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Study of Monte Carlo Methods for Generating Self-Avoiding Walks

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The concept of fractal dimensionality is used to study different statistical methods for generating self-avoiding walks (SAWs). The reliability of SAWs traced by the enrichment technique and the dynamic Monte Carlo technique is verified. The number of dynamic cycles which represent a single independent SAW of N_0 steps is found to be about $0.1N_0^3$. We show that the enrichment process for generating SAWs may be presented as a critical phenomenon.

KEY WORDS: Fractal dimensionality; enrichment Monte Carlo; dynamic Monte Carlo; critical phenomena, self-avoiding walks.

1. INTRODUCTION

The statistical configurational properties of long self-avoiding walks (SAWs) have been of considerable interest.[1-3] Exact enumeration of chains and Monte Carlo (MC) methods were used in numerical studies.[4-11] Most of the Monte Carlo methods give *approximate* representative ensembles of SAWs. The reliability of these ensembles was checked by measuring quantities such as the mean square end-to-end distance of the chains and the mean square radius of gyrations.[5-7,9] However, these measurements do not provide detailed information about the *internal* structure of the chains. In the present work we make use of local fractal dimensionality[12,13] (LFD), in order to check the structure of chains obtained by different methods and to compare between them.

Following the ideas presented by Mandelbrot,[14] LFD is defined[12,13]

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as

$$D_{N_0}(N) = \ln\left(\frac{N+1}{N}\right) \Big/ \ln\left[\frac{\langle R^2_{N+1}\rangle_{N_0}}{\langle R^2_N\rangle_{N_0}}\right]^{1/2} \tag{1}$$

where $\langle R^2_N\rangle_{N_0}$ is the mean-square distance of all subchains consisting of N steps in a SAW of N_0 steps. The LFD $D_{N_0}(N)$ is a measure of the extent that the walk winds about, on a length scale corresponding to N.

Numerical measurements of LFD recently performed,[12,13] had shown for a large range of scale-lengths that $D_{N_0}(N)$ is nearly constant and its value is $1/\nu$, ν being the known end-to-end exponent. This shows that SAWs have an internal self similarity or a scaling property in agreement with the ideas first presented by de Gennes.[3] LFD was found to be useful in determining the critical exponent ν as well as corrections to scaling with great accuracy.[15,16] This is due to the fact that LFD uses all internal distances of each chain thus improving the statistics significantly.

2. ACCURACY OF STATISTICAL ENSEMBLES

The proper way to simulate an emsemble of SAWs is by the direct Monte Carlo procedure.[6] Start with an arbitrary step. Make a random choice for the direction of the next step (but returning to the previous site is excluded). Continue this procedure until the ultimate length of the SAW is reached or until the walk intersects itself. If the SAW intersects itself before terminating then the whole configuration is not considered and a new start is made. This method gives indeed an equilibrated ensemble of SAWs since it is equivalent to eliminating all intersecting walks from a given ensemble of random walks.

In order to check the magnitude of the fluctuations of LFD measured on such an ensemble, we compare two direct MC ensembles (consisting of 100 and 30,000 SAWs of length $N_0 = 20$ in two-dimensional space $d = 2$) with results obtained from an exact enumeration of these SAWs (Fig. 1). In the small ensemble (100 SAWs) fluctuations for short subchains are quite small. For ensembles with about 10^4 SAWs fluctuations are even smaller, about 0.1%.

By applying the method described above, it is possible to obtain ensembles of SAWs with N_0 bigger than may be obtained by exact enumerations (typically 20). However, the probability that a walk intersects itself increases exponentially with N_0. Thus, the longer N_0 is, the more computer time one needs, so that the method becomes impractical for $N_0 \sim 10^2$ ($d = 2, 3$).

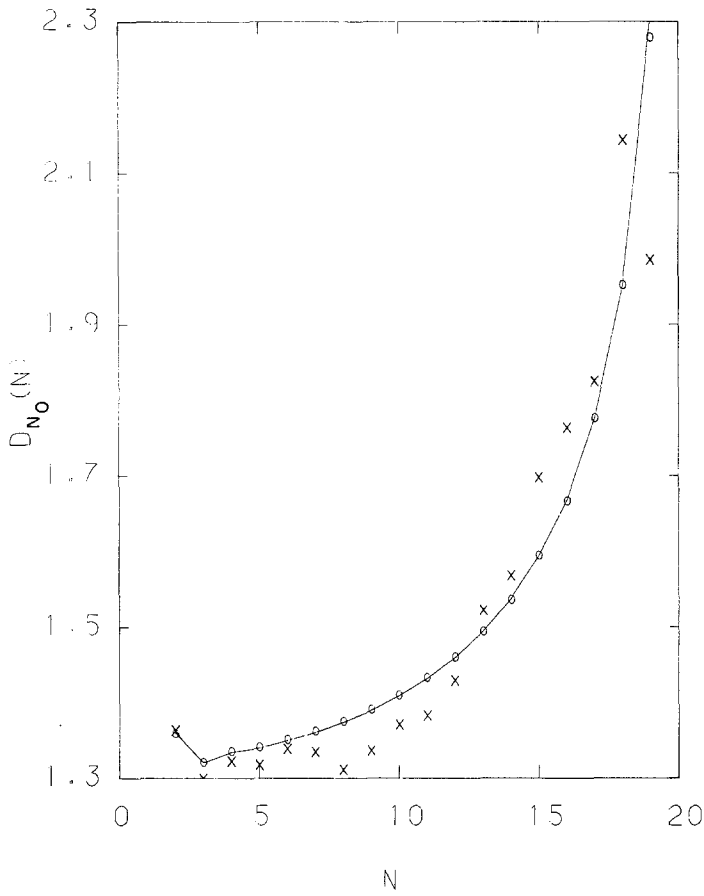

Fig. 1. $D_{N_0}(N)$, the LFD for SAWs, traced on a square lattice, with $N_0 = 20$. The solid line represents exact enumeration data, the circles show the results for a direct MC ensemble containing 3×10^4 SAWs and the crosses those for calculations on a set of 100 configurations.

3. ENRICHMENT METHOD

In order to overcome the attrition described in the first section, Wall *et al.*[6] developed the enrichment technique. In this technique, the sample of walks is enriched by allowing, after each s steps of the walk, p different trials for adding a new section of s nonintersecting steps. The attrition of the samples behaves like $e^{-\lambda N_0}$ (where λ is a lattice-dependent attrition constant). However, this is compensated by an enrichment of $p^{N_0/S}$ so that if $g \equiv pe^{-\lambda S} = 1$ the attrition is exactly compensated. If $g > 1$, the walks

with common first sections are given too much weight. If $g < 1$ the attrition is not fully compensated. Therefore, using $g = 1$ is best.

It had been argued that the enrichment of samples does not bias the ensemble.[6] This was demonstrated by measurements on enriched ensembles of quantities such as the mean square radius of gyration which yielded good results.[2,6] We intend to be more rigorous and check whether the enrichment spoils the internal structure of the SAWs. In spite of the above demonstration nonbias, it might still be possible that some subchain distances are different; and yet they still have the same mean end-to-end

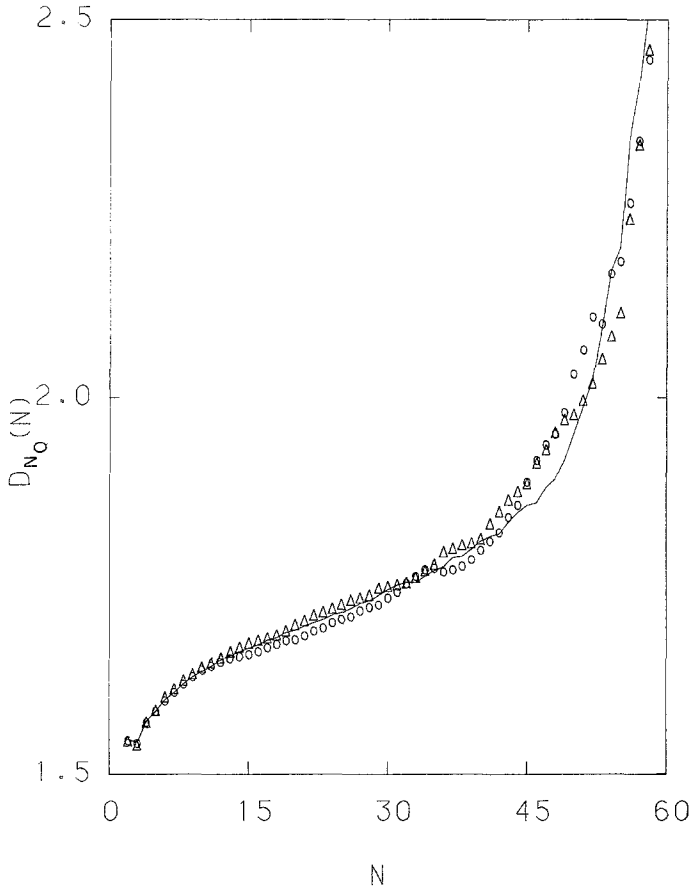

Fig. 2. $D_{N_0}(N)$, the LFD for SAWs, traced on a SC lattice ($d = 3$), for $N_0 = 60$. The full line is the result of direct MC ensemble containing 10^4 SAWs. The circles and triangles show the results for 10^4 SAWs of enrichment ensembles using $s = 20$, $p = 3$ and $s = 30$, $p = 6$, respectively.

distance. We generate an ensemble of 10,000 SAWs with $N_0 = 60$ on a cubic lattice by the direct method of Section 2. Then we compare to the obtained LFD of enriched ensembles with $s = 20$, $p = 3$ and $s = 30$, $p = 6$ (Fig. 2). The results compare favorably showing that if there are any distortions of internal distances they must be very small. There is in fact some influence to the aggregation of s-step sections. In Fig. 3 we show results for an ensemble of 10,000 SAWs traced on a two-dimensional lattice with $p = 13$ and $s = 20$. There seem to be irregularities in the LFD at $N = sl$ $(l = 1, 2, 3)$ which clearly result from the method used. However, these irregularities are minor and they are not a practical obstacle in researching the properties of SAWs.

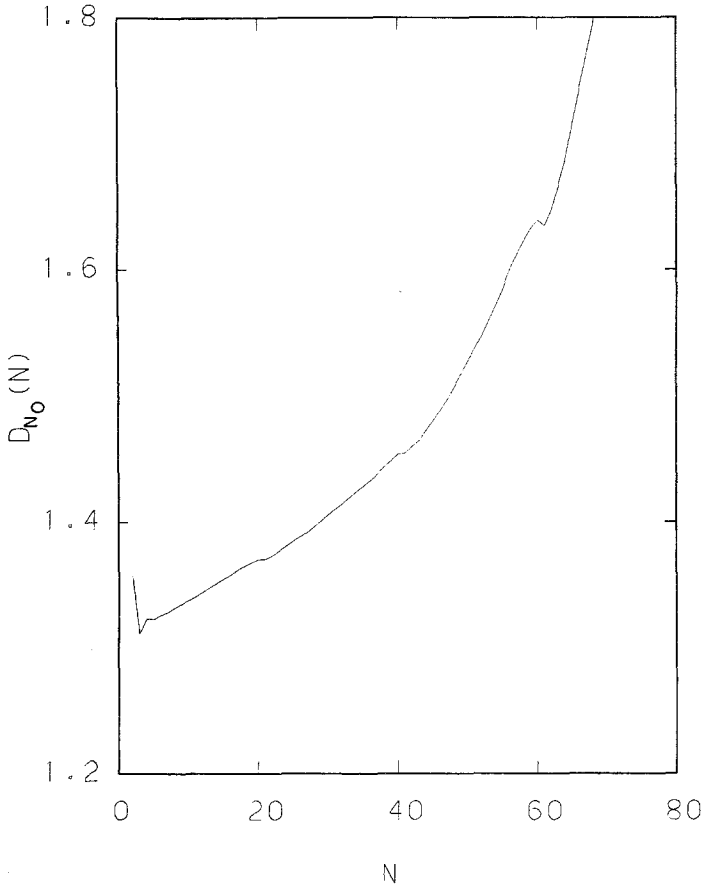

Fig. 3. $D_{N_0}(N)$, the LFD for 10^4 SAWs traced on a square lattice with $N_0 = 80$, using enrichment technique with $s = 20$, $p = 13$.

A similar method to the enrichment technique was proposed by Alexandrowicz,[17] the dimerization technique. His method also consists of joining sections. It would be interesting to have the above-described check done on an ensemble of dimerized SAWs.

4. BIASED ENRICHMENT

In this section we explore the influence of the parameter $g = pe^{-\lambda S}$ on the ensemble. We interpret the two regions of g ($g > 1$, $g < 1$) as two different phases where $g = g_c = 1$ is a critical point separating the two.

When $g < g_c = 1$, there is a net attrition of the samples and thus the method produces SAWs with a finite average $\overline{N}_0$. The SAWs produced that way are representative of an equilibrated ensemble. Indeed, in the limit $p = 1$, $s = \infty$ ($g = 0$) we return to the direct method described in Section 2. The mean end-to-end distance $\langle R^2_{\overline{N}_0} \rangle^{1/2}$ of the SAWs increases as g approaches g_c from below (since $\overline{N}_0$ increases) thus, $\langle R^2_{\overline{N}_0} \rangle^{1/2}$ represents a correlation length ξ diverging at g_c.

The average $\overline{N}_0$ for $g < 1$ can be calculated considering the probability $P(xs)$ of tracing a SAW having $N_0 = xs$ steps,

$$P(xs) \propto \left(pe^{-\lambda s}\right)^x = g^x \tag{2}$$

Then for $g \lesssim g_c$

$$\overline{N}_0 = s \frac{\int_0^\infty x g^x \, dx}{\int_0^\infty g^x \, dx} = -\frac{s}{\ln g} \simeq \frac{s}{g_c - g} \tag{3}$$

so that

$$\xi \sim \langle R^2_{\overline{N}_0} \rangle^{1/2} \sim \overline{N}_\nu^0 \sim (g_c - g)^{-\nu} \tag{4}$$

Thus the usual end-to-end exponent ν gets the meaning of a correlation length exponent.

At the critical point $g = g_c = 1$, $\overline{N}_0 \to \infty$ ($\xi \to \infty$), and this is in fact the only way to build "infinite",[3] nonbiased SAWs. Of course finite SAWs can be built with $g < g_c$ (we show examples later) but with less efficiency, i.e., one gets more diluted ensembles.

For $g > g_c$ one gets biased samples of SAWs. In the limit $p \to \infty$, $s = 1$, ($g \to \infty$) we obtain a sample of maximally biased SAWs whose LFD equals 2 after a small correlation length ξ. This is predicted theoretically[18] and numerically as shown below. When g approaches g_c from above, the steps within the walks are typically correlated up to a correlation length ξ (which diverges at g_c) as for a SAW.[19] Above this correlation length ξ, the correlation between steps is negligible and therefore LFD is 2 as for ideal chains.

[3] In practice one terminates the SAWs at an arbitrary large value of N_0.

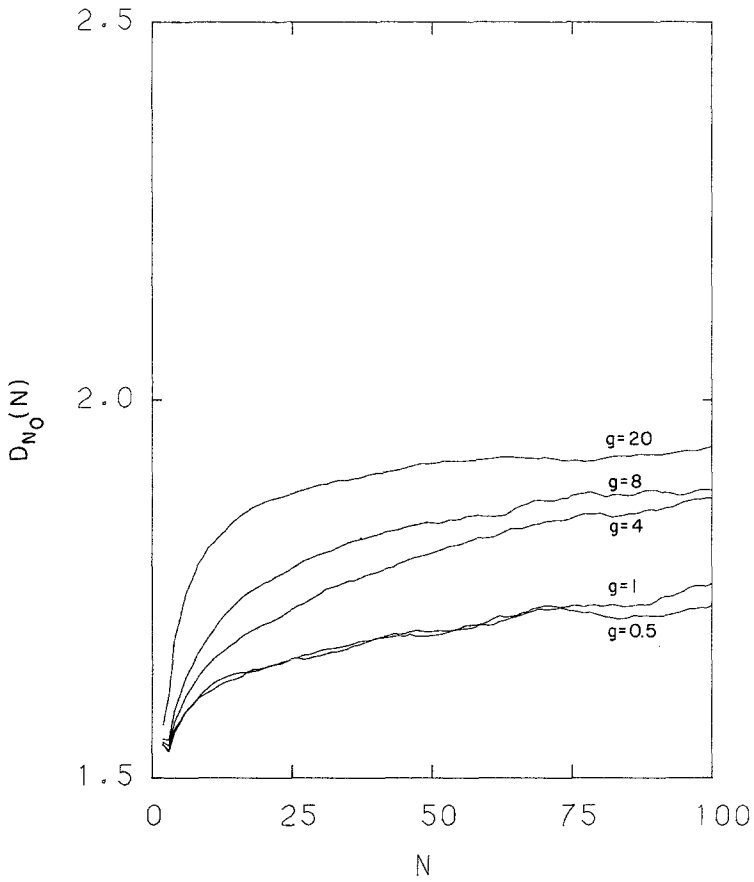

Fig. 4. $D_{N_0}(N)$, the LFD for ensembles of SAWs, containing 10^4 configurations. The SAWs were generated by the enrichment technique with $g = 20, 8, 4, 1, 0.5$.

The effect of g on LFD of SAWs is shown in Fig. 4. For $g \to \infty$ the LFD tends to 2 at a small correlation length. When g decreases but is still above 1, LFD tends to 2 but with an increasing correlation length. Finally for $g \leqslant 1$ LFD tends asymptotically[12,13] to $1/\nu$ (~ 1.7 for $d = 3$).

5. DYNAMIC MONTE CARLO METHOD

We now compare ensembles obtained from the dynamic Monte Carlo[4] method[11] to the static Monte Carlo ensembles discussed above. In Fig. 5

[4] In the dynamical Monte-Carlo method[11] one starts with an arbitrary SAW's configuration: in each *cycle* a group of two or three steps on the walk is randomly chosen and shifted (whenever possible). Equilibrium is expected to be reached after a large number of cycles.

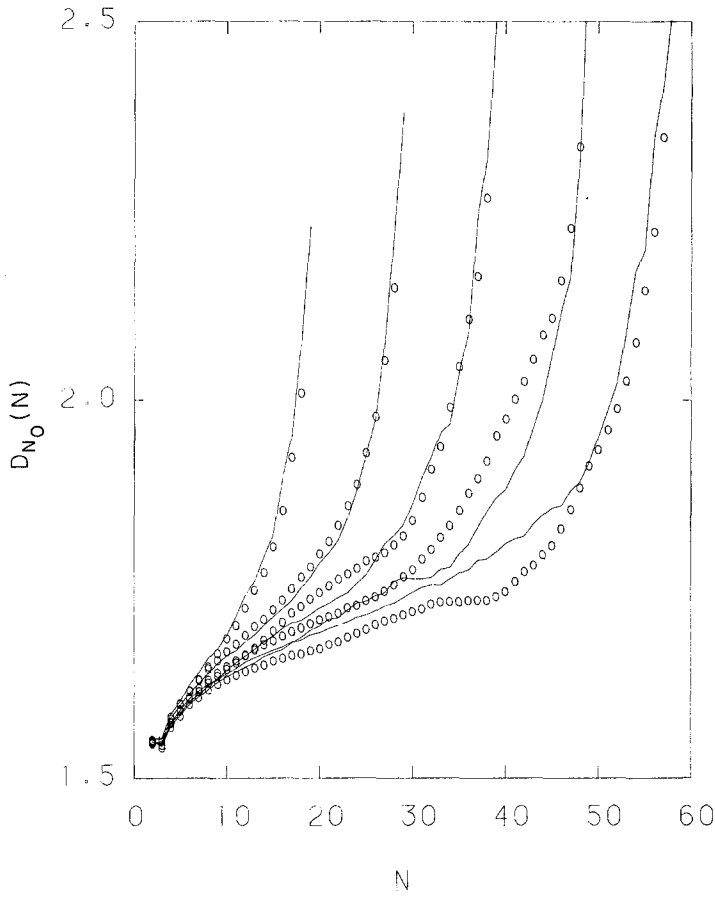

Fig. 5. $D_{N_0}(N)$, the LFD for SAWs traced on SC lattice ($d = 3$), with $N_0 = 20$, 30, 40, 50, and 60. The solid lines are the results for direct MC ensembles each containing 10^4 configurations. The circles show the results for dynamic MC ensembles containing 10^7 cycles each.

we show LFD of 10000 SAWs of length $N_0 = 20, 30, 40, 50, 60$ ($d = 3$) analyzed using static Monte Carlo ensembles as well as the LFD of SAWs obtained from dynamic Monte Carlo ensembles built from 10^7 cycles. Generally the results are in good agreement, as seen in Fig. 5.

From a comparison of the two Monte Carlo methods it is possible to estimate the number of cycles needed in order to represent one independent configuration.[20] For fluctuations of $\langle R_N^2 \rangle_{60}$, we compare in Fig. 6 between static ensembles containing 30 and 50 independent SAWs and dynamic ensembles of 10^6 cycles each. From Fig. 6 it is estimated that for $N_0 = 60$, 10^6 cycles represent 40 ± 10 independent configurations. The same proce-

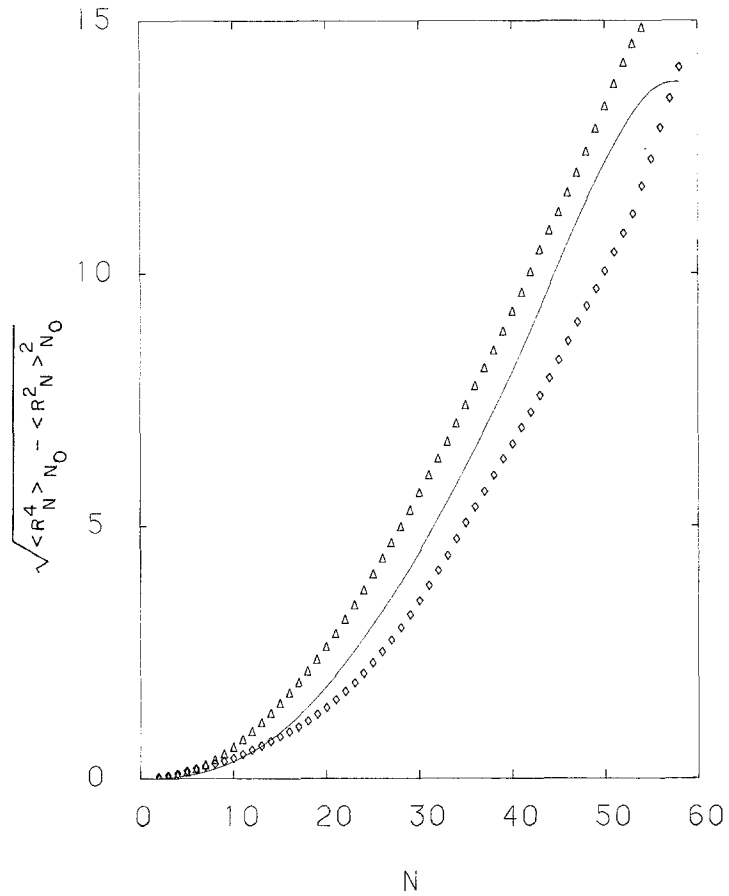

Fig. 6. The fluctuations in $\langle R_N^2 \rangle_{N_0}$ for $N_0 = 60$. The solid line shows the fluctuations between sets of 10^6 dynamic MC cycles. The triangles and diamonds show the fluctuations between sets of 30 and 50 independent SAWs produced by direct MC method, respectively.

dure was also applied for $N_0 = 20$, 30, 40, and 50. We find that the number of cycles representing one independent configuration of an N_0-step SAW is close to $0.1\ N_0^x$ with x close[20] to 3.

6. CONCLUSIONS

We have used LFD to study different statistical numerical methods for tracing SAWs. We find that the accuracy for the LFD of short subchains is about 0.1% for ensembles containing about 10^4 SAWs. This high accuracy is due to the use of all internal distances in each chain.

It is shown that the enrichment technique produces representative ensembles of SAWs except for minor disturbances in the internal distances around $N = sl$ (l = integer). The dynamic Monte-Carlo method also produces the same kind of ensembles. The number of cycles needed for each independent configuration is about $0.1N_0^3$.

The enrichment technique is presented as a critical process. The critical point is at $g_c = pe^{-\lambda s} = 1$. Below g_c, SAWs are created with only a finite average $\bar{N}_0$. This average diverges when g approaches g_c from below ($g \to g_c^-$). Above g_c the SAWs behave like ideal chains (with LFD = 2) for a scale length greater than ξ, while ξ diverges as $g \to g_c^+$. This picture reminds us of the approach of Redner and Reynolds[21] to SAWs as critical phenomena. It seems that g in the enrichment technique is strongly related to the fugacity per monomer p in their approach. They find that $\langle N_0 \rangle \equiv \bar{N}_0/V$, where $V = \langle R(2/N) \rangle^{d/2}$, behaves like $|p_c - p|^{d\nu - 1}$ while in the enrichment technique $\langle N_0 \rangle = |g_c - g|^{d\nu - 1}$, which is effectively the same result. Also for $p < p_c$, in their approach the phase is characterized by finite-length chains just as for $g < g_c$. However, above p_c the phase described by Redner and Reynolds consists of collapsed compact chains with LFD = d rather than the limit of ideal chains (LFD = 2), obtained in the enrichment method for $g > g_c$.

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