"True" self-avoiding walk in one dimension

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The "true" self-avoiding walk in one dimension is studied via extensive Monte Carlo simulations. For any finite and nonzero value of the repulsion parameter g, the asymptotic behavior of the end-to-end distance is characterized by a universal exponent $\nu = 0.67 \pm 0.01$, in close agreement with the value $\nu = \frac{2}{3}$ recently predicted by one of us (L.P.).

It has been common in the last years to identify the problem of the self-repelling polymer chain (SRC) with the expression "self-avoiding walk."[1] Only recently, Amit, Parisi, and Peliti[2] have shown that the problem of a traveler who steps randomly, but tries to avoid places which he has already visited, is actually different from the SRC. They call this problem the "true" self-avoiding walk (TSAW) and show that the upper critical dimensionality (d_c) of such a walk is 2, while for the SRC it is known to be 4. They use renormalization methods to calculate logarithmic corrections to the ordinary random-walk behavior in two-dimensions. This approach has been implemented by Obukov and Peliti[3] who, in addition, construct an ϵ expansion for this problem. One of us (L.P.) has then formulated a simple self-consistent approach that gives, for a TSAW of N steps,[4]

$$\langle x^2 \rangle^{1/2} \simeq N^{\nu} \ , \tag{1}$$

$$\nu = \begin{cases} \frac{1}{2} \text{ for } d \geq d_c = 2 \ , \\ 2/(2+d) \text{ for } d < 2 \ . \end{cases} \tag{2}$$

Here x is the end-to-end distance of the walk and d is the space dimensionality. This result correctly reproduces $d_c = 2$ in agreement with the renormalization analysis, but also gives rise to a prediction for the nonclassical values of ν for dimensions $d < 2$. Of particular interest is the result of $\nu = \frac{2}{3}$ for one dimension, which is quite surprising in view of the fact that the self-repelling chain problem is essentially trivial in one dimension and gives rise to $\nu = 1$. Since the TSAW for $d = 1$ is probably the simplest example of a non-Markovian dynamics with infinitely long memory, we decided to clarify the situation by means of extensive Monte Carlo simulations. It is the purpose of this paper to report these numerical results that give strong support to the predicted exponent of $\nu = \frac{2}{3}$.

The TSAW in one dimension corresponds to a traveler that can move to one of the two nearest neighbors of the site he is at. The probability to move to a site i depends on the number of times, n_i, this site has already been visited and is given by

$$p_i = \frac{e^{-gn_i}}{\sum_{i=1}^{2} e^{-gn_i}} \ . \tag{3}$$

The parameter $g\,(>0)$ measures the intensity with which the path avoids itself. At first sight one may think that in the limit of large g ($g \to \infty$) the traveler always moves in the same direction, giving rise to $\nu = 1$ as for the SRC problem. This is actually *not* true. For any finite value of g (however large) the path will make several consecutive steps in a given direction, but after a large enough number of steps there will be a finite probability for the traveler to go back all the way in the opposite direction for a comparable number of steps. For larger and larger values of g one has to wait longer and longer before the path folds back on itself, but this will always happen. The asymptotic dynamics is therefore highly nontrivial and the exponent can deviate from $\nu = 1$.

According to the self-consistent construction of Ref. 4, a traveler after a certain number of steps has for the next step a probability p_{out} to move away from the origin (starting point) and a probability p_{in} to go toward the origin. Their difference is linked to the gradient of the density of occupation of the various sites

$$\delta p = p_{\text{out}} - p_{\text{in}} \sim -\frac{d\rho(x)}{dx} \ , \tag{4}$$

where it is assumed that for large N the occupancies n_i can be replaced by the smooth (differentiable) function $\rho(x)$. If this assumption is correct, it follows from scaling concepts that $\nu = 2/(2+d)$, and therefore $\nu = \frac{2}{3}$ for $d = 1$ (Ref. 4) *independent of the value of g*. If in one dimension the path would proceed just in one direction the above assumption would be incorrect because $\rho(x)$ would be a step function. As discussed before, however, the situation is actually more complicated because that path always folds back on itself so it is possible that $\rho(x)$ is finally a smooth function and our assumption therefore correct.

Motivated by these questions we have performed Monte Carlo simulations of the dynamics defined by Eq. (3), keeping track of the total number of visits to every site n_i. In Fig. 1 we report the results for three values of the repulsion parameter: $g = 3$, $g = 1$, and $g = 0.1$, corresponding, respectively, to strong, intermediate, and weak repulsion. Each set of data points corresponds to an averge over 1000 Monte Carlo runs of walks up to $N = 10\,000$ steps. It is remarkable to observe that: (i) The initial slopes are quite different, but for large values of N the three slopes become very similar, independent of the value of g. (ii) This asymptotic slope appears to converge to the value $\nu = \frac{2}{3}$,

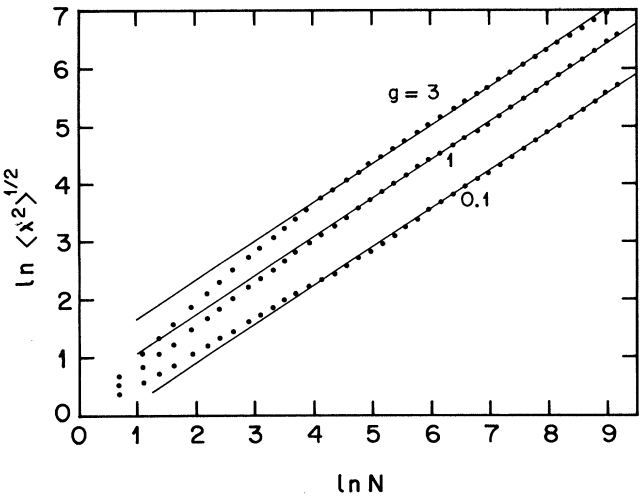

FIG. 1. Monte Carlo simulations of the TSAW for different values of the repulsion parameter g corresponding to strong ($g=3$), intermediate ($g=1$), and weak ($g=0.1$) repulsion. Each set of data is the average over 1000 Monte Carlo runs, each up to 10 000 steps (the error bars in the data are of the order of the size of the dots). Different initial slopes merge into the "universal" slope $\frac{2}{3}$ (indicated by the continuous lines) for large N, independent of the value of g.

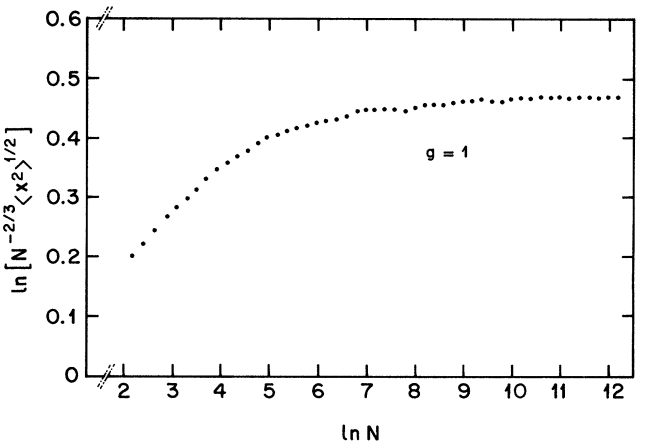

FIG. 2. Extended Monte Carlo simulation (10 000 Monte Carlo runs, each up to 200 000 steps) for $g=1$ plotted in such a way as to enhance eventual deviations from the slope $\frac{2}{3}$. Flat behavior at large N gives strong support for $\nu=\frac{2}{3}$ with an estimated error bar of the order of 1%.

represented by the three continuous lines drawn for comparison. Note that for large g the asymptotic regime is only reached for very large values of N. In addition, the approach to the asymptotic behavior can have an oscillatory part which would be more pronounced for larger values of g. This could be the origin of the somewhat smaller apparent slope of the case $g=3$ in Fig. 1.

In order to obtain a more accurate estimate of the asymptotic exponent, ν, we have performed a much more extended analysis of the case $g=1$. In Fig. 2 we report data corresponding to 10 000 Monte Carlo runs each of 200 000 steps. Without particular program optimization this calculation took about 110 h of CPU (central processing unit) time on a Digital Equipment Corporation VAX-11/780 computer. The data are plotted in such a way as to enhance deviations from the $\frac{2}{3}$ slope. If the real exponent is $\frac{2}{3}$ the data of Fig. 2 should become flat for large N. This is indeed the trend shown by the numerical results, and it should be noted that even a difference of only 1% in the slope is well visible in a plot as that in Fig. 2. Clearly, it is a delicate issue to make statements about asymptotic exponents from numerical results, but we can safely say that our data provide strong support to the value $\frac{2}{3}$, and if the real exponent is actually different from this value the difference should not exceed 1%. In this connection it may be interesting to note that, for example, the Flory exponent for the three-dimensional self-repelling chain $\nu_F=\frac{3}{5}$ seems to be incorrect just by about 1%.[5]

We can now turn back to the self-consistent construction of Ref. 4 and be more confident about the assumptions that were made. In particular, we assumed that the occupation density of the sites $\rho(x)$ can be represented by a continuous differentiable function. Following arguments of the type of Ref. 4 we can now show that this function also satisfies scaling and universality properties. We introduce

$$R=\lambda_g N^{2/3} , \tag{5}$$

where λ_g is a prefactor which depends on the repulsion parameter g. For the end-to-end probability distribution we can write within scaling concepts[1,4]

$$P_N^{(g)}(x)=\frac{1}{R} f_p(x/R) , \tag{6}$$

and the occupation density (that here we normalize to unity) is then given by[4]

$$\rho_N^{(g)}(x)=\frac{1}{N}\int_0^N dn P_n^{(g)}(x)=\frac{1}{R} h(x/R) , \tag{7}$$

where

$$h(z)=\tfrac{3}{2} z^{1/2}\int_z^\infty dy\, y^{-3/2} f_p(y) \tag{8}$$

is a universal function independent of N and g. Equation (7) therefore implies that

$$\frac{1}{\rho_N^{(g)}(0)}\rho_N^{(g)}\left[\frac{z}{\rho_N^{(g)}(0)}\right]=\frac{1}{h(0)}h\left[\frac{z}{h(0)}\right] \tag{9}$$

should be independent of N and g. This result is particularly useful for analyzing numerical data. In Fig. 3 we report Monte Carlo calculations of $\rho_N^{(g)}(x)$ for different values of g. Each set of data corresponds to 10 000 Monte Carlo runs of $N=1000$ steps. The universality property expressed by Eq. (9) is well confirmed by the numerical data. A further check of the scaling and universality properties can be made by considering that asympotically

$$\langle x^2\rangle^{1/2} \propto R=\lambda_g N^{2/3} . \tag{10}$$

By analyzing the data of Fig. 1 we then obtain

$$\begin{aligned} &\frac{\lambda_3}{\lambda_1}=1.8\pm 0.1 , \\ &\frac{\lambda_1}{\lambda_{0.1}}=2.3\pm 0.1 . \end{aligned} \tag{11}$$

On the other hand, using Eq. (7) we can derive the relation

$$\frac{\lambda_g}{\lambda_{g'}} = \frac{\rho_N^{(g')}(0)}{\rho_N^{(g)}(0)} , \tag{12}$$

which links λ_g to the central value of the occupation density. Using Eq. (12), the data of Fig. 3 lead to

$$\frac{\lambda_3}{\lambda_1} = 1.7 \pm 0.1 ,$$
$$\frac{\lambda_1}{\lambda_{0.1}} = 2.4 \pm 0.1 , \tag{13}$$

in good agreement with the values of Eq. (11) obtained directly from Fig. 1.

In summary, we have presented Monte Carlo simulations for the TSAW in one dimension. This dynamical process with infinitely long memory manifests a new type of critical behavior with a universal exponent (independent on the repulsion parameter g) equal to extremely close to the predicted value $\nu = \frac{2}{3}$. In view of the validity of the relation $\nu = 2/(2+d)$ (derived in Ref. 4) both for $d = 2$ ($\nu = \frac{1}{2}$) and for $d = 1$ ($\nu = \frac{2}{3}$) it is now of great interest to check the intermediate region $1 < d < 2$ for systems with fractal dimensionality. Work in this direction is in progress.[6]

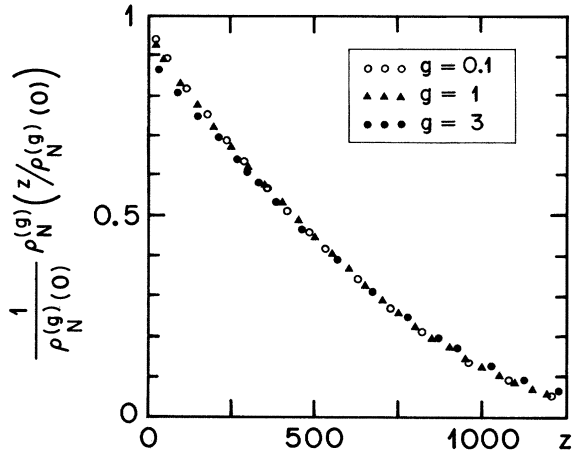

FIG. 3. Universal behavior of the occupation density of the lattice sites. Each set of data for a given value of g corresponds to an average over 10 000 Monte Carlo runs, each consisting of $N = 1000$ steps. With occupation we denote here the total number of times a given site has been visited.

ACKNOWLEDGMENTS

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