Spectrum of self-avoiding walk exponents

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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 having m nearest-neighbor contacts, and performing an energetically weighted averaging over these restricted SAW configurations. Surprisingly, there have been limited studies of the geometrical properties of ''contact-constrained'' SAW configurations, which contrasts with the well studied unrestricted SAW's. Accordingly, we generate Monte Carlo data for the total number of SAW configurations $C_{n,m}$ having a fixed number of contacts m for chains of length n on square and cubic lattices. Applications of the standard ratio method to the $C_{n,m}$ data shows a *unique* connectivity constant μ (NAW), corresponding to neighbor-avoiding walks ($m=0$), and a ''spectrum'' of γ exponents which depend on the contact number m. The asymptotic scaling of the number of contact-constrained SAW's is found to be similar to the number of lattice animals and random plaquette surfaces having a fixed cyclomatic index c and genus g, respectively. The existence of this common structure is promising for the development of an analytic theory of interacting polymers and surfaces. [S1063-651X(97)10101-5]

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I. INTRODUCTION

There have been numerous studies of the properties of self-avoiding walks (SAW's), and many of their properties have become established, at least numerically. For example, an extensive body of theory and numerical data indicates that the total number of SAW configurations C_n of lattice walks of length n scales asymptotically as [1–6]

$$C_n \sim [\mu(\mathrm{SAW})]^n n^{\gamma-1}, \quad n \to \infty, \tag{1.1}$$

where μ(SAW) is the SAW ''connectivity constant,'' and γ is the SAW ''susceptibility'' exponent. Rigorous results include a proof of the existence of μ(SAW) [1], $1/d$ expansions of μ(SAW) [2], and a proof that $\gamma=1$ for high dimensionalities, $d \geqslant 5$ [3]. Moreover, formal conformal invariance calculations indicate $\gamma=43/32$ in the non-trivial case of $d=2$ [7], and it is evident that $\gamma=1$ for $d=1$. Numerical data for μ(SAW) and γ as a function of d for hypercubic lattices have recently been summarized [4–6].

The theoretical treatment of interacting polymers requires further information about the properties of SAW's, however. A short-range interaction is incorporated into the SAW model of polymer chains by partitioning SAW configurations into equivalence classes corresponding to a fixed number m of nearest-neighbor contacts [8]. Chain properties are then calculated by performing an energetically weighted averaging of these constrained SAW configurations [5,8]. This restricted SAW data contain important information such as the location of the θ-temperature, where attractive interactions begin to predominate over repulsive polymer-polymer interactions [9–12]. The θ-point γ exponent and the radius of the gyration exponent ν are also contained in this SAW data, and these quantities have been estimated by a variety of methods [11,13–17].

Surprisingly, there have been few studies of SAW's having a fixed number of contacts m, except for the $m=0$ case corresponding to ''neighbor-avoiding walks'' [18], and usually these types of data are averaged to determine other information about polymers with nearest-neighbor (NN) interactions (critical exponents, connectivity constant, internal energy, specific heat, etc.) [6,8,10,11]. Contact-constrained SAW data are often not even reported.

It seems clear that if we can understand the asymptotic variation of the contact-constrained SAW properties, then this should open the way to further analytical progress on describing interacting SAW's and other closely related lattice models. Accordingly, we generate accurate numerical data for the total number of SAW configurations $C_{n,m}$ having a *fixed* number of contacts m by Monte Carlo (Rosenbluth and Rosenbluth [19]) methods, and analyze these data using the ratio method as for unrestricted SAW data [11,20].

A similar scaling for the $C_{n,m}$ data to Eq. (1.1) is found in our data analysis, except that the connectivity constant corresponds to neighbor-avoiding walks μ(NAW) [5,18] for *all* m, and γ is found to depend on the contact number m. This nontrivial scaling of the contact-constrained SAW's is similar to the asymptotic scaling for the number of lattice animals and random plaquette surfaces having a fixed cylomatic index c and genus g, respectively [21–24], and the connection between these problems is considered in Sec. III.

II. CONTACT-CONSTRAINED SELF-AVOIDING WALKS

Although SAW's have no self-intersections by definition, there can be NN contacts corresponding to adjacent vertices of the SAW path which are not connected by a bond of the chain path. An energetic interaction is incorporated into the SAW model by associating a Boltzmann weight with these

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contacts. Thus we arrive at the general problem of sorting SAW configurations into equivalence classes having a common contact number m, and of counting the number of these contact-constrained SAW configurations by direct enumeration or Monte Carlo (MC) sampling.

In previous papers the exact SAW partition function for interacting chains up to a chain length $n=11$ in d dimensions [5] was calculated, and the partition function Q_n of the NN-interacting SAW is obtained in the form of a polynomial [5,8],

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

where Φ is the dimensionless NN interaction energy describing the polymer self-interaction (Positive values correspond to attractive interactions, while negative values to repulsive ones.). $C_{n,m}$, the number of SAW's of length n having exactly m contacts, are polynomials in d, and the sum in Eq. (2.1) is limited by the maximum number of NN-chain contacts $m_{\max}$ [6].

Some special limits of Eq. (2.1) have been extensively studied. For example, the limit of a vanishing polymer-polymer interaction ($x\to 1$) corresponds to unrestricted SAW's, so that $Q_n(x=1)\equiv C_n$ and the asymptotic scaling prescribed in Eq. (1.1) must be recovered. Known results for C_n provide useful tests of our MC data below. Another well studied limit corresponds to a strongly repulsive interaction ($\Phi\to-\infty$), where the sum in Eq. (2.1) reduces to a single athermal term

$$Q_n(\Phi\to-\infty)\sim C_{n,0}. \tag{2.2a}$$

Asymptotically, the number of chains having no NN contacts, $C_{n,0}$ (''neighbor-avoiding walks''), scales as [18,25]

$$C_{n,0}\sim[\mu(\mathrm{NAW})]^n n^{\gamma_{\mathrm{NAW}}-1}, \quad n\to\infty, \tag{2.2b}$$

where μ(NAW) is the NAW connectivity constant, and arguments have been given that γ_{NAW} equals γ in Eq. (1.1) [18]. [There is a constant of proportionality in Eqs. (1.1) and (2.2b) which is neglected in the present paper; see Ref. [5] for numerical and $1/d$ expansion evaluations of this constant as a function of d.]. Numerical estimates for μ(NAW) for hypercubic lattices were summarized by Nemirovsky *et al.* [5(a)] and Douglas and Ishinabe [6], where it was found that $\mu(\mathrm{NAW})<\mu(\mathrm{SAW})$ for $1<d<\infty$. Formal $1/d$ expansion calculations [27(c)] to leading order in x indicate that the entropy is at a maximum for SAW's, and we conjecture that this result is exact for $1<d<\infty$. This conjecture is consistent with the strict inequality between μ(NAW) and μ(SAW) mentioned above.

Next, we consider the opposite extreme, where the NN interactions are very attractive ($\Phi\to\infty$), so that Eq. (2.1) again reduces to a single term,

$$Q_n(x\to\infty)\sim C_{n,m_{\max}}x^{m_{\max}}. \tag{2.3}$$

The number of compact walks $C_{n,m_{\max}}$ has a finite entropy on a hypercubic lattice, and $C_{n,m_{\max}}$ scales as [6,8,26,27],

$$C_{n,m_{\max}}\sim[\mu(\mathrm{Ham})]^n, \quad n\to\infty, \tag{2.4}$$

where μ(Ham) is the ''Hamilton walk'' connectivity constant. Because of the small fluctuations of such compact SAW's, the $1/d$ expansion [27(b)] and even mean-field theory [27(a)] (the leading order term of the $1/d$ expansion) provide good approximations of μ(Ham) [6,26]. The corrections to scaling for $C_{n,m_{\max}}$ are not presently known for collapsed chains, but a correction of the form $\exp(-\delta^* n^{(d-1)/d})$ has been suggested [28] where δ^* is a constant related to the surface free energy of the compact SAW. The value of γ is also uncertain for collapsed chains, but γ values for Hamilton walks arising in concentrated bulk polymer systems were calculated by Duplantier and co-workers [29] for $d=2$. Questions remain regarding the universality of the γ exponent for isolated collapsed SAW's [28].

The present investigation of $C_{n,m}$ is partly motivated by an observation of Fisher and Hiley [8(c)] about the energetic dependence of the average number of SAW contacts $\langle m\rangle$. They note the intriguing relation between these quantities,

$$\langle m\rangle/n=[C_{n,1}/(nC_{n,0})]x+O(x^2). \tag{2.5}$$

The constancy of the ratio $C_{n,1}/(nC_{n,0})$ for $n\to\infty$ implies that $C_{n,1}$ scales like $C_{n,0}$ in Eq. (2.2b), but the γ exponent for $m=1$ is larger,

$$C_{n,1}\sim[\mu(\mathrm{NAW})]^n n^{\gamma(m=1)-1}, \quad n\to\infty, \tag{2.6a}$$

$$\gamma(m=1)=\gamma(m=0)+1. \tag{2.6b}$$

A numerical examination of the ratio $C_{n,1}/(nC_{n,0})$ shows that it converges rather rapidly to its fixed point value for large n, and a tabulation of the limiting value of this ratio for various d is given by Douglas and Ishinabe [6].

From the discussion above it seems natural to consider the asymptotic variation of the $C_{n,m}$ coefficients according to the assumed relation

$$C_{n,m}\sim[\mu(m)]^n n^{\gamma(m)-1}, \quad n\to\infty, \tag{2.6c}$$

which generalizes cases considered previously. An examination of this scaling is more difficult with increasing m because of the slower increase of $C_{n,m}$ for more compact SAW configurations (m large). We must then resort to a MC calculation, since a direct enumeration of the contact-constrained SAW configurations become computationally prohibitive for large m [this difficulty can be appreciated by observing that C_{50} is on the order $O(10^{34})$]. Once we generate the $C_{n,m}$ data, we directly apply the ratio method to calculate $\mu(m)$ and $\gamma(m)$ based on Eq. (2.6c).

$C_{n,m}$ values are generated using the Rosenbluth and Rosenbluth (RR) method [19], which has been extensively utilized in previous calculations of interacting SAW properties [10(a)]. Each ith chain generated by the RR procedure is given the weight $W_n(m,i)$ which is the ratio of the weight of the RR walk with excluded volume to a random walk (see below). According to the RR method, the weight $W_n(m,i)$ is given by

$$W_n(m,i)=\sum_{r=0}^{2d-2}[2d-1-r]/(2d-1)]^n, \tag{2.7a}$$

where $n_{r,i}$ is the number of segments in the ith, chain, with r contacts. For each chain the total number of NN contacts m is obtained from the relation

$$m=\sum_{r=0}^{2d-2} r n_{r,i}. \tag{2.7b}$$

The weight $W_n(m,i)$ is naturally determined by the RR method [10(a),19], which is its attraction for the present calculations. In an ensemble of N_t total generated chains, the weights of all walks of a fixed m are summed and multiplied by the random walk partition function [30]

$$C_{n,m}(\mathrm{RR})=Q_{\mathrm{NRRW}}\sum_{i=1}^{N_t} W_n(m,i)/N_t, \tag{2.7c}$$

$$Q_{\mathrm{NRRW}}=2d(2d-1)^{n-1}, \tag{2.7d}$$

where Q_{NRRW} is the partition function of a nonreversing random walk.

Monte Carlo estimates of the $C_{n,m}$ for n values in the range 1 to 50 and for $d=3$ and 2 (cubic and square lattice, respectively) were calculated and these results are available through the AIP Physics Auxiliary Publication Service [45]. Exact enumeration data [5(c),11,31] provide an important and independent check of the accuracy of the Monte Carlo data in these tabulations, and these tests led us to impose restrictions on the n values to the limited range indicated to achieve acceptable numerical accuracy. Table I provides a representative comparison between some exact enumeration data and MC data for $C_{n,m}$ having the largest values of n available. (Recently, we generated $C_{n,m}$ data in $d=3$ and 2 up to $n=18$ and 26, respectively, for the purposes of checking our MC data in nontrivial cases.) The comparison shows that errors are largest for the most compact SAW's and for the relatively extended NAW's and that the sampling errors are generally larger in $d=2$. Errors for the total number of SAW's were small for arbitrary n, and further tests of these data are made below between our results and numerical SAW results obtained by more refined data analyses. Our Monte Carlo $C_{n,m}$ data were created through the generation of 5 000 000 million and 7.5 000 000 sample chain configurations in $d=3$ and 2, respectively, using a Convex 3820 computer. Each of these runs took about 5 h.

The standard ''ratio method'' for determining μ and γ is based on the assumed scaling in Eq. (1.1) for SAW's, and for general m we assume Eq. (2.6c) and consider the ratio $C_{n,m}/C_{n-1,m}$ versus $1/n$ as for unrestricted walks [20]. Plots of this ratio for our MC data are shown in Figs. 1 and 2 for $d=3$ and 2, respectively. We observe that the extrapolations have nearly the same intercept for each m, and we average these intercepts to estimate the NAW connectivity constants, $\mu(\mathrm{NAW};d=3)=4.028$ and $\mu(\mathrm{NAW};d=2)=2.315$ (See Refs. [5], [6] for a summary of μ(NAW) data as a function of d, as obtained from direct enumeration data.) The $\gamma(m)$ exponents, determined by a simple least squares fit to the ratio data in Figs. 1 and 2, are shown in Figs. 3 and 4. Solid lines in these figures show best fits to an assumed linear dependence of $\gamma(m)$, while the dashed line indicates the anticipated result

$$\gamma(m)=\gamma(m=0)+m, \tag{2.8}$$

where we take $\gamma(m=0)=\gamma_{\mathrm{SAW}}$. The least-square fit slopes are 0.93 and 0.92 in $d=3$ and 2, respectively, which accord well with Eq. (2.8). Motivation for the linear variation of γ with m is discussed below in comparison with other lattice models of interacting polymers, where similar scaling has been found theoretically and numerically.

The results for $C_{n,m}$ scaling are contrasted with those for the total number of SAW configurations,

$$C_n=\sum_{m=0}^{m_{\max}} C_{n,m}. \tag{2.9}$$

Again we apply the ratio test to our MC data, where $1<n<50$, and an additional set of data (filled circles) for $1<n<100$ is also included in our examination of the C_n scaling, so that we can obtain precise critical parameter estimates. We utilized the ratio method for the C_n and $C_{n,m}$ data, because it exhibits a ''scattering'' when statistical fluctuations are a problem, thus providing an additional test of the quality of our numerical data. Extrapolation of the *least-square fit* to the lattice data for $d=3$ in Fig. 5 gives $\gamma\approx 1.160$ and $\mu(\mathrm{SAW})\approx 4.684$, which agree well with previous, more sophisticated, exponent estimates [32]. Similar consistency is found for the $d=2$ SAW data. These results confirm the accuracy of our MC calculations and our extrapolation methods, and serve to emphasize the change in the connectivity constant μ in restricted SAW's from the value for unrestricted SAW's. Evidently, this change in μ reflects a general feature of the asymptotic variation of $C_{n,m}$ and $m_{\max}$ but the mathematical origin of this μ change is not fully understood (see below). It should also be appreciated that the maximum number of SAW contacts exhibits a nontrivial dependence on the chain length n. Some exact $m_{\max}$ results for $d=2$ and 3 are shown in Fig. 6, and tight bounds on $m_{\max}$ are discussed by Douglas and Ishinabe [6].

We next examine the scaling of the number of Hamilton walks C_{Ham} corresponding to the maximum number of NN contacts,

$$C_{\mathrm{Ham}}\equiv C_{n,m_{\max}}. \tag{2.10}$$

Determination of the connectivity constant for Hamilton walks is complicated by the possibility of other corrections to scaling than the usual γ exponent, as discussed above. In light of Eq. (2.4), we simply take the nth root of C_{Ham} to estimate μ(Ham), and look for convergence to the long chain limit. The result of this procedure for $d=3$ and 2 is shown in Figs. 7 and 8. Some oscillations are observed about a roughly constant value about which the oscillations appear to be slowly damped. Leading order $1/d$ expansion estimates of μ(Ham) (denoted as ''mean field'') are indicated for comparison in these figures. The average values of μ(Ham) indicated from the MC data equals $\mu(\mathrm{Ham},d=3)\approx 2.19$ and $\mu(\mathrm{Ham},d=2)\approx 1.57$, which is compared to the second order $1/d$ expansion estimates [6,27(b)] $\mu(\mathrm{Ham},d=3)\approx 2.22$ and $\mu(\mathrm{Ham},d=2)\approx 1.53$. Our numerical estimates should be considered tentative, since an accurate extrapolation requires an understanding of the type of corrections to scaling exhibited by C_{Ham}. We examine this question briefly in Fig. 9, where

TABLE I. Comparison of exact enumeration and Monte Carlo data of $C_{n,m}$.

$C_{n,m}$ in three dimensions for $n=18$			
m	Exact	Monte Carlo	% Error
0	211 059 485 310	211 032 540 457.32	−0.01
1	413 331 190 896	413 561 837 332.88	0.06
2	468 396 156 360	467 884 259 905.73	−0.11
3	410 931 236 976	410 742 912 946.66	−0.05
4	302 001 979 368	302 073 496 791.33	0.02
5	195 614 670 720	195 338 712 193.01	−0.14
6	115 369 171 224	115 523 265 039.12	0.13
7	63 197 862 432	63 276 679 447.572	0.12
8	32 132 589 576	32 188 795 766.744	0.17
9	15 332 612 976	15 349 712 406.028	0.11
10	6 591 974 304	6 578 745 537.143 1	−0.20
11	2 596 321 248	2 586 337 473.142 8	−0.38
12	849 705 360	854 831 641.535 71	0.60
13	257 779 872	255 771 866.580 36	−0.78
14	46 269 648	45 603 177.392 857	−1.44
15	11 185 152	10 587 390.357 143	−5.34
16	492 672	630 195.1	27.91
C_{18} ($d=3$)	2 237 720 684 094	2 237 304 719 567.6	0.000 186
$C_{n,m}$ in two dimensions for $n=26$			
m	Exact	Monte Carlo	% Error
0	11 284 095 921	11 142 571 461.556	1.25
1	31 911 750 887	31 938 638 276.124	−0.08
2	51 003 659 069	51 025 459 467.918	−0.04
3	58 695 622 132	58 495 084 120.683	0.34
4	54 777 840 664	54 805 994 496.214	−0.05
5	43 910 631 128	43 911 801 631.031	0.00
6	31 307 514 535	31 374 080 727.054	−0.21
7	20 184 660 662	20 213 944 137.053	−0.15
8	11 896 662 099	11 931 738 191.524	−0.29
9	6 517 681 484	6 506 520 160.5201	0.17
10	3 278 616 327	3 286 714 863.0416	−0.25
11	1 535 090 131	1 535 894 702.5736	−0.05
12	662 785 715	659 321 911.42501	0.52
13	256 653 464	257 361 436.57 243	−0.28
14	89 028 548	89 192 448.243 775	−0.18
15	27 288 380	27 332 352.281 892	−0.16
16	5 184 278	5 154 568.7 959 853	0.57
17	276 902	266 631.63 169 372	3.71
C_{26} ($d=2$)	327 345 042 326	327 207 071 584.24	0.000 42

we show MC data for the ratio $C_{\mathrm{Ham}}/(\mu(\mathrm{Ham}))^n$, where the estimated average value of μ(Ham) from Fig. 7 is utilized. These results for $d=3$ seem compatible with a surface free-energy $\exp[-\delta^* n^{(d-1)/d}]$ correction where $\delta^*=-0.94$. Further numerical data are needed to verify this possibility. Gordon, Kapadia, and Malarus [26(a)] presented exact examples of Hamilton walks in $d=2$ with *fixed* boundary geometries where $\mu_{\mathrm{Ham}}=1$ (i.e., zero entropy), and the number of Hamilton walk configurations scale like $\exp(\delta' n^{0.5})$, where δ' is a constant. This example illustrates the strong influence of boundary conditions on compact walk properties. An $\exp(n^{0.5})$ scaling is also found for spiral SAW's in $d=2$, which perhaps has some relation to the Hamilton walk problem [33].

Another complication of the μ_{Ham} estimates is that the MC sampling efficiency for Hamilton walk configurations becomes increasingly poor for longer chains so the results of Figs. 7–9 should be viewed as only qualitative. This is perhaps the most significant limitation of our numerical calculations.

We also note that the existence of the different scaling for C_{Ham} does not violate the scaling of $C_{n,m}$ assumed in Eq. (2.7), since $m_{\max}$ is *not fixed* (see Fig. 6). For large n the maximum number of contacts approaches a linear dependence on n [5,6,8],

$$m_{\max}\sim(d-1)n+O(n^{(d-1)/d}),\quad n\to\infty \qquad (2.11)$$

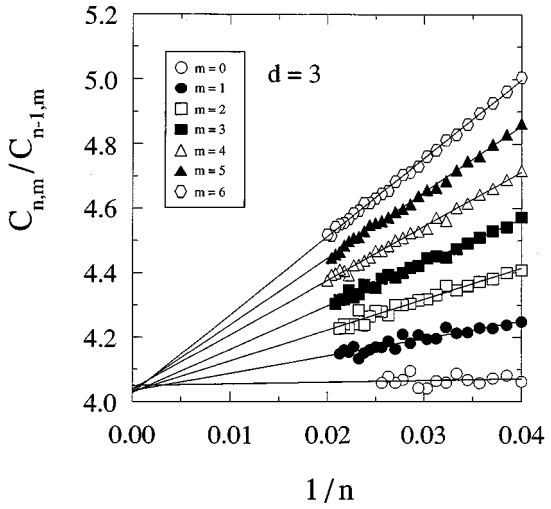

FIG. 1. Ratio extrapolation of contact constrained SAW's in $d=3$. The NAW connectivity constant μ(NAW) is estimated as the average of the intercepts, and $\gamma(m)$ is determined from the slope of the these extrapolations.

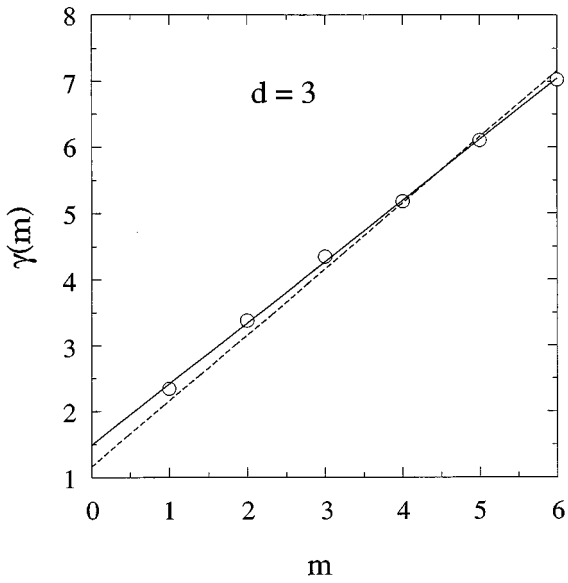

FIG. 3. Exponent spectrum $\gamma(m)$ for contact-constrained SAW's in $d=3$. See Fig. 1.

for a hypercubic lattice (see Fig. 6). This limiting behavior is approached rather slowly, however [6].

The average number of SAW contacts, $\langle m\rangle_{\mathrm{SAW}}=\langle m(\Phi=0)\rangle$, was extensively investigated in Ref. [6] by direct enumeration. $\langle m\rangle_{\mathrm{SAW}}$ is calculated as a average over $C_{n,m}$,

$$\langle m\rangle_{\mathrm{SAW}}=\left(\sum_{m=0}^{m_{\max}} mC_{n,m}\right) \Big/ C_n \qquad (2.12)$$

and this average for our MC data is shown in Fig. 10. The approach of $\langle m\rangle_{\mathrm{SAW}}$ to its linear scaling behavior with n is rapid for this quantity, as noted in our previous direct enumeration study [6]. The slope 0.193 indicated in Fig. 10 is obtained by a simple least-square linear fit, and differs slightly from value given in Ref. [6], where corrections to scaling were included in the extrapolation.

The limits Eqs. (2.11) and (2.3) imply the exact dependence of $\mu(x)$ for the (hypercubic lattice) Hamilton walk limit, $\mu(x\to\infty)\sim\mu(\mathrm{Ham})x^{d-1}$, which determines the free energy, internal energy, and entropy of a collapsed chain in the infinite chain limit by standard thermodynamic relations [5,8].

Figure 11 shows the average number of contacts $\langle m\rangle$ as a function of the NN interaction parameter $x=\exp(\Phi)$, based on our Monte Carlo data. The crossover from the NAW limit ($x\to 0^+$) to the collapsed limit ($x\to\infty$) is exhibited. Notably, the number of contacts per link is very sensitive to the interaction energy in the ''collapsed'' region for finite chains. An estimate of the location of the θ point is readily obtained

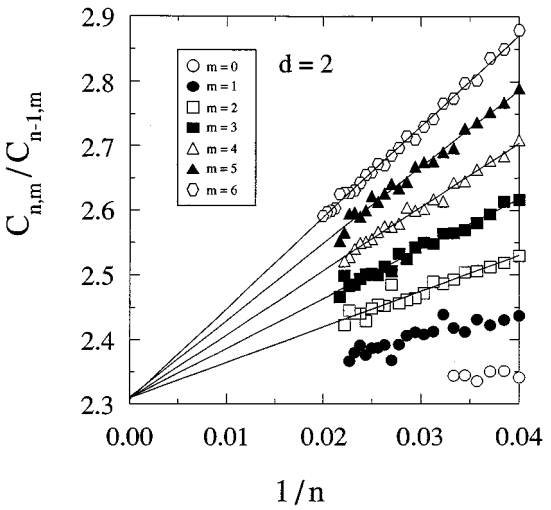

FIG. 2. Ratio extrapolation of contact constrained SAW's in $d=2$. The NAW connectivity constant μ(NAW) is estimated as the average of the intercepts, and $\gamma(m)$ is determined from the slope of the these extrapolations.

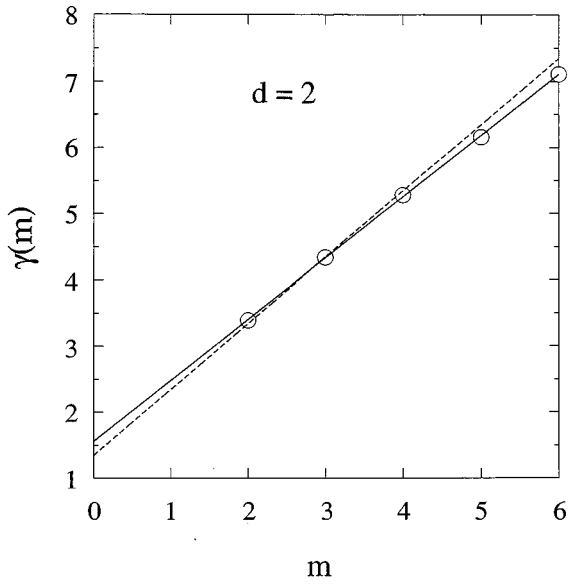

FIG. 4. Exponent spectrum $\gamma(m)$ for contact-constrained SAW's in $d=2$. See Fig. 2.

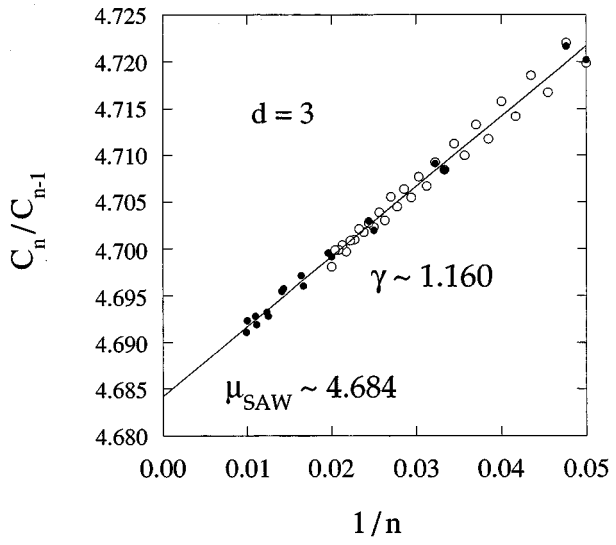

FIG. 5. Ratio extrapolation of unrestricted SAW's in $d=3$. The SAW connectivity constant is obtained from the intercept, and γ(SAW) is determined from the slope. The line was obtained through a least-squares fit to the lattice data. Unfilled circles indicate MC data for $n\leqslant 50$, while the filled circles show the results of a separate calculation with a larger n range, $n\leqslant 100$.

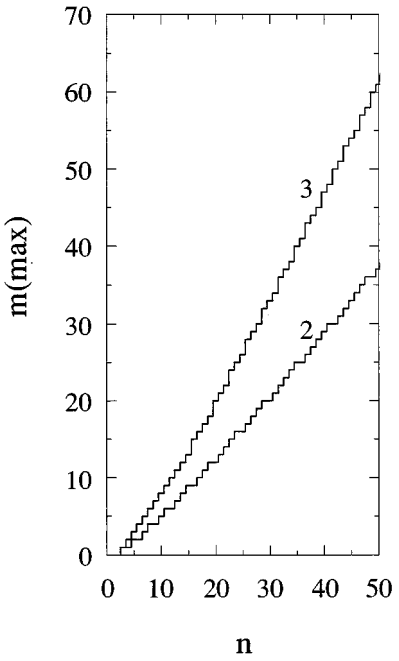

FIG. 6. Estimate of the maximum number of chain contacts $m_{\max}$ as described in Ref. [6]. The upper and lower curves correspond to $d=3$ and 2, respectively. Monte Carlo in $d=2$ agrees with this figure for n in the interval (1, 50), except for a couple of n values where the simulation value is lower by one unit due to inadequate sampling of the most compact SAW configurations. In $d=3$ the Monte Carlo estimates of $m_{\max}$ begin to deviate substantially (greater than four units) from the $m_{\max}$ curve for $n\approx 40$. It should be mentioned that the $d=3$ curve shown is actually a tight *upper bound* (accuracy to within one unit for the range shown) of the number of contacts of a compact spiral SAW. The $d=2$ curve is an exact expression for the number of compact spiral SAW contacts. Since a compact spiral SAW (see Ref. [6]) is a representative compact SAW configuration, its number of contacts is a *lower bound* on the number of contacts of ''collapsed'' chains. In Ref. [6] we suggest that $m_{\max}$ actually equals the number of compact spiral SAW contacts, and numerical data support this conjecture. The simulation values of $m_{\max}$ provide a good qualitative measure of how well compact chain configurations are being sampled.

from the variance of the chain contacts shown in Fig. 12. ($\langle m\rangle$ is proportional to the internal energy and the variance is proportional to the specific heat.) The maxima in this figure correspond to the ''collapse transition'' point for these finite chains, and the θ point is obtained by extrapolation of this maximum to $n\to\infty$.

We mention another value of m which is important for characterizing $C_{n,m}$. In Fig. 13 we indicate the contact number M for which $C_{n,m}$ is at a maximum for all values of m in the range $(0,m_{\max})$. M increases in a curious stepwise fashion, and apparently approaches a linear asymptotic dependence for large n.

The amplitude in Eq. (2.7) also varies with the number of chain contacts m. To examine this quantity, we take the ratio $A(m,n)\equiv C_{n,m}/C_{n,0}n^m$ as a function of m in Figs. 14(a) and 14(b) for $d=3$ and 2. (Note the absolute error in the MC data for this ratio is much smaller for large n than for $C_{n,m}$ because of the large value of $C_{n,0}$.) The $A(m,n)$ ratio becomes nearly independent of chain length for n large $[A(m,n\to\infty)\approx A(m)]$, and decreases monotonically and rapidly with increasing m. We can obtain some insight into this variation by inserting the definition of $A(m,n)$ into Eq. (2.1),

$$Q_n(x)=C_{n,0}\sum_{m=0}^{m_{\max}} A(m,n)(nx)^m. \tag{2.13}$$

Since the connectivity constants μ(NAW) and μ(SAW) rigorously exist [2,25], we can require that Eq. (2.13) reduce to Eq. (1.1) for the SAW limit $x=1$, $n\to\infty$,

$$Q_n(x=1)\sim[\mu(\mathrm{NAW})]^n n^{\gamma(m=0)-1}\sum_{m=0}^{m_{\max}} A(m)n^m$$

$$Q_n(x=1)\sim[\mu(\mathrm{SAW})]^n n^{\gamma-1}. \tag{2.14}$$

The expected relation $\gamma(m=0)=\gamma$ then implies a strong constraint on the amplitude $A(m)$. Equality in these asymptotic relations in the $n\to\infty$ limit implies

$$A(m)=\delta^m/m!,\quad \delta=\ln[\mu(\mathrm{SAW})/\mu(\mathrm{NAW})], \tag{2.15a}$$

where δ is the entropy difference between SAW's and NAW's. Equation (2.15) then reduces to the asymptotic relation for contact constrained SAW's,

$$C_{n,m}\sim[\mu(\mathrm{NAW})]^n\delta^m n^{\gamma(m)-1}/m!,\quad n\to\infty, \tag{2.15b}$$

where $\gamma(m)$ is given by Eq. (2.8). The probability of a chain having m contacts, $P(m)\equiv C_{n,m}/C_n$, asymptotically then becomes a Poisson distribution

$$P(m)\sim\exp(-\delta n)(\delta n)^m/m!,\quad n\to\infty. \tag{2.15c}$$

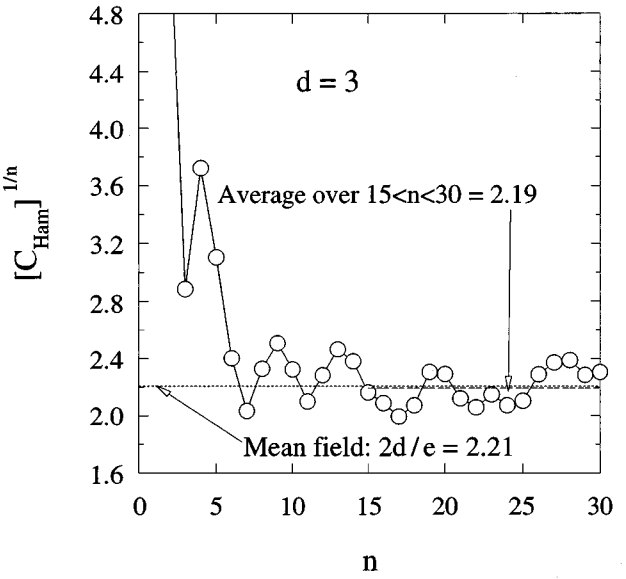

FIG. 7. Rough estimate of Hamilton walk connectivity constant in $d=3$. Estimate is obtained by simply averaging the oscillations as described in the text.

In Eq. (2.15c) we again adopted the expected (but unproven) relation between NAW and SAW susceptibility exponents, $\gamma(m=0)=\gamma$. Note also that the $\exp(-\delta n)$ term arises from the change in the NAW and SAW connectivity constants in Eqs. (1.1) and (2.15b).

The asymptotic expression for the amplitude factor $A(m)$ in Eq. (2.15a) is compared with our MC data in Fig. 14, where we take [5,6; see Figs. 1, 2, 5]

$$\mu(\mathrm{NAW};d=3)=4.065, \quad \mu(\mathrm{NAW};d=2)=2.316, \tag{2.16a}$$

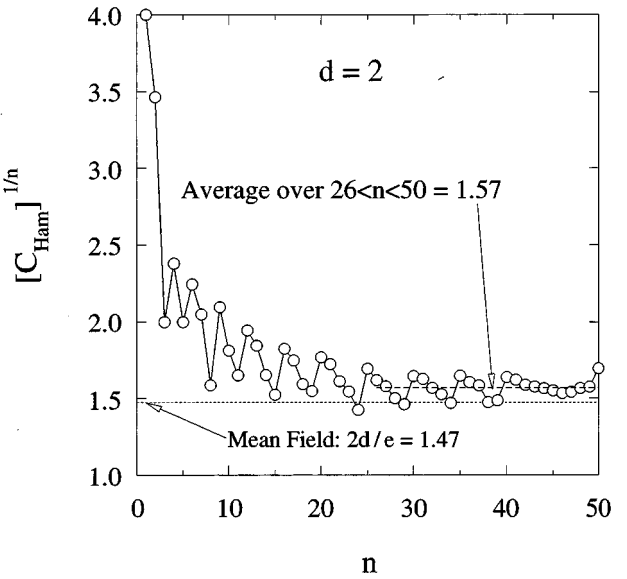

FIG. 8. Rough estimate of Hamilton walk connectivity constant μ(Ham) in $d=2$. An estimate is obtained by simply averaging the oscillations as described in the text.

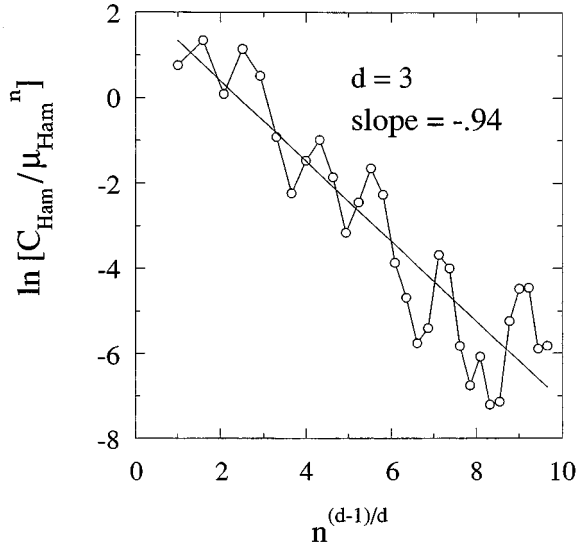

FIG. 9. Check for surface free energy corrections to scaling. See the text for discussion.

$$\mu(\mathrm{SAW};d=3)=4.684, \quad \mu(\mathrm{SAW};d=2)=2.638, \tag{2.16b}$$

so that δ is estimated as

$$\delta(d=3)=0.1301, \quad \delta(d=2)=0.1417. \tag{2.17}$$

Qualitative agreement between Eq. (2.15a) and MC data for $A(m,n)$ is obtained without free parameters, and the fit becomes very good if δ is phenomenologically adjusted to account for finite-size effects on the connectivity constants (see Fig. 14).

The existence of the connectivity constants μ(NAW) and μ(SAW), and the expected exponent equality $\gamma(m=0)=\gamma$ provides important constraints on $C_{n,m}$, and there are additional constraints of this kind which should be useful in refining our knowledge of $C_{n,m}$. For example, the property that $C_{n,m}$ is positive requires that the zeros of the partition function Q_n [12],

$$Q_n(x)=\sum_{m=0}^{m_{\max}} C_{n,m}x^m = C_n(x=0)\prod_{i=1}^{n}(1-x/x_i), \tag{2.18}$$

lie off the real axis for finite chains, and the existence of the θ point and the collapse transition imply that the zero having the smallest magnitude imaginary component approaches the real axis as $n\to\infty$ [12]. The location where the zeros intersect the positive real axis determines the critical energy Φ_c defining the θ point. Figure 15 shows the zeros obtained from our MC data for some selected values of chain length n which illustrates this ''zero-pinching'' effect. A crude extrapolation of the zeros having the smallest magnitude imaginary component for a given n gives a theta point estimate similar to the location of the specific heat maximum in Fig. 12. Unfortunately, the uncertainty of the MC estimates of $C_{n,m}$ for large m makes the accuracy of the θ-point estimation by this method rather unreliable, and we refrain from making a precise estimate here.

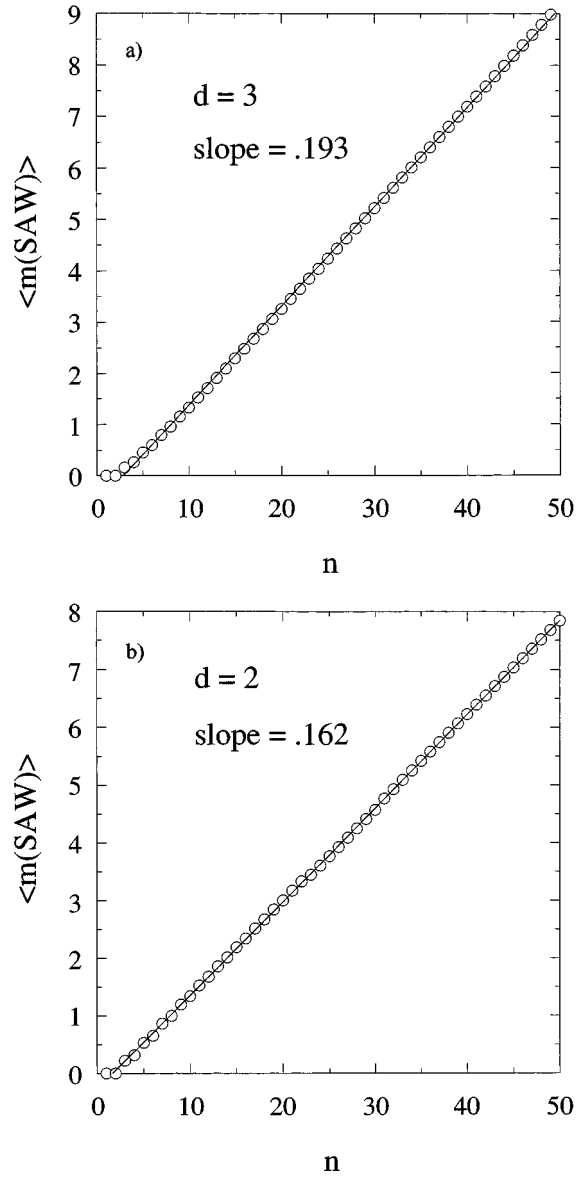

FIG. 10. Average number of contacts for unrestricted SAW's. (a) $d=3$. (b) $d=2$. Slopes indicate simple least-squares fit to lattice data without account of corrections to scaling. See Ref. [6].

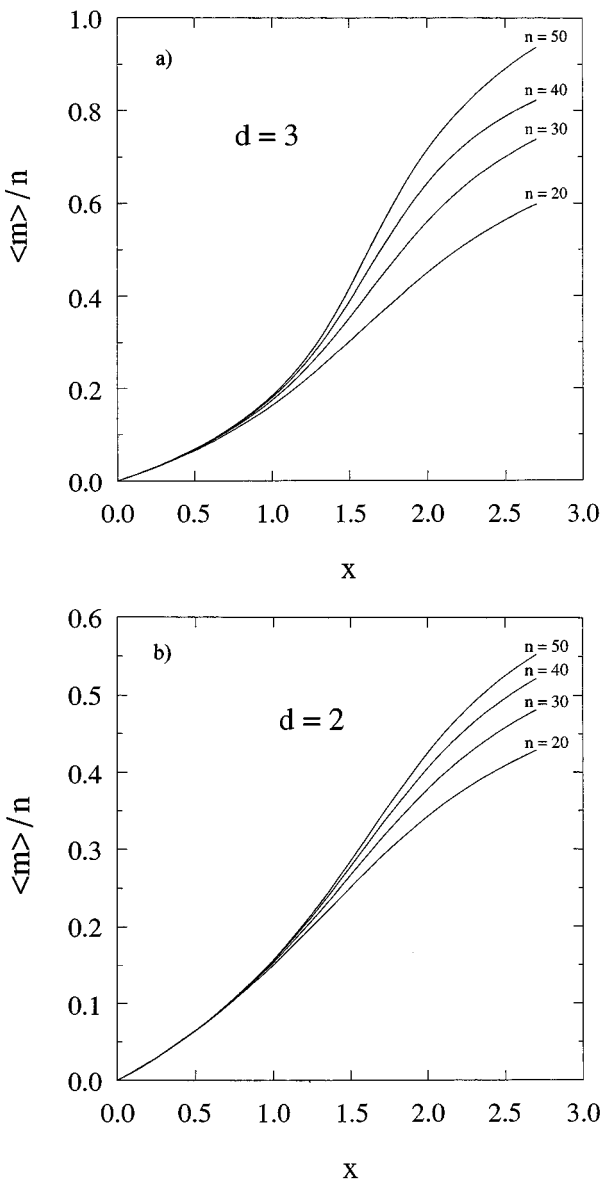

FIG. 11. Average number of SAW contacts as a function of nearest-neighbor energy. Note the sensitivity of average contacts to energy in the collapsed regime for finite chains. (a) $d=3$. (b) $d=2$.

The main point for the present discussion is that the structure of the zeros contains much information about the critical behavior of interacting SAW's, and the interesting question arises of how this information is related to $C_{n,m}$ and the maximum contact number $m_{\max}$. It is well known in the mathematically related Ising model that the transition temperature is likewise determined by the thermal (Fisher) zeros pinching the real axis, and the exponent ν is determined by the rate of approach of the zero closest to the real axis [34]. Important amplitude ratios are determined by the angle at which the zeros intersect the real axis [34], and no doubt more analytical information is contained in the structure of the Fisher zeros. It is difficult to understand how this subtle information can be compatible with the simple relation Eq. (2.15b). Perhaps corrections to the asymptotic scaling in Eq. (2.15b) play an important role in determining these critical parameters. It should be interesting to examine these questions in reverse where the implications of the critical scaling of the partition function for $C_{n,m}$ are investigated. We plan to study this type of question further once we obtain more accurate lattice data for longer chains.

III. DISCUSSION

The main result of the present paper is the suggestion of a spectrum of γ exponents corresponding to SAW's having a constrained number of nearest-neighbor (NN) contacts m. These numerical results must be verified by rigorous calculation before they can be accepted as established, however. Some insight into the conjectured $\gamma(m)$ exponents can be obtained through physical reasoning and comparison with results known for other constrained polymer problems.

As the temperature is lowered below the θ point, the NN interaction energy becomes stronger, and it becomes natural to think of the NN contact as being a ''virtual bond.'' In this

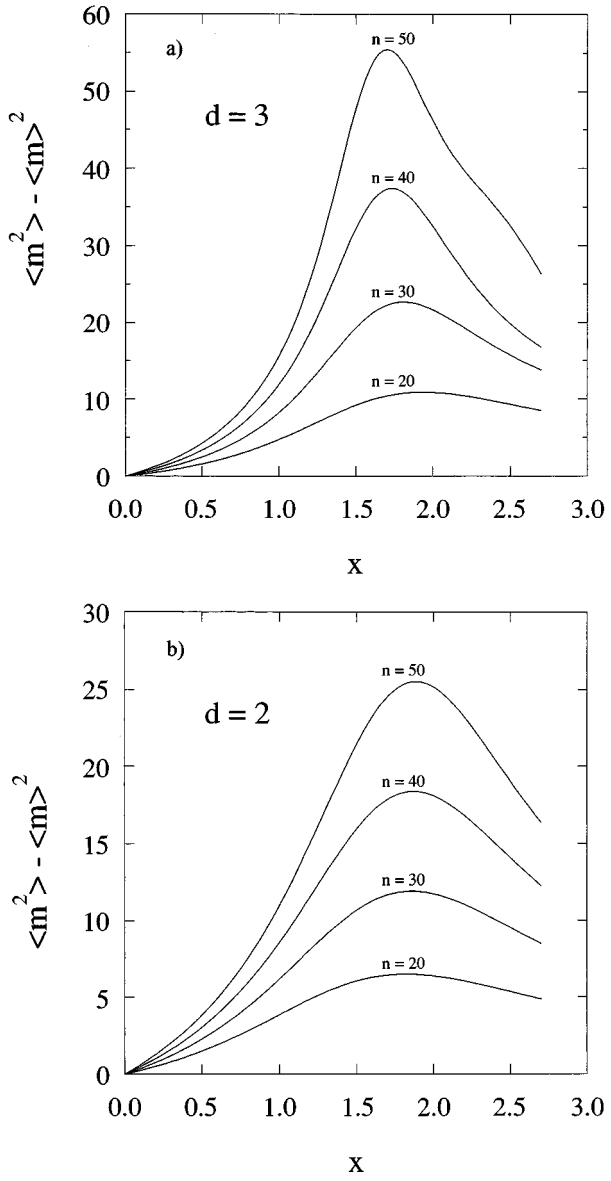

FIG. 12. Specific heat of NN-interacting SAW's. (a) $d=3$. (b) $d=2$.

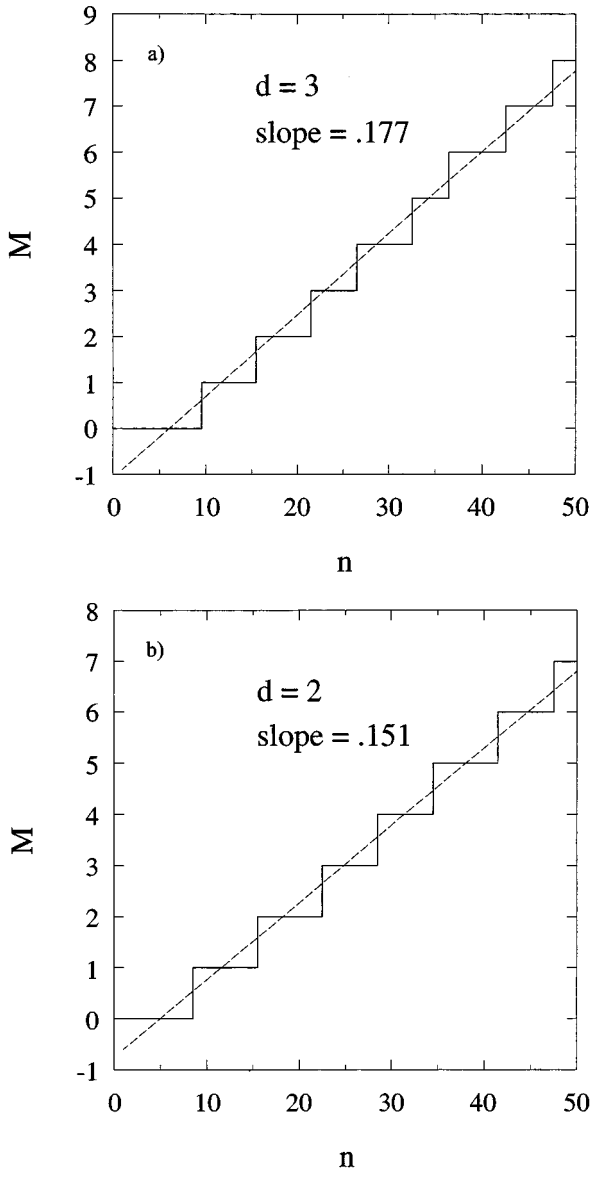

FIG. 13. Contact number M for which the number of SAW configurations is greatest. (a) $d=3$. (b) $d=2$.

physical view, the m-contacting polymers become much like *branched polymers*. Indeed, a number of authors have pointed out the similarity of self-attracting polymers to branched polymers based on other reasoning [35].

Soteros and Whittington [21] have rigorously shown that the number of self-avoiding branched polymers (''lattice animals'' or simply ''animals'') $C_{n,c}$ having a fixed cycle number c (''cyclomatic index'') scales like

$$C_{n,c}(\text{animal}) \sim [\mu(\text{animal})]^n n^{\gamma(c)-1}, \quad n \to \infty \tag{3.1a}$$

$$\gamma = \gamma(c=0) + c. \tag{3.1b}$$

The cyclomatic index c is the maximum number of the edges which can be removed from a lattice animal without breaking the graph up (roughly speaking the number of ''loops'') into disjoint parts. For the SAW the NN contacts are likewise ''bonds'' which can be cut without disconnecting the polymer. We also note that the maximum c of a lattice animal has the asymptotic variation [36],

$$c_{\max} \sim (d-1)n, \quad n \to \infty \tag{3.2}$$

for a hypercubic lattice. The maximum number of SAW contacts notably exhibits the *same* asymptotic scaling [see Eq. (2.11)]. Following the analogy further, we note that an unrestricted sum of the number of lattice animals C_n (animal),

$$C_n(\text{animal}) = \sum_{c=0}^{c_{\max}} C_{n,c} \tag{3.3}$$

exhibits an asymptotic scaling

$$C_n(\text{animal}) \sim [\mu(\text{animal})]^n n^{\gamma-1}, \quad n \to \infty, \tag{3.4}$$

where it has rigorously been shown [37] that

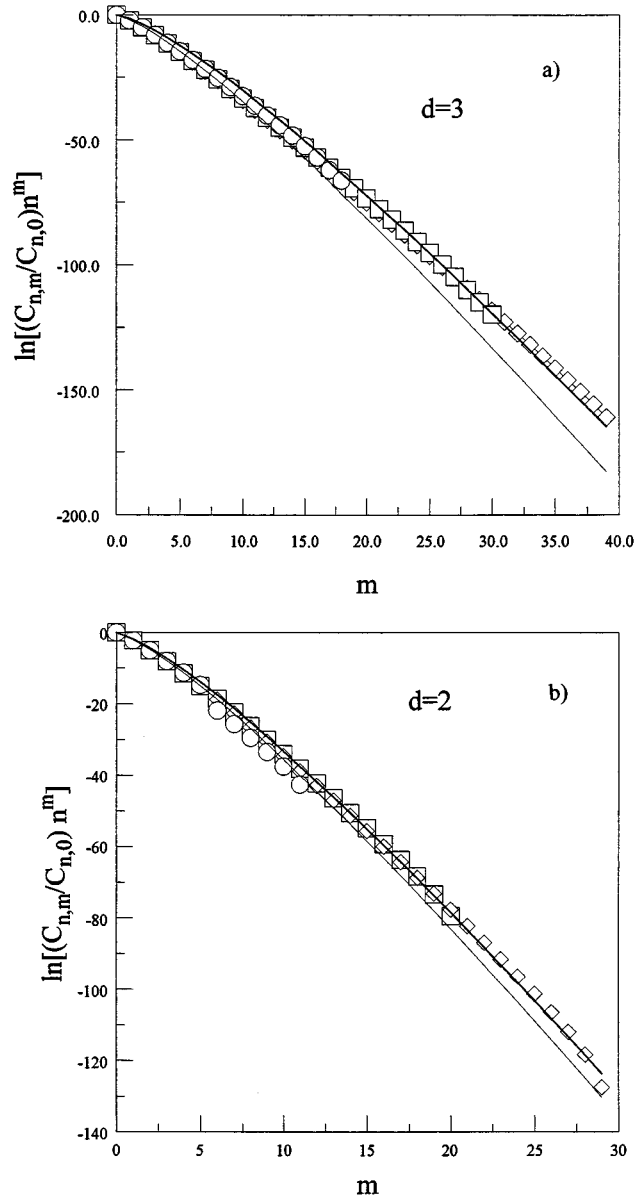

FIG. 14. Amplitude factor $A(m) \equiv C_{n,m}/n^m C_{n,0}$ for contact-constrained SAW's. (a) $d=3$. (b) $d=2$. The light solid line denotes Eq. (2.15a), where δ is fixed by lattice data estimates of the connectivity constant [see Eq. (2.17)]. The dark solid lines are obtained through a least-square fit of Eq. (2.15a) to the MC data, where δ is adjusted as a fit parameter. This fitting procedure led to the δ estimates: $\delta(d=3)=0.224$ and $\delta(d=2)=0.164$. The numerical data are for $n=20$ (○), $n=30$ (□), and $n=40$ (◇).

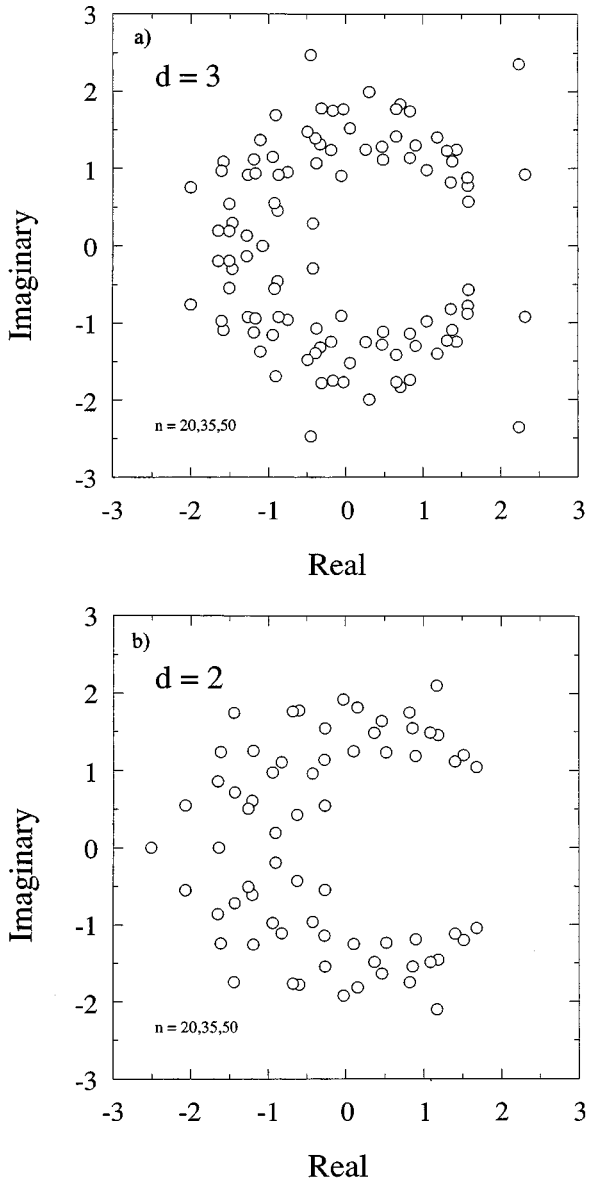

FIG. 15. Zeros of SAW partition function in the complex plane. (a) $d=3$. (b) $d=2$.

$$\gamma = \gamma(c=0). \tag{3.5}$$

Exact formal results for γ(animal) are available in $d=3$ and 4 through the connection between branched polymers and the Yang-Lee edge singularity problem [38]. [Often the exponent γ(animal)-1 is denoted as $-\theta$ in the literature on branched polymers, and the present notation is introduced to stress the analogy between SAW's and branched polymers.]

The connectivity constants for ''treelike'' lattice animals ($c=0$), μ_0(animal), and unrestricted lattice animals, μ(animal), where c is not fixed, have been proven to exist [39], and have been shown to satisfy the strict inequality [36,37]

$$\mu_0(\text{animal}) < \mu(\text{animal}), \quad 1 < d < \infty, \tag{3.6}$$

and μ(animal;c) equals μ_0(animal) independent of c [21(b)]. The corresponding relations for SAW's were discussed in Sec. II (conjectures supported by numerical evidence and incomplete mathematical arguments)

$$\gamma = \gamma(m=0) \equiv \gamma(\text{NAW}), \quad \mu(\text{NAW}) < \mu(\text{SAW}), \quad \mu(\text{NAW}) = \mu(m), \tag{3.7}$$

are compatible with the proposed ''analogy'' between lattice animals and SAW'S. Moreover, the radius of gyration exponent ν is believed to be the same for NAW's and SAW's, and to be m independent (fixed m), and similarly the lattice animal exponent ν has been shown to be independent of c (fixed c) for lattice animals [37(c)]. Finally, we mention the generalization of Eq. (3.3), where a branching fugacity

$y=\exp(-\mu)$ replaces the NN interaction parameter x in the SAW partition function, Eq. (2.1) [40,41],

$$C_n(\text{animal},y)\equiv C_n(y)=\sum_{c=0}^{c_{\max}} C_{n,c}y^c. \tag{3.8}$$

An increase in the number of branched polymer cycles through y leads to a phase transition [40] for a critical value of $y=y_c$, where the critical exponents become altered. Again the analogy with interacting SAW's is striking.

There have apparently been no studies of the amplitude of $C_{n,c}$ for lattice animals, despite the more developed rigorous theory for animals in comparison with interacting SAW's. Equation (2.15a) suggests a c-dependent prefactor $A(c)$,

$$A(c)\sim[\delta(\text{animal})]^c/c!, \quad n\to\infty, \tag{3.9a}$$

$$\delta(\text{animal})=\ln[\mu(\text{animal})/\mu_0(\text{animal})]. \tag{3.9b}$$

We mention numerical estimates of μ(animal) and μ_0(animal) for square and cubic lattices [37(a),37(b)],

$$\mu(\text{animal},d=3)=10.62, \quad \mu_0(\text{animal},d=3)=10.53, \tag{3.10a}$$

$$\mu(\text{animal},d=2)=5.210, \quad \mu_0(\text{animal},d=2)=5.14. \tag{3.10b}$$

A rigorous derivation of the dependence of the lattice animal amplitude $A(c)$ on c would be interesting. In the meantime, it should be useful to check Eq. (3.9) numerically.

Data relating to the amplitude $A(c)$ have recently been given for the closely related problem of self-avoiding random plaquettes surfaces [22–24]. Strong arguments have been given that these surfaces belong to the lattice animal universality class [41], and these arguments are well supported by numerical studies [41,42]. For random surfaces the genus plays a role similar to the number of loops (cyclomatic index) of branched polymers [22], and we would then expect that the number of random surfaces with fixed genus, $Q_{n,g}$ to scale as

$$Q_{n,g}\sim n^{\gamma(g)-1}[\mu_0(\text{surface})]^n, \quad n\to\infty, \tag{3.11a}$$

$$\gamma(g)=\gamma(g=0)+g, \tag{3.11b}$$

where n is the number of surface plaquettes and μ_0(surface) is the surface connectivity constant for a fixed genus. Dotsenko *et al.* [23] suggested a relation of this kind where n is replaced by the surface area A for self-avoiding random plaquette surfaces arising in their investigation into clustering in the Ising model ($d=3$). They also suggest that this scaling relation (or a very similar form) obtains for a wide range of random surface models. Dotsenko *et al.* estimated the genus-dependent amplitude numerically and argued that the probability $P(g)$ of a random surface having a genus g equals [see Eq. (2.15)],

$$P(g)\sim\exp(-\delta A)(\delta A)^g/g!, \tag{3.12}$$

where A is proportional to the surface mass (n). The data for various random surface models show that the slope of $\gamma(g)$ versus g is near 1 as in Figs. 3 and 4 for contact-constrained SAW's. It is not clear whether the small deviations from a unit slope in both these models reflect real deviations or numerical uncertainty [22]. Very similar numerical results and conclusions for random plaquette surfaces have been found by Caselle and co-workers [24].

The physical arguments for the distribution $P(g)$ of the number of self-avoiding surface configurations given by Dotsenko *et al.* and Caselle and co-workers also provide a motivation for the SAW contact distribution function Eq. (2.15a), where the genus of the random surface is replaced by the SAW contact number m. These physical arguments complement the deduction of Eq. (2.15c) in Sec. III, based on analytical self-consistency.

Finally, we mention that other aspects of the relation between the SAW contact number m and the genus number g carry over as in the discussion between m and the cyclomatic index c. The connectivity constant is different for surfaces with an unconstrained genus number from those with a fixed genus [22,43], the linear exponent spectrum $\gamma(s)$ [23,24], the transition for a critical fugacity [44], etc., are common features of these problems.

In summary, the scaling of the number of SAW's having a fixed number of contacts m, the number of branched polymers with a fixed cyclomatic index c and the number of random surfaces having a fixed genus g exhibit similar scaling behavior with polymer mass n. This suggests that many results, which are known properties for SAW's, should hold for those more complex polymer structures and some interesting properties of contact-constrained SAWs such as a spectrum of contact $\gamma(m)$ exponents. These analogies also work in reverse, and interesting results are also implied for SAWs.

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