PHYSICAL REVIEW A VOLUME 26, NUMBER 3 SEPTEMBER 1982

# Theoretical and numerical study of fractal dimensionality in self-avoiding walks

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(Received 4 August 1981; revised manuscript received 29 March 1982)

It is shown that the concept of fractal dimensionality, recently proposed by Mandelbrot, provides a useful characterization of the configurational properties of a single polymer. From numerical studies of self-avoiding walks, computer generated by Monte Carlo methods, we find that a single-chain configuration possesses a statistical self-similarity property and therefore has a well-defined fractal dimensionality. The fluctuations in fractal dimensionality measured on a single-chain configuration vanish as the number of steps increases. It is shown that renormalization-group theory provides a theoretical basis for the concept of fractal dimensionality in polymers, as well as for its relation to the end-to-end exponent $\nu$.

## I. INTRODUCTION

Polymers represented by self-avoiding walks (SAW's) have been the focus of extensive theoretical and numerical investigations.[1-4] The usual quantities that are studied are the mean-square end-to-end distance and the mean radius of gyration.[4-10] These quantities are very useful in characterizing a statistical ensemble of polymer chains. However, they exhibit large fluctuations when measured on different configurations.[11,12] For instance, one can think of a regular polymer chain for which bending about the middle does not change its general shape (i.e., it remains a regular polymer), but such bending leads to a considerable change in the mean-square end-to-end distance or in the mean radius of gyration. On the other hand, we argue that, in spite of the large fluctuations in these quantities, there must be a parameter related to the degree of winding of the chain which is nearly the same for the majority of the different configurations. In this work, we find that the concept of fractal dimensionality (FD), recently introduced by Mandelbrot,[13] is useful in characterizing a single polymer chain. Indeed, the FD represents the degree of winding of the chain, and for each configuration it is shown to be nearly equal to the average value of the entire ensemble of polymers. The concept of FD has already proved fruitful for analyzing different physical problems.[13-19]

We show that renormalization-group theory provides a theoretical basis for the existence of FD in polymer chains as well as a relationship between the FD and the end-to-end exponent $\nu$.

The outline of the paper is as follows. In Sec. II we present the concept of FD as defined for polymer chains. In Sec. III we present the theoretical basis for FD in SAW's. Numerical results for SAW's traced out on two- and three-dimensional lattices are discussed in Sec. IV.

## II. FRACTAL DIMENSIONALITY OF POLYMER CHAINS

Consider a polymer traced out by a long self-avoiding walk. The polymer can be viewed on different scales of length (Fig. 1). Choose a section of length $a_0$ and count the number $b_0$ of details apparent in that section. Suppose that upon inspecting a longer section of length $a_1$ one can see $b_1$ details. Let us define $D$ by the relationship

$$(b_1/b_0)=(a_1/a_0)^D . \tag{1}$$

If $D$ is independent of the magnification factor $a_1/a_0$ for some range of scales, i.e., range of $a_0$, the quantity $D$ is called the fractal dimensionality of the polymer in this range. This definition is in accordance with the ideas developed by Mandelbrot.[13] The assumption that $D$ is independent of $a_0$ expresses a self-similarity property of the polymer for different scales. The quantity $D$ represents the extent to which the polymer is winding. If the polymer is a straight line, then clearly $D=1$, whereas for ideal random chains, $D$ can be easily shown equal to 2.

In the following we present a definition for a practical concept, the local fractal dimensionality

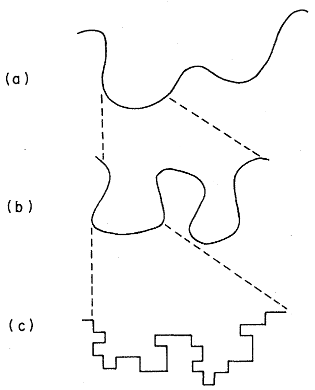

FIG. 1. Different scales of length of polymers. (a) End-to-end scale of length. (b) Upon magnification, exhibiting internal statistical self-similarity (main range) of the chain. (c) Geometrical scale.

(LFD) of polymer chains. The mean-square separation of the end points of a segment containing $N$ links in a polymer consisting of $N_0$ links is defined by

$$\langle R_N^2 \rangle_{N_0} = \frac{1}{N_0 - N + 1} \sum_{i=1}^{N_0 - N + 1} \langle R_{i,i+N}^2 \rangle_{N_0} , \quad (2)$$

where $\langle R_{i,i+N}^2 \rangle_{N_0}$ is the mean-square separation between the $i$th and the $(i+N)$th elements of the chain. The quantity $(\langle R_{N+1}^2 \rangle_{N_0} / \langle R_N^2 \rangle_{N_0})^{1/2}$ plays the role of $a_1/a_0$ in (1). Further, we expect that $b_0$ should be proportional to $N$ and that $b_1$ should be proportional to $N+1$. Thus, we define and measure the value of the LFD by

$$D_{N_0}(N) = \ln \left[ \frac{N+1}{N} \right] \Bigg/ \ln \left[ \frac{\langle R_{N+1}^2 \rangle_{N_0}}{\langle R_N^2 \rangle_{N_0}} \right]^{1/2}$$

$$\underset{N \gg 1}{\simeq} \frac{\partial \ln N}{\partial \ln (\langle R_N^2 \rangle_{N_0})^{1/2}} . \quad (3)$$

The subscript $N_0$ emphasizes the fact that we are considering finite polymers. $D_{N_0}(N)$ is the LFD of a length scale corresponding to $N$.[20] It should be noted that if $D_{N_0}(N) = D$ is independent of $N$, then (3) is equivalent to

$$[(\langle R_N^2 \rangle_{N_0})^{1/2}]^D = A' N , \quad (4)$$

where $A'$ is a constant of proportionality. If such is the case, then (4) may be used as the definition of $D$.

FD is indeed a measure of the degree of winding of the chain. Define $\theta_{1/2}$ as the mean angle between two neighboring segments $\vec{R}_N, \vec{R}'_N$, each containing $N$ steps (Fig. 2). Then

$$\begin{aligned} \langle (\vec{R}_{2N})^2 \rangle &= \langle (\vec{R}_N + \vec{R}'_N)^2 \rangle \\ &= \langle \vec{R}_N^2 \rangle + \langle \vec{R}'^2_N \rangle - 2 \langle \vec{R}_N \cdot \vec{R}'_N \rangle \\ &\equiv 2 \langle \vec{R}_N^2 \rangle - 2 \langle \vec{R}_N^2 \rangle \cos\theta_{1/2} . \end{aligned} \quad (5)$$

Using Eq. (4)

$$\cos\theta_{1/2} = 1 - 2^{2/D - 1} . \quad (6)$$

When $D$ increases, $\theta_{1/2}$ decreases, implying that the chain is more winding.

It is reasonable to expect that if the polymer is very long, it has the same degree of winding in most length scales in which it is observed. Thus, we expect it to have a fractal dimensionality independent of scale. However, when we inspect the polymer in the smallest scales, $N \sim 1$ (the geometrical scale), we see that the polymer is forced to bend according to the lattice geometrical constraints [Fig. 1(c)]. This might spoil the self-similarity, thus changing the LFD in this range. Finally, in the largest scales, $N \sim N_0$ (the end-to-end range), the polymer is more free to bend than in smaller scales. This follows because in smaller scales, the exclusion of volume arising from different parts of the polymer has to be considered, while in the end-to-end range of scales, there is no such constraint. Thus, in view of (6), we expect LFD to increase in the end-to-end range.

## III.THEORY

We now present the theoretical background for the FD, as well as a relation between the value of $D$ defined in this work and the known end-to-end exponent. We base our treatment on renormalization-group ideas developed for polymers by de Gennes.[1]

It is well known that for an ideal random-walk chain,

$$\langle R_{N+1}^2 \rangle_{N_0} / \langle R_N^2 \rangle_{N_0} = (N+1)/N \equiv g_N . \quad (7)$$

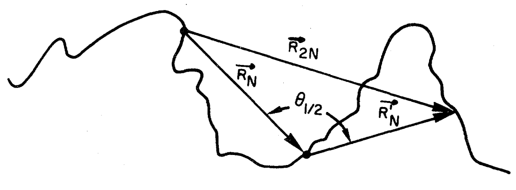

FIG. 2. Definition of the angle $\theta_{1/2}$.

However, in self-avoiding chains, the excluded volume interaction swells the polymer. We describe this swelling by a factor $(1+h)$, where $h$ depends[1] in general on $g_N$ and on a dimensionless coupling constant $u_N$. That is,

$$\langle R^2_{N+1}\rangle_{N_0}=\langle R^2_N\rangle_{N_0} g_N[1+h(g_N,u_N)]\ . \tag{8}$$

The main idea of renormalization-group theory is to repeat this transformation many times, starting with $N \sim 1$, until $N \gg 1$. It is assumed that for large enough $N$, the coupling constant $u_N$ reaches a finite limit $u^*$, which is called the "fixed point." Using the semigroup property of the transformation, Eq. (10) yields

$$\langle R^2_{N+1}\rangle_{N_0}/\langle R^2_N\rangle_{N_0}=[(N+1)/N]^{2\nu}\ , \tag{9}$$

that is,

$$\langle R^2_N\rangle_{N_0}=AN^{2\nu}\ , \tag{10}$$

from which (4) follows if $\nu=1/D$. Thus, we see that renormalization-group ideas lead to the concept of FD. It should be noted that (9) holds only for $N \gg 1$ (i.e., not in the geometrical range), a result which is consistent with our numerical data. Moreover, when $N$ is of the order of $N_0$, another edge effect appears, that is, the effective coupling constant $u_N$ tends to change again because of the decrease in the excluded volume interaction. Equation (9) is thus correct only in the main range, because only then $u_N \simeq u^*$. In spite of this, a similar approach can be applied for the mean-square end-to-end distance $\langle R^2_{N_0}\rangle$, showing that

$$\langle R^2_{N_0}\rangle=BN_0^{2\nu}\ , \tag{11}$$

that is, the same exponential law results for $\langle R^2_{N_0}\rangle$ and for $\langle R^2_N\rangle_{N_0}$. The only difference might be in the constants of proportionality $A$ and $B$. The fact that the exponents are equal in (10) and (11) is by no means obvious. Moreover, the usual end-to-end exponent does not represent an *internal* self-similarity of the polymer and therefore it does not have the meaning of fractal dimensionality.

A general function which predicts internal self-similarity and the same exponential law for both internal and the end-to-end distances is

$$\langle R^2_N\rangle^{1/2}_{N_0}=N^{\nu}\rho(x)\ ,\quad x=\frac{N}{N_0}\ . \tag{12}$$

This relation is typical of scaling relations. Indeed, if

$$\rho(x)=\begin{cases}A^{1/2}, & x \ll 1\\ B^{1/2}, & x=1\end{cases} \tag{13}$$

we regain (10) and (11). Using the definition (3) of LFD and (12) leads to

$$D_{N_0}(N)=\left[\nu+x\frac{d\ln\rho(x)}{dx}\right]^{-1}\ . \tag{14}$$

This expression predicts that $D_{N_0}(N)=1/\nu\equiv D$ for finite segments of $N$ steps in an infinite chain, that is, an internal self-similarity. Moreover, if for quite a wide range of $x$ $\rho(x)$ is nearly constant, then $D_{N_0}(N)$ is nearly constant in this range. We show in Sec. IV that such a range exists, and we call it the "main range." On the other hand, $\rho(x)$ should decrease when $x$ approaches unity. This is due to the fact mentioned above that for the entire chain, the excluded volume effect is weaker than for internal segments (this implies $A>B$). Thus, it follows from (14) that $D_{N_0}(N)$ increases when $x \rightarrow 1$.

An interesting result is the universality property of $D$. Adopting (12) yields that the LFD is a function of $x$ and not of $N_0$ (it also depends, of course, on the lattice dimensionality $d$). The above predictions are confirmed by the numerical results that will be presented in Sec. IV.

The exponential behavior of $\langle R^2_N\rangle_{N_0}$ may also be obtained by a different approach by making a simple assumption about the correlation function. The mean-square average $\langle R^2_{i,i+N}\rangle_{N_0}$ over all possible configurations of $N_0$ steps can be written[5] in terms of the correlation function as

$$\langle R^2_{i,i+N}\rangle_{N_0}=N+2\sum_{m=1}^{N}\sum_{j=1}^{i+N-m}\langle \vec{u}_j\cdot\vec{u}_{j+m}\rangle_{N_0}\ . \tag{15}$$

If the polymer is long enough and $m$ is finite, a reasonable assumption is that $\langle \vec{u}_j\cdot\vec{u}_{j+m}\rangle_{N_0}$ will not depend on $j$ and will be of the form[5]

$$\langle \vec{u}_j\cdot\vec{u}_{j+m}\rangle_{N_0}\sim\frac{C}{m^{2-2\nu}}\ . \tag{16}$$

Similar assumptions are commonly used in other interacting systems, e.g., spin systems.[21]

Using (2), (15), and (16) and assuming that $N \gg 1$ and $2\nu>1$ yields

$$\langle R^2_N\rangle_{N_0}\simeq AN^{2\nu}\ . \tag{17}$$

This is exactly the same as (4) if we identify $\nu$ with $1/D$. This result shows that the assumption made regarding the correlation function leads to the existence of the FD concept in polymers.

## IV. NUMERICAL RESULTS

We have carried out numerical studies of self-avoiding walks performed on two- and three-dimensional lattices. The walks were computer generated by the enrichment technique.[7,22] In the enrichment mehtod, two parameters $p$ and $s$ are introduced which satisfy the condition $pe^{-\lambda s}=1$, where $\lambda$ is the attrition constant and $p$ is the number of trials used to generate $s$ subsequent steps without intersections. We used $p=11$, $s=20$ for the square lattice; $p=35$, $s=20$ for the triangular lattice; and $p=11$, $s=40$ for the cubic lattice. We note that using slightly different values of $p$ and $s$ hardly affects the results. In most cases, we use ensembles consisting of about $10^4$ polymers.

We present our results for the LFD $D_{N_0}(N)$ measured according to (3), beginning from the case of $d=2$ (other dimensions are discussed later). In Figs. 3 and 4, we present a plot of $D_{N_0}(N)$ as a function of $N$ for square and triangular lattices, respectively. For both cases, the same picture results, a fact that stresses the universality property of LFD. The three ranges discussed at the end of Sec. II are seen in the figures. As $N_0$ increases, there is a wider region in which $D_{N_0}(N)$ is nearly constant (the main range). The constant value of LFD in the main range is defined as the FD of the chain. When $N \simeq N_0$ (the end-to-end range), there is an abrupt increase in LFD, as proposed earlier. Finally, the geometrical range, $N \sim 1$, is displayed in Fig. 5 on an enlarged scale for SAW's on triangular and square planar lattices. For $N \lesssim 10$, the LFD is different, as expected, but as $N$ increases, the LFD coincides for both types of lattices.

In Fig. 6, it is shown how $D_{N_0}(N)$ scales as a function of $x=N/N_0$. The fact that for different $N_0$ the results fall on nearly the same curve confirms (12) and (14).

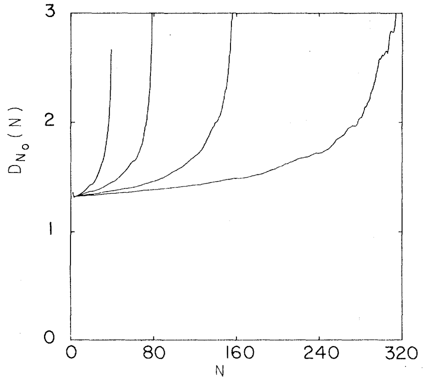

FIG. 3. Plot of the LFD $D_{N_0}(N)$ as a function of $N$ for SAW's traced on a square two-dimensional lattice, for $N_0=40,80,160,320$.

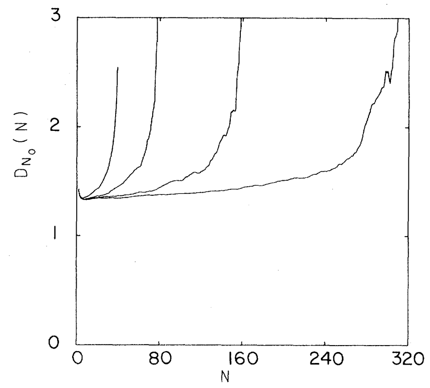

FIG. 4. Plot of the LFD $D_{N_0}(N)$ as a function of $N$ for SAW's traced on a triangular two-dimensional lattice for $N_0=40,80,160,320$.

The FD is measured according to (4) by plotting $\ln N$ as a function of $\ln(\langle R_N^2 \rangle_{N_0})^{1/2}$. The slope at each point on the resulting curve is the LFD and the part corresponding to the main range is a straight line. We calculated a best fit for this part and obtained $D=1.36 \pm 0.04$.

The difference between FD and the usual end-to-end exponent $\nu$ can be clearly understood from Fig. 7. In this figure, we plot $\ln N$ as a function of $\ln(\langle R_N^2 \rangle_{N_0})^{1/2}$ for different values of $N_0$. FD is obtained from internal distances as described above, whereas the end-to-end exponent $\nu$ is obtained from the slope of the line connecting the end points of the curves (the broken line). Thus $\nu$, in contrast to

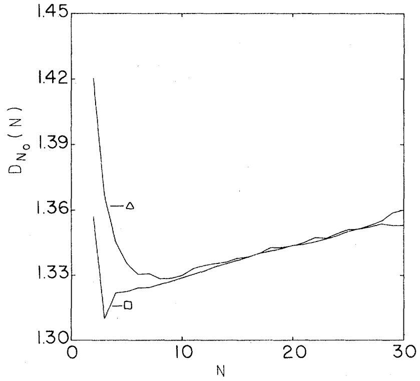

FIG. 5. Geometrical range for SAWs traced on two-dimensional square and triangular lattices.

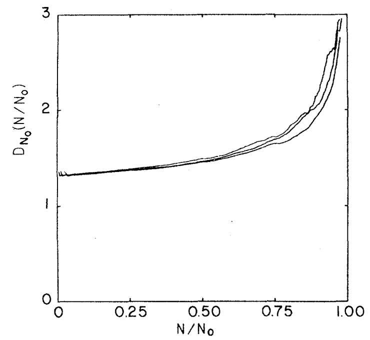

FIG. 6. Plot of $D_{N_0}(N)$ as a function of $x = N/N_0$ for 10 000 SAW's on a two-dimensional square lattice for $N_0 = 80$, 160, and 320.

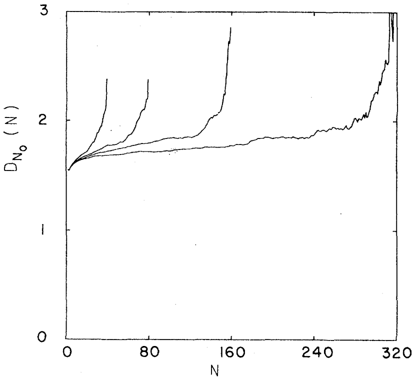

FIG. 8. Plot of the LFD $D_{N_0}(N)$ as a function of $N$ for SAW's traced on a cubic lattice for $N_0 = 40, 80, 160, 320$.

the FD, does not represent an internal self-similarity. However, the numerical value obtained for $1/D$ equals, to within numerical uncertainty, that of the usually measured end-to-end exponent $\nu$, in agreement with our theoretical prediction.

The case of $d = 3$ is not much different from that of $d = 2$. In Fig. 8, we present plots of the LFD for SAW's in a cubic lattice as a function of $N$ for different values of $N_0$. The picture is similar to Fig. 3. As $N_0$ increases, there is a wider region for which $D_{N_0}(N)$ is nearly constant.

In Fig. 9, we plot $D_{N_0}(N)$ as a function of $N/N_0$ for different values of $N_0$. It seems that LFD does not scale for small values of $x$ as well as it does in the two-dimensional case. However, the deviations from scaling are small and therefore may be neglected in the present discussion.[23] The same analysis for obtaining the FD as described for the two-dimensional case yields for $d = 3$ the value $D = 1.68 \pm 0.04$. This result is in agreement with the value $D = 1.67$, which is obtained when applying our method to the results given by Alexandrowicz.[24] The deviations from scaling are found[25] to be even larger in the case of $d = 4$.

*Fractal dimensionality of a single configuration.* One of the main results of this work is the success in defining and measuring a quantity which is nearly the same for almost *each* of the configurations of a single chain. In Fig. 10, we present a typical single configuration (chosen at random) of a SAW ($N_0 = 400$) traced on a square lattice, as obtained by computer simulation. The LFD of this chain is measured according to (3) and is shown in Fig. 11. It resembles the general picture given in Fig. 3. The fractal dimensionality of a single configuration is

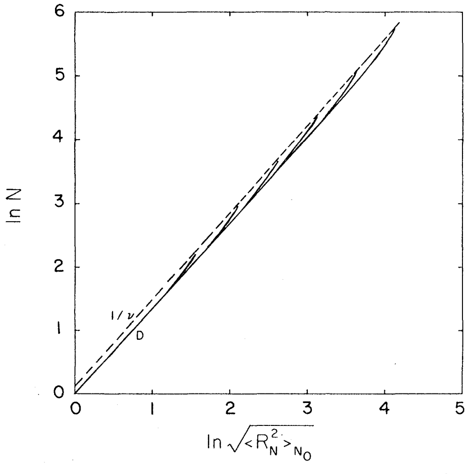

FIG. 7. Plot of $\ln N$ as a function of $\ln(\langle R_N^2 \rangle_{N_0})^{1/2}$ averaged on sets of polymers for several values of $N_0$. The dashed line represents the end-to-end exponent.

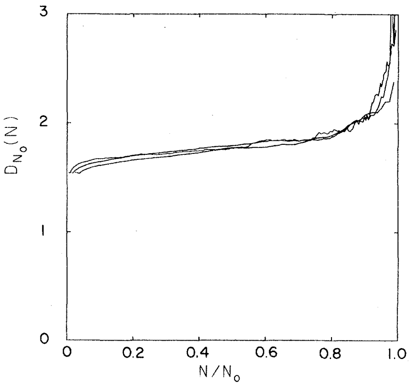

FIG. 9. Plot of $D_{N_0}(N)$ as a function of $x = N/N_0$ for 10 000 SAW's on a three-dimensional cubic ($d = 3$) lattice for $N_0 = 80$, 160, and 320.

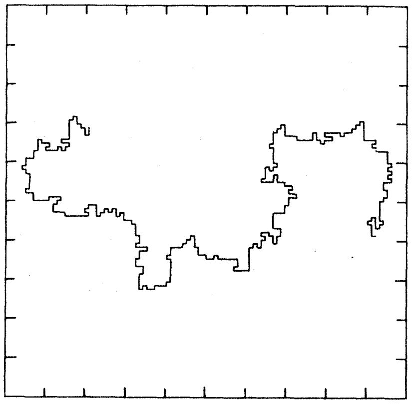

FIG. 10. Example of a single configuration of a polymer ($N_0=400$) as simulated by the computer.

obtained from a plot of $\ln N$ as a function of $\ln(\langle R_N^2 \rangle_{N_0})^{1/2}$ as described above. Using this method, we have measured the FD of single configurations of chains for different values of $N_0$. For each value of $N_0$, we calculated the average FD (overall configurations with the same $N_0$) and the fluctuations from this average. These fluctuations vanish as $N_0$ increases, as shown in Fig. 12. Thus, we can obtain the FD characteristic of an ensemble from a single configuration of a chain, provided that it is long enough.

## V. SUMMARY AND CONCLUSIONS

Polymer chains exhibit an internal statistical self-similarity, a fact that enables us to use the FD as a parameter characterizing a single configuration. The FD behaves like a macroscopic quantity in the sense that its uncertainty vanishes as $N_0$ increases. By contrast, the end-to-end distance behaves like a microscopic quantity, since its relative fluctuations remain finite even in the thermodynamic limit $N_0 \rightarrow \infty$. The reason for the special behavior of FD is that FD is a measure of the degree of winding of the chain for most lengths of scale.

We have shown that there is a direct relation between FD and the end-to-end exponent $\nu$. It is well known from the analogy of SAW's to the $n=0$ vector model[1,26,27] of a ferromagnet that there exist corrections to scaling[28] related to the exponent $\nu$. Indeed, a more detailed analysis of SAW's using the concept of LFD would permit one to treat these corrections.[29]

## ACKNOWLEDGMENTS

The authors wish to thank Professor C. Domb, Professor M. Luban, Professor B. B. Mandelbrot, Professor Z. Alexandrowicz, Dr. M. Lax, and Dr. C. Brender for stimulating discussions and I. Dayan, J. Hashkes, and S. Simhon for valuable assistance in the computer programming.

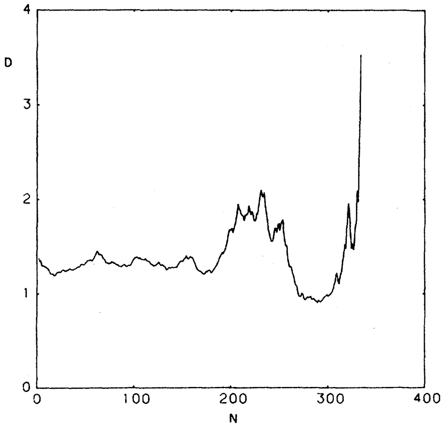

FIG. 11. The LFD of the configuration shown in Fig. 10.

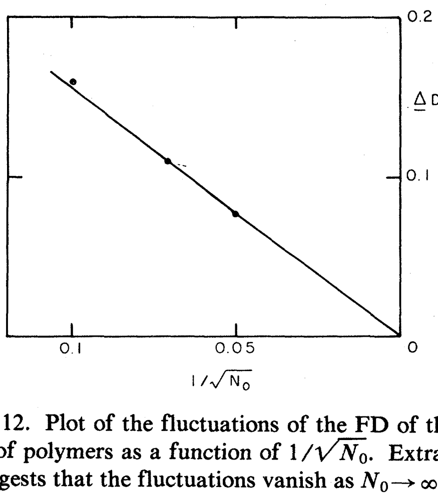

FIG. 12. Plot of the fluctuations of the FD of the ensemble of polymers as a function of $1/\sqrt{N_0}$. Extrapolation suggests that the fluctuations vanish as $N_0 \rightarrow \infty$.

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