONFIGURATIONAL CALCULATIONS

In this section we outline the way in which the coefficients p_n, c_n, g_n, and a_n have been calculated for arbitrary d up to $n=11$. The reader who is prepared to take the results on trust [see Eqs. (6), (10), (14), (19), (20), (23) to (25) and Tables I to VI] and who is uninterested in the combinatorial details will lose little by omitting this section.

The most difficult nonreducible lattice constant to calculate is probably p_n the number of n-step polygons. We have used the method devised by Domb and Sykes.[3,24] First, we calculate $r_n(d)$ the number of returns of a walk which is allowed to make all possible self-intersections. Then

$$r_n(d)=\text{Coefficient of 1 in }\Big[\sum_{i=1}^{d}(x_i+x_i^{-1})\Big]^n \tag{4.1}$$

and so

$$r_{2m}(1)=\binom{2m}{m}, \quad r_{2m}(2)=\binom{2m}{m}^2. \tag{4.2}$$

The recurrence relation

$$r_{2m}(d+1)=\sum_{t=0}^{m}\binom{2t}{t}\binom{2m}{2t}r_{2(m-t)}(d) \tag{4.3}$$

and a similar one for $r_{2m}(d+2)$ in terms of $r_{2m'}(d)$ follows easily from the generating function (4.1) and provides the simplest method of computing the $r_{2m}(d)$ for higher d.

Second, we require $q_n(d)$ the numbers of n step returns with no immediate reversals (but other self-intersection allowed). These may be calculated recursively from $r_{2m}(d)$ by the relation

$$q_{2m}(d)-2(d-1)$$
$$=r_{2m}(d)-\sum_{s=1}^{m}\binom{2m}{s}\sigma^s[q_{2(m-s)}(d)-2(d-1)] \tag{4.4}$$

established by Domb and Fisher.[24] The number of polygons (or self-avoiding returns) can now be derived by subtracting off the relatively few possible types of intersections included in the q_n. The simplest of these consist of chains of lower order polygons touching at vertices and are reducible in terms of products of the q_l $(l<n)$. There remain a few nonreducible possibilities such as the star figure eights [(3.10) and Fig. 1(d)]. The appropriate reduction formulas as far as p_{10} on a general 'loose-packed' lattice have been given explicitly by Sykes (see p. 311 of the review article by Domb.[3])

Fortunately, many of the irreducible lattice constants for the hypercubical lattices are zero because the fundamental stars $p_{6a}=(2,2,2)_S$ and $p_{8r}=(2,2,2,2)_S$ vanish (using the notation of Domb.[3]) These constants are nonzero, for example, on the body-centered cubic lattice. Thus, the only nonvanishing constant required to calculate p_4 to p_{10} is the star $(2,2,4)_S$. By the type of argument used to calculate p_4 in Eq. (3.5) it is not difficult to see that

$$p_{8c}=(2,2,4)_S=24\binom{d}{3}. \tag{4.5}$$

Alternatively, since from the results of the previous section, the constant cannot extend into a space of more than three dimensions, this formula could be written down from the known results for the plane square $(d=2)$ and simple cubic $(d=3)$ lattices.[26]

In this way the values of $p_4(d)$ to $p_{10}(d)$ have been calculated numerically for $d=2$ to 8. The values for $d=2$ to 5 suffice to calculate the binomial expansion coefficients in the analog of Eq. (3.3) and these may then be checked by the values for larger d. We obtain

[26] Tables of lattice constants for many two- and three-dimensional lattices are tabulated by Domb (Ref. 3), pp. 345–360.

TABLE I. Number of self-avoiding returns, $u_n(d)$.

n	$d=2$	3	4	5	6
2	4	6	8	10	12
4	8	24	48	80	120
6	24	264	912	2160	4200
8	112	3 312	22 944	82 720	216 720
10	560	48 240	652 320	3 737 120	13 594 320
12	2976	762 096			
14	16 464	12 673 920			

[in addition to Eq. (3.5)]

$$p_6=2\binom{d}{2}+16\binom{d}{3},$$

$$p_8=7\binom{d}{2}+186\binom{d}{3}+648\binom{d}{4},$$

$$p_{10}=28\binom{d}{2}+2328\binom{d}{3}+23136\binom{d}{4}+47616\binom{d}{5}. \quad (4.6)$$

The corresponding numerical values of the returns $u_n=2np_n$ are given in Table I for $d=2$ to 6. The tabulated values $u_2(d)=2d$ are, of course, purely conventional. The results for $n=12$ and 14 are taken from the known results for $d=2$ and 3 which extend to $u_{16}(2)=94\,016$, $u_{18}(2)=549\,648$, and $u_{16}(3)=218\,904\,768$.[15,27]

To calculate the coefficients $g_n(d)$ for the partition function expansion we need, in addition to the polygons $p_n(d)$, the contributions from separated and touching polygons. These may be reduced in terms of the p_n and a few further stars. The general formulas up to $n=10$ have also been given by Sykes.[28] In our case the only further stars required are

$$p_{7a}=(3,1,3)_S=2\binom{d}{2}+12\binom{d}{3}, \quad (4.7)$$

$$p_{9k}=(3,1,5)_S=12\binom{d}{2}+288\binom{d}{3}+768\binom{d}{4}, \quad (4.8)$$

and

$$p_{10b}=(3,1,3,3)_S=0\binom{d}{2}+12\binom{d}{3}+32\binom{d}{4}. \quad (4.9)$$

Although the last two of these have contributions from configurations which can arise only in four dimensions they are quite easy to calculate combinatorially since essentially one merely has to find the number of ways of placing a square 'flap' on the side of a hexagon (for p_{9k}) or on the 'hinge' joining two similar flaps (for p_{10b}). The constant p_{7a} can be calculated by either of the methods previously described for p_{8c}. The explicit results for the nonzero g_n are found to be

$$g_4=\binom{d}{2},$$

$$g_6=2\binom{d}{2}+16\binom{d}{3},$$

$$g_8=4\tfrac{1}{2}\binom{d}{2}+174\binom{d}{3}+648\binom{d}{4},$$

$$g_{10}=12\binom{d}{2}+1944\binom{d}{3}+22304\binom{d}{4}+47616\binom{d}{5}. \quad (4.10)$$

The configurational energy of the Ising lattice has the high-temperature expansion

$$-U(T)/J=\sum_{n=1}^{\infty} h_n v^n, \quad (4.11)$$

where the coefficients $h_n(d)$ may be derived by differentiating the partition function (2.11) with respect to v and multiplying by $(1-v^2)$. The numerical values of the nonvanishing $h_n(d)$ are presented in Table II for $d=2$ to 6. The series $h_n(2)$ could be continued indefinitely by using Onsager's exact solution.[1] The terms $h_n(3)$ are, of course, already known.[3]

TABLE II. Coefficients $h_n(d)$ for the high-temperature expansion of the energy [see Eq. (4.11)].

n	$d=2$	3	4	5	6
1	2	3	4	5	6
3	4	12	24	40	60
5	8	120	432	1040	2040
7	24	1368	10 512	39 120	104 040
9	84	18 300	290 552	1 746 760	6 487 020
11	328	268 728			
13	1372	4 180 860			

To calculate the number c_n of open self-avoiding walks we follow Sykes and Fisher[14,25] and use the counting theorem which expresses c_n in terms of lower order walks, polygons, simple and star figure eights and dumbbells [see Eqs. (3.6) to (3.10)]. This is derived by adding a step in σ ways to one end of an n-step self-avoiding walk thus forming either an $(n+1)$-step walk, a tadpole, or a closed walk (polygon). In a similar way adding a step to the tail of a tadpole yields either a tadpole of higher order, a dumbbell, or a figure eight. Collecting terms yields the relations

$$c_n=2\sigma c_{n-1}-\sigma^2 c_{n-2}+d_n, \quad n=3,4,5,\cdots$$
$$c_1=\sigma+1, \quad c_2=\sigma(\sigma+1), \quad (4.12)$$

[27] G. S. Rushbrooke and J. Eve, J. Math. Phys. 3, 185 (1962).
[28] Ref. 3 page 321. Our g_n is denoted $p(n)$.

where the 'correction coefficients' are

$$d_n = 8\sum_n (r,s,t)_D + 8\sum_n (r,s)_8 + 12\sum_n (r,s,t)_S + u_{n-1} - u_n, \quad (4.13)$$

in which the sums are over all graphs of specified type with $r+s+t=n$.

For large n the most important lattice constants are the dumbbells, in particular the leading dumbbells $(4, n-8, 4)_D$ which extends at most into $n-4$ dimensions, and $(6, n-10, 4)_D$ which extends into $n-5$ dimensions. For $n>9$ none of the other graphs extend as far. Consequently, we may write

$$d_n(d) = \sum_{l=2}^{n-4} \bar{d}_{nl} 2^l l! \binom{d}{l}, \quad (n \geqslant 7), \quad (4.14)$$

where the factor $2^l l!$ has been included for convenience in order to keep the coefficients relatively small. When $n=4$, 5, or 6 the formula still applies but with upper limits 2, 2, and 3, respectively. (For any loose-packed lattice we have $d_3 \equiv 0$.)

To illustrate the technique of calculating the dumbbells and to obtain a result needed in the following section consider the dumbbell $(4, n-8, 4)_D$. It can be described from either end and by (3.5) we have a factor $\binom{d}{2}$ for the number of ways of choosing the square. Onto one of the four corners of this square we may attach a self-avoiding walk of $n-8$ steps (and hence of lower order) which, however, can only set out in $2d-2$ directions. On the last point of the walk we may fix the second square. If one side of this square is in the same direction as the last step, there are $2(d-1)$ possibilities for the plane of the square, but if the square is orthogonal to the last step there are $\frac{1}{2}(d-1)(d-2)\times 2\times 2$ distinct possibilities making $2(d-1)^2$ in all. Collecting up factors we obtain

$$(4, n-8, 4)_D = \tfrac{1}{2}\binom{d}{2} 4\times 2(d-1)\frac{c_{n-8}}{2d} 2(d-1)^2 - \Sigma^* \quad (4.15)$$

where Σ^* is the weighted sum of all those configurations of n or fewer lines which can be formed by the possible interactions or overlaps of the walk with either square, or of the squares with each other, etc. Since such configurations will have at least one extra closed loop of at least four steps they can extend at most into $n-4-\frac{1}{2}(4)$ dimensions and, hence, are of order d^{n-6} or less. To corresponding order we may similarly replace c_{n-8} by $2d(2d-1)^{n-9} = q\sigma^{n-9}$. From (4.15) we thus derive for general n

$$(4, n-8, 4)_D = \tfrac{1}{8} q\sigma^{n-5}\{1 - (4/\sigma) + O[1/\sigma^2]\} \quad (n \geqslant 9). \quad (4.16)$$

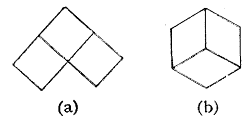

FIG. 2. p_{10s} and p_{9q}.

An entirely parallel analysis yields

$$(6, n-10, 4)_D = q\sigma^{n-6}\{1 + O(1/\sigma)\}, \quad (n \geqslant 11). \quad (4.17)$$

The factors $q=2d$ are left in front for later convenience.

For large n the complete enumeration of all the terms in Σ^* and their weights is difficult but for $n=11$ (or even 12) it is accomplished quite easily by careful exhaustion of the possibilities. There are in fact relatively few realizable cases and the task is eased by first constructing the tadpole $(4, n-8)_T$. For $n=10$, for example, we need only the constants

$$p_{10s} \text{ and } p_{9q} \text{ (see Fig. 2)} \quad (4.18)$$

which are easy to calculate directly.

The most troublesome configurations are the higher order stars $(r,s,t)_S$ since these, being relatively more open, are more numerous than configurations like (4.18). At order $n=11$ the star $(3,1,7)_S$ may be calculated by placing a square flap on a polygon p_8 and subtracting off possible intersections. Along similar lines $(5,1,5)_S$ is obtained by considering all possible configurations of two hexagons hinged onto a common bond. (There are three 'space types' of hexagon, namely 'flat', 'bent' and 'twisted'!) Finally, $(3,3,5)_S$ can be calculated by careful drawing of all five-step 'bridges' across the main diagonals of all types of hexagon.

In total the numbers of nonzero lattice constants needed to order $n=11$, in addition to the polygons, are 1 of order seven, 2 of order eight, 4 of order nine, 9 of order ten, and 10 of order eleven. (These numbers include a few lattice constants needed only for the susceptibility; see below.)

Collecting the relevant terms, after expressing each lattice constant in binomial form, yields the correction coefficients $\bar{d}_{n,l}$ and, thence, by (4.12) the number of walks c_n. To economize space only the coefficients $\bar{d}_{n,l}$ are tabulated (in Table III) while the numerical values of the $c_n(d)$ for $d=2$ to 6 are given in Table IV.

TABLE III. Values of the coefficients $\bar{d}_{nl}$ for calculating $c_n(d)$. See Eqs. (4.14) and (4.20).

n	$l=2$	3	4	5	6	7
4	−1					
5	1					
6	−3	−4				
7	6	7				
8	−12	−52	−26			
9	40	167	64	1		
10	−33	−605	−941	−219	1	
11	263	3671	4261	915	40	1

TABLE IV. Number of self-avoiding walks, $c_n(d)$.

n	$d=2$	3	4	5	6
1	4	6	8	10	12
2	12	30	56	90	132
3	36	150	392	810	1452
4	100	726	2696	7210	15 852
5	284	3534	18 584	64 250	173 172
6	780	16 926	127 160	570 330	1 887 492
7	2172	81 390	871 256	5 065 530	20 578 452
8	5916	387 966	5 946 200	44 906 970	224 138 292
9	16 268	1 853 886	40 613 816	398 227 610	2 441 606 532
10	44 100	8 809 878	276 750 536	3 527 691 690	26 583 605 772
11	120 292	41 934 150	1 886 784 200	31 255 491 850	289 455 960 492

From (4.13), (4.16), and (4.17), it follows that the leading contributions to the correction coefficients are

$$d_n(d)=q\sigma^{n-5}+4q\sigma^{n-6}+O(q\sigma^{n-7})\,,\quad (n\geqslant 11). \tag{4.19}$$

By solving the recurrence relation (4.12) generally the walks are given explicitly in terms of the d_n by

$$c_n(d)=q\sigma^{n-1}+\sum_{k=4}^{n} d_k(n+1-k)\sigma^{n-k}. \tag{4.20}$$

The summation runs only from $k=4$ since $d_3\equiv 0$.

To calculate the susceptibility expansion coefficients $a_n(d)$ we need the n-step self-avoiding walks (or chains) but, in addition, we need all dumbbells, single and 'double-tailed' tadpoles, star figure eights etc., of order n, and combinations of similar connected graphs of lower order with one or more separated polygons. In analogy with the counting theorem (4.12) we may write

$$a_n=2\sigma a_{n-1}-\sigma^2 a_{n-2}+b_n\,,\quad n=3,4,5,\cdots$$
$$a_1=\sigma+1\,,\quad a_2=\sigma(\sigma+1)\,, \tag{4.21}$$

TABLE V. Values of the coefficients $\bar{b}_{nl}$ for calculating $a_n(d)$. [See Eqs. (4.24) and (4.25).]

n	$l=2$	3	4	5	6	7
4	-1					
5	0					
6	-2	-4				
7	2	2				
8	0	-42	-26			
9	26	$97\frac{1}{3}$	$30\frac{2}{3}$	1		
10	59	$-251\frac{1}{3}$	-837	-217	1	
11	242	$2979\frac{1}{3}$	$3077\frac{1}{3}$	654	42	1

where each new correction coefficient b_n will be a weighted sum of *closed* lattice constants (i.e., graphs with 'tails' will *not* appear). General rules for the lattice constants required and expressions for their weights have been found by Sykes.[25] The leading terms for large d again come from dumbbells of order n but dumbbells of two lower orders also occur. Thus, in general,

$$b_n=8\sum_{n}(r,s,t)_D+16\sum_{n-1}(r,s,t)_D+8\sum_{n-2}(r,s,t)_D+\cdots\,, \tag{4.22}$$

where the higher order terms are more closely connected.[29] By (4.16) and (4.17) we then have, in analogy to (4.19),

$$b_n(d)=q\sigma^{n-5}+6q\sigma^{n-6}+O(q\sigma^{n-7})\,,\quad (n\geqslant 11). \tag{4.23}$$

The explicit detailed breakdown of the b_n for $n=1$ to 9 have been published.[30] The formulas for b_{10} and b_{11} follow from the rules given by Sykes.[31] As before, we may write

$$b_n(d)=\sum_{l=2}^{n-4}\bar{b}_{nl}2^l l!\binom{d}{l}\,, \tag{4.24}$$

except that for $n=4$, 5, and 6 the upper limit should be 2, 2, and 3. Further, since $b_3\equiv 0$, we also have

$$a_n(d)=q\sigma^{n-1}+\sum_{k=4}^{n} b_k(n+1-k)\sigma^{n-k}. \tag{4.25}$$

The coefficients $\bar{b}_{nl}$ are presented in Table V while the numerical values of $a_n(d)$ for $d=2$ to 6 will be found in Table VI.

5. EXPANSIONS IN $1/\sigma$ AND $1/q$

Partition Function

The Bethe approximation[3] for an Ising lattice of coordination number $q=\sigma+1$ yields a transition at a critical point given by

$$\tanh(J/kT_c)=v_c=1/\sigma. \tag{5.1a}$$

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[29] The coefficients 8, 16, 8 in Eq. (4.22) find their origin in the factor $8(1+v)^2$ in Eq. (23) of Ref. 25. We are grateful to Dr. M. F. Sykes for confirming this point.

[30] Ref. 3, pp. 323–4. Our b_n is denoted d_n.

[31] We are indebted to Dr. M. F. Sykes for checking the detailed symbolic expressions for b_{10} and b_{11}.

TABLE VI. Expansion coefficients $a_n(d)$ for the susceptibility (note: for $n<5$ $a_n(d)=c_n(d)$, see Table V).

n	$d=2$	3	4	5	6
5	276	3510	18 536	64 170	173 052
6	740	16 710	126 536	568 970	1 884 972
7	1972	79 494	863 720	5 044 810	20 532 252
8	5172	375 174	5 873 768	44 649 930	223 437 852
9	13 492	1 769 686	39 942 184	395 180 650	2 431 526 492
10	34 876	8 306 862	271 009 112	3 494 051 130	26 447 593 812
11	89 764	38 975 286	1 838 725 896	30 893 156 970	287 669 976 492

In terms of the rescaled variable

$$x=\sigma v=\sigma\tanh(J/kT)\,, \qquad (5.1\text{b})$$

the Bethe critical equation is simply $x_c=1$. General considerations suggest that Bethe's approximation might be more accurate the higher the coordination number q and we may test this idea conveniently by re-expressing the true partition function in terms of the variable x.

Now by Eqs. (2.11) and (4.10) we may write down the high-temperature expansion of the partition function in powers of v for general d. (Of course, we are considering only the simple hypercubical lattices.) By the argument of Sec. 3 the coefficient of v^{2m} can be expanded as a polynomial in σ of degree m. Thus,

$$\ln Z=\ln 2+\tfrac{1}{2}(\sigma+1)\ln\cosh(J/kT)+\sum_{m=2}^{\infty}v^{2m}\sum_{t=0}^{m}G^{\sigma}{}_{m,t}\sigma^{t}\,, \qquad (5.2)$$

where the coefficients $G^{\sigma}{}_{mt}$ follow directly from (4.10). On making the substitution $v=x/\sigma$, we thus obtain an expansion in powers of x in which the coefficient of x^{2m} is a polynomial in *inverse* powers of σ of degree $2m$, the lowest order term, however, being of degree m. Regarding the series as a double series in x and $(1/\sigma)$ we may rearrange to obtain an expansion of the partition function in powers of $(1/\sigma)$. (This rearrangement may, of course, be invalid in a region where the double series is not absolutely convergent.) Performing these manipulations we readily derive the result

$$\begin{aligned}\ln Z=\ln 2&+\tfrac{1}{2}(\sigma+1)\ln\cosh(J/kT)\\&+\frac{1}{8}x^4(1/\sigma)^2+\frac{1}{3}x^6(1/\sigma)^3\\&+\left(-\frac{1}{8}x^4-\frac{3}{4}x^6+1\tfrac{11}{16}x^8\right)(1/\sigma)^4\\&+\left(-\frac{1}{3}x^6-9\tfrac{7}{8}x^8+12\tfrac{2}{5}x^{10}\right)(1/\sigma)^5\\&+\left(\frac{3}{4}x^6+13\tfrac{5}{16}x^8-127\tfrac{11}{12}x^{10}+120^{*}x^{12}\right)(1/\sigma)^6\\&+\left(9\tfrac{7}{8}x^8+443\tfrac{5}{6}x^{10}+\cdots\right)(1/\sigma)^7\\&+\left(-15x^8-422\tfrac{5}{6}x^{10}+\cdots\right)(1/\sigma)^8\\&+\left(-456\tfrac{7}{30}x^{10}+\cdots\right)(1/\sigma)^9\\&+\left(550\tfrac{3}{4}x^{10}+\cdots\right)(1/\sigma)^{10}\\&+\cdots,\end{aligned} \qquad (5.3)$$

which is correct to order x^{10} and to order $(1/\sigma)^5$. (The asterisk on the coefficient of x^{12} in the $(1/\sigma)^6$ term indicates that this value is an approximate estimate.)

The first line of this formula, corresponding to $(1/\sigma)\to 0$, is just the result of the Bethe approximation for $T>T_c$ $(x<1)$. In as far as the truncated series in $(1/\sigma)$ is a good representation of $\ln Z$ we are justified in concluding that the Bethe approximation becomes more accurate as $\sigma\to\infty$. It is notable that the first correction term is of order $(1/\sigma)^2$ rather than of order $(1/\sigma)$. If one sets $(1/\sigma)=1$ one discovers that the coefficient of each power of x vanishes identically. This corresponds to the fact that the Bethe approximation is exact for the one dimensional linear chain ($\sigma=1$, $q=2$, $d=1$).

Evidently the coefficient of $(1/\sigma)^p$ is a polynomial in x^2 the term of lowest degree being x^p for p even or x^{p+1} for p odd, and that of highest degree being x^{2p}. Although each coefficient is merely a finite polynomial in x and, hence, is a *nonsingular* function of T, it is clear that the series in $(1/\sigma)$ can only represent the partition function *above* the critical temperature T_c, i.e., only for $x<x_c=x_c(\sigma)$. This suggests strongly that the series in $(1/\sigma)$ for fixed x is divergent if x is large enough. However, we will postpone further discussion of the convergence of (5.3).

The mean-field or Bragg-Williams approximation[3] is even less accurate than the Bethe approximation but is also expected to improve as the coordination number q increases. The Bragg-Williams critical point is given by

$$kT_c/qJ=\theta_c=1\,, \tag{5.4}$$

which suggests expressing the partition function in the variable $\theta=(1/q\tanh^{-1}v)$ and considering an expansion in inverse powers of θ and q [rather than in powers of x and $(1/\sigma)$]. From (5.3), or directly from (2.11) and (4.10), we then find the '$(1/q)$-expansion'

$$\begin{aligned}\ln Z=\ln 2&+\frac{1}{4}\theta^{-2}(1/q)+\frac{1}{8}\theta^{-4}(1/q)^2\\&+\left(-\frac{7}{24}\theta^{-4}+\frac{1}{3}\theta^{-6}\right)(1/q)^3\\&+\left(-1\frac{11}{12}\theta^{-6}+1\frac{11}{16}\theta^{-8}\right)(1/q)^4\\&+\left(2\frac{46}{90}\theta^{-6}-17\frac{7}{24}\theta^{-8}+12\frac{2}{5}\theta^{-10}\right)(1/q)^5\\&+\left(56\frac{57}{80}\theta^{-8}-194\frac{5}{12}\theta^{-10}+120^*\theta^{-12}\right)(1/q)^6\\&+\cdots,\end{aligned} \tag{5.5}$$

which is correct to order $(1/q)$.[5] (As before the asterisk indicates an approximate value.)

As expected the term independent of q is the constant ln2 which is just the Bragg-Williams result *above* T_c (corresponding to a constant configurational energy and zero specific heat). Note, however, that the leading correction term is now of first order.

The coefficient of $(1/q)^p$ is a polynomial in θ^{-2} of degree p but with leading term of order $\theta^{-(p+1)}$ for p odd or $\theta^{-(p+2)}$ for p even. As a function of T the coefficients are thus nonsingular to all orders (except for poles at $T=0$). If we put $1/q=\frac{1}{2}$ and regroup in powers of $(1/\theta)$, we recapture the expansion of $\ln\cosh(1/2\theta)$, the exact result for the linear chain. Similarly putting $1/q=\frac{1}{4}$ and regrouping yields the expansion for the plane-square lattice which is known to converge up to $\theta^{-1}=\theta_c^{-1}=1.762\,747\cdots$ but to display a singularity of type $(\theta-\theta_c)^2\ln|\theta-\theta_c|$ at θ_c.[1]

Self-Avoiding Walks

It is clear that we may perform parallel manipulations on the generating function for self-avoiding polygons. The resulting formulas, however, are not of special interest. Instead we consider now the generating function $C(z)$ for self-avoiding walks [Eq. (2.5)]. The analog of the Bethe approximation for the excluded volume problem is the neglect of all self-intersections except those due to immediate reversals (or 'digons'). This yields the first-order approximation $c_n\simeq q\sigma^{n-1}$ and hence, for the generating function, the approximation

$$\begin{aligned}C(z)&\simeq 1+qz+q\sigma z^2+q\sigma^2z^3+\cdots\\&\simeq 1+[qz/(1-\sigma z)].\end{aligned} \tag{5.6}$$

This function has a simple pole at $z_c=1/\sigma$, which indicates that the first-order approximation for the walk limit is $\mu\simeq\sigma$, corresponding to the Bethe critical point (5.1a). In analogy with (5.1b) we may introduce the new variable

$$y=\sigma z. \qquad (5.7)$$

Since, by (3.2) the nth coefficient in the expansion of $C(z)$ in z is a polynomial in σ of degree n, the coefficients in the expansion in y will be polynomials in *inverse* powers of σ, the leading terms being constant. On regrouping we will obtain an expansion of $C(z)$ in powers of $(1/\sigma)$ in which we expect the zero order term to correspond to (5.6).

It is convenient to start with the expression (4.20). Multiplication by $(\sigma/q)z^n$ followed by summation from $n=1$ to ∞ yields

$$\frac{\sigma}{q}[C(z)-1]=\frac{\sigma z}{1-\sigma z}+\frac{\sigma}{q}\sum_{n=1}^{\infty}\sum_{k=4}^{n} d_k(n-k+1)z^n\sigma^{n-k}. \qquad (5.8)$$

On writing $z=y/\sigma$, interchanging the order of summation and summing on $j=n-k$ (assuming $|y|<1$) we get

$$\frac{\sigma}{q}[C(z)-1]=\frac{y}{1-y}+\sum_{k=4}^{\infty}(d_k/q\sigma^{k-1})\frac{y^k}{(1-y)^2}. \qquad (5.9)$$

Using the expression (4.14) and the coefficients $\bar{d}_{nl}$ given in Table III we may expand each term $(d_k/q\sigma^{k-1})$ in inverse powers of σ. Thus,

$$\begin{aligned}
d_4/q\sigma^3 &= -\sigma^{-2}+\sigma^{-3}\\
d_5/q\sigma^4 &= \quad +\sigma^{-3} \quad -\sigma^{-4}\\
d_6/q\sigma^5 &= \quad -4\sigma^{-3} \quad +13\sigma^{-4} \quad -9\sigma^{-5}\\
&\cdots \qquad \cdots\\
d_{10}/q\sigma^9 &= \sigma^{-4}-244\sigma^{-5}+2793\sigma^{-6}+\cdots\\
d_{11}/q\sigma^{10} &= \sigma^{-4}+4\sigma^{-5} \quad +420\sigma^{-6}+\cdots \qquad (5.10)
\end{aligned}$$

and by (4.19) the first two terms in $d_k/q\sigma^{k-1}$ remain unchanged for $k\geqslant 11$. On collecting up terms in $1/\sigma$ and performing the infinite sums for the terms in $(1/\sigma)^4$ and $(1/\sigma)^5$, which yield extra factors $(1-y)^{-1}$ (for $|y|<1$), we finally obtain

$$\begin{aligned}
\frac{\sigma}{q}[C(y/\sigma)-1]
&=\frac{y}{1-y}-\frac{y^4}{(1-y)^2}(1/\sigma)^2\\
&+y^4\left[1+\frac{3y}{(1-y)}-\frac{2y^2}{(1-y)^2}\right](1/\sigma)^3\\
&-y^5\left[1-11y-\frac{30y^2}{(1-y)}+\frac{7y^3}{(1-y)^2}-\frac{y^4}{(1-y)^3}\right](1/\sigma)^4\\
&-y^6\left[9+40y-111y^2-\frac{310y^3}{(1-y)}\right.\\
&\qquad\left.+\frac{45y^4}{(1-y)^2}-\frac{4y^5}{(1-y)^3}\right](1/\sigma)^5+\cdots. \qquad (5.11)
\end{aligned}$$

As anticipated the term independent of σ corresponds precisely to the first-order approximation (5.6) and has a simple pole at $y=1$. The first correction term is of second order but has a double pole at $y=1$. The coefficient of $(1/\sigma)^m$ has the form

$$y^{m+1}\{k_0+k_1y+\cdots+k_my^m\}(1-y)^{-1-[m/2]}, \qquad (5.12)$$

(where $[w]$ denotes the integer part of w) and, hence, diverges increasingly strongly at $y=1$ as m increases.

Of course the fact that the expansion in $(1/\sigma)$ diverges to all orders at $y=1$ does *not* imply that $C(y/\sigma)$ has any singularity at $y=1$. Indeed the upper bound[14]

$$\mu(2)<\nu=2.712 \qquad (5.13)$$

for the plane-square lattice proves that $C(y/\sigma)$ is bounded and regular for $y<\sigma/\nu=1.106$ when $\sigma=3$. Generally, by considering walks in which only immediate reversals and square loops (4-step self-intersections) are forbidden, one may show[32] that $\mu(d)\leqslant\nu(d)$ where $\nu(d)$ is the real positive root of

$$\nu^3-(\sigma-1)\nu^2-(\sigma-1)\nu-1=0. \qquad (5.14)$$

It is easy to establish that $\sigma/\nu(d)\geqslant 1+\epsilon(d)$ with $\epsilon(d)>0$ (for $d<\infty$). This proves that $C(y/\sigma)$ is regular at $y=1$ for *all* finite σ. The divergence of the expansion in $(1/\sigma)$ at $y=1$ is evidently a mere 'artifact' but it apparently prevents us from locating, even approximately, the true singularity in $C(y/\sigma)$ and, thence, estimating $\mu(d)$.

This difficulty can, however, be circumvented in the following manner. By re-expanding (5.11) in powers of y, or directly from (4.20) and the polynomials (5.10), we find that the number of walks for $n\geqslant 11$ can be written

$$\begin{aligned}
(1/q)c_n(d)=\sigma^{n-1}[1&-(n-3)\sigma^{-2}-(2n-13)\sigma^{-3}\\
&+(\tfrac{1}{2}n^2-14\tfrac{1}{2}n+107)\sigma^{-4}\\
&+(2n^2-83n+895)\sigma^{-5}+O(\sigma^{-6})], \qquad (5.15)
\end{aligned}$$

where for $n>n_0=n_0(m)$ the coefficient of σ^{-m} will be a definite polynomial in n of degree $[\frac{1}{2}m]$. If, formally, we take the logarithm of this expression we find

$$\begin{aligned}
\ln(c_n/q)=(n-1)\ln\sigma&-(n-3)\sigma^{-2}\\
&-(2n-13)\sigma^{-3}-(11\tfrac{1}{2}n-102\tfrac{1}{2})\sigma^{-4}\\
&-(64n-856)\sigma^{-5}+O(\sigma^{-6}). \qquad (5.16)
\end{aligned}$$

It is remarkable that the terms in n^2 have cancelled identically. It seems probable, although we have as yet no proof, that this cancellation will continue in the general mth term [for $n>n_0(m)$] so that the logarithm will be formally linear in n to all orders. We may now use the definition (2.4)

$$\ln\mu(d)=\lim_{n\to\infty} 1/n \ln c_n(d) \qquad (5.17)$$

[32] One must construct a recurrence relation for the number of walks divided into classes according to the least number of extra steps needed to complete a square. See the Appendix to Ref. 14.

to derive an expansion in powers of $(1/\sigma)$ for the limit μ, namely

$$\ln\mu(d)=\ln\sigma-\sigma^{-2}-2\sigma^{-3}-11\tfrac{1}{2}\sigma^{-4}-64\sigma^{-5}+O(\sigma^{-6}) \tag{5.18a}$$

or, taking exponentials,

$$\mu=\sigma[1-\sigma^{-2}-2\sigma^{-3}-11\sigma^{-4}-62\sigma^{-5}+O(\sigma^{-6})]. \tag{5.18b}$$

The leading terms in these expressions correspond, as expected, to the first-order approximation $\mu=\sigma$. The first correction term is again of second order and is negative confirming that $C(y/\sigma)$ is regular at $y=1$ for $1/\sigma>0$. The question of the convergence of (5.18) will be discussed later.

Susceptibility

Returning to the Ising model it is now clear how the susceptibility may be expanded in powers of $(1/\sigma)$. We start with the expression (4.25) for the expansion coefficients, multiply by v^n and sum. The correction coefficients b_n defined by (4.24) and Table V, are then expanded in powers of σ. On making the substitution $v=x/\sigma$, rearranging and summing we finally obtain, in analogy with (5.11),

$$\frac{\sigma}{q}[\xi-1]=\frac{x}{1-x}-\frac{x^4}{(1-x)^2}(1/\sigma)^2 +x^4\left[1+\frac{2x}{1-x}-\frac{3x^2}{(1-x)^2}\right](1/\sigma)^3 +x^5\left[14x+\frac{30x^2}{(1-x)}-\frac{10x^3}{(1-x)^2}+\frac{x^4}{(1-x)^3}\right](1/\sigma)^4 +x^6\left[-10-26x+150x^2+\frac{340\frac{2}{3}x^3}{(1-x)}-\frac{51\frac{1}{3}x^4}{(1-x)^2}+\frac{6x^5}{(1-x)^3}\right](1/\sigma)^5+\cdots, \tag{5.19}$$

where the reduced susceptibility is

$$\xi=(kT/m^2)\chi(T). \tag{5.20}$$

The term independent of σ yields

$$\chi(T)\simeq\frac{m^2}{kT}\left[1+\frac{qx}{\sigma(1-x)}\right]=\frac{m^2}{kT}\frac{1+v}{1-\sigma v}, \tag{5.21}$$

which is the well-known Bethe approximation for the susceptibility[3] (Firgau formula). This exhibits a simple pole at the Bethe critical point $x_c=1$ as is to be expected. The leading correction term is again second order but has a double pole. In general, the coefficient of $(1/\sigma)^m$ is of the form (5.12) (with x replacing y) and thus diverges at $x=1$ as $(1-x)^{-1-[m/2]}$. As previously the divergence in all orders does *not* imply that the susceptibility diverges at $x=1$. Indeed since generally[14]

$$\omega(d)=1/v_c\leqslant\mu(d), \tag{5.22}$$

the argument based on Eq. (5.14) shows that $\xi(x)$ or $\chi(T)$ is bounded and regular at $x=1$ for all $1/\sigma>0$.

To compare with the mean-field or Bragg-Williams approximation we carry the expansion one stage further as for the partition function. Writing for convenience,

$$t=1/\theta=J_0/kT, \tag{5.23}$$

we obtain from (5.19) the $(1/q)$ expansion of the susceptibility in the form

$$(J_0/m^2)\chi(T)=\frac{t}{1-t}-\frac{t^3}{(1-t)^2}(1/q) -t^4\left[\frac{\frac{1}{3}}{(1-t)}+\frac{\frac{4}{3}t}{(1-t)^2}-\frac{1}{(1-t)^3}\right](1/q)^2 +t^5\left[1+\frac{2t}{(1-t)}+\frac{1\frac{2}{3}-3t^2}{(1-t)^2}+\frac{2\frac{2}{3}t}{(1-t)^3}-\frac{1}{(1-t)^4}\right](1/q)^3+\cdots, \tag{5.24}$$

where the exact terms to order $(1/q)^5$ follow from (5.19) but are omitted to save space. The term independent of q yields the mean-field result (Curie-Weiss law)

$$\chi(T)\simeq\frac{m^2}{J_0}\frac{T_c}{T-T_c}\quad(t_c=J_0/kT_c=1). \tag{5.25}$$

In this case, however, the leading correction term is of first order in $(1/q)$. Furthermore, the divergence in each term, which now occurs at $t=1$, is sharper than in the $(1/\sigma)$-expansion. This arises merely from the expansion of the Bethe result (5.21) in powers of $(1/q)$ which necessarily yields a pole of order $(m+1)$ in the coefficient of $(1/q)^m$.

To obtain expansions for the critical point we must again abandon the complete expansions and examine the expansion coefficients themselves. From (4.25), (4.24), the coefficients in Table V and the general expression (4.23), or by expanding (5.19), we find for $n\geqslant 11$

$$a_n(d)=q\sigma^{n-1}[1-(n-3)\sigma^{-2}-(3n-17)\sigma^{-3} +(\tfrac{1}{2}n^2-17\tfrac{1}{2}n+128)\sigma^{-4} +(3n^2-108\tfrac{1}{3}n+1072\tfrac{2}{3})\sigma^{-5}+O(\sigma^{-6}). \tag{5.26}$$

On taking the logarithm, formally, the terms in n^2 again cancel so that

$$\ln(a_n/q)=(n-1)\ln\sigma-(n-3)\sigma^{-2} -(3n-17)\sigma^{-3}-(14\tfrac{1}{2}n-123\tfrac{1}{2})\sigma^{-4} -(82\tfrac{1}{3}n-1021\tfrac{2}{3})\sigma^{-5}+O(\sigma^{-6}). \tag{5.27}$$

Dividing by n and taking the limit $n \to \infty$ then yields by (2.13)

$$\ln\omega(d) = -\ln\tanh(J/kT_c) = \ln\sigma - \sigma^{-2} - 3\sigma^{-3} - 14\tfrac{1}{2}\sigma^{-4} - 82\tfrac{1}{3}\sigma^{-5} + O(\sigma^{-6}), \quad (5.28a)$$

and, on taking exponentials,

$$\omega = \sigma[1 - \sigma^{-2} - 3\sigma^{-3} - 14\sigma^{-4} - 79\tfrac{1}{3}\sigma^{-5} - \cdots]. \quad (5.28b)$$

We have thus obtained an expansion for the critical point of the Ising problem, the zero order term being the result of the Bethe approximation. Comparison with the expansion (5.18) for the walk limit shows that

$$(\mu - \omega)/\sigma = \sigma^{-3} + 3\sigma^{-4} + 17\tfrac{1}{3}\sigma^{-5} + \cdots > 0 \quad (5.29)$$

in agreement with (5.22). It is interesting that the fractional difference is only of third order in $(1/\sigma)$.

By writing $\sigma^{-1} = q^{-1}(1-q^{-1})^{-1}$ and inverting the relation $\tanh(J/kT_c) = 1/\omega$ we can obtain a direct expansion for the critical temperature in powers of $1/q$,

$$\theta_c = kT_c/J_0 = 1 - q^{-1} - 1\tfrac{1}{3}q^{-2} - 4\tfrac{1}{3}q^{-3} - 21\frac{34}{45}q^{-4} - 133\frac{14}{15}q^{-5} - \cdots. \quad (5.30)$$

The term independent of q is now the Bragg-Williams or mean-field result but the leading correction term is again of first order.

We could alternatively have derived this last result directly from the $(1/q)$ expansion (5.24) by calculating the coefficients $f_n(q)$ in the expansion

$$(J_0/m^2)\chi(T) = \sum_{n=0}^{\infty} f_n(q) t^{n+1}. \quad (5.31)$$

It is clear that $f_n(q)$ can be expanded in powers of $1/q$. The coefficient of $(1/q)^m$ would now be a polynomial in n of degree m (for n sufficiently large) since the divergence of the $(1/q)^m$ term in (5.24) is $(1-t)^{-m-1}$. On forming $\ln f_n(q)$ we would now find (at least to the fifth order in $1/q$) that the terms in n^2, n^3, n^4, and n^5 would *all* cancel leaving only linear terms. The critical temperature expansion (5.30) would then be derived formally from

$$\ln\theta_c = \lim_{n\to\infty} \frac{1}{n} \ln f_n(q). \quad (5.32)$$

There seems no reason to suppose that the cancellation of the higher powers of n in $\ln f_n(q)$ will not continue indefinitely so that the form of the expansion (5.32) would remain the same to all orders.

Convergence

We cannot state any definite conclusions regarding the nature of the convergence of the $(1/\sigma)$ and $(1/q)$ expansions derived above. The coefficients in the series (5.18), (5.28), and (5.30) for μ, ω, and θ_c increase rapidly with n and at first sight the series appear unsuitable for numerical evaluation unless q is rather large. On general grounds one might expect the series to be only asymptotic.[33] This is supported by the ratios of successive terms in (5.30) which are

$$1,\ 1.3333,\ 3.2500,\ 5.0205,\ 6.1563,\ \cdots.$$

These increase roughly linearly with n in a fashion reminiscent of the ratios

$$1,\ 2,\ 3,\ 4,\ 5,\ 6,\ \cdots,$$

derived from the well-known asymptotic series $\sum n!x^n$.[34]

If the series *are* asymptotic, truncation at the smallest term for given q should yield the optimum approximation. This rule does indeed seem to apply. Thus, with $q=4$ $(d=2)$, the first three terms of (5.30) yield

$$\theta_c(2) \simeq 0.59896, \quad (m=3) \quad (5.33a)$$

which is 5.6% larger than the exact result[1]

$$\theta_c(2) = 0.56730\cdots \quad \text{(exact)}. \quad (5.33b)$$

This error is about $\frac{3}{8}$ of the fourth-order term which yields

$$\theta_c(2) \simeq 0.51398, \quad (m=4). \quad (5.33c)$$

In three dimensions $(q=6)$ we similarly obtain the approximation

$$\theta_c(3) \simeq 0.75945, \quad (m=4) \quad (5.34a)$$

which is only 1.03% higher than the best estimate

$$\theta_c(3) \simeq 0.75172, \quad (\text{'exact'}), \quad (5.34b)$$

which is probably accurate to 1 part in 10^4 or better. The error is just under one half the fifth-order term which yields

$$\theta_c(3) \simeq 0.74222, \quad (m=5). \quad (5.34c)$$

The mean of (5.34a) and (5.34c) is accurate to 0.1%.

In four dimensions the fifth-order term is probably the smallest (although we do not know the next term). The corresponding estimate is

$$\theta_c(4) \simeq 0.8363, \quad (m=5) \quad (5.35a)$$

the last term being about 0.5% of this value. In analogy with two and three dimensions, one would expect (5.35a) to be about 0.3% high which is confirmed by the estimate

$$\theta_c(4) \simeq 0.8340, \quad (\text{'exact'}) \quad (5.35b)$$

obtained from the series in the next section. For optimum accuracy in higher dimensions more terms are

[33] Thus, the expansions (5.15) and (5.26) should be accurate when $n\sigma^{-2}$ is small or $1/\sigma \ll 1/n^{1/2}$. As $n \to \infty$ in (5.17) and (5.28), however, the range of convergence would seem to shrink to zero as would be expected if the limiting series where only asymptotic.

[34] The constant sign of the terms suggests, in any case, that there is a singularity on the real positive axis. If the series were asymptotic this would be at $1/\sigma = 0+$.

required. The approximations for $\theta_c(5)$ and $\theta_c(6)$ must thus be expected to be some 0.1 to 0.2% high as is confirmed by the direct series estimates (see Table VII below).

The $(1/\sigma)$ expansions for $\omega(d)$ and for $\mu(d)$ behave in a very similar fashion. In all cases the error appears to be roughly one half the smallest term (see Table VII).

The convergence of the $(1/\sigma)$ and $(1/q)$ expansions for the susceptibility and partition function (and for the corresponding walk generating functions) is a rather different problem. For small enough x or t, i.e., high-enough temperatures, it seems likely that the series have a finite radius of convergence in $1/\sigma$ and $1/q$. However, as $(1/\sigma)$ and $(1/q)$ approach zero, we have found that the positions of the singularities in χ and the partition function approach $x=1$ and $t=1$ (from above) which suggests that the series will have a zero radius of convergence if $x\geqslant 1$ or $t\geqslant 1$, respectively. This heuristic conclusion is supported by the divergence of each term in the susceptibility expansions *at* $x=1$ or $t=1$. The individual coefficients in the partition-function expansion are well behaved at $x=1$ or $t=1$ but we expect the free energy to have some singularity for all q (even if the specific heat is finite, see below) so that the argument still applies.

6. NUMERICAL EXTRAPOLATIONS

In this section we use the first eleven explicit coefficients of the series expansions (Tables I, II, IV, and VI) to estimate the Ising critical points $\omega(d)$ and $\theta_c(d)$ and the self-avoiding walk limit $\mu(d)$ for the hypercubical lattices. Following the analyses of the two- and three-dimensional cases we study the ratios[6,14,15]

$$\omega_n = a_n/a_{n-1}, \quad \mu_n = c_n/c_{n-1} \tag{6.1}$$

as a function of $1/n$ and the behavior of the related Padé approximants.[7,18]

At the same time, and more importantly, we will estimate the indices $\delta(d)$ and $\alpha(d)$ in the asymptotic relations

$$\chi(T)\approx C/(T-T_c)^{1+\delta}, \quad (T\to T_c+) \tag{6.2a}$$

$$a_n \approx C' n^{\delta}\omega^n, \quad (n\to\infty) \tag{6.2b}$$

and

$$c_n \approx A n^{\alpha}\mu^n, \quad (n\to\infty) \tag{6.3}$$

which are observed to hold.[6,14] In two and three dimensions we have[6,15,17] $\delta(2)=\frac{3}{4}$, $\alpha(2)=\frac{1}{3}$ and $\delta(3)=\frac{1}{4}$, $\alpha(3)=\frac{1}{6}$ (to quite high accuracy). Furthermore, these results have been found to be *independent* of the lattice structure for fixed dimension. We are confident that the same will be true in four and more dimensions so that it is sufficient to consider only the simple hypercubical lattices.[19] The only danger is that these lattices are not "typical" when d is large. Thus, for example, lattices are known for $d=8$, 12, and 16, with coordination numbers 240, 756, and 2160, respectively, compared with merely 16, 24, and 32 for the hypercubical lattices.[35] Furthermore, the previous arguments suggest that until $n>d$ the configurations counted by the coefficients do not "sample" the lattice fully in all its dimensions. For these reasons we have restricted our extrapolations to $d=4$, 5, and 6 this being sufficient, in any case, to exhibit the trend with increasing dimension.

Since the extrapolation procedures are now standard and have been discussed in detail elsewhere[6,7,14,15,18] we will give only an outline account. Examination of the ratios $\omega_n(d)$ and $\mu_n(d)$ on a plot versus $1/n$ shows that, allowing for the odd-even alternation, they quite rapidly approach linearity as $n\to\infty$. One observes, however, a slight curvature which increases with dimensionality. This is almost totally removed by regarding the ratios as a function of $1/n'=1/(n-k)$ where $k=\frac{1}{2}(d-3)$. The asymptotic forms for large $n\simeq n'$ are, of course, not altered. Linear extrapolation of odd and even pairs of ratios to the $1/n'=0$ axis then yields first estimates for ω and μ. For example, for self-avoiding walks in four dimensions the last few intercepts are 6.7810, 6.7582, 6.7765, 6.7605, 6.7742, 6.7642, while successive means are 6.7696, 6.7674, 6.7685, 6.7674, and 6.7692. These indicate that the limit $\mu(4)$ is close to 6.768 and the corresponding slopes suggest that $\alpha(4)\simeq 0.071$. This value is close to $1/14=0.07143$ which index may be used to obtain from the modified ratios $\mu_n^*=n'\mu_n/(n'+\alpha)$ the refined estimate $\mu(4)\simeq 6.7680 \pm 0.0015$. This, in turn, leads to a refined estimate for the index based on the sequence $\alpha_n=n'(\mu_n-\mu)/\mu$ which yields $\alpha(4)=0.0715\pm 0.0010$.

The poles of the successive Padé approximants to $(d/dz)\ln C(z)$ indicate a value of 6.7677 ± 0.0010 for $\mu(4)$. The corresponding residues are in the region $1+\alpha(4)\simeq 1.073$ in agreement with the analysis of the ratios. Removing the critical factor from the series for $(d/dz)\ln C(z)$ using $\mu(4)\simeq 6.7680$ and estimating α by direct evaluation of the approximants yields $\alpha(4)\simeq 0.0722\pm 0.0010$ again in satisfactory agreement.

A similar procedure has been applied to the terms c_n and a_n for the other dimensions. Generally we have found that with regular series such as these the ratio method is more sensitive, displays steadier trends and thus yields more accurate estimates. In a number of cases, notably the susceptibility series for $d=4$ many of the Padé approximants suffer from the defect of a "split singularity," i.e., an expected simple pole with residue R is represented as a pair of close but displaced poles with residues R_1 and R_2 such that $R_1+R_2\simeq R$. This behavior may be an indication of more complex analytic behavior in the true function but is also quite typical of the "noiseness" of the sequence of Padé approximants. Usually the estimates for α and δ obtained from the approximants are some 0.001 to 0.002 higher than the series estimates. In absolute terms

[35] See H. S. M. Coxeter and J. A. Todd, Can. J. Math. 5, 384 (1951) and the references quoted in footnote 19.

TABLE VII. Estimates for critical parameters.

d	2	3	4	5	6
$\mu(d)$	2.6390	4.6826	6.7680±0.0015	8.8313±0.0020	10.8720±0.0015
$\mu^{(\sigma)}(d)$	2.5556	4.6760	6.7714	8.8397	10.8800
μ/σ	0.8797	0.9365	0.9669	0.9813	0.9884
$\alpha(d)$	0.333	0.166	0.0715±0.0010	0.0310±0.0015	0.0138±0.0015
$1/\alpha(d)$	3	6	14±0.3	32±1.5	72±7
$\omega(d)$	2.414 214	4.5840	6.7220±0.0015	8.8072±0.0010	10.8580±0.0015
$\theta_c(d)$	0.567 296	0.751 72	0.834 01	0.876 94	0.902 27
$\theta_c^{(q)}(d)$	0.598 96	0.759 45	0.836 30	0.878 82	0.903 31
$\delta(d)$	0.750	0.250	0.094±0.0025	0.0375±0.0010	0.016±0.001
$3/\delta(d)$	4	12	32±1	80±2	188±12

this is a rather small discrepancy but since $\alpha(d)$ and $\delta(d)$ fall sharply as d increases the percentage uncertainties naturally increase.

Our final best estimates for $\mu(d)$, $\alpha(d)$, $\omega(d)$, $\theta_c(d)$, and $\delta(d)$ are presented in Table VII. In all cases the values of μ are consistent with the upper bounds derived from Eq. (5.14) and with the lower bounds which can be found by extending previous methods.[14,36] It must be stressed, however, that the indicated uncertainties are not rigorous bounds but correspond to reasonable fitting limits. [The two- and three-dimensional results, which are not new, are given for completeness without any indication of uncertainty.]

The row labelled $\mu^{(\sigma)}(d)$ represents approximations to $\mu(d)$ computed from the $(1/\sigma)$ expansion (5.18b) by retaining terms up to order $(1/\sigma)^d$ plus one-half the term in $(1/\sigma)^{(d+1)}$ [except for $d=5$ and 6 where all available terms are utilized]. Similarly, the row labelled $\theta_c^{(q)}(d)$ is calculated from the $(1/q)$ expansion truncated after the term in $(1/q)^{(d+1)}$ except for $d=5$ and 6 where all terms are retained. As mentioned before, the asymptotic series estimates are quite close to the more accurate numerical estimates.

In two and three dimensions the reciprocal indices $1/\alpha(d)$ and $3/\delta(d)$ appear to be exact integers. From Table VII it is plausible that this is true also for self-avoiding walks in four dimensions where $1/\alpha(4)\simeq 14$ but, unfortunately, the accuracy of the extrapolations is not sufficiently great to confirm such a conjecture in the other cases. It is clear, however, that the indices are rapidly approaching zero as d increases. Indeed the sequences of ratios (for $d=2, 3,\cdots$)

$$\alpha(d)/\alpha(d+1)\simeq 2.000,\quad 2.333,\quad 2.286,\quad 2.25,\quad \cdots$$

and

$$\delta(d)/\delta(d+1)\simeq 3.00,\quad 2.67,\quad 2.50,\quad 2.35,\quad \cdots$$

suggest that, for large d, the indices $\alpha(d)$ and $\delta(d)$ behave as $1/\lambda^d$ with $\lambda\simeq 2.0$. In conformity with the inequality[14] $\mu(d)>\omega(d)$ we also observe that $\alpha(d)<\delta(d)$ appears to hold generally.

[36] B. C. Rennie, Magy. Tud. Akad. Mat. Kuk. Inetz **6A**, 263 (1961)—generalizes the technique of Ref. 14 and obtains the lower bounds $\mu(4)\geqslant 5.718$, $\mu(d)\geqslant 2d-\ln d+O(1)$ $(d\to\infty)$.

Since we have obtained accurate estimates for the limit $\mu(d)$, we may endeavor to determine the asymptotic behavior of the number of self-avoiding returns,[14,37] i.e., the index $\zeta(d)$ in the expression[21]

$$u_n(d)\approx Un^{-\zeta}\mu^n \quad (n\to\infty). \tag{6.4}$$

The ratios $(u_n/u_{n-2})^{1/2}/\mu$ will approach unity as $n\to\infty$ and are observed to do so almost linearly in $1/n$. As before the slope yields an estimate for ζ. Unfortunately there are only four or five significant nonzero terms in higher dimensions and these are not very large numerically. Consequently only limited accuracy is possible. We estimate tentatively that in $d=2, 3, 4, \cdots$ dimensions

$$\zeta(d)\simeq 1.46,\quad 1.75,\quad 2.07,\quad 2.38,\quad 2.70,\quad \cdots. \tag{6.5}$$

To within the uncertainties of 0.01 to 0.03 these results are consistent with the formula

$$\zeta(d)\simeq(4d+11)/13. \tag{6.6}$$

The probability $\mathcal{P}_n$ of an n-step self-avoiding walk returning to the vicinity of the origin will vary as $1/n^{\alpha+\zeta}$. The formula (6.6) thus suggests roughly that $\mathcal{P}_n\sim 1/n^{(4/13)d+1}$ when d is large compared with $\mathcal{P}_n\sim 1/n^{\frac{1}{2}d}$ for unrestricted random walks. Firm conclusions on the value of $\zeta(d)$ for $d\geqslant 4$, however, require further data.

We may in similar fashion investigate the behavior of the specific heat of the Ising model in higher dimensions. In two dimensions we know that the specific heat diverges as[1]

$$(d=2)\quad C(T)\approx D_2|\ln(T-T_c)|,\quad (T\to T_c+) \tag{6.7}$$

while in three dimensions extrapolation of the results for the three cubic lattices[3,38,39] suggests a sharper infinity, namely,

$$(d=3)\quad C(T)\approx D_3/(T-T_c)^{0.2}\quad (T\to T_c+). \tag{6.8}$$

Examination of the ratios $(h_n/h_{n-2})^{1/2}/\omega$ formed from the expansion of the energy (see Table II) suggests,

[37] M. F. Sykes and B. J. Hiley, J. Chem. Phys. **34**, 1531 (1961).
[38] C. Domb and M. F. Sykes, Phys. Rev. **108**, 1415 (1957).
[39] M. E. Fisher, J. Math. Phys. **4**, 278 (1963).

however, that in four and more dimensions the specific heat will approach a finite value as T approaches T_c from above. We expect

$$(d\geqslant 4)\quad C(T)\simeq C_c-E(T-T_c)^{\eta},\quad (T\to T_c+),\qquad (6.9)$$

where the parameters C_c, E and η depend on d. Tentative extrapolations indicate, for $d=4$, 5, and 6,

$$\eta(d)\simeq 0.17,\quad 0.40,\quad \text{and}\quad 0.75,\qquad (6.10)$$

but these values may well be too large. Appreciably more data is needed if more certain estimates are to be made.

7. CONCLUSIONS

By considering a sequence of lattices of dimensionality d and coordination $q=2d$ we have been able to obtain expansions in powers of $(1/q)=\frac{1}{2}(1/d)$ for the critical points and other properties of the nearest-neighbor Ising model of spin $\frac{1}{2}$ and for corresponding self-avoiding walks. It should be noted that the same principles can be used to obtain $(1/d)$-expansions for the Ising model of general spin and also for the Heisenberg model of general spin. In these cases detailed calculations are somewhat more involved since the weight associated with a given lattice constant is no longer so simple but the general nature of the results should be similar. (We hope to discuss these extensions in a future report.)

The zeroth order terms in our expansions are the Bragg-Williams or mean-field results (or their analogs). This is also the case for Brout's 'high-density' or $(1/z)$-expansion.[9–13] However, the specific heat remains analytic as $T\to T_c+$ to all orders in our expansions whereas in the $(1/z)$ type expansions the first-order terms yield specific heat singularities at T_c.[13] From our susceptibility expansions we were able to derive $(1/d)$-expansions for the critical points: corresponding $(1/z)$-expansions have not been derived.

We feel that the present expansions should be viewed essentially as expansions for short-range forces in inverse dimensionality rather than in inverse coordination number. Indeed similar results should be obtainable with other sequences of lattices in which the coordination numbers q have different dependences on d. The $(1/z)$-expansions, on the other hand, are probably best regarded as expansions in the inverse range of long-range forces for lattices of fixed dimension.[12,13] It is then a matter of interest that the zeroth order terms of both expansions agree but not surprising that higher terms differ.

For short-range forces the dependence on dimensionality seems to be of primary importance, coordination number and detailed lattice structure having only a secondary effect. This can be seen from the similarity of the θ_c, ω/σ, and μ/σ results for different lattices of fixed dimension and from the corresponding invariance of the indices δ and α. The numerical extrapolations indicate that the 'classical' Bragg-Williams limit is approached quite rapidly as d increases although the singularities in the susceptibility and specific heat apparently remain 'nonclassical' for all finite d.

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