Critical dimensionality and exponent of the "true" self-avoiding walk

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(Received 18 February 1983)

A simple, self-consistent method is formulated to compute the critical dimensionality d_c and the exponent ν of the "true" self-avoiding walk as defined by Amit *et al.* There results $d_c = 2$, in agreement with the renormalization analysis. In addition, we obtain $\nu = 2/(2+d)$ for $d < 2$. The present method applied to the problem of the self-repelling chain reproduces the Flory exponent.

Recently Amit, Parisi, and Peliti[1] have introduced the "true" self-avoiding walk (TSAW) as the problem of a traveller who steps randomly but tries to avoid places he has already visited. They show that this problem is different from that of the self-repelling chain (SRC). In particular, they find that the upper critical dimensionality (d_c) of such a walk is two, while for the SRC it is known to be four.[2] They also study the logarithmic corrections with the use of renormalization methods. These methods are then implemented in Ref. 3.

We discuss here a simple self-consistent approach that gives, for a TSAW of N steps,

$$R = \langle |r|^2 \rangle^{1/2} \simeq N^{\nu} , \tag{1}$$

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

Here r is the end-to-end distance of the walk and d is the space dimension. This result correctly reproduces the upper critical dimensionality $d_c = 2$ but also gives rise to a prediction for the nonclassical values of ν in the case of dimensions $d < 2$. The same method applied to the SRC reproduces the Flory exponent: $\nu_F = 3/(2+d)$ for $d \leq 4$ and $\nu_F = \frac{1}{2}$ for $d > 4$.

The TSAW is defined in Ref. 1 as follows: In a d-dimensional lattice a traveller may move to one of the K nearest neighbors of the site he is at. The probability of moving to a site i depends on the number of times n_i this site has already been visited and is given by

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

The sum runs over all K nearest neighbors and g measures the intensity with which the walk avoids itself. For the self-repelling chain instead the relative probability of a given configuration depends only on the number of self-intersections. As discussed in Ref. 1 the two statistical problems are different. This depends on the fact that the stepping recipe given by Eq. (3) has no strategy for avoiding embarrassing situations such as the one shown in Fig. 1(a) corresponding to a two-dimensional space. On the other hand, because of the normalization property $\sum_{i=1}^{K} p_i = 1$ (the traveller must move) Eq. (3) also allows for escape out of the central point of Fig. 1(a) at the price of creating a self-intersection [Fig. 1(b)]. Since Eq. (3) does not make any effective attempt to minimize the number of self-intersections it is clear that its statistical properties will be different from those of the SRC. Equation (3) provides, in fact, just a *local* criterion to avoid crowded areas similar to the driving force of a diffusion problem.

In order to make use of this fact it is useful to consider the problem of the standard random walk (in a given direction) with asymmetric jump probabilities. The probability distribution for the end-to-end distance after N steps is

$$P_N(r) = \frac{1}{\sqrt{2\pi N}} \exp\left[-\frac{(r-r_0)^2}{2N} \right] , \tag{4}$$

$$r_0 = N(p_+ - p_-) = N\delta p . \tag{5}$$

Here r is the distance from the origin (initial point) and $\delta p = p_+ - p_-$ represents the difference between the probabilities of moving in the positive or negative

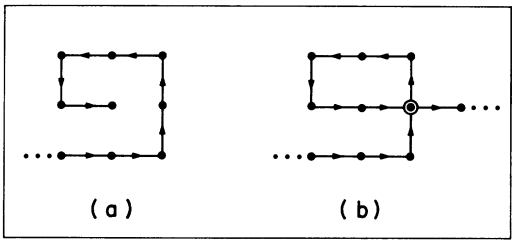

FIG. 1. (a) Example of a path for a two-dimensional walk that leads to a situation without a simple way out. (b) The stepping recipe of Eq. (3) always allows for getting out at the price of creating a self-intersection.

directions. Without considering geometrical details one can look at Eqs. (4) and (5) as the radial portion of the walk. In this case δp is the difference between the probability to go far from the center (initial point) or toward the center. We now assume that Eq. (3) effectively couples δp to the local density gradient (see Fig. 2)

$$\delta p = p_{\text{out}} - p_{\text{in}} \sim -\left.\frac{d\rho(r)}{dr}\right|_R , \tag{6}$$

where $\rho(r)$ represents the probability that a site at distance r from the origin has been visited. $\rho(r) = \langle n_i \rangle_{|\vec{r}_i| = r}$, where the average is on all the sites at distance r. We can then relate the density $\rho(r)$ to the end-to-end probability distribution $P_N(r)$ by the convolution over paths of all lengths $\tilde{N}$ up to N:

$$\rho(r) = \int_0^N P_{\tilde{N}}(r)\, d\tilde{N} . \tag{7}$$

Within scaling concepts we can write, for a generalized random walk[2] (also self-avoiding),

$$P_N(r) = \frac{1}{R^d} f_p(r/R) , \tag{8}$$

$$f_p(x) = f_1(x) e^{(-x^{\delta})}, \quad \delta = (1-\nu)^{-1} , \tag{9}$$

where $R \sim N^{\nu}$ is defined in Eq. (1) and f_1 is a smooth function for large x. From Eq. (7) we then have

$$\rho(r) \simeq \int_0^N \tilde{N}^{-\nu d} f_p(r/\tilde{N}^{\nu})\, d\tilde{N} , \tag{10}$$

$$\frac{d\rho(r)}{dr} \simeq \int_0^N \tilde{N}^{-\nu d} \left[\frac{d}{dr} f_p(r/\tilde{N}^{\nu})\right] d\tilde{N} . \tag{11}$$

Introducing

$$x = \frac{r}{\tilde{N}^{\nu}} , \tag{12}$$

$$\frac{dx}{dr} = \frac{1}{\tilde{N}^{\nu}} , \tag{13}$$

$$y = \frac{\tilde{N}}{N} , \tag{14}$$

$$x_0 = \frac{R}{\tilde{N}^{\nu}} = y^{-\nu} , \tag{15}$$

we obtain

$$\left.\frac{d\rho(r)}{dr}\right|_R = \int_0^N \tilde{N}^{-\nu(d+1)} \left[\frac{d}{dx} f_p(x)\right]_{x_0} d\tilde{N}$$

$$= N^{1-\nu(d+1)} \left[\int_0^1 y^{-\nu(d+1)} g(y^{-\nu})\, dy\right] , \tag{16}$$

where

$$g(y^{-\nu}) = g(x_0) = \left.\frac{d}{dx} f_p(x)\right|_{x_0} . \tag{17}$$

Now comes the construction of a self-consistency condition. After a walk of N steps we perform ΔN additional steps. The change in R is from Eq. (1):

$$\Delta R \sim \frac{dR}{dN} \Delta N \sim N^{(\nu-1)} \Delta N . \tag{18}$$

This has to be compatible (same behavior with respect to the power of N) with the extra contribution to R due to the asymmetry δp [see Eqs. (5), (6), and (16)]:

$$\Delta R_a \sim \delta p \Delta N \sim N^{1-\nu(d+1)} \Delta N , \tag{19}$$

this, of course, only if ΔR_a is larger than the purely Gaussian contribution ΔR_g that can be obtained from Eq. (4) with $\delta p = 0$:

$$\Delta R_g \sim N^{-1/2} \Delta N . \tag{20}$$

We have then two cases:

$$\text{(a)} \quad -\tfrac{1}{2} > 1 - \nu(d+1) ;$$

in this case $-\frac{1}{2} = \nu - 1$ leads to the classical exponent $\nu = \frac{1}{2}$.

$$\text{(b)} \quad -\tfrac{1}{2} < 1 - \nu(d+1) ;$$

the condition is then $1 - \nu(d+1) = \nu - 1$ that leads to $\nu = 2/(2+d)$.

Reversing these results we see that (a) applies for $d \geq 2$ and (b) for $d \leq 2$. The critical dimensionality is then

$$d_c = 2 \tag{21}$$

and

$$\nu = 2/(2+d) \tag{22}$$

for $d < 2$.

The value of d_c agrees with the renormalization analysis.[1] The case $d = 1$ for which we predict $\nu = \frac{2}{3}$ should be considered with caution. Our method is based on a relation between δp and the gradient of

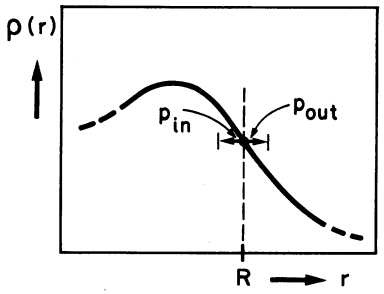

FIG. 2. Schematic picture of the radial density of the sites that have been already visited. R indicates the average end-to-end distance. p_{in} and p_{out} indicate, respectively, the probability that the next step will go toward or far from the center.

$\rho(r)$. In the limit $g \to \infty$ in one dimension $\rho(r)$ is a step function and our method does not apply. The problem is in this case trivial and $\nu = 1$. On the other hand, for any finite value of g the path can go back on itself and it is plausible that $\rho(r)$ is again analytic. In this case our result $\nu = \frac{2}{3}$ should apply. Preliminary computer simulations actually support this value of ν for any finite value of g.[4] At the critical dimensionality $d_c = 2$ one expects logarithmic corrections to the classical exponent behavior. These corrections have been studied in Refs. 1 and 3. In Ref. 3 the behavior of the exponent for small deviations from $d_c = 2$ (ϵ expansion) has also been studied. The results of this expansion are not in agreement with our formula for ν [Eq. (22)]. With respect to this point one should keep in mind that the Flory exponent $\nu_F = 3/(2+d)$ is virtually exact for the self-repelling chain but it is also in disagreement with the corresponding ϵ expansion.[5]

We now sketch how the method discussed in the present paper can be applied to the self-repelling chain to recover the Flory exponent. For the TSAW the "driving force" of the asymmetry $\delta\rho$ is the *local* density gradient. In the case of the SRC we would instead like to minimize the *total* number of self-intersections. A chain of length N has a size of the order of the average end-to-end distance[2] $R \sim N^{\nu}$ and it occupies a volume of the order of $V \sim R^d$. The average density within such a volume is

$$\bar{\rho} \sim \frac{N}{V} = NR^{-d} , \tag{23}$$

and the total number of self-intersections is of the order of

$$N_s \sim N\bar{\rho} = N^2 R^{-d} . \tag{24}$$

Considering one end of the chain, this is at a distance of order R from the other end (origin). If we add an extra element to the chain in the out-going radial direction the end-to-end distance increases by an amount ΔR. The opposite happens for the in-going direction. The difference between the *total* number of self-intersections corresponding to the two cases is

$$\delta N_s \sim N^2(R+\Delta R)^{-d} - N^2(R-\Delta R)^{-d} \sim N^2 R^{-(d+1)} \Delta R . \tag{25}$$

We assume this difference to be the new "driving force" for the probability asymmetry

$$\delta p \sim \delta N_s \sim N^{2-\nu(d+1)} . \tag{26}$$

Inserting Eq. (26) into Eq. (19) and using the previous arguments we directly obtain, for the exponent ν.

$$\nu = \frac{3}{(2+d)} , \tag{27}$$

that is, the Flory result.

ACKNOWLEDGMENTS

It is a pleasure to thank Luca Peliti for interesting discussions and correspondence. The author is also grateful to David Nelson for the hospitality at Harvard University, supported by Grant No. DMR82-07431, where this work was completed.

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[5] The author is grateful to L. Peliti for a discussion about this point.