

Self-Avoiding Random Walks on the Hexagonal Lattice

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We use the algorithm recently introduced by A. Berretti and A. D. Sokal to compute numerically the critical exponents for the self-avoiding random walk on the hexagonal lattice. We find

$$\gamma = 1.3509 \pm 0.0057 \pm 0.0023$$

$$\nu = 0.7580 \pm 0.0049 \pm 0.0046$$

$$\alpha = 0.519 \pm 0.082 \pm 0.077$$

where the first error is the systematic one due to corrections to scaling and the second is the statistical error. For the effective coordination number μ we find

$$\mu = 1.84779 \pm 0.00006 \pm 0.0017$$

The results support the Nienhuis conjecture $\gamma = 43/32$ and provide a rough numerical check of the hyperscaling relation $d\nu = 2 - \alpha$. An additional analysis, taking the Nienhuis value of $\mu = (2 + 2^{1/2})^{1/2}$ for granted, gives

$$\gamma = 1.3459 \pm 0.0040 \pm 0.0008$$

KEY WORDS: Self-avoiding walk; critical exponents; Monte Carlo.

1. INTRODUCTION

The study of random walks, both ordinary and self-avoiding, has gained great interest. The behavior of a single ordinary random walk (ORW) is well understood, but the intersection properties of two or more ORWs are highly nontrivial.^(1,11,17,18)

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Symanzik⁽²³⁾ introduced a representation of continuum field theory in terms of random walks, and this idea proved very fruitful. This representation was later adapted to lattice field theory by Brydges *et al.*⁽⁶⁾ These representations involve walks with rather complicated (and nonlocal) weight factors, which are neither ordinary nor precisely self-avoiding. The Symanzik–Brydges–Fröhlich–Spencer representation has been used to obtain useful rigorous inequalities,^(3,5–7,12) which imply, among other things, the triviality of φ_d^4 field theory for $d > 4$,^(1,3,12) and the nontriviality of φ_d^4 field theory for $d < 4$.^(5,7,8)

Self-avoiding walks (SAW) were first studied as models for organic polymers. De Gennes^(13,54) first discovered, in perturbation theory, that SAWs are equivalent to the field theory obtained as the $N \rightarrow 0$ limit of $O(N)$ model. Later, it was shown that the SAW also arises as the $N \rightarrow 0$ limit of the Symanzik random-walk representation of the $O(N)$ model.⁽³⁾ Some rigorous results on closely related models can be found in Refs. 9 and 16.

On a less rigorous level, the SAWs are used to test theories of critical phenomena. Using the $N \rightarrow 0$ limit equivalence, Nienhuis⁽¹⁹⁾ obtained very beautiful results for the critical exponents of thermodynamic quantities for the SAW on the hexagonal lattice. Other methods include extrapolation of exact enumeration results for short chains⁽¹⁵⁾ and renormalization group methods.⁽¹⁰⁾ Finally, Berretti and Sokal⁽⁴⁾ introduced a very efficient Monte Carlo algorithm to generate SAWs. They used it to calculate critical exponents, describing their error analysis in detail in Ref. 4.

In this paper, we use the algorithm introduced by Berretti and Sokal to generate the SAW on the hexagonal lattice (very often called a honeycomb in the literature). Although their algorithm is described briefly in Section 2, the interested reader is referred to their very detailed paper, since the discussion about estimating statistical and systematic errors is not reproduced here.

Our choice of the hexagonal lattice was dictated by the following considerations:

1. Nienhuis, under some plausible assumptions, obtained results on the effective coordination number μ and the critical exponents γ and ν for the hexagonal lattice thanks to the low value of the coordination number ($q = 3$) for this specific lattice. However, no direct simulation has performed to test the plausibility of Nienhuis' conjecture.³

2. The more difficult parts in a numerical experiment are the data analysis and the correct estimation of errors. However, here we have two

³ Nienhuis' value for μ has very recently been confirmed by an exact solution of Baxter (to appear in *J. Phys. A*). However, this work does not shed any light on γ and ν .

alternative approaches. First, we can ignore completely the prediction for μ and perform a maximum likelihood estimate for both μ and γ from the experimental data. Second, we can take for granted the value of μ and use it as input to extract the value of the critical exponent γ from the data. Both approaches are used and the results are compared.

3. Our ultimate goal is to check the hyperscaling relations in three dimensions, which involve two other critical exponents α and Δ_4 . Here we try to measure α in two dimensions and check the first of these relations, $d\nu = 2 - \alpha$. It is still an open question whether the second hyperscaling relation, which is almost rigorously established in two dimensions, fails in three dimensions. Hence, besides the interest per se of the present simulation for checking the correctness of the Nienhuis conjecture, this relatively easy case provides a consistent check of our methodology.

In Section 2 we describe briefly the algorithm use and give the details of the simulation. In Section 3, the method of data analysis is described and the results are presented. In Section 4, the results are compared with the literature and some considerations for further developments are given.

2. THE ALGORITHM

Let q denote the coordination number ($q=3$ for the hexagonal lattice). Fix a real number β , called the monomer activity, for reasons that will become apparent later. Then, the algorithm⁽⁴⁾ (see Ref. 20 for a distinct, but closely related algorithm) goes as follows:

Start from the walk of length $L=0$ (empty walk) anchored at the origin. Repeat many times:

Choose a random number r uniformly distributed in $[0, 1]$ and compare this number with $r_0 = (1 + q\beta)^{-1}$.

If $r > r_0$
 then choose with probability $1/q$ one of the q *a priori* possible directions and try to append a bond in this direction;
 if the corresponding walk is self-avoiding
 then effectively append the bond;
 else consider the previous walk once more;
 else try to delete the last bond;
 if the initial walk is empty
 then consider the empty walk once more;
 else effectively delete the last bond.

The elementary moves of the algorithm are thus extremely simple. Clearly, this algorithm produces SAWs starting at the origin and ending anywhere

on the lattice. Let c_L denote the number of such SAWs with length L and let $\Xi(\beta)$ be the corresponding grand partition function at monomer activity β , i.e.,

$$\Xi(\beta) = \sum_{L=0}^{\infty} \beta^L c_L \quad (2.1)$$

It is easy to show that the elementary moves of the algorithm satisfy the detailed balance condition and that the algorithm is ergodic. Hence, it admits (2.1) as its unique equilibrium probability distribution.

There exists a positive real β_c for which the mean length $\langle L \rangle$ computed from (2.1) diverges. Hence, for $\beta \rightarrow \beta_c$, very long chains i.e., $L \rightarrow \infty$, are very probable. Scaling behavior is expected for $L \rightarrow \infty$. To be precise, c_L is believed to behave as

$$c_L \sim \mu^L L^{\gamma-1} \quad \text{for } L \rightarrow \infty \quad (2.2)$$

where μ is the effective coordination number. The Cartesian end-to-end distance r_L [defined precisely in Eq. (2.6) below] is believed to behave as

$$\langle r_L \rangle \sim L^{\nu} \quad \text{for } L \rightarrow \infty \quad (2.3)$$

The number $c_L(x)$ of walks of length L starting at the origin and ending at x is believed to behave as

$$c_L(x) \sim \mu^L L^{\alpha-2} \quad \text{for } L \rightarrow \infty \quad (2.4)$$

It should be stressed that the β dependence of the problem is fully specified in (2.1), and that c_L , r_L , etc., are purely geometrical constants.

In relations (2.2) and (2.3), γ and ν are critical exponents. The numbers μ and ν have a very simple intuitive interpretation, which can be clarified by comparison with ordinary random walks. For an ordinary random walk all q directions are equally probable for appending a bond at the end of the walk. Hence, in that case we must have $\mu = q$. Here, due to the self-avoidance condition, there is a kind of self-repulsion of the walks. On the average, there are $\mu < q$ (actually $\mu < q - 1$) possible directions for appending a bond; hence, μ is called the effective coordination number. Similarly, for an ordinary random walk, the exponent ν has the well-known value $1/2$ (drunkard walk). On the other hand, for a deterministic walk, ν must have the value 1. Here, the value of ν must interpolate between these two extreme values.

The mean length can be computed from (2.1) and (2.2) and is given by

$$\langle L \rangle \approx \frac{\beta \gamma}{\beta_c - \beta} \quad \text{as } \beta \uparrow \beta_c \quad (2.5)$$

This relation exhibits the divergence of $\langle L \rangle$ mentioned at the beginning of this section.

The only relevant feature of the hexagonal lattice for that simulation is its topology uniquely characterized by its coordination number. Hence, we used a mapping of the hexagonal lattice to a rectangular one with the same coordination number, as shown in Fig. 1. This trick saves computing time by handling computer integers instead of floating point coordinates. The Cartesian distance r in terms of integer coordinates x and y is expressed easily by the following formula:

$$r = \left(\frac{3}{2}x^2 + \left\{ \frac{3}{2}y - \frac{1}{2}[(x+y) \bmod 2] \right\}^2 \right)^{1/2} \quad (2.6)$$

In order to test the self-avoidance condition, a site occupation map was stored in memory, i.e., a 1024×1024 bit matrix. Each matrix element corresponds to a point of the rectangular lattice of Fig. 1 and is set to 0 or 1 according to the nonoccupation or occupation of the corresponding site. The occupation map is updated at every Monte Carlo step. The essential advantage of this method is that testing the self-avoidance condition needs a short time independent of the actual length L of the walk.

Computers used for this simulation include an Olivetti PC without math-coprocessor programmed in assembly language, a Norsk-Data 500, and the CRAY-1S at CCVR near Paris, programmed in FORTRAN. The mean time for an elementary step of the algorithm is $2.3 \mu\text{sec}$ on the CRAY-1S, $60 \mu\text{sec}$ on the Norsk-Data, and $85 \mu\text{sec}$ on the Olivetti PC.

The main run was performed at $\beta = 0.54$ and the mean length found to be 635 at that monomer activity. The price to pay for being so close to the critical activity is that the autocorrelation time is very large. Berretti and Sokal⁽⁴⁾ observed that the autocorrelation time for the square lattice behaves as $\tau \sim 5\langle N \rangle^2$. If a similar behavior holds for the hexagonal lattice, the autocorrelation time must be 2×10^6 . Sokal and Thomas⁽²²⁾ have

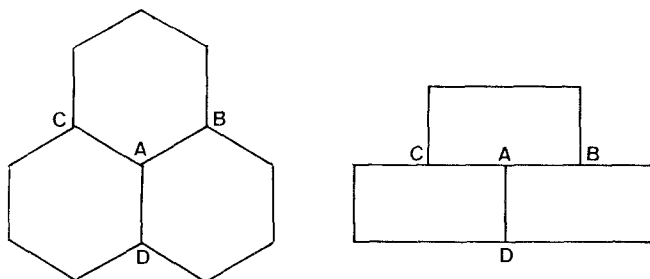


Fig. 1. The mapping of the hexagonal into the rectangular lattice.

recently proven that the autocorrelation time for the hexagonal lattice must behave as $\tau \gtrsim 5.81 \langle N \rangle^2$. It proved extremely difficult to determine this quantity from our data in order to decide how sharp is the bound found by Sokal and Thomas⁽²²⁾; in any case, $\tau > 10^6$.

We performed 10,146,120,000 iterations and data for the coordinates of end points and length of the walk were stored on disk every 30,000 iterations, thus giving 338,204 records. We used periodic boundary conditions, but the map matrix was so huge that it is highly unlikely that the walk touched the boundary even once during the 10^{10} iterations. During all the subsequent analysis the first 38,024 records were always discarded. This corresponds to approximately 600 autocorrelation times; hence, the system may be considered as having reached thermal equilibrium.

3. DETERMINATION OF THE CRITICAL EXPONENTS

In analyzing the data, we followed the article of Berretti and Sokal.⁽⁴⁾ We used their method to determine the critical exponents. In all subsequent analysis when we have to estimate probabilities $p(C)$ for a condition C we estimate it by sample probabilities

$$p(C) = |S(C)|/|S| \quad (3.1)$$

where $S(C)$ is the subset of the sample S satisfying condition C and $|\cdot|$ denotes cardinality.

3.1. Estimating the Exponent ν

The relation (2.3) is expected to hold only asymptotically for $L \rightarrow \infty$. However, in any computer experiment L is finite; hence (2.3) is only approximately valid. Some corrections to scaling must be taken into account. The deviations from exact scaling were taken into account by using one of the following forms:

$$\log(\langle r_L^2 \rangle + k_1) = a + 2\nu \log(L + k_2) \quad \text{for } L > L_{\min} \quad (3.2)$$

or

$$\log(\langle r_L^2 \rangle + k'_1 L^{2\nu_0}) = a' + 2\nu' \log(L + k'_2) \quad \text{for } L > L_{\min} \quad (3.3)$$

Here, $\langle r_L^2 \rangle$ is the observed mean value of r_L^2 for chains in the sample having length exactly L , ν_0 is a guess for ν (in our case $\nu_0 = 3/4$), and k_1 ,

k'_1, k_2, k'_2 are positive constants, which take into account deviations from (2.3) phenomenologically. We tried various values of these parameters, the best choice being the one that makes the result ν as independent as possible of the value of L_{\min} .

Using (3.2) or (3.3), we performed a two-parameter least-squares fit; the results are

$$\nu = 0.7580 \pm 0.0049 \pm 0.0046 \tag{3.4}$$

$$\nu' = 0.7420 \pm 0.0055 \pm 0.0052 \tag{3.5}$$

The first error in (3.4) and (3.5) represents the systematic error, taken equal to the difference between extreme values of ν and ν' obtained for various k and L_{\min} . The range of L_{\min} used to determine the systematic error is 25–100, The central value reported corresponds to $L_{\min} = 50$. The next error is the statistical one. It is chosen to provide 95% confidence limits and is computed by using $L_{\min} = 50$ data. The method suggested in Ref. 4 to extract the autocorrelation time of the algorithm by checking the exponential decay of the autocorrelation function proved impracticably noisy. Therefore, we resorted to binning our results to ten bins of 30,000 data points (i.e., 9×10^8 Monte Carlo iterations) each, which were considered independent.

It is worth noting that the value of ν predicted by Nienhuis ($\nu = 3/4$) lies within one *total* standard deviation from both central values ν and ν' . Besides, it seems that formula (3.2) has a tendency to systematically overestimate ν and (3.3) to underestimate it.

3.2. Estimating μ and the Exponent ν

The algorithm used produces SAWs distributed according to the grand canonical ensemble (2.1) at monomer activity β ; hence,

$$\text{Prob}(\text{length} = L) = \text{const} \times \beta^L c_L \tag{3.6}$$

Using relation (2.2), this expression becomes

$$\text{Prob}(\text{length} = L) = \text{const} \times (\beta\mu)^L L^{\nu-1} \tag{3.7}$$

Now, Eq. (3.7) is expected to hold only asymptotically for $L \rightarrow \infty$. In order to take into account the corrections to scaling, we introduce a phenomenological parameter k and we estimate the probability by the sample probability as in (3.1). Thus, instead of (3.7), we use the relation

$$p(\text{length} = L | L \geq L_{\min}) = \text{const} \times (\beta\mu)^L (L + k)^{\nu-1} \tag{3.8}$$

to extract information from the experimental data. Now we have two alternatives. Either assume the correctness of Nienhuis' prediction for $\mu = (2 + 2^{1/2})^{1/2}$ and make a one-parameter maximum likelihood fit with 3.8 to extract γ , or make a two-parameter fit to compute both μ and γ . The two alternatives were used and the results are, respectively,

$$\begin{aligned}\mu &= (2 + 2^{1/2})^{1/2} = 1.847759\dots \\ \gamma &= 1.3459 \pm 0.0040 \pm 0.0008\end{aligned}\tag{3.9}$$

and

$$\begin{aligned}\mu &= 1.84779 \pm 0.00006 \pm 0.00017 \\ \gamma &= 1.3509 \pm 0.0057 \pm 0.0023\end{aligned}\tag{3.10}$$

These relations must be interpreted as a confirmation of the Nienhuis conjecture. The systematic and statistical errors are computed as previously.

For completeness, we plot in Fig. 2 the curve $\langle r_L^2 \rangle + k$ versus $L + k'$

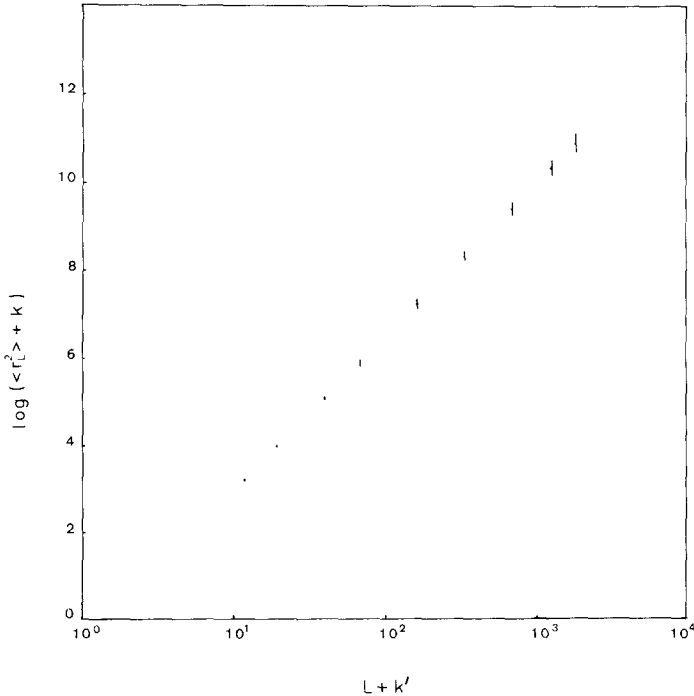


Fig. 2. Plot of $\log(\langle r_L^2 \rangle + k)$ versus $L + k'$.

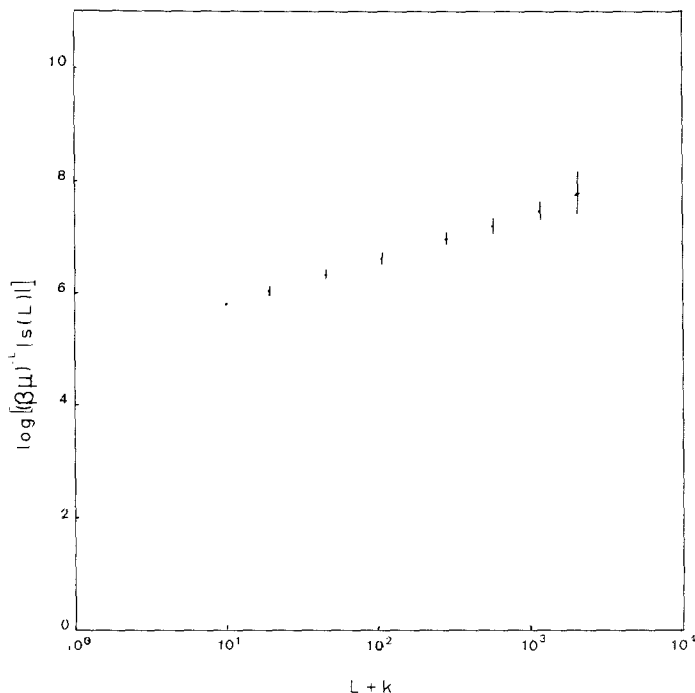


Fig. 3. Plot of $\log[(\beta\mu)^{-L}|S(L)|]$ versus $L+k$.

on a log-log scale for $k = k' = 2.5$, where $\langle r_L^2 \rangle$ is the observed mean value of r_L^2 for chains in the sample having length exactly L . In Fig. 3 we plot $(\beta\mu)^{-L}|s(\text{walks } L)|$ versus $L+k$ on a log-log scale for $k = 2$.

3.3. Estimating the Exponent α

In principle, α can be estimated from (2.4) by considering a subsample of walks with a fixed end-to-end distance $|x|$. Such a subset, however, proves too small for statistical purposes, and does not make use of most of the Monte Carlo information. Actually, the algorithm used is not the best one for extracting information about α ; a much more efficient algorithm for computing this particular exponent is described in Ref. 3.

However, in order to have some rough estimation of the exponent α , we used the following trick. Instead of considering walks with fixed end-to-end distance $|x|$, we consider the set of walks with $|x| \leq r_{\max}$.

Now, (2.4) is expected to hold only for $L \rightarrow \infty$; therefore, we introduce phenomenological corrections by fitting $|s(|x| \leq r_{\max})|$ to the form

$$|s(|x| \leq r_{\max})| \sim f(x) \mu^L L^{\alpha-2} \quad \text{for } L \rightarrow \infty \quad (3.11)$$

where for $f(x)$ we choose $f(x) \sim x^\delta$. The parameter δ is adjusted to make the fitted value of α as independent as possible of r_{\max} .

There is no strong argument to choose this special form for $f(x)$, nor do we claim that it is the best one. It is, however, plausible, since, if hyperscaling $d\nu = 2 - \alpha$ is assumed, then

$$c_L(|x|)/c_L \sim L^{-d\nu} f(|x|/L^\nu) \tag{3.12}$$

and

$$f(y) \sim y^\delta \quad \text{for } y \rightarrow 0 \tag{3.13}$$

$$f(y) \sim \exp(-y^\rho) \quad \text{for } y \rightarrow \infty \tag{3.14}$$

Therefore, we choose ad hoc the form

$$|s(|x| \leq r_{\max})| \sim x^\delta \mu^L L^{\text{some power}} \tag{3.15}$$

The parameter δ is adjusted to make the estimate of the power of L as independent as possible of r_{\max} . In this way we obtain

$$\alpha = 0.519 \pm 0.082 \pm 0.077 \tag{3.16}$$

r_{\max} is chosen in the range 4–12 and central value and statistical errors are obtained for $\delta = 0.22$ and $r_{\max} = 8$. In this fitting procedure μ and ν were fixed to the values $\mu = (2 + 2^{1/2})^{1/2}$ and $\nu = 3/4$.

4. DISCUSSION AND FURTHER DEVELOPMENTS

The results obtained so far are in agreement within less than one standard deviation with Nienhuis' conjecture. Table I compares different results

Table I. Comparison of Results

Method	μ	γ	ν	α
Extrapolation	1.8477	1.344	0.747 ± 0.001	—
Renormalization group	—	1.352	0.7603 ± 0.0002	—
Exact result conjectured	1.84779	1.3438	0.7500	0.5000
Present Monte Carlo	1.84779 ± 0.00066 ± 0.00017	1.3509 ± 0.0057 ± 0.0023	0.7580 ± 0.0049 ± 0.0046	0.519 ± 0.082 ± 0.077

in the literature. This table is not exhaustive. More complete results can be found in Ref. 4. We believe that these results completely support Nienhuis' conjecture, and provide rough numerical evidence for the first hyperscaling relation

$$dv = 2 - \alpha \quad (4.1)$$

However, we want to pursue our work to check the second hyperscaling relation,

$$dv - 2\Delta_4 + \gamma = 0 \quad (4.2)$$

A hyperscaling inequality of the form $dv - 2\Delta_4 + \gamma \leq 0$ is established⁽¹⁾ for the two-dimensional SAW. The other half of the inequality, namely $dv - 2\Delta_4 + \gamma \geq 0$, is not established, but is generally accepted as true. No proof exists generally in three dimensions. It is even believed by some (probably a minority) that it fails for $d=3$. In any case, Sokal has proven⁽²¹⁾ that it fails if $dv > 2$, which is believed to occur for $d > 4$ (and only then). The central problem is therefore the calculation of the critical exponent Δ_4 . The exponent Δ_4 is associated with the probability of intersection of two independent random walks of length L starting at different sites. The number d_L of such intersecting walks behaves as

$$d_L \sim \mu^{2L} L^{2\Delta_4 + \gamma - 2} \quad \text{for } L \rightarrow \infty \quad (4.3)$$

Calculations for Δ_4 , as well as μ , v , γ , and α , are in progress for the three-dimensional cubic lattice.

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