Self-avoiding-walk contacts and random-walk self-intersections in variable dimensionality

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The average number of nearest-neighbor (NN) contacts $\langle m \rangle$ of self-avoiding walks (SAW's) on a hypercubic lattice is calculated using direct enumeration and $1/d$ expansion methods, where d is the spatial dimension. These calculations are compared with exact analytic determinations for the asymptotic number of random-walk (RW) self-intersections in the limit of long chains $n \to \infty$. The number of RW (binary, ternary, etc.) self-intersections is a function of the probability C_d^* that a RW escapes from the origin to infinity and an accurate tabulation of C_d^* is given in the dimension range $2 < d < 10$. We find that the number of SAW NN contacts $\langle m \rangle_{\rm SAW}$ has an asymptotic behavior ($\langle m \rangle_{\rm SAW} \sim a_\infty n$) similar to that for the number of RW self-intersections ($\langle m \rangle_{\rm RW} \sim a_{\rm RW} n$), as first suggested by Domb, but the corrections to this leading scaling differ for the RW and SAW problems. The "contact amplitude" a_∞, determined from direct enumeration data and ratio extrapolation, exhibits a *maximum* near $d=3$ dimensions as does $a_{\rm RW}$. Comparison of the numerical estimates for a_∞ to the $1/d$ expansion calculation of a_∞ shows significant deviation for $d<5$, reflecting the strong fluctuations in contacts that arise in lower dimensions. The correction to the scaling exponent Δ_m for SAW NN contacts exhibits a maximum near $d=2$ dimensions, a behavior similar to previous observations for the SAW exponent γ. Estimates of the θ point for interacting SAW's, the critical temperature of the O(m) model, and other lattice constants (e.g., bond and site percolation thresholds) are obtained in terms of SAW and RW lattice parameters.

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I. INTRODUCTION

A short-range interaction is incorporated into the self-avoiding-walk (SAW) model of polymer chains by partitioning SAW's into equivalence classes of chain configurations of length n having m nearest-neighbor (NN) contacts [1–11]. Chain properties are then calculated as an appropriately weighted average over these configurations (see Sec. II).

The present paper describes the average number of SAW contacts $\langle m \rangle_{\rm SAW}$ and compares these results with the number of unrestricted random-walk (RW) binary self-intersections $\langle m \rangle_{\rm RW}$. Domb first suggested the analogy between these SAW and RW properties, but his predictions [12] have apparently never been tested before.

Domb has shown that many aspects of the critical behavior of spin models (e.g., Ising, Heisenberg, spherical models) can be understood in terms of the geometry of self-avoiding paths [12]. Two parameters are primary in these relations—the SAW connectivity constant μ (SAW) and the number of SAW contacts $\langle m \rangle_{\rm SAW}$. The connectivity constant governs the asymptotic growth of the number of SAW chain configurations Q_n with chain length n [13],

$$\lim_{n \to \infty} (Q_n)^{1/n} \sim \mu({\rm SAW}) \ . \tag{1.1}$$

The existence of this limit has been established [13] and many numerical estimates of μ (SAW) have been made for a variety of lattices [14]. The number of NN contacts $\langle m \rangle_{\rm SAW}$ has been subject to more limited investigation, although the importance of this parameter was recognized in the earliest studies by Orr [1], Fisher and Skyes [2], and Fisher and Hiley [3a]. Apart from the fundamental interest in the number of SAW contacts in the estimation of the critical temperature of spin models [12] and other applications (see Sec. VI), the number of SAW contacts is important in modeling the thermodynamic properties of polymers in solution. The average chain internal energy and specific heat are proportional to the average and variance of m, respectively [3,5,15]. There are also practical applications of $\langle m \rangle$ to modeling fluorescence decay experiments in polymer solutions [16]. SAW contacts have been of recent interest in the context of protein folding and knotting in polymers [17,18]. There are, thus, a variety of motivations for the study of $\langle m \rangle_{\rm SAW}$.

Domb noted that the average number for self-intersections of a random walk $\langle m \rangle_{\rm RW}$ obeys a simple scaling relation for long chains [12],

$$\langle m \rangle_{\rm RW} \sim a_{\rm RW} n + b_{\rm RW} n^{\phi} + c_{\rm RW}, \quad n \to \infty \ , \tag{1.2a}$$

where the exponent ϕ describes "fluctuation corrections" to the leading extensive term, and $a_{\rm RW}$, $b_{\rm RW}$, and $c_{\rm RW}$ are constants. The exponent ϕ exhibits the dimensional dependence

$$\phi = (4-d)/2 \ , \tag{1.2b}$$

and can be recognized as the "Gaussian crossover ex-

ponent" in a renormalization group context [19]. Application of (1.2a) is restricted to $d>2$ and $d\neq 4$. Domb further argued [12] that "the structure of contacts on a SAW follows the same pattern as on a random walk...," but with a changed crossover exponent corresponding to ϕ in (1.2a). Specifically, he suggested that $\langle m\rangle_{\mathrm{SAW}}$ should have the asymptotic scaling [12,13]

$$\langle m\rangle_{\mathrm{SAW}}\sim a_\infty n + b_\infty n^{\Delta_m} + c_\infty, \quad n\to\infty , \tag{1.3a}$$

where a_∞, b_∞, and c_∞ are constants. The SAW crossover exponent Δ_m is estimated by Domb [12] as,

$$\Delta_m(d=2)\approx\tfrac{1}{2}, \quad \Delta_m(d=3)\approx\tfrac{1}{4} . \tag{1.3b}$$

The decreased Δ_m for SAW's relative to ϕ for RW's is attributed to the *decreased probability of ring closure* in SAW's [12].

Section II presents calculations of a_∞ for a range of dimensions $d\geq 1$, including noninteger values. The "contact amplitude" a_∞ is found to have an unanticipated maximum near three dimensions. The maximum number of SAW contacts $m_{\max}$ for a chain of length n is also estimated and approximations relating a_∞ to other lattice constants are introduced. A $1/d$ expansion for a_∞ is given and compared to the lattice extrapolation value. The correction to scaling exponent Δ_m is estimated numerically, and the corresponding exponent Δ_c for compact SAW's is determined. Section III considers the number of RW self-intersections. Exact values of a_{RW} are calculated, and we find that a_{RW} also exhibits a maximum near $d=3$. The calculation of a_{RW} necessitates evaluating the escape probability C_d^* of a RW from the origin to infinity; C_d^* is tabulated since accurate estimates of this quantity have independent interest in other applications (see Appendix A). In short, the scaling (1.3a) suggested by Domb is found to be satisfied, although the specific numerical values of the constants, such as Δ_m in (1.3b), are different than Domb's estimates. Section IV briefly considers the role of lattice variation on SAW contacts, and Section V discusses the estimation of the "fluctuation exponents" (Δ_m and ϕ) in some detail. Finally, the SAW and RW lattice parameters are applied in Sec. VI to develop approximations to other fundamental lattice parameters. In particular, the critical temperature of the O(m) model for all m ($0\leq m\leq\infty$) and $d\geq 3$ is approximated in terms of μ (SAW) and C_d^* and compared to numerical data for the critical temperature of the Ising model. The θ point of SAW's is then estimated based on this information and some additional assumptions. Other basic lattice parameters are approximated by RW data, such as the bond and site percolation thresholds on hypercubic lattices.

II. NUMBER OF SAW CONTACTS

Although a SAW by definition has no self-intersections, there are NN contacts corresponding to adjacent vertices of the SAW path, which are not connected by a bond. The energetic interaction in the SAW model is introduced by associating a Boltzmann weight to these NN contacts [1–11]. The average number of SAW contacts $\langle m\rangle$ is obtained by counting all SAW configurations having n bonds and classifying these configurations into "equivalence classes," which share a common number of contacts m.

In a previous paper [9], we obtained the exact SAW partition function of interacting SAW's in d dimensions for chains up to $n=11$. The partition function $Q_n(x)$ is the weighted sum

$$Q_n(x)=\sum_{m=0}^{m_{\max}} C_{n,m}x^m, \quad x=\exp(\Phi) , \tag{2.1}$$

where the $C_{n,m}$ correspond to the number of SAW's of length n having exactly m contacts. The $C_{n,m}$ are polynomials in the spatial dimension d, which can be treated as continuously variable [9]. Baker and Benofy [20] have shown that this type of analytic continuation in dimensionality is equivalent to the dimensional continuation of continuum field theories, so that a comparison between the two approaches is appropriate. (Reference [9] tabulates the $C_{n,m}$ coefficients for $2<d<6$.) The generating function parameter x in (2.1) is the Boltzmann weight for SAW configurations, and Φ is the associated dimensionless NN interaction energy in k_BT units. A positive value of Φ implies an attractive NN interaction.

The $C_{n,m}$ coefficients in Eq. (2.1) contain a wealth of information relating to polymer chain thermodynamic properties. For example, the "susceptibility exponent" γ in dimension d has been numerically estimated from the $C_{n,m}$ in a previous paper [10]. The SAW exponent γ is defined as a correction to the leading approximation Eq. (1.1),

$$Q_n(\Phi=0)\sim[\mu(\mathrm{SAW})]^n n^{\gamma-1} . \tag{2.2}$$

Another paper [11] begins with the $C_{n,m}$ coefficients and evaluates thermodynamic properties such as the specific heat and the energetic dependence of $\mu(\Phi)$. Some of these prior results are utilized below in our discussion of $\langle m\rangle$.

The average number of contacts for NN interacting SAW's $\langle m\rangle$ equals

$$\langle m\rangle = d[\ln Q_n(x)]/d(\ln x) , \tag{2.3a}$$

and Eqs. (2.1) and (2.3a) allow us to express $\langle m\rangle$ directly in terms of the $C_{n,m}$ and the energy parameter x,

$$\langle m\rangle=\sum_{m=0}^{m_{\max}} mC_{n,m}x^m/Q_n(x), \quad \langle m(\Phi=0)\rangle\equiv\langle m\rangle_{\mathrm{SAW}} . \tag{2.3b}$$

In the limit of a highly attractive interaction, $\langle m\rangle$ approaches its maximum value

$$\lim_{x\to\infty}\langle m\rangle\sim m_{\max} , \tag{2.3c}$$

corresponding to the number of contacts of "compact" SAW's. (See below for explicit estimates of $m_{\max}$.)

A. Direct enumeration estimates of SAW contacts

The asymptotic variation of $\langle m\rangle_{\mathrm{SAW}}$ for n large is estimated by assuming the scaling form Eq. (1.3a) suggested

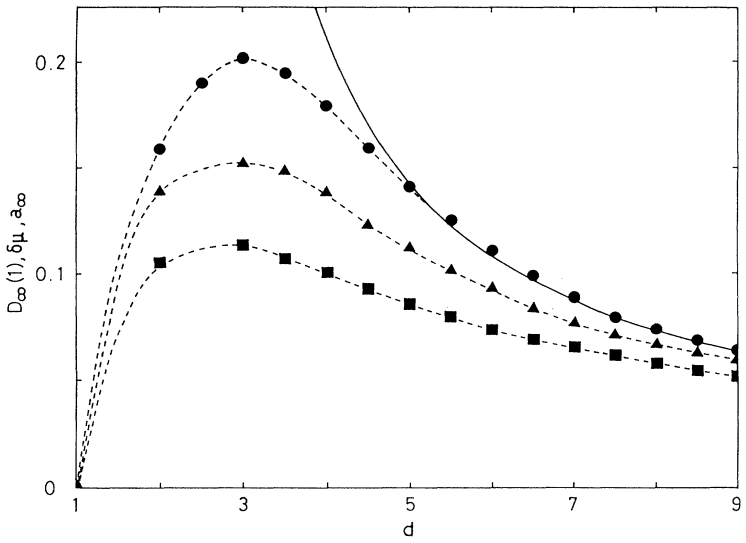

FIG. 1. SAW contact parameters as a function of dimension where (●) denotes extrapolation estimates of the contact amplitude a_∞ [see Eq. (2.4)], (▲) denotes the connectivity constant decrement $\delta\mu=[\mu(\text{SAW})-\mu(\text{NAW})]\mu(\text{NAW})$ [see Eq. (2.15)], and (■) denotes $\text{Lim}_{n\to\infty}(C_{n,1}/nC_{n,0})$ [see Eq. (2.11c)]. The solid curve represents the $1/d$ expansion Eq. (2.14) of a_∞.

by Domb for the infinite chain limit of $\langle m \rangle_{\text{SAW}}$,

$$\lim_{n\to\infty}(\langle m \rangle_{\text{SAW}}/n)=a_\infty \ . \tag{2.4}$$

This procedure is summarized elsewhere [1,2,7] for lattices in $d=2$ and $d=3$ and, consequently, we do not reproduce these details. Figure 1 displays the a_∞ values obtained from Eq. (2.4) for a range of d values. (The circles in Fig. 1 and the dashed line denote an interpolation of the lattice data estimates.) The estimates of a_∞ from Eq. (2.4) are summarized in Table I. Below we make a refined estimate of a_∞ in the process of determining the corrections to scaling in Eq. (1.3a).

The calculation of a_∞ reveals an interesting and unanticipated behavior. The coefficient a_∞ exhibits a *maximum* near $d=3$ dimensions. Apparently, the number of contacts for a long SAW chain is maximal in three dimensions because of two competing effects. In high di-

TABLE I. SAW contact parameters: $a_\infty, b_\infty, c_\infty, \Delta_m, D_\infty(1), \delta\mu$.

d	a_∞ [Eq. (2.4)]	b_∞	c_∞	Δ_m	a_∞ [Eq. (2.9)]	$D_\infty(1)$[f]	$\delta\mu$[f]
2[a]	0.1592±0.0008	0.18	−0.56	$0.25^{+0.10}_{-0.05}$	0.1585±0.0005	0.105±0.001	0.138 9
2.5	0.19±0.02						
3[b]	0.201±0.001	−0.55	0.06	0.15±0.05	0.2014±0.0008	0.113±0.001 5	0.152 0
3.5	0.1940.005	−4.0	3.5	$0.05^{+0.05}_{-0.03}$	0.1948±0.0010	0.107±0.0004	0.148 0
4[c]	0.174±0.0015	−0.005[d]			0.176±0.0015[d]	0.100±0.002	0.138 6
		−0.001[e]			0.179±0.0015[15]		
4.5	0.160±0.0015		−0.40		0.159±0.0015	0.0926±0.001 5	0.122 7
5	0.141±0.001		−0.38		0.140±0.001	0.0862±0.001 0	0.112 3
5.5	0.125±0.001		−0.33		0.124±0.001	0.0802±0.000 8	0.101 7
6	0.111±0.001		−0.28		0.110±0.001	0.0747±0.000 6	0.092 9
6.5	0.099±0.001					0.0697±0.000 6	0.084 5
7	0.0892±0.0008					0.0654±0.000 4	0.077 8
7.5	0.0814±0.0008					0.0615±0.000 3	0.071 9
8	0.0744±0.0006					0.0580±0.000 3	0.067 1
8.5	0.0691±0.0004					0.0549±0.000 2	0.063 07
9	0.0642±0.0004					0.05209±0.000 15	0.059 56
9.5	0.0600±0.0004					0.04948±0.000 15	0.055 55
10	0.0561±0.0003					0.04721±0.000 10	0.052 80
∞	$1/2d$						

[a] $n \le 22$.
[b] $n \le 16$.
[c] $n \le 12$.
[d] $\langle m \rangle_n/n = a_\infty + b_\infty/\ln n$.
[e] $\langle m \rangle_n/n = a_\infty + b'_\infty \ln n$.
[f] From our previous estimates [9] of μ(SAW) and μ(NAW). $D_\infty(m)=\lim_{n\to\infty}D_n(m)$, $D_n(m)=C_{n,m}/[C_n, o^n]$, $\delta\mu=[\mu(\text{SAW})/\mu(\text{NAW})]-1$.

mensions, a_∞ is governed by the probability R_d^* of the walk returning to origin (see below), so that there is a well-defined average "period" between successive excluded volume interferences (see Appendixes A and B). The number of SAW contacts decreases in lower dimensions ($d \to 1+$) because the possibility of contacts diminishes as the chain becomes "stiffer" from spatial constraints (see Sec. IV). This tendency is obvious in the extreme rod limit of a SAW ($d=1$) where there are no self-contacts. The maximal contacts occur for an intermediate dimension of $d \approx 3$.

Once a_∞ is estimated from Eq. (2.4), conventional extrapolation techniques provide refined estimations of the parameters in Eq. (1.3a). We form, prior to the determination of Δ_m, the difference $y_n \equiv \langle m \rangle_{\rm SAW} - a_\infty n$ and get rough estimates of c_∞ (and b_∞) by examining the linearity of y_n versus n^{Δ_m} for suitable Δ_m. We then evaluate the ratios

$$\Delta_n = n(y_n'/y_{n-2} - 1)/2 , \tag{2.5}$$

where $y_n' \equiv \langle m \rangle_{\rm SAW} - a_\infty n - c_\infty$ and we determine Δ_m using Neville tables for linear and quadratic extrapolants of Δ_m. Somewhat refined values of the prefactors can be estimated by exploiting the Δ_n versus n^{Δ_m} plots with the use of this modified Δ_m. Lattice constants obtained from this procedure are given in Table I. The exponent Δ_m is expected to be negative for $d > 4$. Thus, the contribution n^{Δ_m} becomes negligible, and b_∞ is assumed to vanish for $d > 4$. Hence, the constant c_∞ in Eq. (1.3a) is the leading asymptotic correction in high dimension $d > 4$. Numerical examination of $\langle m \rangle_{\rm SAW}$ in high dimensions ($d > 4$) is found to be consistent with the simple asymptotic relation

$$\langle m \rangle_{\rm SAW} \sim a_\infty n + c_\infty . \tag{2.6}$$

We see that the values of c_∞ in Table I slowly decrease with increasing dimension. The magnitude of c_∞ can be roughly appreciated by noting that a SAW on a hypercubic lattice cannot have a contact unless $n \geq 3$. Applying the exact result $\langle m \rangle_{\rm SAW} = 0$ for the extreme case of $n=2$ to the asymptotic limit Eq. (2.6) yields the rough approximation for $d > 4$,

$$c_\infty \approx -a_\infty/2 . \tag{2.7}$$

The qualitative validity of Eq. (2.7) (see Table I) reflects the rapid approach of Eq. (2.6) to its asymptotic limit.

The estimation of fluctuation corrections to $\langle m \rangle_{\rm SAW}$ requires special care at the "critical dimension" of $d=4$ (see Ref. [10]). The fluctuation corrections [21,22] for the analogous problem of RW self-intersections are on the order of $O(\ln n)$ in $d=4$ (see Appendix B), so we first consider the relation

$$\langle m \rangle_{\rm SAW} \sim a_\infty n + b_\infty' \ln n , \tag{2.8a}$$

under the assumption that SAW's are in the RW "domain of attraction" for $d=4$. [SAW's in high dimension ($d \geq 5$) have been shown to behave similarly to RW's with short-range interaction [23], but the situation at $d=4$ is still uncertain.] Equation (2.8a), however, appears inconsistent with the lattice data, so we must consider other possibilities. We also tried the alternative scaling relation

$$\langle m \rangle_{\rm SAW} \sim a_\infty n + b_\infty / \ln n , \tag{2.8b}$$

which is suggested to us by renormalization group theory [19]. The "regularized part" ($\langle m \rangle_{\rm SAW} - a_\infty n$) of the binary contacts might be expected to scale as the dimensionless renormalized binary interaction coupling constant [19] as $d \to 4+$. Estimates of a_∞ and b_∞ based on Eq. (2.8b) extrapolate reasonably, and the resultant lattice constants are given in Table I and Fig. 1. Although this estimate seems reasonable, the treatment of the contact fluctuation correction in $d=4$ requires further attention.

Improved estimates of a_∞ are obtained through the extrapolation

$$\lim_{n \to \infty} (\langle m \rangle_{\rm SAW} - b_\infty n^{\Delta_m} - c_\infty)/n \equiv a_\infty , \tag{2.9}$$

using Neville tables [6,7] where b_∞, Δ_m, and c_∞ are determined as indicated above. The new estimates of a_∞ obtained in this manner are also included in Table I. The resulting revision is small, but such corrections are important in obtaining refined estimates of a_∞.

The final numerical estimates of Δ_m are shown in Fig. 2. We observe that the fluctuation exponent Δ_m exhibits a maximum near $d=2$. This observation is quite similar to our previous numerical investigation [10] of the SAW exponent γ [see Eq. (2.2)], and below we exploit this observation to obtain a phenomenological estimate of $\Delta_m(d)$.

An alternative expression for SAW NN contacts is obtained by formally expanding $\langle m(\Phi) \rangle$ in a Taylor expansion in x,

$$\langle m \rangle = \sum_{j=0}^{\infty} (d^j \langle m \rangle / dx^j)|_{x=0} x^j / j! . \tag{2.10}$$

It should be noted that small x corresponds to a repulsive NN interaction and $x=0$ corresponds to the neighbor-

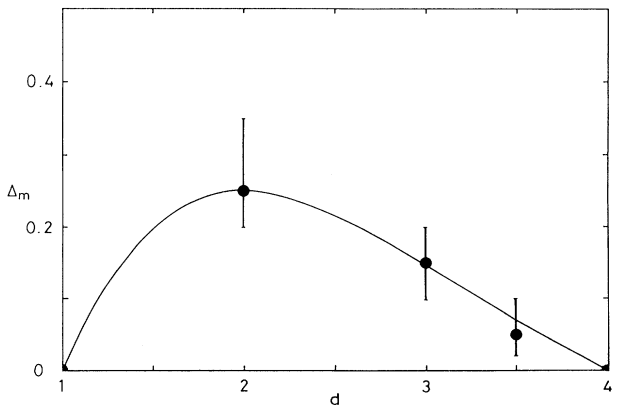

FIG. 2. Correction to the scaling exponent Δ_m for SAW contacts where (●) denotes extrapolation estimates from Table I and the solid curve indicates Eq. (5.10) with ν obtained from Eqs. (3.4b) and (3.4c) (see Fig. 9).

avoiding walk (NAW) limit where $\langle m \rangle = 0$. The leading term in the expansion Eq. (2.10) equals [3]

$$\langle m \rangle = D_\infty(1) n x + O(x^2), \quad x \to 0+ , \tag{2.11a}$$

$$D_\infty(1) = \lim_{n\to\infty} (C_{n,1}/nC_{n,0}) . \tag{2.11b}$$

The constant $D_\infty(1)$ was estimated by Orr [1] and Fisher and Hiley [3a] for square and cubic lattices and was found to have a value of roughly $\frac{1}{8}$. The new estimates of $D_\infty(1)$ in Fig. 1 show a similar variation with d as a_∞. This connection is natural if we note that $D_\infty(1)$ corresponds to a_∞ for $x = 1$ (i.e., SAW's) when higher order x contributions are neglected in Eq. (2.11a).

The ratio $C_{n,1}/nC_{n,0}$ approaches its asymptotic limit rather rapidly and this remarkable behavior led us to study the generalized ratios

$$D_\infty(m) = \lim_{n\to\infty} (C_{n,m}/n^m C_{n,0}) , \tag{2.11c}$$

which require longer chains and the Monte Carlo evaluation of the $C_{n,m}$. This numerical study will be reported elsewhere [24].

Although our primary focus in the present paper is $\langle m \rangle_{\mathrm{SAW}}$, we note that a similar scaling relation to Eq. (1.3) holds for the *maximum* number of SAW contacts. Orr [1] and Fisher and Hiley [3a] found that $m_{\max}$ [see Eq. (2.3b)] obeys the simple asymptotic relation for long chains,

$$m_{\max} \sim a_c n, \quad n \to \infty, \quad a_c = (q-2)/2 , \tag{2.12a}$$

where q is the lattice coordination number. For hypercubic lattices, $a_c = d - 1$. This asymptotic estimate of $m_{\max}$ neglects surface sites, which yield a reduced number of NN contacts. Since the number of surface sites of a compact object scales with mass n as $n^{(d-1)/d}$, we should then have the more general scaling relation for $m_{\max}$,

$$m_{\max} \sim a_c n + b_c n^{\Delta_c} + c_c, \quad \Delta_c = (d-1)/d . \tag{2.12b}$$

The expression for $m_{\max}$ in Eq. (2.12b) can be quantified by observing that a spiral configuration in $d = 2$ maximizes the number of SAW contacts (see Fig. 3) at each step n. We have checked this observation for Monte Carlo generated SAW's up to $n = 50$ [24] in $d = 2$ and find agreement between $m_{\max}$ and the number of spiral SAW contacts. The spiral configuration is not the only configuration that maximizes the SAW contacts, but it is apparently a *representative* configuration. A rigorous proof of this conjecture would be useful, since it is easy to write a numerical program to count the contacts of these ideal compact spiral configurations.

Analytic calculation of m for the compact spiral SAW is not trivial, however. We have consulted colleagues at NIST and have obtained two results for the number of spiral SAW contacts m_{spiral}. Witzgall [25] determined a recursion relation relating m_{spiral} for successive n, which yielded an *exact* solution for $d = 2$ [see Fig. 3(a)],

$$m_{\mathrm{spiral}} = n - \mathrm{Int}[-\tfrac{1}{2} + (n+\tfrac{1}{2})^{1/2}] - \mathrm{Int}[\sqrt{n}\,] , \tag{2.13a}$$

where Int denotes the integer part of the number in parentheses. A bound on m_{spiral}, generalized to higher dimensions was found by McCrackin [26] as

$$m_{\mathrm{spiral}} \le \mathrm{Int}[a_c n - d(n+1)^{\Delta_c} + d] , \tag{2.13b}$$

which becomes *exact* at periodic points at which the spiral completes a hypercube configuration [see Fig. 3(b)]. Numerical data indicate that Eq. (2.13b) is a rather tight bound; this approximation for m_{spiral} is presented in Fig. 4. The bound Eq. (2.13b) is exact in $d = 2$, so that the different looking expressions in Eqs. (2.13a) and (2.13b) (where $\le$ is replaced by equality) are actually *equivalent* in $d = 2$. The number of spiral contacts m_{spiral} is rigorously a lower bound for $m_{\max}$, since a spiral is a particular SAW configuration. We believe that

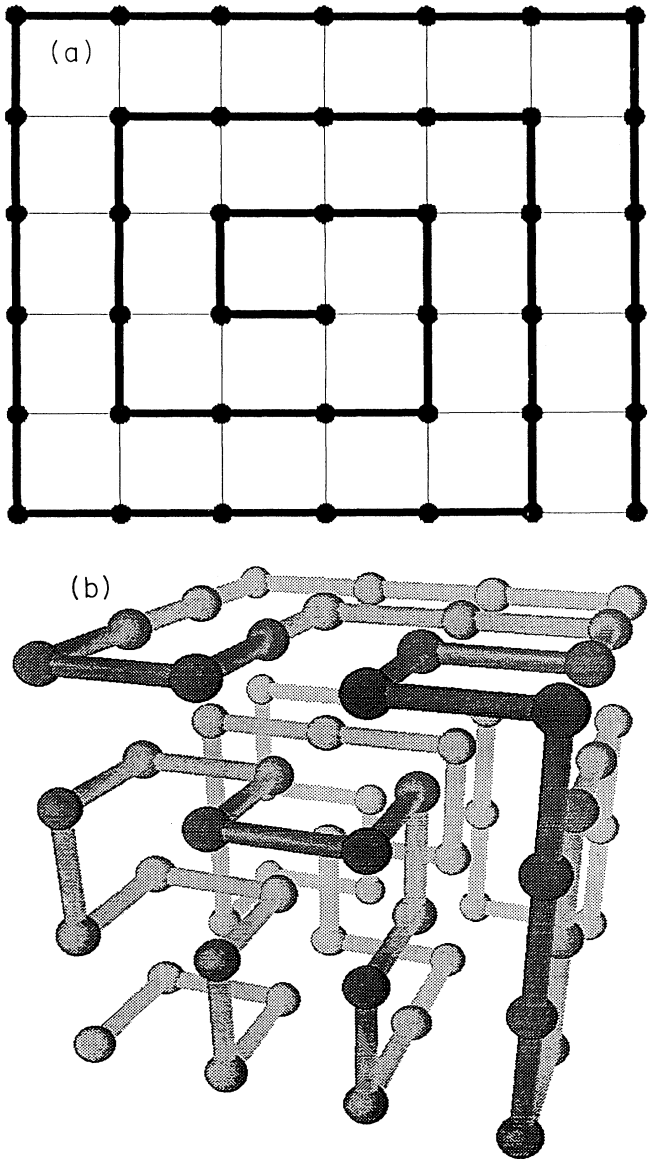

FIG. 3. Compact SAW spiral. (a) Graph of compact spiral SAW (thick line) in $d = 2$ with nearest-neighbor contacts (thin lines) indicated. (b) Compact SAW spiral in $d = 3$ where $n = 64$.

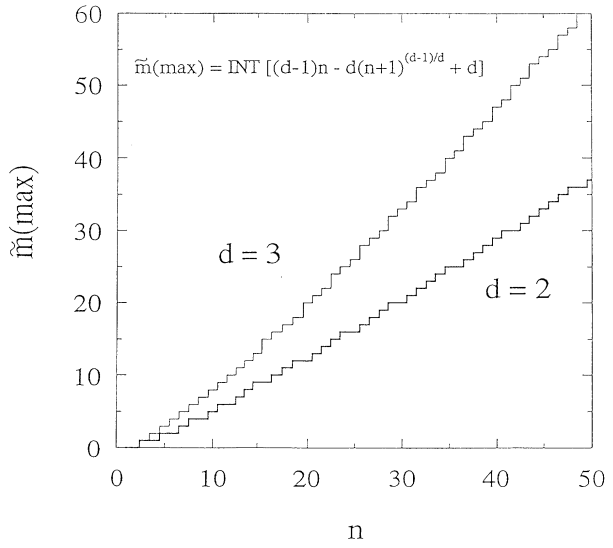

FIG. 4. The estimate of the maximum number of SAW contacts, $m_{\max}$. The curves represent the approximation of Eq. (2.13c) derived from a tight bound on the contacts of a compact SAW spiral. Monte Carlo data also produce these characteristic step patterns [24]. The asymptotic limit in Eq. (2.12a) is only approached for long chains, $n \sim O(10^3-10^4)$.

$m_{\max}=m_{\text{spiral}}$ and numerical evidence is consistent with this identification. [There is some uncertainty at higher chain lengths from the inability of conventional Monte Carlo (MC) methods to sample configurations having maximal contacts for large n so that MC estimates are found to be *less than* or equal to m_{spiral}.] Further efforts are needed to establish the limitations of the approximation

$$m_{\max}\approx \text{Int}[a_c n - d(n+1)^{\Delta_c}+d] ,$$
$$a_c = d-1 , \tag{2.13c}$$
$$\Delta_c=(d-1)/d ,$$

for hypercubic lattices.

The maximum number of SAW contacts is important because it governs the internal energy of compact polymers (e.g., proteins [17]) and $m_{\max}$ is important from a technical standpoint in the testing MC simulations of SAW's. It is generally difficult to sample compact chain configurations using conventional sampling methods. The discrepancy between $m_{\max}$ and numerical estimates of $m_{\max}$ gives a measure of how well these compact configurations are being sampled. A better description of contacts is also a necessary ingredient in developing improved theories of polymer solution phase separation, and this problem is a primary motivation for our examination of SAW contacts (see Sec. VI).

B. $1/d$ expansion of the SAW contact amplitude $a_\infty(d)$

In previous papers, we developed $1/d$ expansions for the partition function and mean-square end-to-end distance of interacting SAW's [9]. (Earlier $1/d$ expansion calculations consider the SAW connectivity constant and other lattice constants [27,28].) Similarly, we can develop $a_\infty(d)$ in a $1/d$ expansion ($\sigma \equiv 2d-1$)

$$a_\infty(d)=\sigma^{-1}+\sigma^{-2}+7\sigma^{-3}+35\sigma^{-4}+250\sigma^{-5}+O(\sigma^{-6}) \tag{2.14}$$

from our exact expansion of the partition function in Eqs. (2.1) and (2.3). The $1/d$ expansion for $a_\infty(d)$ is compared in Fig. 1 with the lattice extrapolation estimates. This comparison exhibits good agreement in higher dimensions ($d \geq 5$), but substantial deviations are found in lower dimensions, reflecting strong fluctuation effects.

The accuracy of the $1/d$ expansion treatment of configurational properties can be improved, however, by combining these calculations with physical reasoning. For example, if we consider the "connectivity constant" in Eq. (1.1) as an effective coordination number of the chain and denote μ in the $x\to 0+$ and $x\to 1$ limits as μ(NAW) and μ(SAW), respectively, then we can expect the average number of contacts per unit chain length a_∞ to be related to the change of the effective coordination number, $\mu(\text{SAW})-\mu(\text{NAW})$. From the $1/d$ expansion of $\mu(\text{SAW})-\mu(\text{NAW})$ and Eq. (2.6), this intuition can be developed into a specific relation between a_∞ and the lattice connectivity constants [μ(NAW), μ(SAW)], which is consistent with the $1/d$ expansion. Explicitly, we find

$$a_\infty=\delta\mu+O(\sigma^{-2}),$$
$$\delta\mu=[\mu(\text{SAW})-\mu(\text{NAW})]/\mu(\text{NAW}) , \tag{2.15a}$$
$$a_\infty \approx \delta\mu . \tag{2.15b}$$

This approximation is also motivated by the observation [3]

$$\mu(\Phi)\sim\mu(\text{NAW})[1+D_\infty(1)x+O(x^2)], \quad x\to 0+ , \tag{2.15c}$$

and the approximate relation between a_∞ and $D_\infty(1)$ suggested above. Extrapolation estimates of μ(SAW) and μ(NAW) over a range of dimensions ($1\leq d\leq 10$) are given in our previous papers [9,11], and Fig. 5 presents these results graphically in a new form. The connectivity constants in high dimensionality approach a simple limiting behavior

$$\mu(\text{SAW})\sim q-1, \quad \mu(\text{NAW})\sim q-2, \quad d\to\infty . \tag{2.16}$$

In high dimensions, μ(SAW) then approaches μ for a nonreversing random walk. The $1/d$ expansion corrections to the asymptotic relations in Eq. (2.16) are shown to order σ^{-5} by a solid line in Fig. 5. Again, the expansion breaks down for lower dimensionality ($d\leq 5$) and we observe the tendency of the connectivity constants to approach a common limit as $d\to 1+$

$$\mu(\text{SAW})\sim\mu(\text{NAW})\sim 1, \quad d\to 1+ . \tag{2.17}$$

It seems likely that the $1/d$ expansion could be substantially improved if the limit in Eq. (2.17) were enforced on the expansion [29].

The estimate of SAW contacts obtained from the con-

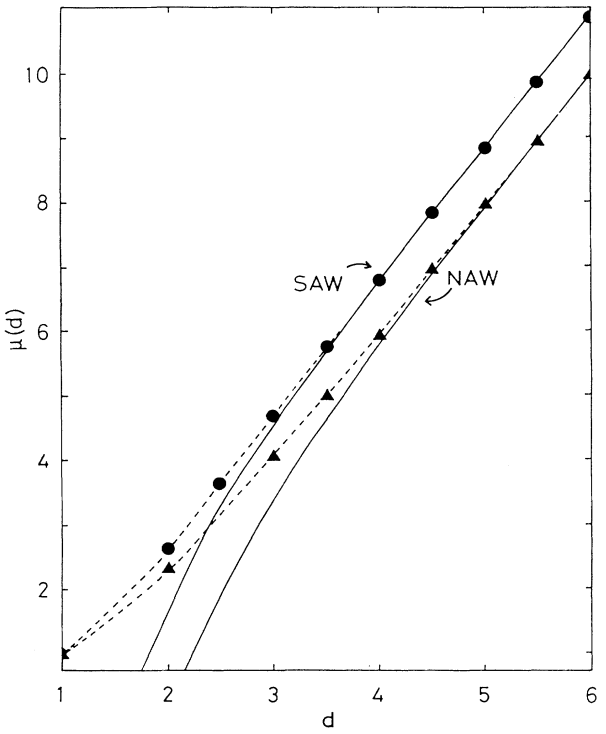

FIG. 5. The SAW connectivity constants as a function of dimension where (●) and (▲) correspond to SAW's and NAW's, respectively. The solid lines denote fifth order $1/d$ expansions for the connectivity constants, and the dashed lines are an interpolation of the lattice data.

nectivity constant decrement $\delta\mu$ [see Eq. (2.15)] is compared with extrapolation estimates of a_∞ in Fig. 1. We observe improved agreement between the $1/d$ expansion and the extrapolation data, but the relation between a_∞ and $\delta\mu$ is not quantitative in lower dimensions. Comparison of a_∞ and $\delta\mu$ is given in Sec. IV for other lattices.

For completeness we note that $\mu(\Phi)$ can also be calculated by $1/d$ expansion in the limit of strong attraction [30]. The compact walks in the $\Phi\to\infty$ limit are Hamilton walks, and the $1/d$ expansion of $\mu_{\rm Ham}$ equals

$$\mu_{\rm Ham}\equiv\mu(\Phi\to\infty)=qe^{-1}[1+\sigma^{-2}/6+O(\sigma^{-3})]\ , \tag{2.18a}$$

This expansion is presented only in an implicit form in previous work [30]. The leading order σ^{-1} correction vanishes [31] and the approximation

$$\mu_{\rm Ham}\approx qe^{-1} \tag{2.18b}$$

gives accurate numerical estimates even in $d=2$ [32–34]. This success is natural given the small fluctuations exhibited by these compact lattice walks.

We further exploit this method of developing nonperturbative approximations for lattice constants in Sec. VI, where estimates of the critical temperature of the Ising model, the θ point of SAW's, and other basic lattice constants are obtained.

III. NUMBER OF RW SELF-INTERSECTIONS

The self-intersection properties of random walks have been studied extensively by both mathematicians and physicists. Erdös and co-workers [21,22,35] pioneered the rigorous theory of geometrical RW properties. Montroll and Weiss [36] and others made further contributions to the quantitative theory and initiated applications [37] of RW "recurrence properties," which showed the physical significance of RW fluctuations. The present section relies heavily on these previous contributions.

The leading order contribution to the number of RW self-intersections can be obtained from the fundamental works of Erdös and Taylor [21] and Montroll and Weiss [36]. Erdös and Taylor first proved that the average number of points $\tilde{V}_m$ visited by a RW at least m times (i.e., m-multiple points) asymptotically equals

$$\tilde{V}_m\sim C_d^*(1-C_d^*)^{m-1}n,\quad d>2,\quad n\to\infty\ , \tag{3.1a}$$

where C_d^* is the probability that an infinite random walk does not return to the origin. (The "escape probability" C_d^* is a fundamental RW property whose evaluation is discussed in Appendix A.) Later, Montroll and Weiss [36,39] formally showed that the number of RW points visited *exactly* m-times V_m has an additional C_d^* factor

$$V_m\sim(C_d^*)^2(1-C_d^*)^{m-1}n,\quad d>2,\quad n\to\infty \tag{3.1b}$$

and this relation was rigorously proven by Pitt [38].

The number of random-walk points where intersection occurs *exactly twice* $\langle m\rangle_{\rm RW}$ then asymptotically equals ($V_{m=2}=\langle m\rangle_{\rm RW}$)

$$\langle m\rangle_{\rm RW}\sim(C_d^*)^2(1-C_d^*)n,\quad d>2,\quad n\to\infty \tag{3.2a}$$

or

$$a_{\rm RW}=(C_d^*)^2(1-C_d^*)\ . \tag{3.2b}$$

The prefactor suggested by Domb [12] is not consistent with this exact result, however.

There are apparently no exact tabulations of C_d^* for variable d that allow a direct estimation of $a_{\rm RW}$. Montroll [39] (see Appendix A) derived a widely cited asymptotic $1/d$ expansion for C_d^*, but this expansion is unreliable for low dimensionality as in the case of a_∞ expansion discussed in the previous section. Gerber and Fisher [27a] developed a formal perturbation expansion (see Appendix A) of the equivalent of C_d^* about $d=2$ dimensions. This expansion is rather badly behaved, however, since $d=2$ is a point of nonanalyticity for C_d^* (see Appendix A). Table II presents our calculated values of C_d^* for a hypercubic lattice over the range $2<d<10$ in dimensional increments of 0.1 based on the numerical evaluation of an integral defining C_d^* (see Appendix A) and C_d^* is plotted as a solid line in Fig. 6. We observe that C_d^* is approximated to within about 1% accuracy by the simple approximant (dashed line in Fig. 6)

$$C_d^*\approx 2(d-2)/[1+2(d-2)],\quad d\geq 2\ , \tag{3.3a}$$

$$C_d^*=0,\quad d\leq 2\ . \tag{3.3b}$$

The escape probability for a simple cubic lattice C_d^* in

$d=3$ is known exactly in terms of Γ functions [40]

$$C_3^* = 32\pi^3/6^{1/2}\Gamma(\tfrac{1}{24})\Gamma(\tfrac{5}{24})\Gamma(\tfrac{7}{24})\Gamma(\tfrac{11}{24}) \approx 0.6595\cdots , \tag{3.3c}$$

and a rapidly convergent expansion and numerical evaluation of the integral defining C_3^* was given by Watson [41] (see also Joyce [42]).

The calculation of C_d^* in variable dimension in combination with (3.2b) then allows the determination of a_{RW}. Figure 7 depicts the *exact* values of a_{RW}. As in the "analogous" case of a_∞, a maximum is observed near $d \approx 3$. Figure 7 also provides the number of RW points occupied exactly m times. It is emphasized that the fluctuation term in Eq. (1.3) becomes large as $d \to 2+$ and this term *predominates* for $d < 2$ (see Appendix B). Figure 8 presents $\tilde{a}_{\mathrm{RW}} \equiv C_d^*(1-C_d^*)$, corresponding to the RW points occupied *at least* twice. This contact amplitude $\tilde{a}_{\mathrm{RW}}$ is more sharply peaked and has a maximum between $d=2$ and $d=3$.

Although the dimensional variation of a_{RW} and a_∞ is similar for high d, there is an important difference in lower d. The RW contact amplitude a_{RW} vanishes for $d \to 2+$, while a_∞ vanishes as $d \to 1+$. This effect can be understood from the increased "swelling" of SAW chains in lower dimensions. It is well known that mean-square dimensions $\langle \mathbf{R}^2 \rangle$ of SAW chains numerically obey the scaling relation

$$\langle \mathbf{R}^2 \rangle \sim n^{2\nu}, \quad n \to \infty , \tag{3.4a}$$

TABLE II. Escape probability of a RW in d dimensions.

d	C_d^*	d	C_d^*
0.0	0.0		
2.0	0.0		
2.1	0.139 343 167 321 667	6.1	0.897 557 907 581 660
2.2	0.249 784 577 109 877	6.2	0.899 729 641 244 915
2.3	0.338 781 361 513 679	6.3	0.901 806 574 846 221
2.4	0.411 531 535 324 035	6.4	0.903 794 975 719 400
2.5	0.471 751 480 834 671	6.5	0.905 700 562 597 621
2.6	0.522 156 543 992 630	6.6	0.907 528 568 654 530
2.7	0.564 768 297 750 299	6.7	0.909 283 790 676 521
2.8	0.601 116 760 617 114	6.8	0.910 970 632 999 663
2.9	0.632 376 874 454 916	6.9	0.912 593 147 129 646
3.0	0.659 462 670 449 368	7.0	0.914 155 065 915 371
3.1	0.683 093 523 276 651	7.1	0.915 659 834 299 400
3.2	0.703 841 586 138 598	7.2	0.917 110 636 535 314
3.3	0.722 166 287 348 678	7.3	0.918 510 420 410 504
3.4	0.738 439 774 241 148	7.4	0.919 861 918 845 346
3.5	0.752 965 922 012 112	7.5	0.921 167 669 189 067
3.6	0.765 994 701 893 923	7.6	0.922 430 030 489 467
3.7	0.777 733 158 441 878	7.7	0.923 651 198 976 838
3.8	0.788 353 879 116 902	7.8	0.924 833 221 970 940
3.9	0.798 001 588 655 984	7.9	0.925 978 010 392 889
4.0	0.806 798 326 773 548	8.0	0.927 087 350 040 607
4.1	0.814 847 545 430 144	8.1	0.928 162 911 752 269
4.2	0.822 237 374 786 415	8.2	0.929 206 260 678 894
4.3	0.829 043 244 310 804	8.3	0.930 218 864 473 517
4.4	0.835 329 999 767 192	8.4	0.931 202 100 989 095
4.5	0.841 153 623 315 606	8.5	0.932 157 265 069 071
4.6	0.846 562 639 013 749	8.6	0.933 085 574 802 418
4.7	0.851 599 267 370 396	8.7	0.933 988 177 207 667
4.8	0.856 300 378 525 860	8.8	0.934 866 153 417 009
4.9	0.860 698 282 929 189	8.9	0.935 720 523 410 817
5.0	0.864 821 390 179 332	9.0	0.936 552 250 347 290
5.1	0.868 694 760 369 504	9.1	0.937 362 244 526 960
5.2	0.872 340 567 360 247	9.2	0.938 151 367 027 440
5.3	0.875 778 489 567 597	9.3	0.938 920 433 039 938
5.4	0.879 026 040 835 594	9.4	0.939 670 214 935 725
5.5	0.882 098 851 578 119	9.5	0.940 401 445 087 726
5.6	0.885 010 882 507 973	9.6	0.941 114 818 469 775
5.7	0.887 774 759 519 103	9.7	0.914 810 995 053 775
5.8	0.890 401 689 981 293	9.8	0.942 490 602 022 884
5.9	0.892 901 873 295 648	9.9	0.943 154 235 817 074
6.0	0.895 284 504 370 825	10.0	0.943 802 464 025 732

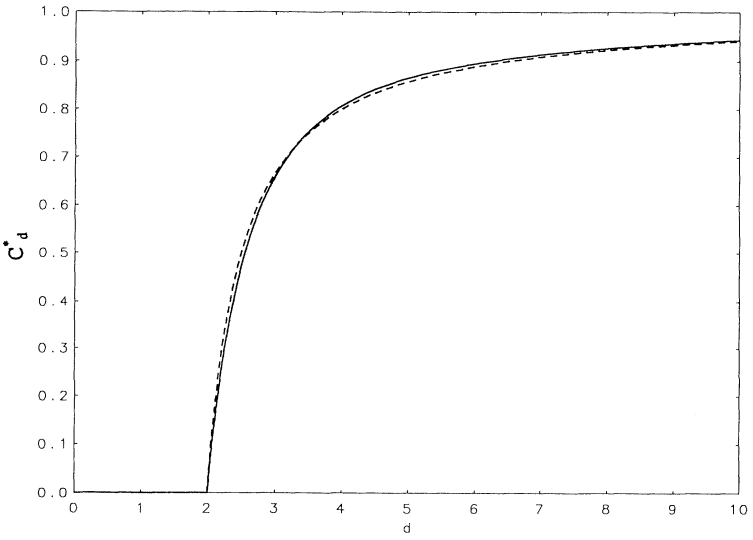

FIG. 6. The escape probability of a simple RW in d dimensions, C_d^*. Solid line denotes exact values (Table II) and the dashed line corresponds to the approximation from Eq. (3.3). C_d^* is also the reduced critical temperature of the spherical model [see Eq. (6.1a)].

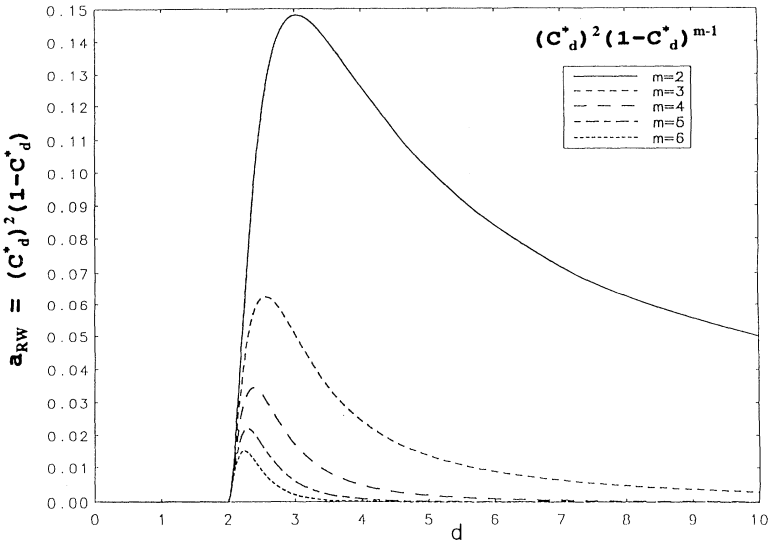

FIG. 7. The self-intersection amplitude for RW's, $a_{\mathrm{RW}}=(C_d^*)^2(1-C_d^*)$. Asymptotically, the number of RW double points $\langle m\rangle_{\mathrm{RW}}$ scales as $\langle m\rangle_{\mathrm{RW}}\sim a_{\mathrm{RW}}n$, $n\to\infty$. We also plot$(C_d^*)^2(1-C_d^*)^{m-1}$, corresponding to the number of m-body contacts per unit chain length. The number of higher order contacts is appreciable in high dimensionality. Compare $m=2$ case with a_∞ data in Fig. 1.

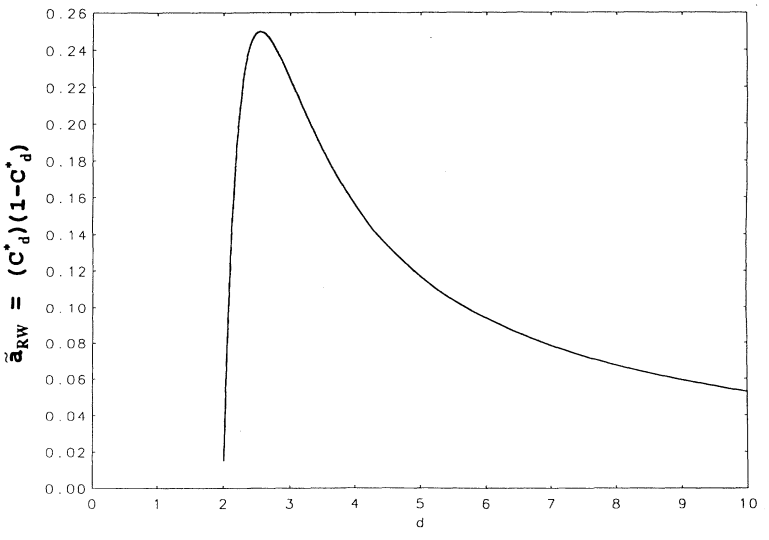

FIG. 8. The self-intersection amplitude for RW's, $\tilde{a}_{\mathrm{RW}}=C_d^*(1-C_d^*)$. The number of binary intersection points that are occupied *at least* twice scales asymptotically as, $\tilde{V}_{m=2}\sim\tilde{a}_{\mathrm{RW}}n$, $n\to\infty$. Notice the maximum becomes sharper and moves closer to $d=2$ in comparison with a_{RW} in Fig. 7.

where ν is apparently piecewise analytic in d [10]. We recently obtained estimates of the SAW exponent ν in variable dimension as [10], $\phi=(4-d)/2$,

$$\nu=\tfrac{1}{2}, \quad d\geq 4 , \tag{3.4b}$$

$$\phi/(2\nu-1)\approx 4[1-2\phi/3+\phi^2/6], \quad 1\leq d\leq 4 , \tag{3.4c}$$

Figure 9 displays the dependence of ν on dimension from Eq. (3.4) in comparison with our extrapolated lattice enumeration estimates of ν [10]. The variation of ν for $d<4$ can be expected to change the escape probability C_d^* for the self-avoiding paths from the RW value (see Appendix A).

Nothing is known about C_d^*(SAW), but exact calculations are possible for generalized RW's (e.g., Lévy flights), which also have ν variable. For example, C_d^* for Lévy flights with a range of ν values have been calculated by Joyce [43a] for $d=1$ and $d=2$ in connection with the spherical model with long-range interactions (see Table III and Sec. VI). Interpolation of Joyce's results for different ν, yields the estimate $C^*(d=2;\nu=\frac{3}{4})\approx 0.77$ for Lévy flights with ν taken as the SAW value. This corresponds to $a_{\mathrm{RW}}\approx 0.14$ for these generalized random walks, which is contrasted with the vanishing of a_{RW} for ordinary NN RW's in $d=2$. Joyce's calculation also indicates that $C^*(d=1;\nu\rightarrow 1^+)$ vanishes (Table III); thus, $a_{\mathrm{RW}}(d=1;\nu\rightarrow 1^+)$ should likewise vanish as for SAW's. These observations are consistent with the vanishing of a_∞ in a lower d than a_{RW} because of the increase in ν as d is lowered (see Sec. IV). A numerical calculation of the escape probability C_d^* for SAW's in $d=2,3,4$ and of Lévy flights having variable ν in $d=3$ would be useful in obtaining a better understanding of the observed dimensional variation of a_∞. In summary, apart from the "stiffening effect" on SAW's in lower dimensionality, a_∞ and a_{RW} vary similarly, and the observed differences are a natural consequence of the variation of ν for SAW's in lower dimensions.

Figure 7, however, indicates a remarkable difference between lattice RW and continuum RW self-intersection properties. The lattice RW's have an appreciable number of many-body ($m>2$) self-intersection points in $d=3$ and higher dimensions. Continuous RW models are rigorously known to have no triple and higher order intersection points [35] (with probability one) in $d\geq 3$. This fundamental difference between lattice and continuum RW's arises because the escape probability of a continuous RW does not gradually increase with spatial dimension as for lattice walks. Indeed, the probability of a continuum limit RW (Wiener path) to "escape" C_d^*

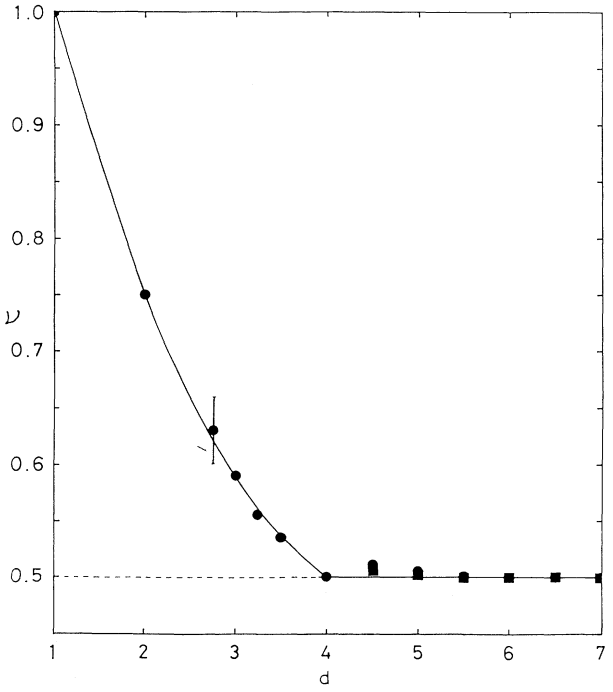

FIG. 9. The extrapolation estimates of SAW size exponent ν. The lattice data (●) for ν in variable d is obtained in a previous paper [9]. The solid curves indicates Eq. (3.4c) and the (■) points for $d>4$ indicate extrapolation estimates, which include analytic corrections to scaling calculated from a $1/d$ expansion while the other points do not include the corrections. See Ref. [10] for further details.

TABLE III. Generalized escape probability $C(d,\nu)$, Lévy Flights.

$x=1/d\nu$	$C(d=1,\nu)$[a]	$(1-x^2)^{4/5}$	$C(d=2,\nu)$[a]	$(1-x^2)^{7/15}$
0.0	1.000	1.000	1.000	1.000
0.1	0.992	0.992	0.994	0.995
0.2	0.968	0.968	0.977	0.981
0.3	0.927	0.927	0.950	0.957
0.4	0.870	0.870	0.914	0.922
0.5	0.796	0.794	0.868	0.874
0.6	0.702	0.700	0.812	0.812
0.7	0.585	0.584	0.744	0.730
0.8	0.439	0.442	0.66	0.621
0.9	0.252	0.265		
1.0	0.0000	0.0000	0.0000	0.0000

[a]See Ref. [43].

jumps discontinuously from zero for $d \leq 2$ to unity for $d > 2$ (see Appendix A). The higher order self-intersections for continuum RW's, thus, have no measurable consequence for $d \geq 3$. The Wiener path model is, thus, somewhat unreliable for discussing many-body interactions [44] in lattice chains and for *presumably real polymer chains,* which are spatially extended objects rather than volumeless filaments. In light of this observation, the higher order m-body contact interactions should be examined more closely in the lattice SAW model to see if these interactions are likewise more significant than continuum model calculations have led us to believe.

IV. LATTICE DEPENDENCE OF SAW CONTACTS

The lattice constant a_∞, which governs the average frequency of NN contacts, depends sensitively on lattice structure. We briefly indicate this effect in Table IV using literature estimates of a_∞ for various lattices. The $1/d$-expansion calculations of a_∞ on hypercubic lattices [see Eqs. (2.14) and (A9)] show that a_∞ approaches the return probability R_d^* of the random walk to the origin in high dimensions,

$$a_\infty \sim R_d^* \sim 1/2d, \quad d \to \infty \ , \tag{4.1}$$

and a_{RW} also approaches this same asymptotic behavior [see Eq. (3.2b)] since $R_d^* = 1 - C_d^*$. From Eq. (4.1), we might naively expect that a_∞ should be smaller for higher coordination number lattices since R_d^* varies inversely to the coordination number q on a hypercubic lattice $R_d^* \sim 1/q$ ($q = 2d$) for high dimensionality. The tabulation of a_∞ data in Table IV *does not* agree with this expectation, however. In fact, a_∞ has a relatively small value ($a_\infty \approx 0.064$) for the low coordination number diamond lattice and a relatively large value ($a_\infty \approx 0.72$) for the high coordination number fcc lattice. Evidently, the variation of the SAW contact amplitude a_∞ is dominated by other factors in lower d.

We can obtain some insight into the observed variation of a_∞ by considering the minimum number of steps necessary for a walk to produce a NN contact $\lambda_{\min}$. The "minimum contact length" $\lambda_{\min}$ is 3 for hypercubic lattices ($d > 1$). Apparently, if $q > 2d$, then $\lambda_{\min} < 3$, while if $q < 2d$, then $\lambda_{\min} > 3$ (see Table IV). We also define $\lambda_\infty \equiv 1/a_\infty$ as the "average period" of NN interferences. (See Appendix B for discussion of this periodicity in the RW case.) The tabulation of $\lambda_{\min}$ and λ_∞ values (Table IV) shows these parameters vary in a qualitatively similar fashion. Thus, the increased persistence length over which excluded volume interferences occur becomes larger for lower coordination number lattices. This increased persistence length for "coarse" (low coordination number) lattices acts very much like an increased chain "rigidity." This important effect deserves further discussion.

The influence of such short-range chain correlations on the escape probability of RW's has been investigated by Daley [45a], who considers the calculation of C_d^* for RW's with a modification in the persistence of the RW to take a step along the direction of the proceeding step. A parameter α is introduced, which when taken to approach $-1+$, corresponds to walks that never have two consecutive steps in the same direction, while the limit $\alpha \to 1-$ produces an enhanced probability of continuing a step in the direction of the previous step. The case $\alpha = 0$ corresponds to a simple unrestricted RW. If we denote the escape probability of the unrestricted walk as $C_3^* \equiv C_3^*(\alpha = 0)$, then the escape probability of Daley's correlated walk equals [45a]

$$C_3^*(\alpha) = q_c C_3^* / [q_c + 2\alpha - \alpha C_3^*], \quad q(\text{cubic}) \equiv q_c = 6 \tag{4.2a}$$

for "cubic-type" lattices (simple cubic, fcc, bcc). The limits $\alpha \to -1+$ and $\alpha \to 1-$ for a simple cubic lattice give limiting modified escape probabilities,

$$C_3^*(-1) = 6C_3^* / [4 + C_3^*] \approx 0.8492 \cdots \ , \tag{4.2b}$$

$$C_3^*(1) = 6C_3^* / [8 - C_3^*] \approx 0.5390 \cdots \ , \tag{4.2c}$$

where the exact value of C_3^* is given in Eq. (3.3c). The exact C_3^* for the tetrahedral lattice equals [46]

$$C_3^*(\text{tet}) = (\tfrac{3}{4}) 2^{11/3} \pi^4 / 9 [\Gamma(\tfrac{1}{3})]^6 \approx 0.5578 \cdots \ , \tag{4.3a}$$

while the cubic-type lattice escape probabilities are larger [36,40,42,46]:

$$\begin{aligned} &C_3^*(\text{simple cubic}) \approx 0.6595 \cdots \\ &C_3^*(\text{fcc}) = 4C_3^*(\text{tet})/3 \approx 0.7437 \cdots \\ &C_3^*(\text{bcc}) = 4\pi^3 / [\Gamma(\tfrac{1}{4})]^4 \approx 0.7177 \cdots \ . \end{aligned} \tag{4.3b}$$

TABLE IV. SAW lattice constants for various lattices.

Lattice	coordination q	a_∞	$\lambda_\infty = 1/a_\infty$	$\lambda_{\min}$	$\delta\mu$	μ(SAW)	μ(NAW)
fcc	12	0.74[a],0.72[d]	1.4	2	0.55	10.035[e]	6.46
Cubic	6	0.18[b],0.201	5.3	3	0.15	4.6835	4.065
Diamond	4	0.064[c]	16	5	0.05	2.8790	2.73
Triangular	2	0.59[d]	1.7	2	0.46	4.152[e]	2.84
Square	3	0.16[c,d]	6.3	3	0.14	2.6385	2.316

[a]See Ref. [15a].
[b]See Ref. [3a].
[c]See Ref. [7].
[d]See Ref. [12].
[e]See Ref. [104].

We then observe that the change of C_d^* from simple cubic lattice to the tetrahedral lattice is similar to the change of C_d^* observed for the cubic lattice in the $\alpha \to 1-$ limit in Daley's correlated random-walk model [see Eq. (4.2)]. Similarly, the increased chain rigidity (lattice induced short-range correlations) upon lowering the dimension ultimately causes a_∞ to approach zero as $d \to 1+$, since the SAW reduces to a nonintersecting rod in this limit. High coordination lattices such as the fcc lattice in $d=3$ exhibit an *opposite* tendency to the low coordination lattices. The high coordination number of the fcc lattice, for example, leads to a tendency for greater chain "coiling" and a_∞ achieves a remarkably high value 0.72 [12]. This effect is similar to taking α negative in Daley's model where an increase in C_d^* is obtained [see Eqs. (4.2b) and (4.3b)]. Finally, we mention that the connectivity constant decrement $\delta\mu$ [see Eq. (2.15) and Table IV] for various lattices generally follows the variation of a_∞ with lattice type, confirming the qualitative approximation Eq. (2.15a).

The "granularity" of the lattice structure, which has a profound effect on lattice parameters (see Sec. VI) [μ(SAW), T_c(Ising), a_∞, $\cdots$], is a caricature of the packing constraints on molecular positioning. Real polymer chains, for example, have constrained bond angles and constraints arising from the presence of surrounding molecules (solvent molecules in the idealized SAW model). The optimal choice of lattices to model the small scale granularity of real condensed phases requires further study.

V. FLUCTUATIONS IN RW SELF-INTERSECTIONS AND SAW CONTACTS

The calculation of corrections to scaling for $\langle m \rangle_{\rm SAW}$ in Sec. II is based on the analogy between SAW contacts and RW self-intersections suggested by Domb [12] [see Eqs. (1.2) and (1.3)]. This relation is potentially quite useful because the recurrence properties of random walks can be calculated *exactly* [21,47], and it might be possible to extend a similar theory to SAW's (see Sec. VII). In this section we reconsider the form of the fluctuation corrections for $\langle m \rangle_{\rm RW}$ where ν is variable (Lévy flights) and we compare these results to our numerical estimates of the fluctuation corrections to $\langle m \rangle_{\rm SAW}$ obtained in Sec. II. In the final part of the section, we briefly discuss the dependence of fluctuation corrections of $\langle m \rangle_{\rm RW}$ on chain topology and the relation of these corrections to the polymer excluded volume problem.

In leading order, the number of RW binary self-intersections $\langle m \rangle_{\rm RW}$ depends on the RW escape probability C_d^* [see Eq. (3.2a)] and, more generally, the calculation of the fluctuation corrections for $\langle m \rangle_{\rm RW}$ requires the determination of the "survival probability" $C(d,n)$—the probability that a RW does not return to the origin before the nth step (see below). Unfortunately, the exact calculation of $C(d,n)$ is difficult and we resort to considering the simpler problem of calculating the leading order fluctuation corrections for $C(d,n)$. This task is made simpler by exploiting an *exact* relation between $C(d,n)$ and the number of distinct sites visited by a RW, $\langle S_n \rangle$, a quantity investigated extensively [21,22, 35,36]. Calculations of the fluctuation corrections for $\langle S_n \rangle$ are not available for variable d and ν and results relating to these cases are found by considering the continuum analog of $\langle S_n \rangle$, the volume of the Wiener sausage $\langle \mathcal{V}_n \rangle$ (defined below). Exact calculations for the fluctuation corrections for $\langle \mathcal{V}_n \rangle$ with d and ν variable are known and these results allow us to estimate the $\langle m \rangle_{\rm RW}$ fluctuation corrections for variable d and ν. Domb's previous suggestion [12] for these corrections are recovered by these arguments and in the process we obtain some geometrical insight into the fluctuation corrections to RW self-intersections.

Fluctuation corrections to many random-walk properties are naturally expressed in terms of the RW survival probability $C(d,n)$ and an exact discrete integral equation [21] for $C(d,n)$ is discussed in Appendix A. The escape probability C_d^* of the previous section corresponds to the limit [21,22]

$$C_d^* = \lim_{n\to\infty} C(d,n) , \tag{5.1}$$

since the paths that "survive forever" are those that "escape to infinity." Erdös and Taylor [21] discuss the order of magnitude of the leading order corrections to the asymptotic scaling in Eq. (5.1) in integer dimensions.

Precise estimates of fluctuation corrections have been studied for the related random variable $\langle S_n \rangle$. These results are relevant to the present problem because $\langle S_n \rangle$ is simply an average of $C(d,n)$ [22],

$$\langle S_n \rangle = \sum_{k=1}^{n} C(d,k) . \tag{5.2}$$

This relation exists because $C(d,k)$ is also the probability that the nth step takes the RW to a previously unvisited site (see Appendix B). The average $\langle S_n \rangle$ has been calculated for a variety of lattices in $d=3$ because of associated physical applications: Here we mention Joyce's calculation [42] of $\langle S_n \rangle$ for a simple cubic lattice, $d=3$,

$$\langle S_n \rangle \sim C_3^* n + 4[(3/2\pi)^{3/2} n^{1/2}](C_3^*)^2 + [81(C_3^*)^2/8\pi^2 + \tfrac{7}{16}]C_3^* + O(n^{-1/2}) , \tag{5.3}$$

where C_3^* is given by Eq. (3.3c). Some liberty has been taken in rewriting Joyce's results in our own more concise notation involving C_3^*. (Joyce also gives the $O(n^{-1/2})$ term explicitly, but this term is unnecessary for the present discussion.) Inserting the numerical value of C_3^* into Eq. (5.3) gives

$$\langle S_n \rangle \sim 0.659n + 0.574n^{1/2} + 0.450 + O(n^{-1/2}) . \tag{5.4a}$$

Monte Carlo estimates [48] of $\langle S_n \rangle$ are rather consistent with this asymptotic series estimate,

$$\langle S_n(\text{num}) \rangle \sim 0.662n + 0.525n^{1/2} + 0.501 . \tag{5.4b}$$

A connection between RW self-intersections and $\langle S_n \rangle$ is obtained by noting that the number n of steps taken minus $\langle S_n \rangle$ equals the number of points of multiple occupation M_n ("redundant points"):

$$\langle M_n \rangle \equiv n - \langle S_n \rangle \ . \tag{5.5a}$$

Since binary self-intersections are the predominant type of multiple occupation point for $d>2$, the average $\langle M_n \rangle$ is closely related to $\langle m \rangle_{\mathrm{RW}}$. For long chains $\langle M_n \rangle /n$ and $\langle S_n \rangle$ have the limiting behavior

$$\lim_{n\to\infty} (\langle M_n \rangle /n) = (1-C_d^*) \ ,$$
$$\lim_{n\to\infty} \frac{\langle S_n \rangle}{n} = \lim_{n\to\infty} \left[\frac{1}{n} \sum_{k=1}^{n} C(d,k) \right] = C_d^* \ . \tag{5.5b}$$

This result holds generally in d dimensions, $d>2$. Equation (4.3) implies that the fluctuation corrections to $\langle M_n \rangle$ in $d=3$ are on the order $O(n^{1/2})$ in accord with Domb's suggestion, Eq. (1.1). Figure 10 presents the contact amplitude $(1-C_d^*)$ for redundant points. Bleris and Argyrakis [48b] show numerically that the fluctuations of RW self-intersections can be estimated accurately by formally replacing C_d^* in Eq. (3.2) by $\langle S_n \rangle /n$ for finite chains. This is a natural approximation given the close relation between $\langle M_n \rangle$ and $\langle m \rangle_{\mathrm{RW}}$.

Calculation of fluctuation correction in d dimensions ($d>2$) is complicated by the difficulty of calculating of $\langle S_n \rangle$ in d dimensions. Exact calculation is possible, however, for the continuum analog of $\langle S_n \rangle$, the volume of the Wiener sausage [49] (see Appendix B). The Wiener sausage corresponds to the average volume $\langle \mathcal{V}_n \rangle$ swept out by an object undergoing Brownian motion where the volume of previously visited regions is not counted [49a, 50]. In the limit of vanishing time n, the sausage volume $\langle \mathcal{V}_n \rangle$ reduces to the particle volume, but $\langle \mathcal{V}_n \rangle$ follows Spitzer's limit theorem, $d>2$,

$$\lim_{n\to\infty} \langle \mathcal{V}_n \rangle /n \sim \hat{C}n + (d/2\pi)^{d/2} n^{\phi} \hat{C}^2/\phi(1-\phi) + O(\mathrm{const}) \tag{5.6}$$

for large n where $\hat{C}$ is proportional to the capacity of the diffusing body [49a, 49b]. Spitzer [35e,49a] notes that C_d^* is the lattice analog of the continuum capacity, which explains the origin of our notation for the RW escape probability. We observe that the leading order fluctuation correction to $\langle S_n \rangle$ in Eq. (5.3) corresponds to the simple fluctuation correction to $\langle \mathcal{V}_n \rangle$ for $d=3$, and this relation should hold generally for hypercubic lattices. [Daley's discussion of the leading order fluctuation corrections to $\langle S_n \rangle$ [45a] shows that the constant $(d/2\pi)^{d/2}$ must be modified for other lattices.] Equation (5.6) then implies that fluctuation exponent (crossover exponent) for random-walk self-intersections should equal $\phi=(4-d)/2$, as suggested before by Domb [12].

Extension of the Wiener sausage calculation to generalized random walks (Lévy flights) with variable ν provides an exact estimate of the exponent $\phi(\nu)$, which is useful in comparison with SAW's where ν is also variable. The exponent $\phi(\nu)$ for Lévy flights equals [51]

$$\phi(\nu) = 2 - d\nu, \quad d > 1/\nu \ . \tag{5.7}$$

Moreover, Eq. (5.6) still applies with $\phi(\nu)$ replacing ϕ, the return probability constant $(d/2\pi)^{d/2}$ suitably modified for Lévy flights, and the capacity $\hat{C}$ also modified for this class of paths [51,52]. The exponent $\phi(\nu)$ for Lévy flights can be recognized as the "specific heat" exponent (more properly the "virial coefficient" exponent in a polymer context [19]),

$$\alpha = 2 - d\nu, \quad d \le 4$$
$$\alpha = 0, \quad d \ge 4 \ . \tag{5.8}$$

Domb estimated α and Δ_m for SAW's in $d=3$ and $d=2$ and found these exponents to be *equal*, as in the case of Lévy flight RW's. Equations (5.7) and (5.8) then suggest an approximation for the SAW fluctuation exponent

$$\Delta_m \approx 2 - d\nu, \quad d < 4 \ . \tag{5.9a}$$

The leading order ϵ-expansion estimate of ν [see Eq. (3.4)] in conjunction with Eq. (5.9a) yields an estimate of Δ_m in accord with Domb's values [see Eq. (1.3b)] in $d=2$ and $d=3$,

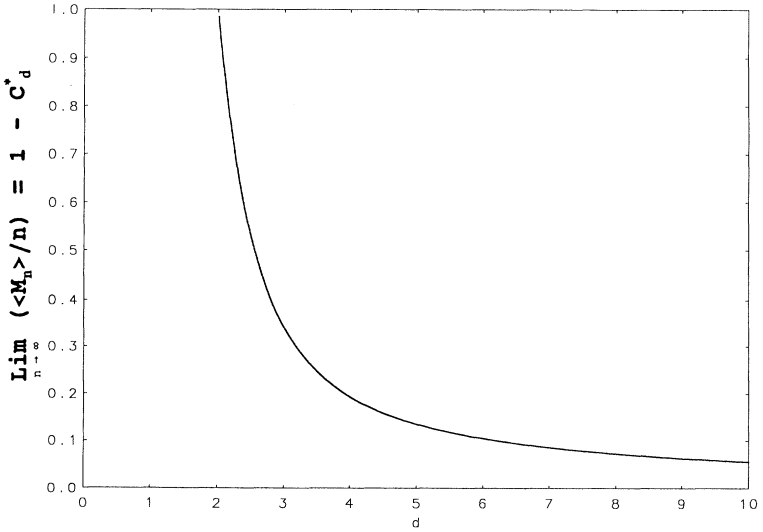

FIG. 10. The amplitude for number of redundant points, $\lim(\langle M_n \rangle /n) = 1-C_d^*$, which equals the number of points a RW occupies more than once divided by the chain length for large n and the return probability of a simple random walk to the origin. The difference $1-C_d^*$ also corresponds to the spherical model estimate of p_c(site) [80] (see Sec. VI).

$$\Delta_m = \phi/2 + O(\phi^2), \quad \phi = \epsilon/2 \ . \tag{5.9b}$$

Using ν from Eq. (3.4c) in Eq. (5.9a) yields

$$\Delta_m(d=3) \approx 0.235, \quad \Delta_m(d=2) \approx \tfrac{1}{2} \ . \tag{5.9c}$$

Unfortunately, these estimates of Δ_m based on the RW analogy are only roughly consistent with the lattice enumeration data in Table I and Fig. 2 and the dependence of Δ_m on d evidently requires further thought.

Simple considerations show that Eq. (5.9a) cannot be correct in lower dimensions where there are important qualitative differences between SAW's and RW's on account of the rigidity effect discussed in Sec. IV. A SAW in $d=1$ is perfectly extended so that Δ_m must vanish, while RW's in $d=1$ do not have this constraint and self-intersect intensely. An improved estimate of Δ_m can be obtained by relating Δ_m to other SAW exponents, which similarly reflect the increased rigidity of SAW's in lower d. The SAW exponent $\gamma - 1$ vanishes as $d \to 1+$ for similar reasons as Δ_m [10] and Ref. [10] suggests the approximation $\gamma \approx (d/2)(3\nu - 1)$, which is exact in both the $d \to 1+$ and $d \to 4-$ limits. Based on these previous arguments, we introduce an *ad hoc* approximation for Δ_m,

$$\Delta_m \approx d(3\nu - 1)/2 - 1, \quad 1 < d < 4 \ , \tag{5.10}$$

corresponding to $\Delta_m = \frac{5}{34} \approx 0.147$ and $\frac{1}{4}$ for $d=3$ and $d=2$, respectively (see Fig. 2). We conclude that the contact fluctuation exponent Δ_m varies quite differently than the fluctuation exponent for RW self-intersections, even in the case where ν is taken to have SAW values. This discrepancy is expected because of the non-Markov nature of SAW's and in Sec. VII we discuss a generalized theory of Feller [47a], which can be applied to the fluctuation corrections of correlated RW's. In the final part of this section, we make some comments regarding some applications of RW self-intersection fluctuations to the problem of excluded volume interaction in flexible polymers and the dependence of self-intersection fluctuations on the RW chain topology.

The average number of "redundant points" in the continuum model $\langle M(n) \rangle = n - \langle \mathcal{V}_n \rangle$ can be directly expressed in terms of a notation conventional in polymer physics,

$$\langle M(n) \rangle \sim (1-C)n + C^2 \left\langle \frac{1}{2!} \int_0^n d\tau \int_0^n d\tau' \delta(\mathbf{R}(\tau) - \mathbf{R}(\tau')) \right\rangle + O(\text{const}) \ , \tag{5.11}$$

which is useful in generalizations to RW's having restricted topology (see below). The average $\langle\ \rangle$ is taken with respect to continuous Gaussian chains (Wiener measure), $\delta(\ )$ is a δ function, and $\mathbf{R}(\tau)$ denotes the position vector of the continuous chain path at a contour point τ along the chain. This configurational average arises in the calculation of the polymer chain partition function Q_n in leading order perturbation theory for the excluded volume interaction [53]. The result for the configurational average for a linear chain is presented in Eq. (5.6). The configurational integral in Eq. (5.11) is sensitive to chain topology, and this term for a ring polymer even has a different sign than the corresponding linear polymer term. These configurational integrals have been investigated extensively because the leading order ϵ-expansion estimates of the susceptibility exponent γ [see Eq. (2.2)] are also determined by the configurational average in Eq. (5.11), and results for various cases are summarized by Cherayil, Douglas, and Freed [53] (ring, chain constrained to begin and end on a surface, star). Our main point for the present discussion is that the fluctuation correction to $\langle m \rangle_{\mathrm{RW}}$ is sensitive to chain topology, and the same can be expected for $\langle m \rangle_{\mathrm{SAW}}$. The contact amplitudes a_{RW} and a_∞ $(d \geq 2)$ should be *invariant* to these topological variations, however. These topological effects deserve further investigation.

VI. RW AND SAW CRITICAL CONSTANTS, CRITICAL PHENOMENA, THE θ POINT OF INTERACTING SAW'S

It is well known that the universal critical behavior of many systems undergoing phase transitions can be related to the geometrical properties of RW's and SAW's. The present paper is largely motivated by Domb's calculations [12] of O(m) spin model ($m=1$, Ising; $m=2$, XY, $\cdots$) properties in terms of the geometrical properties of SAW's and we briefly mention some theoretical results relating these walk properties to various kinds of critical phenomena, including the θ point of self-interacting SAW's and the critical temperature of the Ising model for hypercubic lattices.

The critical temperature of the spherical model T_c(spherical) can be expressed in terms of the Green's function [43,54] for lattice random walks. Translating into our notation, T_c(spherical) equals

$$k_B T_c(\text{spherical})/J = C_d^* q \ , \tag{6.1a}$$

where J is the magnetic NN exchange energy. Equation (6.1a) is exact and reduces to the mean-field (Bragg-Williams or Bethe approximation [27b], Gaussian model [54(b)]) in high dimensions

$$k_B T_c(\text{MF})/J = q \ , \tag{6.1b}$$

since $C_d^*(d \to \infty) = 1$ (see Fig. 6).

The physical origin of the shift of T_c from its mean-field (MF) value deserves comment. Near the critical point of a fluid mixture there is a clustering phenomenon of the phases and the phase within these diffuse "droplets" has a reduced coordination number for interactions with the other phase [55–57]. This effect can be appreciated by considering linear chain "clusters" as an idealization. The extended chain modification of Eq. (6.1b) amounts to simply replacing q by $q-1$ as noted by Flory [58a] in his modeling of T_c for polymer solutions. The counting becomes more involved for self-intersecting random-walk "clusters," which are closer to the physical situation of real critical clusters. The extensive RW self-intersection produces a reduction of the average coordination number. The fraction of RW points occupied at least once asymptotically equals $C_d^* n$ so that C_d^* times

the coordination number of each lattice site provides an estimate of "mean coordination number" per segment for the RW chain. This geometrical estimate of the effective coordination number corresponds to the spherical model T_c in Eq. (6.1a). With this qualitative physical picture in mind, we next consider the critical temperature of the O(m) model in terms of an effective coordination number related to SAW and RW parameters.

The O(m) model encompasses a wide range of physical models of phase transitions and other critical phenomena [12,27]. The SAW model corresponds to $m \to 0$, the Ising model ($m=1$), the XY model ($m=2$), the Heisenberg model ($m=3$), and the spherical model ($m \to \infty$). We generalize Eq. (6.1) by defining the "effective coordination number" $\mu(m)$ of the O(m) model

$$\mu(m) \equiv [J/k_B T_c(m)]^{-1} , \tag{6.2}$$

which follows naturally from Domb's treatment [12] of the O(m) model in terms of SAW's with NN interactions weighted with topological factors reflecting the order parameter dimension m.

Gerber and Fisher [27a] obtained the $1/d$ expansion for the equivalent of $\mu(m)$, and *combining* this result with the $1/d$ expansion for C_d^* (see Appendix A) gives

$$\mu(m) = C_d^* q \{1 + [1 - m/(m+2)]\sigma^{-2} + O(\sigma^{-3})\}, \quad \sigma = 2d - 1 \tag{6.3}$$

for hypercubic lattices. [Equation (6.3) can be thought of as an expansion about the spherical model limit rather than the usual Bragg-Williams limit.] The SAW connectivity constant corresponds to the $m \to 0$ limit and we have the identity

$$\mu(m=0) \equiv \mu(\text{SAW}) \tag{6.4a}$$

and the spherical model limit ($m \to \infty$) corresponds to

$$\mu(m \to \infty) = C_d^* q . \tag{6.4b}$$

Since accurate estimates of μ(SAW) are known, it is useful to reexpress Eq. (6.3) to include this nonperturbative information. Using the $1/d$ expansion of μ(SAW) [9,27] allows us to rewrite Eq. (6.3) as

$$\mu(m) = \mu(\text{SAW}) \times \{1 + [m/(m+2)][C_d^* q - \mu(\text{SAW})]/\mu(\text{SAW}) + O(\sigma^{-3})\} , \tag{6.5}$$

which gives an explicit approximation to the critical temperature of the O(m) model entirely in terms of the *geometrical properties of random and self-avoiding walks.* Equation (6.5) is constructed to be exact in the $m \to 0$ and $m \to \infty$ limits, and Fig. 11 shows that $\mu(m)$ is a rather slowly varying function of m. The data points in Fig. 11 provide estimates for the critical temperature of the Ising model in various dimensions, and the corresponding numerical estimates [59] are given in Table V.

The expansion about the spherical model limit in Eqs. (6.3) and (6.7a) becomes problematic in $d=2$ dimensions since simple RW's become recurrent in this dimension. Indeed, $T_c(m>2)=0$ for $d \leq 2$ because of this recurrence property [60]. Domb [12] and Domb and Smart [61] has developed an alternative expansion about the SAW limit ($m \to 0$), which is useful in lower dimensionality. If we denote the high temperature series expansion parameter as ω,

$$\omega = I_{m/2}(J/k_B T)/I_{m/2-1}(J/k_B T) , \tag{6.6}$$

where $I_{m/2}$ is a modified Bessel function, then Domb's estimate of the critical temperature for the O(m) model is determined as a series in μ(SAW) and SAW contact parameters

$$\omega_c^{-1} = \mu(\text{SAW})\{1 - 3f(m)a_\infty/\mu^2(\text{SAW}) + O(\mu^{-3}(\text{SAW}))\} , \tag{6.7a}$$

$$f(m) = m^2/(m+2), \quad m = 1,2,3 . \tag{6.7b}$$

The leading order term in Eq. (6.7a) has been conjectured

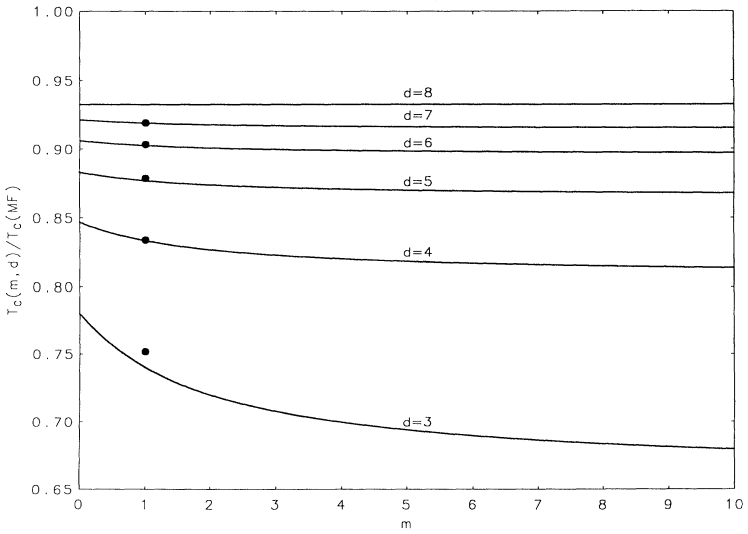

FIG. 11. The critical temperature of the O(m) model in variable dimension where (●) denotes lattice model estimates of T_c from Table III. The solid lines denote approximant Eq. (6.5). Data and curves correspond to hypercubic lattices.

TABLE V. Basic lattice constants.

d	p_c(bond) Ref. [78]	$\frac{T_c(\text{Ising})}{T_c(\text{MF})}$ Ref. [59]	$\frac{T_c(\text{Ising})}{T_c(\text{MF})}$ Eq. (6.5)	$\mu(\text{SAW})/q$ Ref. [59]	$\mu(\text{NAW})/q$ (see Fig. 5)
2	1/2[a]	0.567 296		0.659 539 6	0.579 13
3	0.248 8	0.751 904 0	0.740	0.780 651 2	0.677 5
4	0.160 05	0.835 210	0.834	0.846 500	0.739
5	0.118 19	0.877 832	0.877	0.883 86	0.794 0
6	0.094 20	0.902 912	0.902	0.906 567	0.829 1
7	0.078 685	0.919 22[b]			
8	0.067 70				
9	0.059 50				

[a]See Ref. [105]. [b]See Ref. [106].

to be exact by Temperly [62a] on the basis of numerical evidence, and this conjecture is discussed critically by Fisher and Sykes [2], who show that Temperley's conjecture $\omega_c^{-1}=\mu(\text{SAW})$ is not exactly true. The factor $f(m)$ in Eq. (6.7) is evidently poorly behaved for large m, and we resort to the approximation $f(m)\approx 1$ for the interesting case of the Ising model ($m=1$). Our *ad hoc* modification of Domb's expression Eq. (6.7) then becomes

$$\omega_c^{-1}\approx \frac{\mu(\text{SAW})}{1+3a_\infty/\mu^2(\text{SAW})}, \quad \text{Ising model} . \tag{6.8}$$

Table VI shows that Eq. (6.8) gives good estimates of the critical temperature of the Ising model even in $d=2$. Estimates for other types of lattices are included in Table VI, and all the data agree with Eq. (6.8) to within 2% accuracy. Again we find a representation of the critical temperature of the Ising model in terms of the geometry of SAW paths.

The arguments above for the critical temperature of the O(m) model can be developed further to obtain a useful estimate of the θ point temperature T_θ for NN interacting polymers. There are strong arguments (not rigorous proof, however) that the phase separation of polymers in a small molecule solvent is described by the Ising universality class [63]. Our approximation for T_θ assumes this relation is true. The θ temperature T_θ for long isolated polymers in solution equals the critical temperature for polymer solution phase separation T_c in the Flory-Huggins theory. This theoretical prediction holds to a good approximation experimentally [64], and we also assume $T_c=T_\theta$ for long chains $n\to\infty$. The critical temperature for a binary mixture of NN interacting molecules having identical sizes follows from Eq. (6.5) as

$$\delta = T_c(\text{Ising})/T_c(\text{MF}) , \tag{6.9}$$

since there is an exact mapping between the Ising model and the binary mixture problem [65]. Table V shows that δ is nearly $\frac{3}{4}$ in $d=3$. Equation (6.9) simultaneously describes the phase separation of small molecule binary mixtures, the liquid-vapor phase transition and magnetic Ising models on hypercubic lattices, where each atom is idealized to occupy a lattice position [66]. Moreover, the ratio in Eq. (6.9) is rather *insensitive* to lattice type for the common lattices [27,67] and corresponding ratios for the SAW connectivity constant are summarized by Cherayil, Douglas, and Freed [53]. [The ratio δ in Eq. (6.9) approaches unity with increasing range of the interaction potential and experimental estimates of this ratio in real systems could provide information on the range of the local pair potential.]

Equation (6.9) certainly requires modification of $T_c(\text{MF})$ when passing from the small molecule mixture to

TABLE VI. T_c(Ising) as a function of SAW lattice constants.

d	$1/\omega_c=\tanh(J/k_BT_c)$ Ref. [27]	a_∞ (see Table IV)	$\frac{\mu(\text{SAW})}{[1+3a_\infty/\mu^2(\text{SAW})]}$ Eq. (6.8)	$\mu(\text{SAW})$ Ref. [14]
		Hypercubic lattice		
2	$1+\sqrt{2}=2.41\cdots$	0.1592	2.47	2.6382
3	4.58	0.201	4.56	4.683
4	6.72	0.174	6.70	6.775
5	8.83	0.141	8.82	8.832
6	10.87	0.111	10.86	10.873
		Other lattices		
fcc	9.828[a]	0.72	9.824	10.035
Diamond	2.83[a]	0.0638	2.81	2.878
Triangular	3.732 05[a]	0.59	3.77	4.1515

[a]See Ref. [104] and Fig. 5.

a polymer solution. The effective coordination number μ(SAW) of the chain in high dimensions is reduced due to chain connectivity (see Fig. 5)

$$\mu(\text{SAW},\ d\to\infty)=q-1\ , \tag{6.10a}$$

thus explaining the physical basis of the mean-field result for the θ-point energy Φ_θ of interacting SAW's [68]

$$\Phi_\theta(\text{MF})=1/(q-1)\ . \tag{6.10b}$$

We modify the exact result Eq. (6.9) for small molecule phase separation by requiring that the mean-field result Eq. (6.10b) is recovered as $d\to\infty$, which leads to the approximation

$$\Phi_\theta\approx 1/(q-1)\delta,\quad T_c=T_\theta\ ,\quad n\to\infty \tag{6.11}$$

where δ is defined by Eq. (6.9). The estimate δ for a cubic lattice from Table V yields $\delta(\text{cubic})\approx 0.7519$, and Eq. (6.11) then implies

$$\Phi_\theta(\text{cubic})\approx 0.266\ . \tag{6.12}$$

This estimate of the θ point agrees very well with numerical determinations [4,69,70] of the SAW θ point, Φ_θ(cubic; num)$\approx$0.269. We further observe that since δ is nearly constant [27] ("quasiuniversal" [53]) for the common three-dimensional lattices $\delta(d=3)\approx\frac{3}{4}$, we may obtain the simpler approximation

$$\Phi_\theta\approx 4/3(q-1),\quad d=3\ , \tag{6.13a}$$

which compares favorably with the MC estimate of Φ_θ, found by Mazur and McCrackin [15a],

$$\Phi_\theta(\text{MC})\approx 1.375/(q-1) \tag{6.13b}$$

for a variety of three-dimensional lattices. Estimates of the critical energy Φ_θ for other dimensions follow from Eqs. (6.9) and (6.11).

The escape probability C_d^* governs the critical temperature in other phase transitions. For example, the critical temperature for adsorption of a polymer (RW) onto a penetrable surface of dimension $d_\parallel$ is determined [71] by $C^*_{d-d_\parallel}$. The description of polymer adsorption onto impenetrable surfaces of dimension $d_\parallel$ involves a generalization of C_d^* for walks in the presence of an absorbing boundary [72]. There are also a variety of localization-delocalization transitions determined by C_d^*. Examples include the critical binding of electrons to defect sites in lattices [73], the binding of defect atoms to a lattice position due to a critical mass difference [74], the localization of spin waves by lattice defects [75], and electron localization in disordered materials [76].

There is also a natural relation between the geometrical properties of RW's and SAW's, and lattice percolation. As in the case of the O(m) model, we can define an effective coordination number for lattice percolation [53] and develop the $1/d$ expansion about the spherical model limit. For example, consider bond percolation on a hypercubic lattice and define μ(bond) as the reciprocal of the bond percolation threshold [53]:

$$\mu(\text{bond})\equiv[p_c(\text{bond})]^{-1}\ . \tag{6.14}$$

The $1/d$ expansion for p_c(bond) is known [77], and we can combine this expansion with that for C_d^* (Appendix A) to obtain the modified $1/d$ expansion

$$\mu(\text{bond})=(C_d^*q)[1-\sigma^{-2}/2+\cdots]\ . \tag{6.15a}$$

We observe that the leading order $1/d$ corrections *vanishes* [see Eq. (2.18)] for μ(bond), and we can expect the approximation

$$\mu(\text{bond})\approx C_d^*q \tag{6.15b}$$

to be accurate for $d>2$. This expectation is borne out in Fig. 12, where the best numerical estimates [78] of μ(bond) for hypercubic lattices are compared with Eq. (6.15b). Excellent agreement is observed for $d\geq 3$, but the approximation breaks down for $d\to 2+$ as in Eq. (6.3). The approximation Eq. (6.15b) evidently suggests a relation between the fraction of RW paths that escape to infinity and the number of "percolating paths" that span

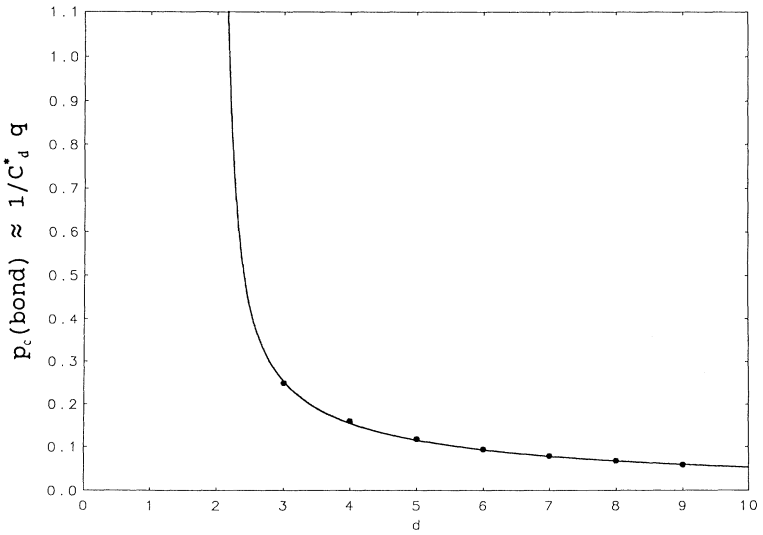

FIG. 12. The estimate of the hypercubic lattice bond percolation threshold where (●) denotes precise numerical estimates [78] of p_c(bond) and the solid line denotes the approximation Eq. (6.15b), $p_c(\text{bond})\approx 1/C_d^*q$.

the system. The leading order "mean-spherical model approximation" for μ(bond) in Eq. (6.15b) was obtained previously by Given and Stell [79].

Similar arguments can be made for site percolation. By inspection of the $1/d$ expansions for bond and site percolation [77], we observe a simple relation between the bond and site percolation thresholds:

$$p_c(\text{site}) = [q - \mu(\text{bond})]/q + O(\sigma^{-3}) . \tag{6.15c}$$

A further simplification of our estimate for p_c(site) can be obtained by introducing the additional approximation Eq. (6.15b) into Eq. (6.15c) to obtain

$$p_c(\text{site}) \approx 1 - C_d^* . \tag{6.15d}$$

Equation (6.15d) (see Fig. 10) is known to be a rather good approximation in high dimensionality ($4 \leq d$) and corresponds to the mean-spherical model approximation for p_c(site) [80].

The resistance properties of regular resistor networks in d dimensions also exhibits a striking relation to μ(bond) and RW properties. Vineyard [81a] has shown that the resistance R between a node at the origin and another at a great distance on a cubic lattice of resistors equals

$$R = (1/C_d^* q)\Omega, \quad d > 2 , \tag{6.16a}$$

where Ω denotes ohm units. Each resistor in the network, situated on the "edges" of the lattice, is taken to have unit resistance (1Ω). We, thus, obtain the numerical approximation of R from Eq. (6.15b)

$$R \approx p_c(\text{bond})\Omega, \quad d \geq 3 , \tag{6.16b}$$

which links the resistance properties of regular resistor networks to percolation theory. This relation is very interesting when generalized to defective lattices, where R_d^* (or C_d^*) becomes a function of bond dilution. Equation (6.16) also has basic significance in polymer physics when the equivalence between network resistance and the dimensions of Gaussian polymer networks is recognized [82,83]. Eichinger [83] has shown that a d_m-dimensional network of RW chains of equal length has the mean-square radius of gyration $\langle S^2 \rangle$ [see Eq. (6.16a)]:

$$\langle S^2 \rangle = \langle \mathbf{R}^2 \rangle_0 / C_{d_m}^* q, \quad q = 2d_m, \quad d_m > 2 , \tag{6.17}$$

where $\langle \mathbf{R}^2 \rangle_0$ is the mean-square end-to-end distance of a RW network chain. $\langle \mathbf{R}^2 \rangle_0$ defines the unit of length as the unit resistor defines the resistance scale in the corresponding resistor problem [82].

This section provides a sampling of phase transition phenomena, which can be interpreted in terms of the geometrical properties of RW's and SAW's. Domb's original study of the critical temperature $T_c(m,d)$ of the O(m) spin model in terms of SAW properties [12] suggested to us that this geometrical point of view might give insight into a variety of critical constants, so we examined this possibility. The critical temperature of the spherical model $T_c(m \to \infty, d)$ is first shown to be exactly related to the RW escape probability C_d^*. (This result was found previously by Joyce [54a], but apparently this result is not widely known.) A geometrical interpretation of $T_c(m \to \infty, d)$ is given in terms of an idealized RW model of critical clusters. This point of view is developed further into a nonperturbative expression for the critical temperature $T_c(m,d)$ in terms of RW and SAW parameters. The derivation of this result utilizes a perturbative $1/d$ expansion of $T_c(m,d)$, where improved accuracy is obtained by the procedure of shifting the $1/d$ expansion to be about the spherical model rather than the Bragg-Williams mean-field theory reference point. Very good results were also obtained for the bond and site percolation thresholds by shifting the reference point for the $1/d$ expansion. This idea is simple and effective.

An examination of the critical phenomena literature revealed that a variety of critical constants could be *exactly* related to RW recurrence properties—critical temperature for polymer adsorption, critical binding energies, resistance of networks, radius of gyration of polymer networks, etc. The discussion of these problems from the RW perspective offers new insights into these previously known analytic results; in cases where exact results are not known and this viewpoint suggests new approximations for calculating critical constants. As a nontrivial example of this approach, we make a heuristic calculation of the θ point of SAW's and the critical temperature of high molecular weight polymer solutions, which accords with numerical estimates of these quantities.

VII. DISCUSSION

The average number of nearest-neighbor SAW contacts $\langle m \rangle$ characterizes the average frequency of excluded volume interferences in a swollen chain. The long chain limit of $\langle m \rangle_{\text{SAW}}$ is found to be proportional to chain length $\langle m \rangle_{\text{SAW}} \sim a_\infty n$, and we study the variation of a_∞ with spatial dimension. The contact amplitude a_∞, as estimated from our direct enumeration data, is observed to have a maximum near $d = 3$ and to vanish in the $d \to 1+$ and $d \to \infty$ limits. Our $1/d$ expansion of a_∞ for a hypercubic lattice shows that a_∞ decays for large dimensionality as the return probability R_d^* of a random walk to the origin $a_\infty \sim R_d^* \sim 1/2d$. Agreement with the asymptotic $1/d$ expansion is only obtained for dimensions higher than four, however. Numerical estimates of a_∞ for other lattices are examined and a rather sensitive dependence on lattice structure is found. This sensitivity is associated with RW's on relatively high and low coordination lattices (relative to the simple cubic lattice) adopting relatively coiled and extended configurations, respectively.

Following some basic observations by Domb [12], suggesting a relation between the SAW contact problem and the self-intersections of RW's, we calculate the number of RW self-intersections $\langle m \rangle_{\text{RW}}$ on a hypercubic lattice exactly for $d > 2$. The number of RW intersections follows a similar pattern to the SAW's. The intersection amplitude a_{RW} in the asymptotic relations $\langle m \rangle_{\text{RW}} \sim a_{\text{RW}} n$ for binary self-intersections is observed to have a maximum near $d = 3$ and to vanish as $a_{\text{RW}} \sim R_d^* \sim 1/2d$ for high dimensionality. The constant a_{RW} vanishes for $d = 2$ for RW's, however. This effect can be understood from the

change of the polymer size exponent ν in lower dimensions, and, indeed, if we consider generalized random walks (Lévy flights) with ν taken to have the values estimated for non-Markov lattice SAW's, then a_{RW} for these generalized RW's approaches zero as $d \to 1+$ rather than as $d \to 2+$. This accords with the extrapolated SAW data (Fig. 1).

The fluctuation exponents Δ_m and ϕ for SAW contacts and RW self-intersections are estimated by numerical extrapolation and by analytical methods, respectively. The RW "crossover exponent" equals $\phi = 2 - d/2$ for $2 < d < 4$ so that ϕ monotonically increases toward 1 as $d \to 2+$, reflecting the increased self-intersections in lower dimensionality. This variation is natural given the (rigorous) geometric interpretation of ϕ in terms of an intersection dimension as discussed by Rosen [84a]. The SAW exponent Δ_m, on the other hand, vanishes both as $d \to 4-$ and $d \to 1+$ and has a maximum near $d \approx 2$. The SAW exponent γ has a similar dimensional variation [10], leading us to introduce a phenomenological approximation consistent with our lattice extrapolation data, $\Delta_m \approx d(3\nu - 1)/2 - 1$, $1 < d < 4$. Simple scaling arguments suggest that Δ_m should approximately equal the specific heat exponent $\alpha = 2 - d\nu$ for $1 < d < 4$, but this estimate (see also Domb [12]) is found to be too large in comparison with the extrapolated lattice data. We briefly discuss the chain topology dependence of the fluctuation corrections to SAW contacts and RW self-intersections.

The lattice data for SAW's and RW's (connectivity constants, a_∞, C_d^*, $\cdots$) are applied to the calculation of various important lattice constants. We obtain an approximation of the critical temperature $T_c(m)$ of the $O(m)$ model in general dimensionality and compare this general result to available lattice data. An alternative estimate of the Ising model T_c involving a_∞ is examined and is found advantageous in $d = 2$ dimensions. A rather good estimate is thereby produced for Ising critical temperatures for a variety of lattices. These preliminary results for the estimation of T_c(Ising) in various dimensionalities culminate in an estimate of the θ temperature of SAW's and the critical temperature for phase separation in solutions of a high molecular weight polymer and a small molecule solvent. Comparison with experiment are again rather favorable. The bond percolation threshold of hypercubic lattices $2 < d < 9$ is found to be approximated accurately ($d \geq 3$) in terms of the RW escape probability C_d^*; other related lattice parameters are discussed such as the resistance of a lattice network.

The Appendixes examine the relation between continuum and lattice random walks and the interrelations of different analytic treatments of the recurrence properties of RW's. Appendix A shows that the escape probability of a continuum random walk varies as a unit step function, which jumps at $d = 2$, while the escape probability of lattice RW smoothly increases for $d > 2$ towards 1 as $d \to \infty$. This difference in continuum and discrete RW's leads to significant differences in the intersection properties of continuum and discrete RW chains, and these differences are discussed in Sec. III.

Domb's analogy between RW self-intersections and SAW NN contacts potentially has other important consequences, which have not been pursued in the present paper. RW self-intersections and their fluctuations can be exactly described by Feller's "fluctuation theory of recurrent events" [47a]. The return of the random walk to the origin, which is related to $\langle m \rangle_{\mathrm{RW}}$, is a classical renewal process discussed by Feller to illustrate his general theory. The scaling of $\langle m \rangle_{\mathrm{SAW}}$ with chain length obtained from our lattice data extrapolations is consistent with the asymptotic scaling of a renewal process. Feller's theory of recurrent events is notably *not restricted* to random walks having uncorrelated steps: Lamperti [85] and Stone [86] have illustrated the general theory for a class ("semistable" [85]) random walks having long-range correlations.

Semistable walks are simply defined by the existence of a limit end-to-end vector distribution function for long chains and the property of invariance (in distribution) of the random-walk curves under the rescaling of the contour length [85]. These scaling properties are often *assumed* (implicitly or explicitly) in the discussion of SAW properties based on formal calculational methods such as the renormalization group method. If we presume that SAW's are "attracted" to a universal (semistable) limit distribution for long chains, then it is quite natural to hypothesize that SAW contacts can be described as a renewal process. This hypothesis (equivalent to the assumption that the chain length distance between SAW contacts is an independent random variable) leads to the prediction that the probability distribution for SAW contacts is in the domain of attraction of a stable process [47] of index $2 - \Delta_m$ for $1 < d < 4$ and should be normally distributed and be centered about the average $\langle m \rangle_{\mathrm{SAW}}$ for $d > 4$. The distribution function for contacts and its moments are fixed by the critical exponent Δ_m ($2 - \alpha$ in Feller's notation) characterizing the contact fluctuations. It should be useful to compare the probability distribution for SAW NN contacts from Monte Carlo data for long chains with the distribution suggested by Feller's renewal theory. The theory of recurrent events appears promising for characterizing the fluctuations of self-avoiding chains, which are responsible for the nonclassical critical exponents for $1 < d < 4$. The functional limit theorems of this theory are especially interesting because they provide a *mathematical mechanism* explaining the existence of universality for the SAW exponents—provided the formulation of the SAW contact problem as a renewal process can be established.

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APPENDIX A: ASYMPTOTIC PROPERTIES OF THE SURVIVAL PROBABILITY

The description of the self-intersection number $\langle m \rangle_{\mathrm{RW}}$ and other properties related to the geometric structure of RW paths are naturally constructed by considering the recurrence of a RW to a specified point on an infinite lattice. Without loss of generality, this specified point is taken as the origin. If we generate a RW path of n steps, taken in the available directions with equal probability $(1/2d)$ at each step, then the probability $C(d,n)$ that the RW survives (does not return to origin) its first $n-1$ steps is a monotone decreasing function of chain length[22]

$$C(d,1)=1\geq C(d,2)\geq C(d,3)\geq C(d,4)\geq \cdots >0 . \quad \text{(A1)}$$

Erdös and Taylor [21], and Dvoretzsky and Erdös [22a] prove that $C(d,n)$ for a RW approaches a limiting "fixed point" value

$$\lim_{n\to\infty} C(d,n)\to C_d^*, \quad d>2 . \quad \text{(A2)}$$

The return of a RW to a point is classic "renewal" process [47], and a discrete integral equation for $C(d,n)$ is obtained by a sum of probabilities (see Eq. (2.11) of Erdös and Taylor [21] and Feller [47a]),

$$C(d,n)+\sum_{k=1}^{[n/2]} U(d,2k)C(d,n-2k)=1 , \quad \text{(A3)}$$

where $U(d,n)$ is the probability that the path return at the nth step and [ ] denotes the "integer part." Erdös and Taylor [21] and Dvoretzsky and Erdös [22a] describe order of magnitude estimates for the rate at which the limit in Eq. (A2) is approaches, i.e., the fluctuation terms. Feller [47a] in 1949 introduced the term "critical exponent" to describe these corrections to scaling exponents in his general fluctuation theory of recurrent events.

The survival probability $C(d,n)$ represents the fraction of the lattice paths with length n that do not return to the origin after the $n-1$ step. The analog of the lattice RW "renewal equation" Eq. (A3) for the return to a point in the limit of continuous paths (Wiener paths) is recently given by Douglas [87] and solved exactly for general d using methods of fractional calculus. The exact solution of Eq. (A3) for various lattices is a more difficult matter, but the continuum limit calculation illustrates certain asymptotic results and physical features of lattice RW models. The survival probability for Brownian paths $\hat{C}(d,n)$ with a short-range interaction and with an endpoint attached to a "boundary" (a point in the present discussion), is described by a Volterra integral equation [87],

$$\Psi(x)=1-\zeta_p\int_0^x [(x-t)^{\phi_p-1}/\Gamma(\phi_p)]\Psi(\tau)d\tau , \quad \text{(A4a)}$$

$$\hat{C}(d,n)=\Psi(x=1), \quad \zeta_p=(z_p/u_p^*)\Gamma(1+\phi_p) , \quad \text{(A4b)}$$

$$\phi_p=1-d/2, \quad u_p^*=\phi_p, \quad z_p=(d/2\pi)^{d/2}n^{\phi_p} , \quad \text{(A4c)}$$

which is the continuum limit of Eq. (A3). The generalization of Eq. (A4) to an interacting (penetrable) hyperplane [87] of dimension $d_\parallel$ simply involves replacing ϕ_p by $\phi_s=(2+d_\parallel-d)/2$, and the generalization to Lévy flight walks with variable ν involves replacing ϕ_p by $\phi_s=(d_f+d_\parallel-d)/d_f$, where d_f is the Hausdorff dimension of the Lévy flight, $d_f\equiv 1/\nu$ [87]. The return probability constant $(d/2\pi)^{d/2}$ in Eq. (A4c) also has to be changed to the value appropriate for the Lévy flight [87]. The transition from RW recurrence to transience (see Appendix B) is reflected analytically in the kernel of Eq. (A4a), which exhibits a corresponding transition from "weakly singular" to "strongly singular" type [87].

We briefly mention the importance of Eqs. (A3) and (A4) for a wide class of physical problems. The survival probability $\hat{C}(d,n)$ for Brownian paths in Eq. (A4) has a direct physical interpretation in terms of the partition function of a polymer chain interacting with a surface, and this model exhibits a phase transition when the coupling parameter ζ_p (or ζ_s) changes sign [87]. The order of the transition depends on ϕ_p (or ϕ_s). A formal extension of Eq. (A4) has also been made for fractal boundaries using the geometric interpretation of ϕ_p as the dimension of (fractal) the Brownian path intersections with the boundary [88] in the contour coordinate. The integral equation Eq. (A4) also arises in modeling relaxation in disordered materials [87c]. Feller [47a] and Darling and Kac [89a] have shown that Eq. (A4) describes the asymptotic survival probability of Brownian paths subject to general interactions so that the renewal Eqs. (A4) and (A3) have applicability to a wide class of quantum mechanical and diffusion problems [87], especially ones involving complicated boundaries.

The exact solution [87] of Eq. (A4) defines the Mittag-Leffler function:

$$\hat{C}(d,n)=\sum_{k=0}^{\infty} (-\zeta_p)^\kappa/\Gamma(1+k\epsilon_p/2) . \quad \text{(A5)}$$

This function is monotone in ζ_p as required by Eq. (A1). Now if we consult the tabulation of the properties of this classical transcendental function summarized by Douglas, Wang, and Freed [87b], we find that $\hat{C}(d,n\to\infty)$ is piecewise analytic in d. It is easily shown that $\hat{C}(d,n\to\infty)$ for $\zeta_p>0$ equals

$$\hat{C}(d,n\to\infty)=\begin{cases} 0, & 0<d\leq 2 \quad \text{(A6a)} \\ 1, & d>2 . \quad \text{(A6b)} \end{cases}$$

Equation (A6) implies that the return of a typical continuum RW (Wiener path) to the origin is certain for $d\leq 2$, while escape of the path to infinity is certain for $d>2$. This result is just the continuum limit analog of Pólya's famous theorem for lattice random walks (see Fig. 6):

$$C(d,n\to\infty)=\begin{cases} 0, & 0<d\leq 2 \quad \text{(A7a)} \\ C_d^*, & 0<C_d^*\leq 1, \quad d>2 . \quad \text{(A7b)} \end{cases}$$

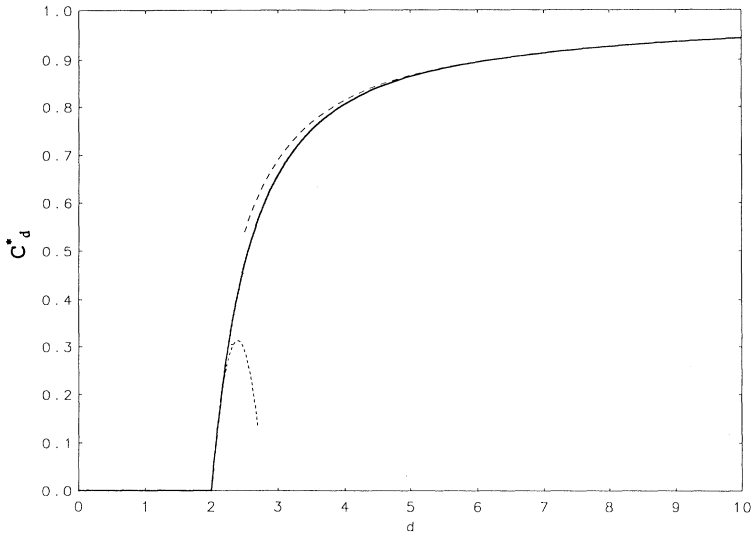

FIG. 13. The escape probability of a RW from the origin, C_d^* where dashed lines denote expansions about $d=2$ and $d\to\infty$.

Lattice RW's return to origin (paths are recurrent) for $d<2$, and some *fraction* of the discrete RW paths "leak to infinity" for $d>2$. C_d^* is this fraction. Explicit calculation of C_d^* for lattice RW's shows that the escape probability depends on the local lattice structure (see Sec. IV) and the spatial dimensionality. The hypercubic lattice C_d^* has the simple integral representation [39]

$$C_d^*=1/d\int_0^\infty [e^{-x}I_0(x)]^d dx\ , \tag{A8}$$

where $I_0(x)$ is a modified Bessel function. [Note that $e^{-x}I_0(x)\sim x^{-1/2}$ for large x, so the integral in Eq. (A8) diverges for $d\le 2$, thereby implying $C_d^*(d\le 2)=0$.] Analytic calculation of the equivalent of Eq. (A8) in $d=3$ is a classical problem [40–42], and the result is given in Eq. (3.3c). Montroll [39] has developed a $1/d$ expansion for C_d^*,

$$C_d^*\sim 1-(1/2d)[1+2/(2d)+7/(2d)^2+35/(2d)^3 +215/(2d)^4+\cdots],\quad d\to\infty \tag{A9}$$

for the hypercubic lattice by simply expanding the Bessel function in Eq. (A8). The probability that the RW returns to the origin equals $R_d^*\equiv 1-C_d^*$. Gerber and Fisher [27a] have also developed [rediscovered independently by us before realizing the relation between T_c(spherical) and C_d^* discussed in Sec. VI] a formal expansion for the equivalent of C_d^* about $d=2$,

$$C_d^*\sim(\pi/2)(d-2)-(\pi/4)[1+8\ln(8/\pi)+\hat{\gamma}](d-2)^2 +O((d-2)^3),\quad d\to 2+\ , \tag{A10}$$

where $\hat{\gamma}$ denotes Euler's constant. Figure 13 compares the leading order expansion of C_d^* about $d=2$ and the fifth order $1/d$ expansion with exact numerical results (solid line). The error involved in truncating the series (A9) is discussed by Gerber and Fisher [27a]. Their discussion of the convergence properties of C_d^* is instructive because it is one of the few cases where the infinite order $1/d$ expansion is known. The formal series in Eq. (A10) about $d=2$ is particularly poorly behaved because $d=2$ is a nonanalytic point for C_d^* (see Fig. 13).

The escape probability C_d^* can also be calculated [91,92] from an average of the return probability $U(d,n)$ to the origin at the nth step [see Eq. (A3)],

$$C_d^*=1\Big/\sum_{n=0}^{\infty} U(d,n),\quad U(d,0)=1\ . \tag{A11}$$

Figure 14 represents the *exact* [93,94] $U(d,n)$ in $d=1$, $d=2$, $d=3$ for $n\le 22$, which shows how the probability of the RW to return to the origin at the nth step (regardless of its previous history) decays with increasing n [see Eq. (A12)]. The lower the dimensionality, the higher the return probability and the longer the tail of the curve. Indeed, C_d^* vanishes for $d\le 2$ because the sum of $U(d,n)$ in Eq. (A11) diverges because of this slow decay for $d\le 2$.

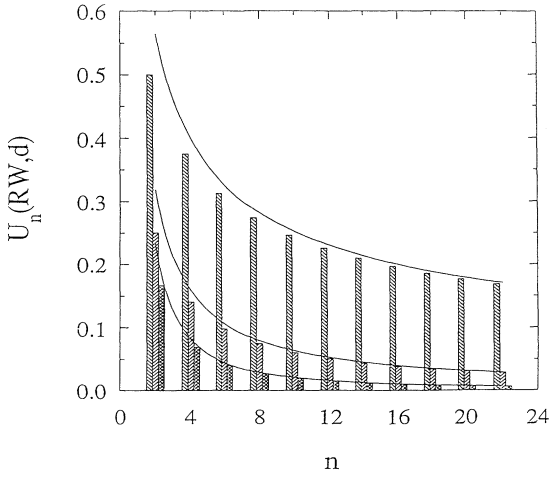

FIG. 14. The probability that a RW will return to origin at the nth step, $U_n(RW,d)$. Histograms are exact lattice data and continuous curves correspond to asymptotic power laws ($n^{-d/2}$) [92] for $d=1$, $d=2$, $d=3$ (top to bottom). Note that the return probability is zero for odd n.

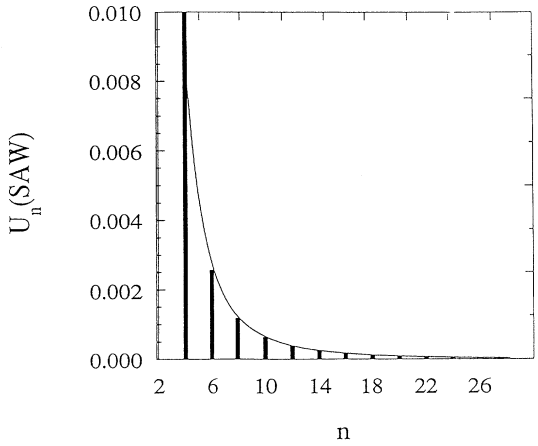

FIG. 15. The fraction of ring SAW's relative to linear SAW's in $d=2$, $U_n(\mathrm{SAW},d=2)$. Ring fraction vanishes for odd n as in the RW analog (see Fig. 14). Solid line denotes the asymptotic power law scaling. Direct enumeration data is taken from Ref. [95].

Figure 15 presents the "ring closure probability" $U_n(\mathrm{SAW})$ for SAW's in $d=2$ (square lattice) obtained from direct enumeration [95]. $U_n(\mathrm{SAW})$ is defined as the number of self-avoiding rings of length n divided by the number of self-avoiding chains without the ring closure restriction. The sum in Eq. (A11) with $U_n(\mathrm{SAW})$ replacing $U(d,n)$ would seem to be convergent, so that it seems likely that the escape probability of a SAW is nonzero in $d=2$. This question deserves further consideration since this geometrical property of SAW's probably is important for understanding the finiteness of $a_\infty(d=2)$ (see Fig. 1).

An approximation to C_d^* can be obtained by utilizing an asymptotic expansion for $U(d,n)$ given by Domb [92a]. The leading order relation

$$U(d,n)\sim 2(d/2\pi)^{d/2}(2n)^{-d/2}+O(n^{(-d+2)/2}) \qquad \text{(A12)}$$

is presented as the solid curves in Fig. 14. This asymptotic limit is approached rapidly with increasing n. We then insert Eq. (A12) into Eq. (A11) to obtain the rough estimate

$$C_d^*\approx 1/[1+f_d\zeta(d/2)],\quad f_d\equiv 2(d/2\pi)^{d/2}2^{-d/2}, \qquad \text{(A13)}$$

where $\zeta(x)$ is the Riemann ζ function. Inclusion of the higher order corrections to Eq. (A13) leads to a power series sum of the Riemann ζ functions [96]. The leading order estimate of Eq. (A13) in $d=3$ equals 0.621 rather than the exact value $0.659\cdots$ from Table II. It should be possible to refine this direct approach of calculating C_d^* from the return probability $U(d,n)$. This should be very useful in the case of Lévy flights in $d=3$ where general results for C_d^* are unknown and asymptotic results for $U(d,n)$ are available [43].

APPENDIX B: THE PERIODICITY OF RW RECURRENCE

The frequency of RW self-intersections is directly related to the average period between RW intersection points along the chain contour. Many of the interesting properties of RW's are associated with the fluctuations in this recurrent random process. The periodicity of RW recurrences is necessarily considered separately for "recurrent" walks ($C_d^*=0$) and "transient" walks ($C_d^*>0$) since in the latter case a fraction of the paths never revisit a given point of the RW path. We calculate the average recurrence period and briefly discuss the relation between various methods for evaluating recurrence properties of RW's.

1. Recurrent walks, $C_d^*=0$

Since recurrence to the origin is certain, the period of recurrence can be expected to correspond to the number of distinct sites visited $\langle S_n\rangle$ by the RW. This relation is exact for a deterministic periodic orbiting trajectory of any kind for a time longer than the orbital period. We show that the corresponding average "period" for a recurrent random walk scales like $\langle S_n\rangle$ for large n.

To obtain the asymptotic behavior of $\langle S_n\rangle$ for large n, it is useful to pass formally to the continuum limit of the discrete sum [22] by defining $\langle S(n)\rangle$ as

$$\langle S_n\rangle=\sum_{k=1}^{n}C(k,d)\rightarrow\langle S(n)\rangle=\int_0^n\hat{C}(\tau',n)d\tau', \qquad \text{(B1)}$$

where $C(n,d)$ is given by Eq. (A5). $\hat{C}(\tau',d)$ is an entire function, so that the integral in Eq. (B1) can be performed term-by-term to give

$$\langle S(n)\rangle=n\sum_{k=0}^{\infty}\{(z_p/u_p^*)\Gamma(1+\phi_p(\nu))]\}^k/\Gamma(2+k\phi_p(\nu)), \qquad \text{(B2a)}$$

where z_p, u_{p*}, and $\phi_p(\nu)$ are defined in general for Lévy flights (ν variable) as

$$z_p=p(0)n^{\phi_p(\nu)},\quad \phi_p(\nu)=1-d\nu,\quad u_p^*=\phi_p(\nu),$$
$$0<\phi_p(\nu)\le 1,\quad 1\le 1/\nu\le 2. \qquad \text{(B2b)}$$

The constant is determined by the probability that the walk returns to the origin at the nth step and for ordinary continuum RW's $p(0,\nu=\frac{1}{2})$ equals $(d/2\pi)^{d/2}$. The large n asymptotic expansion ($0<\phi_p(\nu)\le 1$) of $\langle S(n)\rangle$ equals

$$\langle S(n)\rangle\sim\{\sin[\pi\phi_p(\nu)]/\pi[1-\phi_p(\nu)]\}$$
$$\times nz_p^{-1}[1+O(z_p^{-1})+\cdots],\quad z_p\rightarrow\infty, \qquad \text{(B3a)}$$

which reduces for ordinary RW's ($\nu=\frac{1}{2}$) in $d=1$ to the asymptotic limit

$$\langle S(n)\rangle\sim(2/\pi)nz_p^{-1}=(8/\pi)^{1/2}n^{1/2},\quad n\rightarrow\infty, \qquad \text{(B3b)}$$

which is the well known Pólya result [36,81,90] for discrete RW's ($\nu=\frac{1}{2}$) on a $1-d$ lattice. More generally, $\langle S_n\rangle$ in Eq. (B3a) scales as n^ν for large n in $d=1$, an asymptotic result of Gillis and Weiss [97] under the conditions ($0<\phi_p(\nu)<1$, $1<1/\nu<2$). They do not obtain the prefactor explicitly, however.

Treatment of the $\phi_p(\nu)\rightarrow 0+$ limit for $\langle S_n\rangle$ is delicate. Note the divergent character of the expansion coefficients

of Eq. (B2a) in this limit. There are log$n$ corrections in the $\phi_p(\nu)\to 0+$ limit associated with the transition between the point recurrence and point transience of RW paths and analytically corresponding to a change from weakly singular to a strongly singular kernel in Eq. (A4). Renormalization group calculations [88] show that $C(n,d)$ vanishes logarithmically as

$$C(n;\phi_p\to 0+)\sim A_1/\ln n, \quad n\to\infty , \tag{B4}$$

where A_1 is a nonuniversal constant. Thus, the number of distinct sites visited $\langle S_n\rangle$ scales in the $\phi_p\to 0+$ (or $\phi_s\to 0+$) limit as [36,98]

$$\langle S_n\rangle\sim A_2 n/\ln n, \quad n\to\infty , \tag{B5}$$

where A_2 is a lattice-dependent constant.

A relation between $\langle S_n\rangle$ and the mean recurrence time $\langle \tau_n\rangle$ for a random walk to return to the origin is established through a renewal equation. Renewal equations come in pairs, and the complementary equation to Eq. (A3) is given by

$$U_n=\sum_{k=0}^{n-1} f_{n-k}U_k, \quad U_0=1, \quad 0\le U_{k+1}\le U_k , \tag{B6}$$

where U_n is the probability that the RW returns to the origin at the nth step (regardless of its past history), and f_n is the probability that the return occurs (first passage process) at *exactly* the nth step. Equation (B6) is a superposition principle for point return probabilities and provides the starting point of lattice RW calculations for $\langle S_n\rangle$ and other RW properties by Montroll and Weiss [36,39], and many others following them. Equation (B6) is also the fundamental equation of Feller's fluctuation theory for recurrent events [47a] and, thus, has a significance beyond the particular RW applications discussed here.

The meaning of transience and recurrence terminology can be appreciated by considering the number of visits to the origin, which equals [21,22] (see Appendix A for discussion of U_k),

$$N_n=\sum_{k=0}^{n} U_k, \quad U_0=1 . \tag{B7}$$

Since $U_n=U(n,d)$ asymptotically ($n\to\infty$) scales as $U_n\sim n^{-d\nu}$ for random walks, the average number of visits N_n diverges as $n\to\infty$ for $d<1/\nu$ and is *finite* [see Eq. (B18)] for $d>1/\nu$ as a consequence of the properties of the Riemann ζ function. Thus, $d=2$ is a critical dimension above which $\lim_{n\to\infty}N_n$ approaches a constant value $N^*(d)>0$.

The number of renewals N_n-1 of a walk to the origin is contrasted with the mean period (loop length) of the RW path lengths between recurrences to the origin. To calculate this quantity, we first note a theorem of Feller [47], which indicates that if N_n approaches a fixed point value $N^*>0$ for large n, then the associated renewal process is uncertain. In other words, some RW paths under these conditions *never* return to the origin, so that a renormalization of the renewal probabilities f_k is necessary. Specifically, we define the "norming constant" R_n:

$$R_n=\sum_{k=1}^{n} f_k . \tag{B8}$$

The limit $\lim_{n\to\infty}R_n$ equals unity if return to the origin is certain ($d<1/\nu$) and equals the fixed point value R_d^* ($0<R_d^*<1$) if the return to the origin is uncertain. The mean recurrent time $\langle \tau_n\rangle$ is then defined as

$$\langle \tau_n\rangle=\sum_{k=1}^{n} kf_k\Big/\sum_{k=1}^{n} f_k=\sum_{k=1}^{n} kf_k/R_n . \tag{B9}$$

This is a conditional mean recurrence time because of the presence of the norming constant in the denominator [99]. In other words, the average in Eq. (B9) is limited to those paths that return to origin while escaping paths are disregarded.

We establish a connection between Eq. (B9) and the survival function $C(d,n)$ by noting that the escape probability $C(d;n\to\infty)=C_d^*$ equals [21,22]

$$C_d^*=1-R_d^*, \quad C_d^*=1\Big/\sum_{k=0}^{\infty} U_k \tag{B10}$$

and, more generally,

$$C(d,n)=1-\sum_{k=1}^{n} f_k . \tag{B11}$$

Thus, we observe the "first passage probability" f_n is the discrete derivative of $C(d,n)$,

$$f_n=-[C(d,n)-C(d,n-1)]\equiv-\Delta C_n , \tag{B12}$$

so that the mean recurrence time $\langle \tau_n\rangle$ can be rewritten as

$$\langle \tau_n\rangle=\sum_{k=1}^{n} k\Delta C_k\Big/\sum_{k=1}^{n}\Delta C_k . \tag{B13}$$

The limiting behavior $\langle \tau_n\rangle$ of recurrent walks ($R_d^*=1$) can be formally obtained by taking the continuum limit of Eq. (B9)

$$\langle \tau_n\rangle\sim\int^n t(dC(n)/dt)dt . \tag{B14}$$

We relate this average to the number of distinct sites visited through Eq. (B1) to obtain

$$\langle \tau_n\rangle\sim\int^n t(d^2S_n/dt^2)dt\sim A_3 n^{d\nu} , \tag{B15}$$

which scales as $\langle S_n\rangle$ ($d<1/\nu$) [see Eq. (B3)]. Thus, the number of distinct sites visited $\langle S_n\rangle$ for recurrent RW's and characterizes, roughly speaking, the average period of the random-walk recurrences. This period grows with increasing chain length, reflecting the strong fluctuations of recurrent RW's.

2. Transient walks ($0<C_d^*<1$)

For d greater than $1/\nu$, the RW's are transient [$C_d^*>0$; see Eq. (A11)], and $\langle S_n\rangle$ is expected to have the same asymptotic variation as the Wiener sausage volume $\langle \mathcal{V}_n\rangle$ [see [49] and Eq. (5.6)]

$$\langle S_n \rangle \sim C_d^* n + \{z_2/\phi(\nu)[1-\phi(\nu)]\} \times (C_d^*)^2 + O(\text{const}), \quad d > 1/\nu , \tag{B16}$$

$$z_2 = p(O) n^{\phi(\nu)}, \quad \phi(\nu) = \epsilon\nu, \quad \epsilon = (2/\nu - d) ,$$

where $p(O)$ governs the probability for the RW to return to the origin $U_n(n,d,\nu) \sim p(O) n^{-d\nu}$. (The constant $p(O)$ depends on the lattice structure [43b, 45].) The continuous chain analog of $\langle S_n \rangle$ in Eq. (B2a) reduces to Eq. (B16) where $C_d^* = 1$.

Evidently, only the fluctuation term survives the second derivative in Eq. (B16) so that we have asymptotically,

$$d^2S(n)/dn^2 \sim n^{\phi(\nu)-2}, \quad \int^n t(d^2S(n)/dn^2)dt \sim n^{2-d\nu} , \tag{B17}$$

where constants of proportionality are unspecified in Eq. (B17). The integral in Eq. (B17) diverges for the intermediate dimension range, $1/\nu < d < 2/\nu$, despite the existence of the finite limit for the number of visits to the origin in this range of dimensions,

$$\lim_{n\to\infty} N_n \to N^*, \quad 1/\nu < d < 2/\nu . \tag{B18a}$$

In the strongly transient [22b] case ($d > 2/\nu$), where the renewal probability U_n decays rapidly, the integral in Eq. (B17) approaches a finite limit

$$\lim_{n\to\infty} \langle \tau_n \rangle \to \tau^* , \tag{B18b}$$

where the correction terms to the scaling in Eq. (B17) are evidently important for calculating τ^* in the strongly transient regime. Thus, the strongly transient RW's return to the origin with a *finite period*. For ordinary RW's ($\nu = \frac{1}{2}$), strong transience corresponds to $d > 4$. The limit in Eq. (B18b), however, diverges for weakly transient RW's ($1/\nu > d > 2/\nu$). Weakly transient walks thus have a well-defined number of visits to the origin, but τ^* diverges because of the large fluctuations. This is the motivation for discriminating weak from strong transience.

The number of visits to the origin of a transient RW is directly related to the survival probability C_d^*. Equations (A11) and (B7) imply the identity

$$N^* = 1/C_d^*, \quad d > 1/\nu . \tag{B18c}$$

Exact values of N^* for ordinary RW's ($\nu = \frac{1}{2}$) are shown in Fig. 16, and the divergence of N^* as $d \to 2^+$ is apparent. The limit $N^*(d \to \infty) = 1$ reflects the first step of the walk. We also observe that N^* is related to the number of distinct sites visited by a transient random walk

$$\lim_{n\to\infty} (\langle S_n \rangle / n) \sim 1/N^* . \tag{B18d}$$

This is the well-known ergodic theorem of Spitzer [49a] and Aldous [100a]. The importance of N^* as a rate of RW exploration also holds for finite lattices. Aldous [100a] considers the average amount of time n for a RW to visit *every point* of a large finite connected set, and Nemirovsky, Martin, and Coutinho-Filho [101] have numerically investigated the fluctuation corrections to this "covering time" numerically. The covering time, similarly to Eq. (B18d), is inversely proportional to N^* and is proportional to $\mathcal{N}\ln\mathcal{N}$, where $\mathcal{N}$ is the number of lattice sites in the confining finite lattice region. ($\mathcal{N}$ corresponds to the volume of the confining region.) The average amount of time $\langle T \rangle$ required to visit any prescribed lattice point in a large and connected finite lattice region of $\mathcal{N}$ lattice sites asymptotically equals [102]

$$\langle T \rangle \sim \mathcal{N}/N^* \tag{B19}$$

for transient walks and $\mathcal{N}$ large. Equation (B19) has important applications [102].

We summarize the results obtained from the above for the conditional mean recurrence time $\langle \tau_n \rangle$:

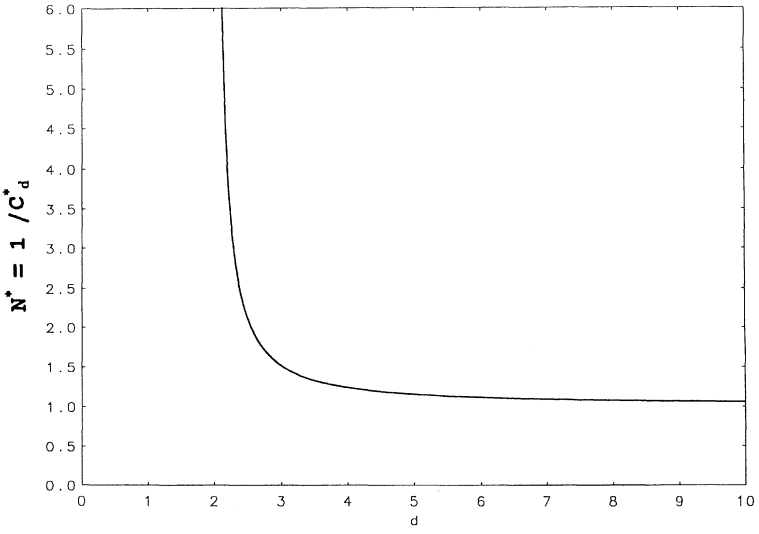

FIG. 16. The number of RW returns to the origin, $N^* = 1/C_d^*$. For high dimensions, the number of returns approaches 1, corresponding to the first step.

$$\langle \tau_n \rangle \sim \begin{cases} n^{dv}, \quad 0<d<d/v \quad \text{(recurrent)} & \text{(B20a)} \\ n^{2-dv}, \quad 1/v<d<d/v \quad \text{(weakly transient)} & \text{(B20b)} \\ \tau^*, \quad d>2/v \quad \text{(strongly transient)}, & \text{(B20c)} \end{cases}$$

where the prefactors are unspecified. These scaling relations are given previously by Hughes [99], but rather different calculational methods are involved. We briefly mention the connection of our computational approach to RW recurrence properties to more conventional approaches in the physics literature.

Following Feller [47a] and Montroll [39], the usual method of solution for the recurrent properties of RW's utilizes discrete Laplace transform methods. We define the generating functions (discrete Laplace transforms)

$$F_n(x)=\sum_{k=0}^{n} f_k x^k, \quad f_0=0, \quad x\equiv e^{-s}, \quad s\geq 0, \tag{B21a}$$

$$U_n(x)=\sum_{k=0}^{n} U_k x^k,$$

$$\lim_{n\to\infty} F_n(x)=F^*(x), \tag{B21b}$$

$$\lim_{n\to\infty} U_n(x)=U^*(x),$$

which upon insertion into the discrete renewal equation Eq. (B6) gives

$$U^*(x)=1+F^*(x)U^*(x). \tag{B22}$$

We then deduce the limiting long chain behavior [103] from the "initial value theorem" of Laplace transform theory

$$F^*(s\to 0+)=R_d^*=1-1/U(s\to 0+)\equiv 1-C_d^* \tag{B23a}$$

and $\langle \tau_n \rangle$ similarly equals

$$\langle \tau_n \rangle = \lim_{s\to 0+} [d \ln F_n(x)/d(\ln x)]$$

$$= \sum_{k=1}^{n} k f_k e^{-sk} \Big/ \sum_{k=0}^{n} f_k e^{-sk} \Big|_{s\to 0+}. \tag{B24}$$

The generating function approach is very economical for calculating the asymptotic properties of RW's, while the discrete integral equation approach has its own advantages, such as the ease with which contact can be made with continuum integral equation and path integral approaches to RW recurrence properties.

As a final comment regarding the continuum limit of the renewal Eq. (B6), it is also useful to observe that this equation can be rearranged as

$$U_{n+1}=f_{n+1}+\sum_{k=0}^{n-1} U_{n+1-k} f_k, \tag{B25a}$$

which has the continuum (Volterra equation) analog [see also Eq. (A4a)]

$$U(n)=f(n)+\int_0^n U(n-\tau)f(\tau)d\tau. \tag{B25b}$$

The limiting variation of continuum random-walk return probability $U(n)$ for large n is governed by the moments of the renewal density function $f(n)$, and distinct "universality classes" exist according to whether the second or first moments of $f(n)$ exist [47].

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