Asymptotic behavior of the "true" self-avoiding walk

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The "true" self-avoiding random walk is defined as the statistical problem of a traveler who steps randomly, but tries to avoid places he has already visited. We show that this problem is different from the problem of a self-repelling chain (polymer problem). Most striking is perhaps the fact that the upper critical dimensionality of such a walk is 2. Renormalization-group theory is applied to compute logarithmic corrections to ordinary random-walk behavior in two dimensions. The theoretical predictions are confirmed by computer simulations.

I. INTRODUCTION

Recent literature has created a situation in which the expression "self-avoiding random walk" is considered synonymous with the problem of polymer statistics (chain with excluded volume). This is due to the fact that this expression has been used uncritically in a number of bona fide studies of polymer statistics, $1-4$ the underlying implicit assumption being that the two problems are very intimately related, if not identical.

A natural definition of a self-avoiding random walk may be a walk in which the traveler tends to make random steps, but avoids regions of space which he has already visited. In the statistics of a self-repelling chain one considers instead all possible configurations of a chain of a given length, giving them as a weight a Boltzmann factor with a potential energy proportional to the number of self-'intersections. (More precise definitions are given in the next section.) We wish to point out in this paper that, contrary to the common belief, these two problems are different and belong to different universality classes; in particular, their upper critical dimensionalities are different. Since the statistics of the self-repelling chain is equivalent to the $n \rightarrow 0$ limit of a $O(n)$ symmetric ϕ^4 field theory,^{4,5} the upper critical dimensionality of this problem is 4. We will show that it is 2 for the self-avoiding walk.

The self-avoiding random-walk problem is defined in Sec. II where it is contrasted with the selfrepelling chain problem. A heuristic identification of the upper critical dimensionality of the selfavoiding walk $(d_c = 2)$ and its comparison with the Flory result for the self-repelling chain $(d_c = 4)$ are expounded in Sec. III.

A continuum approximation to the self-avoiding walk is introduced in Sec. IV and analyzed in the following sections. In Sec. V the relevant parameters are identified on the basis of dimensional analysis; in Secs. VI and VII relevant Ward identities are investigated. A perturbation expansion is introduced in Sec. VIII, where the upper critical dimensionality is derived from a Ginzburg-type criterion. A renormalization scheme for this expansion is proposed and applied in Secs. IX and X to the determination of the asymptotic behavior of the walk in two dimensions. These results are compared with computer simulations in the last section. Appendixes A and B contain some details of the computation.

II. DEFINITIONS

We define the "true" self-avoiding walk as follows: Suppose that the walk takes place on a simple cubic, d-dimensional lattice, with the traveler starting from the origin at step zero. At any step the traveler may move to any of the 2d nearest neigh-

bors of the lattice site he is at. The probability of stepping to site i depends on the number of times n_i this site has already been visited and is given by

$$
p_i = \exp(-gn_i) / \left(\sum_{i=1}^{2d} e^{-gn_i}\right), \qquad (2.1)
$$

where the sum runs over all $2d$ nearest neighbors of the current position of the traveler, and g is a positive parameter which measures the intensity with which the walk avoids itself.

A few comments should be made concerning this apparently simple-looking formula. (a) The sum over i of p_i is equal to 1, meaning that the traveler never stays at the same point. (b) Each time a step is taken the n_i are modified. (c) The p_i 's depend not only on the point where the traveler is, but on the entire past history of the walk. The probability of a given walk of N steps is the product of the p_i 's for each step. It does not just depend on the configuration of the walk; it also depends on where the starting point is (see the example at the end of the section}.

In contrast, the relative probability of a given configuration of a self-repelling chain depends only on the distribution of n_i 's in that configuration. It is simply given by¹

$$
P \propto \exp \left[-g' \sum_i n_i^2\right],
$$

where *i* runs over all the lattice.

To see the difference between the two problems more concretely we consider short walks, of N steps, in two dimensions in the limit $g \rightarrow \infty$. In the selfrepelling chain problem, only configurations which do not intersect themselves are allowed in this limit. Allowed configurations of equal length have equal probabilities.² (See also note added in proof.)

Self-avoiding configurations with their corresponding statistical weights are shown in Fig. 1. Only a quarter of the configurations are shown, since the others might be obtained by a rotation about the origin. Up to $N=3$ the number of alabout the origin. Up to $N=3$ the number of allowed configurations (up to rotations) is $3^{(N-1)}$ for either problem, each configuration having weight either problem, each configuration having weight
 $3^{-(N-1)}$. The difference appears at $N=4$. The two diagrams marked with a star at $N=3$ generate only two self-avoiding configurations of the next step, while all other diagrams generate three configurations each. This is shown in Fig. 2, which shows the fate of the upper five diagrams of the $N = 3$ column of Fig. 1. The total number of configurations is therefore (up to rotations) $2 \times 2 + 3 \times 7 = 25$. In the self-repelling chain problem each such configuration has the same weight, namely $\frac{1}{25}$. In the self-

FIG. 1. Self-avoiding walks (up to rotations) with their statistical weights for $N = 1, 2, 3$.

avoiding walk problem the "starred" configurations have a weight $1/(2)(9) = \frac{1}{18}$, while the remaining di-
agrams have a weight $1/(3)(9) = \frac{1}{27}$. One sees, therefore, that the statistics of the two problems are already different at $N = 4$.

One may also remark that the first diagram on the left of the first row of Fig. 2 differs from the rightmost diagram in the third row of that figure only by a rotation and by the position of the starting point. Their weights are different in the selfavoiding walk problem. Things go in the same way

FIG. 2. Self-avoiding walks generated by the upper five walks of the $N = 3$ case (Fig. 1) with their statistical weights.

for the second diagram of the first row, and the first diagram of the fourth row.

The difference which appears in this example is purely a difference of statistics. There is, of course, another difference between the two problems in the $g \rightarrow \infty$ limit, namely, some self-intersecting configurations are allowed for the self-avoiding walk whereas they are not for the self-repelling chain. In fact, since the traveler must move at each step, if he finds himself at a site whose neighbors have all been already visited, he will have to move to one of these sites at the next step. However, in the example we have shown that such a situation does not arise.

III. HEURISTIC CONSIDERATIONS ON THE ASYMPTOTIC BEHAVIOR

We now estimate the asymptotic behavior of R_N^2 for large N . If the walk were not self-avoiding (free), one would, of course, have $R_N^2 \propto N$. The number $S(N)$ of self-intersections of such a walk is of order N^2/R_N^d . Hence for a free random walk $S(N) \propto N^{2-d/2}$. In the self-avoiding walk we may imagine that the traveler makes a detour each time he would have crossed his steps in a free random walk. This operation is likely to increase R_N^2 . We obtain, therefore, the following estimate:

$$
R_N^2 \propto N + \text{const}[S(N)] = N + \text{const}(N^{2-d/2})
$$
. (3.1)

The correction due to the fact that the walk is selfavoiding is asymptotically negligible for $d > 2$ and may alter the asymptotic behavior for $d < 2$. Equation (3.1) gives the correct asymptotic behavior for $d>2$.

For the self-repelling chain R_N^2 may be obtained by the Flory argument.⁶ In order to obtain R_N^2 one looks for the minimum of a generalized free energy

$$
F \propto R_N^2/N + \text{const}(N^2/R_N^d) \;, \tag{3.2}
$$

where the first term is the entropy contribution, while the second term (proportional to the number of self-intersections) is the energy contribution. Thus one arrives at the Flory result $R_N^2 \propto N^{6/(d+2)}$ for $d < 4$. It is clear that the two problems have rather different properties: Deviations from the free case are obtained when $S(N) \propto N^{\alpha}$ with $\alpha > 0$ for the chain problem, while $\alpha > 1$ is needed for the walk.

IV. THE CONTINUUM APPROXIMATION TO THE WALK

At very long times the density of visited points in the lattice approaches a continuous function, with well-defined gradients at every point. In such a situ-

ation the walk can be approximated by a stochastic process of the variable $\mathbf{R}(t)$, which develops, as a function of the time t , in a space of d dimensions according to

$$
\vec{\mathbf{R}}(t) = \vec{\eta}(t) - g \,\vec{\nabla}\rho(\vec{\mathbf{R}}, t) \;, \tag{4.1}
$$

where $\eta(t)$ is a stochastic d-dimensional vector with a Gaussian distribution of width $D⁷$ Namely, the distribution of $\vec{\eta}$ is

$$
P[\eta]d[\eta] \propto \exp\left[-\frac{1}{4D}\int_0^\infty \eta^2(t)dt\right]d[\eta].
$$
\n(4.2)

The density $\rho(x, t)$ varies whenever the walk crosses the point x at time t . Therefore,

$$
\dot{\rho}(\vec{x},t) = \delta(\vec{x} - \vec{R}(t)) \ . \tag{4.3}
$$

Typical initial conditions would be

$$
\rho(\vec{x},0) = 0, \ \vec{R}(0) = 0 \ . \tag{4.4}
$$

When g vanishes (4.1) and (4.2) describe a free random walk. The presence of the interaction term gives preference to the direction in which ρ decreases.

To make contact with the definition of the walk on the lattice, as given in Sec. II, we consider a discretization of the above equations. Making discrete equal-time steps Eqs. (4.1) and (4.2) give the probability for a step ΔR ,

$$
P(\Delta R) \propto \exp[-K(\Delta \vec{R} + g \vec{\nabla} \rho)^2]. \tag{4.5}
$$

 ΔR are steps to nearest-neighbor sites on the lattice; ρ is proportional to an average of *n* over a few sites.

Expanding the square in the exponent we have

$$
P(\Delta R) \propto \exp{-K[(\Delta R)^2 + g^2(\nabla \rho)^2]}
$$

× $\exp(-2Kg\Delta \vec{R}\vec{\nabla}\rho)$. (4.6)

Since $|\Delta R|$ is fixed, the first factor is independent of the step chosen. It is absorbed in the normalization constant. It is the last factor which will discriminate among the different possible steps.

The exponent in this factor— $\Delta \vec{R} \cdot \nabla \rho$ —is proportional to the difference of ρ across the step,

$$
P(\Delta R) \propto \exp[-K'(\rho_{R+\Delta R} - \rho_R)]
$$

$$
\propto \exp(-K'\rho_{R+\Delta R}),
$$

which is related to Eq. (2.1).

V. DIMENSIONAL ANALYSIS

In natural units, ρ and δ in Eq. (4.3) have the same dimensions L^{-d} . Hence there should have been a rate coefficient on the right-hand side of Eq. (4.3) . This coefficient is absorbed into the units of t. If D is chosen to be dimensionless, comparing the dimensions of η in Eqs. (4.1) and (4.2), one finds that

$$
[t] = L^2, \tag{5.1}
$$

as is common in random walks. One is then left with length as the only scale and with onedimensional parameter g. In fact,

$$
[g] = L^{d-2} \tag{5.2}
$$

Already at this level the special role of $d=2$ is transpiring. It is there that the coupling constant becomes dimensionless. For $d < 2$, g is relevant, and it is irrelevant for $d > 2$. This parlance is appropriate, of course, to a local field theory. Here, since we have not succeeded in constructing such a field theory, which generates the averages of the various quantities associated with the walk, it is used somewhat loosely. But, as we shall see, the expansion in powers of g justifies it.

VI. STATISTICAL AVERAGES AND A WARD IDENTITY

The typical quantities one would like to compute in the problem are the time dependence of averages (over η) of quantities such as $R^2(t)$, $R^4(t)$, $\rho(\vec{x}, t)$, etc. For every distribution of the stochastic vector $\vec{\eta}$ we have, from Eq. (4.3), the identity for the spatial Fourier transform of ρ ,

$$
\dot{\rho}(\vec{\mathbf{p}},t) = \exp[-i\vec{\mathbf{p}}\cdot\vec{\mathbf{R}}(T)].
$$
\n(6.1)

This is our basic Ward identity.

From (6.1) one has, for each walk,

$$
[R^{2}(t)]^{n} = (-\vec{\nabla}_{p} \cdot \vec{\nabla}_{p})^{n} \dot{\rho}(\vec{p}, t) |_{p=0}.
$$
 (6.2)

Taking averages on both sides, one finds

$$
G^{(n)}(t) \equiv \langle [R^2(t)]^n \rangle
$$

= $(-\nabla_p^2)^n \langle \dot{\rho}(\vec{p}, t) \rangle |_{p=0}$ (6.3)
 $\equiv (-\nabla_p^2)^n \Delta(\vec{p}, t) |_{p=0},$

in which the angular brackets indicate average over η . We have, in particular,

$$
G^{(0)}(t) = 1 = \Delta(p = 0, t) , \qquad (6.4)
$$

which will prove quite useful below.

VII. DEPENDENCE ON PARAMETERS

A priori Δ and $G^{(n)}$ are functions of the variables \vec{p} and t, as well as of g and D. In fact, Eqs. (4.1) —(4.3) imply that this dependence on g and D is constrained. One has

$$
\Delta(p,t,g,D) = \Delta(pD^{1/2},t,gD^{-2+\epsilon/2},1)
$$

$$
\equiv \overline{\Delta}(pD^{1/2},t,gD^{-2+\epsilon/2}), \qquad (7.1)
$$

where $\epsilon = 2-d$. Using the identity (6.3), one concludes

$$
G^{(n)}(t,g,D) = D^{n}G^{(n)}(t,gD^{2-\epsilon/2},1)
$$

= $D^{n}\overline{G}^{(n)}(t,gD^{-2+\epsilon/2})$. (7.2)

To prove Eq. (7.1) one makes the transformation

$$
\vec{x} \rightarrow D^{1/2}\vec{x} \text{ or } \vec{p} \rightarrow D^{-1/2}\vec{p} ,
$$

$$
\vec{R} \rightarrow D^{1/2}\vec{R} ,
$$

$$
\vec{\eta} \rightarrow D^{1/2}\vec{\eta} ,
$$

$$
\rho \rightarrow D^{-d/2}\rho .
$$

The new variables satisfy Eqs. (4.1)–(4.4) with $D = 1$ and $g \rightarrow gD^{-2+\epsilon/2}$.

From (7.1) and (7.2) it follows that the actual expansion parameter, in a perturbation expansion, is $gD^{-2+\epsilon/2}$ rather than g. These equations will also serve as a starting point for our renormalization procedure, in the absence of an underlying field theory.

VIII. PERTURBATION EXPANSION AND UPPER CRITICAL DIMENSION

Consider Eqs. (4.1) - (4.3) with $D=1$. The formal expansions of $R(t)$ and of $\rho(p, t)$ are

$$
R(t) = R_0(t) + gR_1(t) + g^2R_2(t) + \cdots, \qquad (8.1)
$$

$$
\dot{\rho}(\vec{p},t) = \dot{\rho}_0(\vec{p},t) + g\dot{\rho}_1(\vec{p},t) + g^2\dot{\rho}_2(\vec{p},t) + \cdots
$$
\n(8.2)

Using (6.1) and (8.1) , one has

$$
\dot{\rho}_0(\vec{p},t) = \exp[-i\vec{p}\cdot\vec{R}_0(t)],
$$
\n(8.3a)

$$
\dot{\rho}_1(\vec{p},t) = -i\dot{\rho}_0(\vec{p},t) [\vec{p}\cdot\vec{R}_1(t)] , \qquad (8.3b)
$$

$$
\dot{\rho}_2(\vec{p},t) = -\dot{\rho}_0(\vec{p},t) [\vec{p}\cdot\vec{R}_2(t) + \frac{1}{2}(\vec{p}\cdot\vec{R}_1)^2].
$$
\n(8.3c)

From Eq. (4.2) we have

$$
\vec{\mathbf{R}}_0(t) = \int_0^t \vec{\eta}(t_1) dt_1,
$$
\n(8.4)

$$
\dot{\rho}_0(\vec{p},t) = \exp\left(-i\vec{p}\cdot \int_0^t \vec{\eta}(t_1)dt_1\right).
$$
 (8.5)

Hence

$$
R_0(t) = \int_0^t \eta(t_1) dt_1, \qquad (8.4)
$$

\n
$$
\dot{\rho}_0(\vec{p}, t) = \exp\left[-i\vec{p} \cdot \int_0^t \vec{\eta}(t_1) dt_1\right]. \qquad (8.5)
$$

\n
$$
\Delta_0(\vec{p}, t) = \left\{ \exp\left[-i\vec{p} \cdot \int_0^t \vec{\eta}(t_1)\right] \right\}
$$

\n
$$
= \exp(-p^2 t) \qquad (8.6)
$$

and the Laplace transform with respect to t is

$$
G^{(2)}(t) = 2dt , \t\t(8.8a)
$$

 $\Delta_0(p,\mu) = (p^2+\mu)^{-1}$. (8.7)

$$
G^{(2)}(\mu) = 2d\mu^{-2} \ . \tag{8.8b}
$$

Substituting into (6.3) one finds the familiar result for the free random walk,

$$
\vec{R}_1(t) = -\int_0^t dt_1 \vec{\nabla}\rho_0[\vec{R}_0(t_1), t_1] = \int dq(-i\vec{q}) \int_0^t dt_1 \int_0^{t_1} dt_2 \exp\left[i\vec{q} \cdot \int_{t_2}^{t_1} \vec{\eta}(t_3) dt_3\right]. \tag{8.9}
$$

Substituting (8.5) and (8.9) into (8.3b) and performing the average over η one has

$$
\Delta_1(\vec{p},t) = -\int dq(\vec{p}\cdot\vec{q}) \int_0^t dt_1 \int_0^{t_1} dt_2 \exp[-p^2t_2 - (p-q)^2(t_1-t_2) - p^2(t-t_1)] . \tag{8.10}
$$

The Laplace transform reads

$$
\Delta_1(p,\mu) = -\frac{p^2}{(p^2 + \mu^2)} \int_q (q^2 + \mu)^{-1} . \tag{8.11}
$$

The notation \int_{q} stands for

$$
\int_{q} = \int \left[2^{d-1} \pi^{d/2} \Gamma(\frac{1}{2}d)\right] d^d q \tag{8.12}
$$

(The powers of the proportionality constant are absorbed in a redefinition of the coupling constant.)

Up to first order in g one finds

$$
\Delta(p,\mu) = (p^2 + \mu)^{-1} - g \frac{p^2}{(p^2 + \mu)^2} I(\mu) , \qquad (8.13)
$$

with

$$
I(\mu) = \int_{q}^{1} (q^2 + \mu)^{-1}
$$

= $\epsilon^{-1} \Gamma(1 - \epsilon/2) \Gamma(1 + \epsilon/2) \mu^{-\epsilon/2}$, (8.14)

where the integral was computed by analytic continuation in $d^{8,9}$. The asymptotic behavior at long times is determined by the behavior of $\Delta(p,\mu)$ for small μ . Hence $\epsilon = 0$ —two dimensions—separates between a theory in which $\Delta(p, \mu)$ is asymptotically dominated by the free term $(d > 2, \epsilon < 0)$ and by a nonclassical one ($d < 2$, $\epsilon > 0$).

From (8.13) and (6.2) one has for $G^{(2)}$, or $\langle R^2 \rangle$,

$$
G^{(2)}(\mu) = 2 d\mu^{-2} [1 + 2gI(\mu)] + O(g^2) . \qquad (8.15)
$$

Here again, $G^{(2)}$ behaves asymptotically as μ^{-2} (as $(\mu \rightarrow 0)$ if $d > 2$. The second term dominates for $d < 2$. To reconstitute the dependence on D one employs (7.1}and (7.2).

IX. RENORMALIZATION OF THE THEORY

The perturbation series can be analyzed, as usual, by considering the dependence on the microscopic length—the ultraviolet divergences. The integral I, in (8.13), has just such a divergence for $d > 2$. It is logarithmic at $d=2$, which is represented by the factor of ϵ^{-1} in (8.14). In second order in g one finds both ϵ^{-2} and ϵ^{-1} singularities (see Appendi B).

At first order Eqs. (4.1) and (4.3) give

To follow a well-trodden path we proceed to remove these ultraviolet singularities by a renormalization of the parameters, and then to derive and solve renormalization-group equations. Since, however, we have not been able to find a field theory (or a path-integral formulation) which would generate $G^{(n)}$ and Δ , the procedure we employ is not firmly established to all orders in g. It is, however, explicitly verified to second order, and it is very plausible that it applies at all orders.

In attempting to renormalize Δ we turn to Eq. (7.1). There are three candidates for multiplicative renormalization: the coupling g, the diffusion constant D, and the scale of Δ . Equation (6.4) excludes a change in the scale of Δ . Hence one is left with two parameters to renormalize.

The structure of the second term in (8.13) dictates a renormalization of D , since the only way to eliminate a pole in ϵ with residue $p^2 (Dp^2 + \mu)^{-2}$ is through

$$
\frac{1}{(D+\delta D)p^2+\mu} = \frac{1}{Dp^2+\mu} - \frac{\delta Dp^2}{(Dp^2+\mu)^2} \ .
$$
\n(9.1)

At first order this is all the renormalization that is required. A renormalization of D, making Δ finite to first order, ensures that all $G^{(n)}$'s are finite at this order, due to (6.3).

At second order one finds that g has to be renormalized as well. The explicit calculation of the renormalization at second order is outlined in Appendix B. The procedure chosen is minimal subtraction of the ϵ poles.^{8,9} The results can be summarized as follows:

$$
gD^{-2+\epsilon/2} = \kappa^{\epsilon/2} u Z_u(u) , \qquad (9.2a)
$$

$$
D = D_R Z_D(u) \tag{9.2b}
$$

In these equations u is a dimensionless renormalized coupling constant (see, e.g., the end of Sec. VII). The parameter κ is arbitrary and has the dimensions

of μ (length⁻²); Z_u and Z_p are the renormalization constants. They are given by

$$
Z_n = 1 + \frac{5}{2\epsilon}u , \qquad (9.3a)
$$

$$
Z_D = 1 - \frac{1}{\epsilon} u \tag{9.3b}
$$

The function

$$
\Delta_R(p,\mu,u,D_R,\kappa) = \Delta[p(D_R Z_D)^{1/2},\mu,\kappa^{\epsilon/2}uZ_u,1]
$$
\n(9.4)

is finite, when considered as a power series in u .

X. RENORMALIZATION-GROUP AND ASYMPTOTIC BEHAVIOR

The functions Δ_R and $G_R^{(n)}$ satisfy The functions Δ_R and $G_R^{(n)}$ satisfy
renormalization-group equations (RGE).^{10,11} Typically,

$$
\left[\kappa \frac{\partial}{\partial \kappa} + \beta(u) \frac{\partial}{\partial u} - \gamma(u)\right] G_R^{(2)}(t, u, D_R, \kappa) = 0,
$$
\n(10.1)

with

$$
\beta(u) = \kappa \left. \frac{\partial u}{\partial \kappa} \right|_{\text{bare}} = -\frac{1}{2} \epsilon u + \frac{5}{4} u^2 \;, \tag{10.2}
$$

$$
\gamma(u) = \kappa \frac{\partial}{\partial \kappa} \ln Z_D \bigg|_{\text{bare}} = \frac{1}{2} u \quad . \tag{10.3}
$$

As has been anticipated from the discussion of Secs. VI and VIII, the form of β is qualitatively similar to that of β of a ϕ^4 theory near four dimensions. The long-time behavior of the theory for $\epsilon > 0$ (d < 2) is dominated by a nontrivial, infrared stable fixed point. Above two dimensions it is free, and at $d = 2$ the walk becomes asymptotically free at a logarithmic rate. One can then expect logarithmic corrections to the classical behavior of the walk, which can be computed exactly.

The solution of the RGE for $\epsilon = 0$ has the $\mathrm{form^{12-14}}$

$$
G_R^{(2)}(t) \sim t(\ln t)^{0.4} \left[1 + A \frac{\ln |\ln t|}{\ln t} \right], \quad (10.4)
$$

where the 0.4 is the ratio of the coefficient of u in $\gamma(u)$ to that of u^2 in β . A is a universal constant, which depends on the coefficient of u^3 in β . It has not been computed.

One can also derive an RGE for the fluctuations of $G^{(2)}$ or $\langle R^2 \rangle$. Namely, one can define

$$
Q = (G^{(4)} - G^{(2)2}) / G^{(2)2} . \tag{10.5}
$$

This function is dimensionless and has no anomalous dimensions. Hence asymptotically, it behaves like the free ratio, with $\ln |\ln t| / \ln t$ corrections. The numerical simulation described in the next section is intended to test two predictions: first, the behavior (10.4) without the correction A and second, the behavior of the fluctuations.

XI. COMPUTER SIMULATIONS

In order to test the validity of our predictions [Eq. (10.4)] we have performed computer simulations on ^a square lattice for the self-avoiding walk—as defined in Sec. II—for different values of g . We have generated walks of $N=2^{14}$ steps starting from the center of a 1600×1600 lattice. We have checked that none of our walks hit upon the boundary of the lattice. Our program (which was not particularly optimized) was rather fast, taking about 3 s of central processor unit time of a VAX 71/780 to generate one walk. We have extracted 4000 walks at $g=0.1$, 2000 at $g=0.3$, 5676 at $g=1$, and 300 at $g = \infty$, and we have computed R_N^2 and R_N^4 averaged over the different walks. We would expect, for very large N,

$$
\ln(R_N^2/N) \sim \alpha \ln \ln N \tag{11.1}
$$

However, although our walks are rather long, $\ln \ln N$ only ranges from 0 to 2.3 and it is not easy to extract the value of α with reasonable accuracy. We have therefore preferred to check whether the data are consistent with (10.4), which implies

$$
(R_N^2/N)^{2.5} \sim \ln(N/N_0)
$$

×[1+A ln ln(N/N_0)/ln(N/N_0) ···], (11.2)

where the prefactor N_0 is an increasing function of g. The data for $g=0.1$, 0.3, and 1 are shown in Figs. 3, 4, and 5, respectively. The agreement with theoretical expectations is rather satisfactory. The asymptotic behavior is reached for values of N which increase with g, thus refiecting the increase of No. The data for $g = \infty$ are better fit by $R_N^2/N \propto \ln N$ in the region we have examined. This is likely to be due to a delayed asymptotic behavior, but the possibility of an unstable fixed point at $g = \infty$ cannot be ruled out.

We have tested the asymptotic freedom of the model in the infrared limit by plotting

$$
(2-Q)\ln N = v(N) , \qquad (11.3)
$$

where Q is defined by Eq. (10.5). In an ordinary random walk Q should be equal to 2; one therefore expects $v(N)$ to go to a constant for large N if the distribution of the endpoints of the walk is essentially Gaussian. The results for $g = 1$ are shown in Fig. 6. The errors can be estimated from the scattering

of the points. The data seem to agree with the prediction $Q \rightarrow 2+$ const/lnN.

Note added in proof. Dr. S. Redner has brought to our attention the paper by M. N. Rosenbluth and A. W. Rosenbluth [Phys. Rev. 23, 356 (1955)], in which the difference between random walks and polymers is recognized. The special features of the random walk are then suppressed and polymer statistics are studied.

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APPENDIX A

In order to obtain the term proportional to u^2 in β one must compute the first nontrivial term in Z_u . In order to do this we chose to calculate $G^{(2)}(\mu)$ to order g^2 (two loops). The structure of the series has the general form

$$
G^{(2)}(\mu) = D\mu^{-2} \left[G_0 + \frac{1}{\epsilon} G_1 (g D^{-2+\epsilon/2}) \mu^{-\epsilon/2} + \frac{1}{\epsilon^2} G_2 (g D^{-2+\epsilon/2})^2 \mu^{-\epsilon} \right].
$$
 (A1)

The procedure we adopt is to eliminate, by minimal subtraction, ϵ poles with residue 1 and with residue $1n\mu$. In $(A1)$ we replace D and g by (9.2) and write

$$
Z_u = 1 + a_u u \tag{A2a}
$$

$$
Z_D = 1 + a_D u + b_D u^2 \tag{A2b}
$$

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The result is

$$
G_R^{(2)} = D_R \mu^{-2} [G_0(1 + a_D u + b_D u^2) + \epsilon^{-1} G_1 u (1 + a_u u)(1 + a_D u)(1 - \frac{1}{2} \epsilon \ln \mu / \kappa)
$$

+ $\epsilon^{-2} G_2 u^2 (1 - \epsilon \ln \mu / \kappa)$]
= $D_R \mu^{-2} \{ G_0 + u (G_0 a_D + G_1 \epsilon^{-1}) + u^2 [G_0 b_D + G_1 \epsilon^{-1} (a_u + a_D) + G_2 \epsilon^{-2}]$
- $\left[\frac{1}{2} G_1 (a_u + a_D) + \epsilon^{-1} G_2 \right] \ln \mu / \kappa \} + \cdots$, (A3)

where the ellipsis represents finite terms.

The term of order u gives

$$
a_D = -\frac{G_1}{G_0 \epsilon} \tag{A4}
$$

The term of order u^2 , and proportional to $\ln \mu / \kappa$, gives a_u ,

$$
a_u = -\frac{2G_2}{G_1 \epsilon} - a_D \ . \tag{A5}
$$

Expansion of $I(u)$ —Eq. (8.14)—in powers of ϵ gives

$$
I(\mu) \sim \frac{1}{\epsilon} \mu^{-\epsilon/2} + O(1) \tag{A6}
$$

Together with (8.15) one has

$$
G_0=4+O(\epsilon)=G_1,
$$
 (A7)

and hence

$$
a_D=-\frac{1}{\epsilon}.
$$

$$
\rho(\vec{R}(t),t) = \rho_0(\vec{R}_0(t) + g\vec{R}_1(t) + \cdots, t) + g\rho_1(\vec{R}_0(t) + \cdots, t) + O(g^2)
$$

= $\rho_0(\vec{R}_0(t),t) + g[\vec{R}_1 \cdot \nabla \rho_0(\vec{R}_0) + \rho_1(\vec{R}_0)] + O(g^2)$. (B2)

 R_0 is given by Eq. (8.4) and $\rho_0(\vec{R}_0(t), t)$ is, by (8.5),

$$
\rho_0(R_0,t) = \int_0^t dt_1 \int \frac{d^d p}{(2\pi)^d} \exp\left[i\vec{p}\cdot \int_{t_1}^t \vec{\eta}(t_2)dt_2\right].
$$
\n(B3)

The function ρ_1 is obtained from (4.4) by expanding the δ function in powers of the g dependence contained in $R(t)$. Hence

$$
\rho_1(x,t) = -\int_0^t dt_1 \vec{R}_1(t_1) \cdot \int_p i \vec{p} \exp\left[i \vec{p} \cdot \left(x - \int_0^{t_1} \vec{\eta}(t_2) dt_2\right)\right].
$$
\n(B4)

Inserting (82) in Eq. (4.1) one finds

$$
\vec{R}_2(t) = -\int_0^t dt_1 \vec{\nabla} [\rho_1(R_0(t_1)) + \vec{R}_1(t_1) \vec{\nabla} \rho_0(R_0)] .
$$
\n(B5)

Inserting (8.9) and (B5) in (B1) one can proceed to calculate $\langle R^2 \rangle$ at second order by computing the average over η .

A lengthy but straightforward computation (Appendix 8) gives

$$
G_2 = -3 + 4\epsilon + O(\epsilon^2) \tag{A8}
$$

Inserting (A8) into (AS) one finds

$$
a_u = \frac{5}{2\epsilon} \tag{A9}
$$

One could proceed to compute b_D from the term $u²$ in (A3), but it is of no interest for our present purposes.

APPENDIX 8

Here we indicate a few of the steps involved in the computation of $G^{(2)}$ to second order in g. From (8.1) one has

$$
R^{2}(t) = R_{0}^{2} + 2g\vec{R}_{0}\cdot\vec{R}_{1} + g^{2}(R_{1}^{2} + 2\vec{R}_{0}\cdot\vec{R}_{2}) + O(g^{3}).
$$
 (B1)

 R_0 is given by (8.4) and R_1 is given by Eq. (8.9).

From Eq. (4.1) it is clear that to compute R to second order in g we need $\rho(\vec{R}, t)$ to first order. This has two contributions. One can write

As an example we follow the calculation of the first of the two terms, namely $\langle R_1^2 \rangle$. The calculation of the second term— $\langle \vec{R}_0 \cdot \vec{R}_2 \rangle$ —is very similar.

$$
\langle R_1^2(t) \rangle = -\int_{q_1} \int_{q_2} (q_1 q_2) \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^t dt_3 \int_0^{t_3} dt_4 \Big\langle \exp \left[i q_1 \int_{t_2}^{t_1} \eta + i q_2 \int_{t_4}^{t_3} \eta \right] \Big\rangle . \tag{B6}
$$

There are six possible time orderings of t_1 , t_2 , t_3 , and t_4 , inside the interval $(0,t)$. They are depicted in Fig. 7. To the right of each time ordering is the corresponding average, which enters (86).

Clearly, when (a) and (f) are integrated over q_i they vanish. The other four terms are convolutions in t_i , and their Laplace transform has a simple form,

$$
\langle R_1^2(\mu) \rangle_b = \langle R_1^2(\mu) \rangle_e = -\mu^{-2} \int_{q_1} \int_{q_2} (q_1 q_2) \frac{1}{(q_2^2 + \mu)(q_1^2 + \mu)[(q_1 + q_2)^2 + \mu]} \tag{B7}
$$

Note that we have taken $D = 1$;

$$
\langle R_1^2(\mu) \rangle_c = \langle R_1^2(\mu) \rangle_d = -\mu^{-1} \int_{q_1} \int_{q_2} (q_1 q_2) \frac{1}{(q_1^2 + \mu)^2 [(q_1 + q_2)^2 + \mu]}.
$$
 (B8)

The integrals in (B7) and in (B8) are dimensionally regularized. Their divergent parts can be expressed in terms of the integral I, defined in Eq. (8.14).

Thus

a
C

$$
(B7) = \mu^{-2} [I^2 + \mu(\cdots)]
$$
 (B9)

where the ellipsis represents finite uv, and

$$
\begin{array}{ccccccccc}\n0 & t_4 & t_3 & t_2 & t_1 & t \\
\hline\nq_2 & & & q_1 & & \n\end{array}
$$
 (a)

$$
\begin{array}{ccccccccc}\n0 & t_4 & t_2 & t_3 & t_1 & t \\
\hline\n & q_2 & q_1 + q_2 & q_1 & \n\end{array}
$$
 (b)

$$
\begin{array}{ccccccccc}\n0 & t_{4} & t_{2} & t_{1} & t_{3} & t_{2} \\
 & & q_{2} & q_{1}+q_{2} & q_{2} & (c)\n\end{array}
$$

$$
\begin{array}{cccccccc}\n0 & t_2 & t_4 & t_3 & t_1 & t \\
\hline\nq_1 & q_1 + q_2 & q_1 & \n\end{array}
$$
 (d)

$$
\begin{array}{ccccccccc}\n0 & t_2 & t_4 & t_1 & t_3 & t_4 \\
\hline\n & q_1 & q_1 + q_2 & q_2 & \n\end{array}
$$
 (e)

$$
\frac{t_2}{q_1} \quad \frac{t_1}{q_2} \quad \frac{t_4}{q_3} \quad \frac{t_3}{q_2} \quad (f) \quad \exp[-q_1^2(t_1-t_2)-q_2^2(t_3-t_4)]
$$

 $(B8) = -\mu^{-2} I \frac{\partial I}{\partial D}$ (810)

where

$$
\frac{\partial I}{\partial D} = \int_{q} q^2 (q^2 + \mu)^{-2} . \tag{B11}
$$

This notation stems from the fact that the reconstitution of D amounts to multiplication by D of the q^2 in the propagators.

The second term entering $G^{(2)}$ at second order in

$$
\exp[-q_1^2(t_1-t_2)-q_2^2(t_3-t_4)]
$$

(b)
$$
\exp[-q_1^2(t_1-t_3)-(q_1+q_2)^2(t_3-t_2)-q_2^2(t_2-t_4)]
$$

(c)
$$
\exp[-q_2^2(t_3-t_1)-q_2^2(t_2-t_4)-(q_1+q_2)^2(t_1-t_2)]
$$

(d)
$$
\exp[-q_1^2(t_1-t_3)-q_1^2(t_4-t_2)-(q_1+q_2)^2(t_3-t_4)]
$$

(e)
$$
\exp[-q_2^2(t_3-t_1)-(q_1+q_2)^2(t_1-t_4)-q_1^2(t_4-t_2)]
$$

FIG. 7. Six possible time orderings of t_1 , t_2 , t_3 , and t_4 , inside the interval $(0, t)$.

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g is the average of $\vec{R}_0 \cdot \vec{R}_2$ —Eq. (B1). Here we write only the final result

$$
\langle \vec{R}_0 \cdot \vec{R}_2 \rangle = -2\mu^{-2} \left[I \frac{\partial^2 I}{\partial D^2} - \frac{1}{d} \left(\frac{\partial I}{\partial D} \right)^2 \right] + \cdots, \tag{B12}
$$

- *Address until June 1983: Institute for Advanced Study, Princeton, NJ 08540.
- ¹S. F. Edwards, Proc. Phys. Soc. London 85, 613 (1965).
- ²C. Domb, J. Gillis, and G. Wilmers, Proc. Phys. Soc. London 85, 625 (1965).
- ³J. des Cloizeaux, J. Phys. (Paris) B 1, 715 (1970).
- 4P. G. de Gennes, Phys. Lett. 38A, 339 (1972).
- 5V.J. Emery, Phys. Rev. B 11, 239 (1975).
- ⁶P. J. Flory, *Principles of Polymer Chemistry*, 7th ed. (Cornell University Press, Ithaca, 1967), Chap. 14.
- 7A similar equation was written down by J. des Cloizeaux [Ref. 3, Eq. (111.32)] in the course of his criticism of Edwards's mean-field treatment (Ref. 1). There ρ is replaced by a spherically symmetric mean-field potential, while here it is a dynamically developing density.
- ⁸G.'t Hooft and M. Veltman, Nucl. Phys. B 44, 189

where the ellipsis stands for uv finite terms and where d is the number of space dimensions, and

$$
\frac{\partial^2 I}{\partial D^2} = \int_q q^4 (q^2 + \mu)^{-3} .
$$
 (B13)

(1972).

- ⁹D. J. Amit, Field Theory, the Renormalization Group, and Critical Phenomena (McGraw-Hill, New York, 1978), Secs. 9 and 10.
- ¹⁰See, e.g., E. Brezin, J. C. Le Guillou, and J. Zinn-Justin, in Phase Transition and Critical Phenomena, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 6.
- ¹¹Reference 9, Chap. 8.
- ¹²F. J. Wegner, Phys. Rev. B 5, 4529 (1972); 6, 1891 (1972); and unpublished.
- $13K$. Symanzik, in Particles, Quantum Fields, and Statistical Mechanics, edited by M. Alexanian and A. Zepeda (Springer, Berlin, 1975).
- ¹⁴See also Ref. 10 and Ref. 9, Sec. 9-6.