Self Avoiding Walks in Four Dimensions: Logarithmic Corrections

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Abstract

We present simulation results for long \( N \leq 4000 \) self-avoiding walks in four dimensions. We find definite indications of logarithmic corrections, but the data are poorly described by the asymptotically leading terms. Detailed comparisons are presented with renormalization group flow equations derived in direct renormalization and with results of a field theoretic calculation.
1 Introduction

Self avoiding walks (SAW’s) are of practical importance since they form a model for randomly coiled linear polymers. But even more important for theoretical physics is that they represent in some sense the simplest critical phenomenon. More precisely, they formally are described by the \( m \to 0 \) limit of the \( O(m) \) Landau–Ginzburg field theory. Other members of this family are the Ising \((m = 1)\) and the Heisenberg \((m = 3)\) models.

The most profound theoretical understanding of these critical phenomena is obtained by the field theoretic renormalization group evaluated near 4 dimensions. Above \( d = 4 \), all \( O(m) \) models show mean field behavior. Below \( d = 4 \), the deviations of the critical exponents from their mean field values are of order \( \epsilon = 4 - d \).

This follows from the fact that the renormalized coupling constant is of order \( \epsilon \) in the infrared limit. The most extensively studied method for estimating critical exponents (the “\( \epsilon \)-expansion”) involves resumming perturbation expansions in \( \epsilon \).

Precisely at \( d = 4 \), the deviation from mean field behavior is given by logarithmic corrections which can be predicted unambiguously by renormalization theory. Specifically, the leading behavior in the limit of long chains is

\[
R_N^2 \sim N \log N^\alpha, \quad \alpha = 1/4
\]

for the average squared end-to-end distance, and

\[
C_N \sim \mu N \log N^\beta, \quad \beta = 1/4
\]

for the number of distinct walks. These predictions are basic results. In particular, they do not suffer from any ambiguities inherent in a resummation of the \( \epsilon \)-expansion. It thus would be extremely useful if one could verify them by independent means. The most obvious candidates for alternative calculations are exact enumerations of short walks and Monte Carlo simulations. Both methods have been applied in the past.

Enumerations of chains with length up to \( N = 18 \) have been used in \([2,3,4]\) to verify eq.(2) \((R_N \) was not computed in these papers\), and recently chains were enumerated with \( N \) up to \( N = 21 \) \([5]\). From this the authors claim excellent agreement with eq.(2): the power of the logarithm in the best fit is \( \beta = 0.250 \pm 0.005 \).

Monte Carlo Simulations, on the other hand, have been used previously for estimating \( \alpha \) in \([3,9]\). In addition, different exponents related to \( \alpha \) and \( \beta \) were
measured in [7, 8]. While refs. [6, 7, 8] claim good agreement with eq.(1) (with e.g. \( \alpha = 0.25 \pm 0.02 \) in [7]) and with eq.(2), serious disagreement was found in [9]: the best fit was obtained there with \( \alpha = 0.31 \). Although no error bars were given in [9], the author obviously considered the value \( \alpha = 1/4 \) to be ruled out. This seems a serious problem since the simulations of ref. [9] are by far more significant statistically than those of [4, 6, 8], both concerning the chain lengths \((N \text{ up to } 2400)\) and the sample size. Also, the method of analysis used in [9] was justly criticized in [9] since it introduces an uncontrolled bias and does not use the data optimally.

The methods used in [7, 8] (in both papers, identical methods were used) are not easily compared to the present one. In different runs, these authors measured the average length \( \langle N_R \rangle_p \) of chains with fixed end-to-end distance \( R \) in grand canonical ensembles at \( p < p_c \) \((p\text{ is the fugacity})\), and the probability \( Q(p) \) that two chains starting at neighboring sites never cross each other. We have not measured \( Q(p) \) ourselves (such measurements will be presented in [10]), but we have measured \( \langle N_R \rangle_p \). From this we shall argue in sec.5 that the analyses of [7, 8] have large systematic errors, and that indeed deviations from mean field behavior is much larger than claimed there.

In view of this situation (and since simulations of theta polymers in 3 dimensions [11] also gave discrepancies with the logarithmic corrections expected there [1]) we decided to perform simulations with much higher accuracy than those done previously.

We find that the numerical results of [9] are correct (though we do not agree with the conclusions drawn from them). In contrast, it seems that the findings of [6, 7, 8] were not completely unaffected by wishful thinking. This means that the leading logarithmic terms of (1) and (2) are not sufficient to describe the behavior at any chain lengths which can be simulated in the foreseeable future (unless we assume, as was done in [9], that the leading terms show a different power of \( \log N \)).

The first corrections to the asymptotic laws (1) and (2) have been calculated by Duplantier [12], but it turns out that even the corrected expressions are not fully consistent with the numerical data. These expressions involve a non-universal parameter (an integration constant from integrating the renormalization group flow) which should be the same for \( R^2_N \) and \( C_N \). But for a good fit two different values have to be chosen for \( R^2_N \) and \( C_N \), which is an internally inconsistent procedure.
However, from our data we can extract logarithmic derivatives $\partial \ln R^2_N / \partial \ln N$, $\partial \ln C_N / \partial \ln N$, which may be compared directly to renormalization group flow equations of an appropriate direct renormalization scheme. Such a comparison does not involve unknown fit parameters. It thus is very pleasing that the flow equations consistently can be put into a form which compares very well to our Monte Carlo data.

Stimulated by that success we use the original data to test another theoretical approach. As has been stressed previously [13, 14], the renormalization approach can be viewed as proceeding in two essentially independent steps. We first determine a mapping from the physical model to its renormalized counterpart, and in a second step we use renormalized perturbation theory to determine the observables, working completely within the renormalized model. It has been suggested that the mapping must be determined most precisely, but in the second step we may be content with low order perturbation theory. We find that this method allows for a consistent determination of the nonuniversal parameters and yields a good quantitative fit to our data.

The paper is organized as follows: In the next section we present our Monte Carlo algorithm and the resulting data. Comparison with renormalization group flow equations derived in the spirit of direct renormalization is given in sec.3, while comparison with field theoretic renormalization is presented in sec.4. We conclude with a discussion of our results in sec.5.

2 Simulations

Aiming at estimates for both $R^2_N$ and $C_N$, we decided not to use the pivot algorithm [16], though it should be the most efficient algorithm for estimating $R_N$ in the limit $N \to \infty$. Instead, we essentially used a recursive and randomized implementation of the old enrichment method [17]. This method is an improvement over the incomplete enumeration or ‘recursive sampling’ method used in [18, 19], and was applied successfully in [14, 20] to polymer adsorption on surfaces, to theta polymers and to off-lattice polymers interacting via Lennard-Jones potentials.

The basic structural element of incomplete enumeration is a subroutine STEP($x$) which marks the site $x$ as occupied and calls itself at all neighboring sites $x \pm e_i$, provided these sites are still free and provided $N < N_{max}$. Before leaving the
subroutine, the site $x$ is marked as free again. If each free neighboring site were visited with probability 1, this would give exact enumeration. In order to obtain a grand canonical distribution of walks where

$$n_N = \text{const} \ C_N p^N$$

is the average number of $N$-step walks, one has to use a random number generator so that only a fraction $p$ of all free neighbors are visited.

The basis of the present improvement is the observation that it is sufficient to visit only one of the neighbors (provided it is free; otherwise the subroutine is left immediately), but in average $(N-1)p$ times. Here $N$ is the coordination number of the lattice, and we have assumed that we do not attempt any back steps as the corresponding site would not be free anyhow. The average chain length diverges when $p \to p_c = 1/\mu$. Since $(N-1)p_c > 1$ for all lattices, this means that we make $>1$ attempts to continue each successful path if $p \approx p_c$. Thus we choose a random neighbor (different from that we had come from), call STEP at this neighbor, and after having returned we call STEP again at the same neighbor with probability $(N-1)p_c-1$. The main difference to the algorithm of [21], e.g., is that we always try at least once to continue the walk.

Like the incomplete enumeration method of [18, 19] and like the method of [21], the present method corresponds essentially to a random walk in the chain length with reflecting boundary conditions at $N = 0$ and $N = N_{max}$. At $p_c$, it takes thus roughly $N^2/D$ steps to obtain one statistically independent SAW of length $N$. Here $D$ is a diffusion constant which is of order unity in the algorithms of [18, 21, 19]. The main advantage of the present algorithm (apart from slightly shorter programs) is that here

$$D \sim 1/\delta, \quad \delta = ((N-1)p_c - 1).$$

Since $\delta \approx 0.033$ for the simple hypercubic lattice in $d = 4$, this gives a very large diffusion coefficient, and the method is more than one order of magnitude faster than those of [18, 21, 19]. Eq.(4) can be understood as follows: in the present algorithm, a step back in $N$ is only needed when the walker hits an occupied site. The chance for this is $\approx \delta$. In simulations near $p_c$, this means that in average $1/\delta$ forward steps are made until one back jump reduces $N$ by $1/\delta$. In each of [18, 21, 19], in contrast, the probability to make a back step is of order 1 (it is $(1-p)^{d}$ for [18, 19], and $1/(1+pN)$ for [21]).
We have simulated SAW’s of length up to $N_{\text{max}} = 4000$. Since it is not possible to store the sites occupied by such long walks in a simple bit map, we used a hashing procedure similar to (but somewhat simpler than) that used in [10]. We made only simulations very close to $p_c$, where $n_N$ is roughly independent of $N$. As explained in [17, 19], this should be most efficient. Our total sample corresponded to $n_N \approx 10^8$. This is also roughly the number of SAW’s of maximal length $N_{\text{max}}$, but all these walks are of course not independent. Often it is stated that this correlation between the walks is the main drawback of the enrichment method. In our version, it is not a big problem because of the ease with which walks are generated. The number of independent walks is given by the number of instances where the algorithm has reached $N = N_{\text{max}}$ between two returns to the main routine (corresponding to $N = 0$). Our sample contained $\approx 1.2 \times 10^6$ such independent walks. The total CPU time was ca. 800 h on a cluster of DEC ALPHA workstations.

Our results for $R^2_N/N$ are shown in fig.1. In order to compare with eq.(1), we plotted its logarithm against $\ln(\ln N)$. To demonstrate the importance of non-leading terms in logarithmic expressions, we show two slightly different quantities. For the solid line, $N$ is defined as the number of bonds, while $N$ is the number of sites for the dotted line. These two definitions differ by one unit and are clearly equivalent for $N \to \infty$. Nevertheless, we see that the difference is still important for $N = 300!$ We show also the results of [9] which have larger error bars but are otherwise in perfect agreement. From eq.(1) we expect our data to fall onto a straight line with slope $1/4$. This is definitely not seen. Instead, the best straight line to the data (where $N$ is interpreted as the number of bonds) has slope $0.311 \pm 0.003$. It would indeed give a perfectly acceptable fit.

Our data for $C_N$ are shown in fig.2. More precisely, we there plotted $C_N p^N$ against $\ln N$ for three different values of $p$. We also show the exact enumeration data of [4] with which we are in perfect agreement. But again we see hardly any sign of the predicted asymptotic behavior. We do not want to discuss in detail why several authors [4, 3, 2] were able to extract the correct asymptotic behavior from enumeration data (for noiseless data there exist very sophisticated methods to extract singularities), but obviously non-leading contributions are very large.
3 Higher Order Terms and Renormalization
Group Flow

Fortunately, the leading corrections to eqs. (1,2) have been calculated in [12]

\[ \alpha_N \equiv R_N^2 / N = r [\ln(N/a)]^{1/4} \left[ 1 - \frac{17 \ln(4 \ln(N/a))}{64 \ln(N/a)} + \ldots \right] \]  (5)

\[ C_N / \mu^N = c [\ln(N/a)]^{1/4} \left[ 1 - \frac{17 \ln(4 \ln(N/a))}{64 \ln(N/a)} - 3 \right. \]  (6)

The constant \( a \) has to be treated here as a free parameter. We thus have two parameters \( (r,a) \) to fit \( R_N^2 / N \), and two more \( (\mu, c) \) if we also want to fit \( C_N \).

The best fit to eq.(5) is obtained with \( r = 1.331 \), \( a = 0.1237 \). It is included in fig.1 (dashed line). Over the range of interest it practically is undistinguishable from a straight line with slope 0.311.

For \( C_N \) it is even more obvious that the leading term \( [\ln(N/a)]^{1/4} \) would give a very poor fit. A fit with eq.(6), using \( a \) again as a free parameter, gives \( c = 1.05, a = 0.055 \). This fit is shown as dotted curve in fig.2. Notice that the values of \( a \) extracted from \( \alpha_N \) and from \( C_N \) differ considerably. No acceptable fit is found with a common value of \( a \).

Neglecting this problem for the moment, our data suggest that the critical value of \( p \) is \( p_c = 0.147622 \pm 0.000001 \). This is to be compared to \( p_c = 0.147625 \pm 0.000002 \) as obtained in [3]. The values accepted in [4, 5] were substantially larger, 0.1490 ± 0.0003 and 0.1493 ± 0.0007, which partly explains why smaller logarithmic corrections were found in these papers (see sec.5).

We have thus been able to produce individual good fits to \( R_N^2 / N \) and to \( C_N p^N \), but the non-leading corrections are very important (in the latter case masking completely the leading behavior), and the fit parameters are not mutually consistent. This can also be seen by plotting the ratio \( (R_N^2 / N) / (C_N p^N) \). Here the dominant terms cancel, and we obtain

\[ \frac{\alpha_N}{C_N p_c^N} = \text{const} \left[ 1 - \frac{17}{32 \ln(N/a)} + \ldots \right] \]  (7)

From fig.3 we see that this ratio is indeed a roughly linear function of \( 1 / \ln(N/a) \), provided we take \( a \approx 0.1 \). The slope of this function has the right sign but is
roughly twice as large as the value predicted by eq. (7). To summarize, even including the leading correction terms we do not find a fully satisfactory explanation of the data.

To proceed we note that eqs. (5, 6) are derived by integrating the renormalization group flow equations, keeping only terms up to one loop order. It therefore is of interest to take a step back and compare the data against the more basic flow equations. We first reconstruct the flow equations from results given in the literature.

Following [13], we start from dimensionally regularized perturbation theory in $d = 4 - \epsilon$ dimensions. Denoting by $b$ the bare coupling constant and by

$$z = \frac{b N^{\epsilon/2}}{(2\pi)^{d/2}}$$

a dimensionless coupling strength, we have up to second order in $z$ [15]

$$\alpha_N = 1 + z\left(\frac{2}{\epsilon} - 1\right) + z^2\left(-\frac{6}{\epsilon^2} + \frac{11}{2\epsilon}\right) + O(z^3), \quad (9)$$

$$C_N/\mu^N = 1 + z\left(\frac{1}{\epsilon} + \frac{1}{2}\right) - z^2\left(\frac{7}{2\epsilon^2} + \frac{4}{\epsilon}\right) + O(z^3). \quad (10)$$

Obviously these expansions are singular at $d \to 4$. We thus introduce a renormalized coupling constant, which in the minimal subtraction scheme of [22] reads

$$z_R = z - \frac{8}{\epsilon}z^2 + \left(\frac{64}{\epsilon^2} + \frac{17}{\epsilon}\right)z^3 + O(z^4). \quad (11)$$

From this we get the Wilson function [12]

$$W[z_R, \epsilon] = N \frac{\partial}{\partial N} z_R|_{b,\epsilon} = \frac{1}{2} \epsilon z_R - 4z_R^2 + 17z_R^3 + \ldots, \quad (12)$$

in which we can take the limit $\epsilon \to 0$ without encountering any problems:

$$W[z_R] = -4z_R^2 + 17z_R^3 + O(z_R^4). \quad (13)$$

While $\alpha_N$ or $C_N/\mu^N$ expressed in terms of $z_R$ still are singular, their derivatives with respect to $\ln N$ are known to be finite. Indeed these derivatives yield flow equations governing the renormalization of the chain length and of the partition function. Defining

$$\sigma_0[z_R, \epsilon] = N \frac{\partial \ln \alpha_N}{\partial \ln N}|_{b,\epsilon}, \quad (14)$$

and

$$\sigma_1[z_R, \epsilon] = N \frac{\partial \ln C_N}{\partial \ln N}|_{b,\epsilon}, \quad (15)$$
we have \[\begin{align*}
\sigma_0[z_R] &= \lim_{\epsilon \to 0} \sigma_0[z_R, \epsilon] = z_R + \frac{7}{2} z_R^2 + \ldots, \\
\sigma_1[z_R] &= \lim_{\epsilon \to 0} \sigma_1[z_R, \epsilon] = z_R - 5 z_R^2 + \ldots.
\end{align*}\] (16) (17)

Equations (16) and (17) were obtained by first integrating eq. (12) at \(\epsilon = 0\), yielding \(z_R\) as a function of \(N\). This was inserted into eqs. (16) resp. (17), and eqs. (14) resp. (15) were integrated again. During these manipulations, only the leading terms were kept, since higher order terms are not completely known anyhow.

Avoiding these integrations we now directly compare our data to eqs. (12)–(17). We first calculate the derivatives (14), (15) as functions of \(N\). Of course, we have to replace derivatives with respect to \(N\) by finite differences (we use \(\Delta \ln N = \ln 2\) for first derivatives, and \(\ln 4\) for second), but this should not present much problems in view of the slow variations of all functions involved.

We thus show in fig.4
\[
\sigma_0(N) \equiv \frac{1}{\ln 2} \ln \frac{R^2_{2N}}{2R^2_N},
\]
while
\[
\sigma_1(N, p) \equiv \frac{1}{\ln 2} \ln \frac{p^N C_{2N}}{C_N}
\]
is plotted in fig.5 for the same three values of \(p\) as before. From these plots, we should be able to obtain the same function \(z_R(N)\) by inverting eqs. (16), (17). A quick test shows that this is not so easy. The problem is that \(z_R(N)\) turns out to be not very small (even for the largest values of \(N\)), and the Taylor expansions (16), (17) obviously are poorly convergent. This is particularly true for \(\sigma_1\), for which truncation in eq. (17) after the quadratic term yields \(\sigma_1 \leq 0.05\), in contradiction to the data for \(N < 30\).

A trick which helps – though its justification is far from obvious – is to change the expansions in eqs. (14), (17) into Padé approximants,
\[
\sigma_0[z_R] = \frac{z_R}{1 - 7z_R/2}, \quad \sigma_1[z_R] = \frac{z_R}{1 + 5z_R}.
\] (20)

These can be inverted to give
\[
z_R = z_R^{(\alpha)} = z_R^{(C)}
\] (21)
with
\[
z_R^{(\alpha)} = \frac{\sigma_0}{1 + 7\sigma_0/2}, \quad z_R^{(C)} = \frac{\sigma_1}{1 - 5\sigma_1}.
\] (22)
In fig.6 we have plotted $z_R^{(\alpha)}$ and $z_R^{(C)}$ as obtained from the finite-difference approximations. We see still some disagreement for small $N$ which may be due to higher order terms in $\sigma_0[z_R], \sigma_1[z_R]$ and/or to $1/N$ corrections. But for large $N$ we find very acceptable agreement, provided we take $p = 1/\mu = 1.476223$.

The final test of the theory consists in checking whether these estimates of $z_R$ satisfy the differential equation $N \frac{d z_R}{d N} = W[z_R]$ or, rather, its finite-difference approximation. Again we find problems due to the slow convergence of the Taylor expansion for $W[z_R]$, and again we take recourse to a Padé approximant,

$$W[z_R] = -\frac{4 z_R^2}{1 + 17 z_R/4}.$$  \hspace{1cm} (23)

In fig.7a we have plotted this form of $W$ with argument $z_R^{(\alpha)}$ against $N$, together with

$$\frac{\Delta z_R^{(\alpha)} (N)}{\Delta \ln N} = \frac{z_R^{(\alpha)} (2N) - z_R^{(\alpha)} (N/2)}{\ln 4}.$$  \hspace{1cm} (24)

We see very nice agreement, in particular for large values $N$ where it is most significant. For small $N$ agreement could indeed be improved by adding a constant of $\mathcal{O}(1)$ to $N$ so that $\alpha_N$ is replaced by $R_N^2/(N + 0.16)$, see fig.7b. Such a $1/N$ correction would also improve the agreement in fig.6 at intermediate values of $N$.

We thus conclude that our data are fully consistent with the renormalization group flow predicted theoretically, though there is some ambiguity related to the use of Padé approximants and – to a much lesser degree – to the treatment of $1/N$ corrections. We want to stress that this analysis is particularly interesting since, except for the size of the nonuniversal $1/N$ corrections, it does involve no fit parameter! Note further, that this analysis uses only the information underlying also eqs.(11) or (12). This suggests that solving the renormalization group equations to one loop order and substituting the result into expressions for higher order corrections we lose meaningful information which still can be identified on the level of the flow equations.

4 Field Theoretic Renormalization

As mentioned in the introduction, the renormalization program may be separated into two steps: We first map the physical ‘bare’ model on a renormalized model which exhibits the scale invariance of long chains. We then calculate $R_N^2, C_N$ perturbatively within the renormalized model.
The bare model depends on the coupling constant $b$, the chain length $N$, and a microscopic length scale $l$ which is of the order of the lattice spacing in the computer experiments. In the renormalized theory these parameters are replaced by the renormalized coupling $u$, the renormalized chain length $N_R$, and a renormalized length scale $l_R$. The mapping takes the general form

$$ b = \text{const} \left( \frac{l}{l_R} \right)^\epsilon Z_u(u, l/l_R) u $$

$$ N = \left( \frac{l_R}{l} \right)^2 Z_n(u, l/l_R) N_R, $$

where the renormalization factors are normalized according to

$$ Z_u(0, 1) = Z_n(0, 1) = 1. $$

The observables of interest here can be expressed as

$$ R_N^2 = 2d l_R^2 N_R A_R(u, N_R) $$

$$ C_N = \text{const} \frac{Z(u, l/l_R)}{Z_n(u, l/l_R)} A_C(u, N_R), $$

where $Z(\ldots)$ denotes another renormalization factor and the amplitudes $A_R, A_C$ are to be calculated by renormalized perturbation theory. In general the renormalization factors have to be chosen to absorb the leading dependence on the microscopic scale $l$: for fixed $l_R$, all observables have to become independent of $l$ up to corrections of order $l^2/l_R^2 N_R \sim 1/N$. Using the scheme of dimensional regularization, defined by taking the limit $l \to 0$ for $d < 4$, factors such as to make the renormalized theory finite in four dimensions.

The length scale $l_R$ is a free parameter of the renormalized theory. Under a change of $l_R$ the other parameters change according to the flow equations

$$ \frac{\partial u}{\partial \ln l_R} = \epsilon u - \tilde{\beta}(u) $$

$$ \frac{\partial \ln Z_n}{\partial \ln l_R} = \zeta_n(u) $$

$$ \frac{\partial \ln Z}{\partial \ln l_R} = \zeta(u), $$

where all derivatives have to be taken at fixed $b, l$ and $\epsilon$. Based on Padé–Borel summation of higher order perturbation theory, a parametrization of the flow functions has been given in [24]:

$$ \zeta_n(u) = -u + \frac{5}{4} u^2 - a_1 u^3 + a_2 u^4 $$

$$ \zeta(u) = \frac{u_0}{u} - \frac{u_1}{u^2} - \frac{u_2}{u^3} + \frac{u_3}{u^4} $$

where $u_0, u_1, u_2, u_3$ are constants.
\[ \zeta(u) = -\frac{u^2}{4} + a_3 u^3 \quad (34) \]
\[ \tilde{\beta}(u) = 4u^2 \frac{1 + a_4 u}{1 + a_5 u} \quad (35) \]

with the constants \( a_1 = 3.6328, a_2 = 3.8953, a_3 = 0.04395, a_4 = 1.555 \) and \( a_5 = 3.5962 \).

(Our notation differs somewhat from that of [24]: \( u = 8u, \zeta_n = -\zeta, \zeta = \zeta_0 \). We further note that recently some mistake has been found [25] in the five loop contributions to the renormalization factors. However, due to the remarkable stability of the Padé–Borel results this is not expected to yield serious changes in the parametrization of (33)–(35).)

Starting from arbitrary initial conditions set at \( l_R = l \) we now integrate the flow equations to find functions \( u(l_R) \) e.t.c. in analytic form. We then fix the final value of \( l_R \) by the condition

\[ N_R = 1 \], \quad (36) \]

which implies that \( l_R \) is of order \( R_N \). There result the expressions

\[ \alpha_N = l_0^2 \frac{e^{1.951u - 1.422u^2 + 0.734u^3}}{u^{1/4}(1 + 1.555u)^{1.369} A_R(u, 1)}, \quad (37) \]
\[ C_N/\mu^N = c_0 \frac{e^{2.101u - 1.434u^2 + 0.734u^3}}{u^{1/4}(1 + 1.555u)^{1.425} A_C(u, 1)}. \quad (38) \]

The renormalized coupling constant is implicitly determined by the equation

\[ N = n_0 \left( 1 + 1.555u \right)^{2.349} u^{-0.790} e^{\frac{1}{2\pi} - (1.951u - 1.422u^2 + 0.734u^3)}. \quad (39) \]

Here \( l_0, c_0, n_0 \) are nonuniversal fit parameters absorbing the initial conditions in the integration of the flow equations.

So far we have been concerned with the renormalization group mapping. Calculation of the amplitudes is a straightforward exercise in renormalized perturbation theory. It yields

\[ A_R(u, 1) = 1 - \frac{u}{2} + O(u^2) \quad (40) \]
\[ A_C(u, 1) = 1 + \frac{u}{2} + O(u^2) \quad (41) \]

Eqs. (37)–(41) constitute our final result. From the derivation it should be clear that the calculation of the amplitudes is a problem well separated from the determination of the renormalization group mapping. Indeed, within the minimal
subtraction scheme it is the singular terms in expressions like eq.(9),(10) which
determine the mapping, whereas the amplitudes result from regular terms.

We now compare to the Monte Carlo data. Fitting $\alpha_N$ in the range $300 \leq N \leq 4000$ we find $l_0 = 1.0436$ and $n_0 = 0.275$ (see fig.8). The same value for $n_0$ together with $c_0 = 0.864$ would also give an acceptable fit to $C_N$. But the best fit to the latter (see fig.9a) is obtained with $n_0 = 0.316$, $c_0 = 0.870$, and

$$p_c = 0.1476223 \pm 0.0000005.$$  \hspace{1cm} (42)

The latter value for $n_0$ gives also an excellent fit to $\alpha_N$, provided $N$ is replaced by $N + n_1$ in the definition of $\alpha_N$, with $n_1 = 0.56$ (see fig.9b). In the latter fit, $l_0 = 1.0466$. A priori, such a change would be well within the uncertainty intrinsic in the definition of $N$. But fig.7 and analogous plots of the dependence of $u$ on $l_R$ in the present scheme suggest that such a value of $n_1$ is somewhat large.

We must note, however, that introducing $n_1$ we can account for $1/N$ corrections only in a very crude way [26]. We thus find agreement with the field theoretic prediction, but there remains some room for further improvement in the region of short chains.

It is of some interest to note the range of the renormalized coupling resulting from our fit: $0.067 < u < 0.15$ for $N$ in the range $4000 > N > 100$. Thus even for $N \approx 4000$ $u$ is not particularly small. On the other hand, it is sufficiently small for the parametrizations of [24] to be justified.

5 Discussion

We have seen that self-avoiding walks on the hypercubic lattice in four dimensions show clear logarithmic corrections. These corrections are in perfect agreement with the predictions of the renormalization group, though they would be very poorly described by the asymptotically leading approximation. Thus claims [3, 7, 8] that exactly these leading terms have been seen in simulations must be viewed with some reservation. On the other hand, our numerical results agree perfectly with simulations reported in [8], although the conclusion drawn in that paper seems to be wrong. Though our data are perfectly fitted by power laws in $\ln N$ — in particular,

$$R^2_N/N \sim [\ln N]^{0.31},$$  \hspace{1cm} (43)

these do not represent the asymptotic behavior.
In order to understand the discrepancy with [7, 8], we have repeated their computation of \( \langle N_R \rangle_p \) and their subsequent analysis, but with several modifications:

(i) using our algorithm, we calculated \( \langle N_R \rangle_p \) not only for a single fixed value of \( R \) (\( R = 7 \) in [7, 8]), but for all \( R < \sqrt{500} \);

(ii) due to the efficiency of our algorithm (and improved hardware) we have much higher statistics;

(iii) we use data much closer to the critical point: \( p_c - p \geq 0.0012 \) compared to \( p_c - p \geq 0.018 \); and

(iv) in the analysis we use our very accurate estimate for \( p_c \).

Assuming that the decay of the two-point function is dominated by the smallest mass \( m \) in the model (the inverse correlation length \( \xi \)), the authors of [7, 8] obtain

\[
\langle N_R \rangle_p \sim R \frac{dm}{dp}
\]

(44)

with

\[
m \equiv \frac{1}{\xi} \sim \sqrt{p_c - p} \left[ \ln(p_c - p) \right]^{-N}, \quad N = 1/8 .
\]

(45)

Thus, \( \langle N_R \rangle_p / R \) should be a function of \( p \) alone, independent of \( R \). Our data shown in fig.10 clearly demonstrate that this is true only for \( R \gg \xi \), while

\[
\langle N_R \rangle_p \sim R \ln R
\]

(46)

for \( R < \xi \). This is not surprising: the decay of the correlation function should be dominated by the smallest mass only for \( R \gg \xi \), while effects of the effective coupling should be visible at shorter distances. Indeed, keeping \( R \) fixed while \( p \to p_c \) we encounter the region where the data should be analysed via a short distance expansion, and eq.(44) is no longer justified. According to fig.10, \( R = 7 \) is not yet in the regime where eq.(44) holds for the range of \( p \) considered in [0].

This gives already a first indication that this coupling is larger than anticipated in [0] (we might add that the fluctuations seen in fig.10 are not statistical, but are lattice effects).

In fig.11 we show our data for \( R = 7, \sqrt{150} \) and \( \sqrt{500} \) together with those of [0], and with the mean-field prediction

\[
\frac{\langle N_R \rangle_p}{R} \propto \frac{1}{\sqrt{p_c - p}}.
\]

(47)

On the one hand we see that the slopes deviate strongly from mean field prediction, much more than they differ between different values of \( R \). On the other hand,
we see the dramatic effect of a wrong choice of $p_c$. Indeed, while we use our value of $p_c$ when plotting our own data, we show the data of [7] twice: once plotted using our $p_c$, and once using their own estimate of $p_c$. We see that the latter reduces the deviation from mean field considerably. Thus we see that the logarithmic corrections are indeed larger than estimated in [7] (in spite of the fact that the too small value of $R$ alone would have led to their overestimation!), but the systematic uncertainties and the lack of higher order predictions from field theory prevent a more detailed analysis. The same comments should hold for the data of [8], as this author used the same values of $R$ and of $p$ as [7], and his estimated $p_c$ was even further from our estimate.

To what chain lengths would we have to go in order to see the asymptotic behavior $R_N^2/N, C_N/\mu^N \sim [\ln N]^{1/4}$? Our renormalization group calculation can easily be extended to larger $N$ and show that eq.(43) no longer would give a good fit above $N = 10^4$, but even at $N = 10^7$ the effective exponent is $\approx 0.285$ instead of $1/4$.

The analysis in the field theoretic framework stresses the importance of a good quantitative form of the renormalization group mapping. For the amplitudes then a low order approximation seems sufficient. This supports previous findings, both in polymer physics [13] and in the physics of liquid helium [14]. If a good form of the mapping were missing, this would justify the often expressed pessimism about the possibility to see logarithmic corrections. Such a situation prevails e.g. for $\theta$-polymers in three dimensions. There only leading terms in the sense of eq.(5),(6) have been computed [27], and they disagree badly with simulations [11]. Although the disagreement there is even worse than the disagreement with the leading terms in the present case, one might suspect that also there the poor representation of the renormalization group mapping employed is at the root of the problem.

The present analysis showed large subleading corrections because of the rather large value of the renormalized coupling constant, even for our longest chains. This raises the question whether the asymptotic behavior could be seen for much shorter chains in models with weaker repulsion between chains. Two such models come immediately into mind: chains with attraction between neighboring sites ($\theta$ polymers above $T_\theta$), and the Domb-Joyce model [28]. In the latter, $n > 1$ monomers can occupy the same site, but the contribution to the partition function gets a weight $(1 - w)^{n-1}$ for each multiple occupancy. For sufficiently small $w$ one is arbitrarily close to the free case, and also the renormalized coupling constant
should be small.

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Figure Captions:

Fig. 1: Plot of the logarithm of the swelling ratio, \( \ln(R^2_N/N) \), against \( \ln(\ln N) \). The solid line are our data with \( N \) taken as the number of bonds; the dotted line represents these data with \( N \) as the number of sites. The diamonds are the data from [9], and the dashed line is the fit with eq.(5). The dashed-dotted line indicates the slope predicted by the leading term given in eq.(1). The statistical errors of our data are roughly \( \propto \sqrt{N} \). They are thus largest for \( N = 4000 \), where \( \Delta \ln R^2_N = 0.0005 \).

Fig. 2: Semi-logarithmic plot of \( C_N p^N \) against \( \ln N \). The plot shows our MC data for 3 different values of \( p \) very near \( p_c \), the fit with eq.(6), and the exact enumeration data from [4]. The statistical error of our data for \( N = 4000 \) is \( \Delta C_N/C_N = 0.0013 \).

Fig. 3: Plot of \( (R^2_N/N)/(C_N p^N) \) against \( 1/\ln(10N) \). According to eq.(7) a straight line with negative slope is expected for \( p = p_c \), with a slope as indicated by the dotted line.

Fig. 4: Function \( \sigma_0(N) \) against \( N \) (full line). Also shown is \( z_R^{(a)}(N) \) as obtained by the Padé approximant eq.(22) (dashed line).

Fig. 5: Function \( \sigma_1(N) \) against \( N \), for the same 3 values of \( p \) as in fig.2.

Fig. 6: Functions \( z_R^{(a)}(N) \) (full line) and \( z_R^{(C)} \) (dashed). The latter is again shown for the same 3 values of \( p \).

Fig. 7: Panel (a): function \( W[z_R^a] \) (full line) and the “derivative” of \( z_R^a \) with respect to \( \ln N \) (dashed line). Both curves should agree up to higher orders in \( z_R \). Panel (b) shows the same data, but in the definition of \( \alpha_N \) we have replaced \( N \) by \( N + 0.17 \).

Fig. 8: Fit to the swelling ratio \( \alpha_N \) with \( l_0 = 1.0436 \) and \( n_0 = 0.275 \).

Fig. 9: (a) Fit to \( C_N/\mu^N \) with \( c_0 = 0.870 \) and \( n_0 = 0.316 \); (b) fit to \( \alpha_N \) with the same \( n_0 = 0.316 \), with \( l_0 = 1.0466 \), and with \( n_1 = 0.56 \).

Fig. 10: Average chain lengths at fixed \( p \) against their end-to-end distance \( R \). Actually, the ratio \( \langle N_R \rangle p/R \) is plotted. The values of \( \ln(1/p) \) (from top to bottom) are: 1.9143, 1.915, 1.916, 1.918, 1.921, 1.925, 1.932, 1.948, 1.966, 1.984, 2.002, 2.021, 2.066, 2.100, and 2.150.
**Fig.11:** Full lines: $\langle N_R \rangle_p / R$ against $p_c - p$ for $R = 7, 12.25, 22.36$ (from bottom to top); dotted line: slope $\langle N_R \rangle_p \propto (p_c - p)^{-1/2}$ predicted by mean field theory; diamonds: data of [8] (for $R = 7$), using our value of $p_c$; crosses data of [7], using their value of $p_c$. 