Journal of Statistical Physics, Vol. 49, Nos. 1/2, 1987

Critical Exponents for the Self-Avoiding Random Walk in Three Dimensions

Ph. de Forcrand[1], F. Koukiou,[2] and D. Petritis[2]

Received March 13, 1987; revision received May 22, 1987

We compute by direct Monte Carlo simulation the main critical exponents α, γ, Δ_4, and ν and the effective coordination number μ for the self-avoiding random walk in three dimensions on a cubic lattice. We find both hyperscaling relations $d\nu = 2 - \alpha$ and $d\nu - 2\Delta_4 + \gamma = 0$ satisfied in $d = 3$.

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

1. INTRODUCTION

The self-avoiding random walk (SAW) provides a nontrivial test for the theory of critical phenomena. First introduced as a model of organic polymers, it was shown by de Gennes[16] to occur as the $N \to 0$ limit of an $O(N)$ field theory with $(\phi \cdot \phi)^2$ interaction. The more interesting features of the SAW arise in two and three dimensions, since the repulsion due to the self-avoidance condition is strong enough to yield a critical behavior falling in a universality class different of that of the ordinary walk. In four dimensions the self-repulsion is much weaker, for topological reasons. The critical behavior of the SAW in $d = 4$ is expected to be essentially the same as for the ordinary random walk,[20] though some weak subdominant corrections to the critical exponents may occur. For $d \geqslant 5$ the behavior of the SAW is conjectured to be trivial, and this has recently been proven by Slade[30] for d sufficiently large. Moreover, Brydges and Spencer[10] have proven triviality for the "weakly self-avoiding" walk in $d \geqslant 5$, i.e., a kind of walk interpolating between ordinary and strict self-avoiding. The "weakly self-avoiding" walk is shown to follow the same trajectories as the ordinary

[1] CRAY Research Inc., Chippewa Falls, Wisconsin 54729.
[2] Institut de Physique Théorique, Université de Lausanne, 1015 Lausanne, Switzerland.

0022-4715/87/1000-0223$05.00/0

822/49/1-2-15

walk[31] in two dimensions, but it follows trajectories not having a density with respect to the Wiener measure in three dimensions, as shown in Ref. 32.[3]

Many methods have been used and even invented to treat this problem. Without being exhaustive, let us mention (in a random order): rigorous methods for a random walk representation of field theory,[2–4,8,9] probabilistic methods,[20–22] duality arguments,[24] extrapolation of exact enumeration of short walks,[17] renormalization group techniques,[12,23] Monte Carlo simulations,[4,6,7] and supersymmetry.[26]

Here we limit ourselves to the Monte Carlo simulation of a strict self-avoiding walk on a cubic lattice in three dimensions. The also nontrivial case of two-dimensional lattices is treated by Monte Carlo simulation by various authors[7,14]. The algorithm we use to generate the SAWs was introduced by Berretti and Sokal[7] and is the most efficient one as far as the autocorrelation time for long walks is concerned.

Since this paper is the continuation of our previous work,[14,15] we only sketch in Section 2 the manner in which critical exponents arise in the problem of SAWs. Then we present in Section 3 the way we did our analysis in order to extract the critical exponents. Finally, in Section 4 we compare our results with previous ones in the literature obtained by different methods.

2. THE CRITICAL EXPONENTS

We use the algorithm introduced in Ref. 7 to generate SAWs. This algorithm is ergodic, satisfies the detailed balance condition, and hence generates SAWs in a grand canonical ensemble at a fixed value of the monomer activity β. The self avoidance condition is tested by using a $200 \times 200 \times 200$ table monitoring site occupation.

We can tune the monomer activity β to obtain ensembles of walks with any value of the mean length $\langle N \rangle$ we wish. We chose $\beta = 0.21$ such that the mean length is approximately 80.

It is desirable to obtain walks as long as possible because in the limit of infinite length, $N \to \infty$, we have the following asymptotic properties:

(i) The number of walks c_N of length N starting at the origin and ending anywhere on the lattice behaves as

$$c_N \sim \mu^N N^{\gamma - 1} \tag{1}$$

[3] We thank Jean-François Le Gall for pointing out Ref. 32.

(ii) The number of walks $c_N(\mathbf{x})$ of length N starting at the origin and ending at point $\mathbf{x}$ behaves as

$$c_N(\mathbf{x}) \sim \mu^N N^{\alpha-2} \tag{2}$$

(iii) The end-to-end mean Euclidean distance $\langle r_N \rangle$ for walks of given length N follows

$$\langle r_N \rangle \sim N^{\nu} \tag{3}$$

(iv) Finally, the number of intersecting pairs d_N of independent SAWs, both walks hakving the same length N and starting anywhere, behaves as

$$d_N \sim \mu^{2N} N^{2\Delta_4+\gamma-2} \tag{4}$$

In these relations μ is a parameter, called the effective coordination number, depending solely on the lattice and dimension. It has to be determined just like the critical exponents α, γ, Δ_4, and ν. These exponents are not all independent, but are believed to obey hyperscaling relations, namely:

$$d\nu = 2 - \alpha \tag{5}$$

and

$$d\nu - 2\Delta_4 + \gamma = 0 \tag{6}$$

Relation (6) has a very controversial history. Using a high-temperature series expansion, Baker claimed that it fails for the Ising model in $d \geqslant 3$.[5] Subsequent work on the Ising model[13,18,25,27,33] attested to the validity of (6) for $d=3$. Aizenman[2] proved the hyperscaling equality $d\nu - 2\Delta_4 + \gamma = 0$ for the two-dimensional Ising model; the same argument proves the inequality $d\nu - 2\Delta_4 + \gamma \leqslant 0$ for the two-dimensional SAW. Des Cloizeaux[11] argued that (6) must fail if $d\nu > 2$ and Sokal[29] proved it. However, it is generally believed that $d\nu > 2$ occurs for $d > 4$ and only then. The rigorous proof of (6) for the SAW in $d < 4$ is still an open problem.

3. SIMULATION AND DETERMINATION OF THE CRITICAL EXPONENTS

We did 103,520,000,000 Monte Carlo steps and data for the end-point coordinates and length of the walk were stored every 10^4 steps. In analyzing our data, the first 352,000 records—corresponding to 3,520,000,000 Monte Carlo steps—were discarded in order to allow the system to thermalize. Moreover, during the last fraction of the simulation the complete walks were saved and sorted by length.

The simulation was performed on a CRAY-XMP computer at CRAY Research and the analysis on a NORSK DATA 570 at Lausanne. The mean time needed for one Monte Carlo step is about $0.5\,\mu sec$.

We did an extensive study of the autocorrelation time τ for various observables. This parameter plays an important role in computing the statistical errors and is crucial for the validity of the method for determining Δ_4.

The use of the autocorrelation time for a sequence of random variables presupposes that the truncated correlation function of this sequence decays exponentially, asymptotically for large time. For instance, to determine τ for the random variable length N, we use the asymptotic exponential decay of the truncated correlation function $C_{NN}(t) = \langle N_i N_{i+t} \rangle - \langle N \rangle^2$. Using our data $\{N_i\}$, $i = 1,..., n_{\max}$, we compute an unbiased estimator of the truncated correlation function $C_{NN}(t)$, namely $\hat{C}_{NN}(t)$ given by

$$\hat{C}_{NN}(t) = \frac{1}{n_{\max} - t} \sum_{i=1}^{n_{\max}} N_i N_{i+t} - \langle N \rangle^2 \tag{7}$$

Applying the hypothesis of asymptotic exponential decay, we get for the autocorrelation time τ:

$$\tau \approx -\lim_{t \to \infty} \frac{t}{\ln[\hat{C}_{NN}(t)/\hat{C}_{NN}(0)]} \tag{8}$$

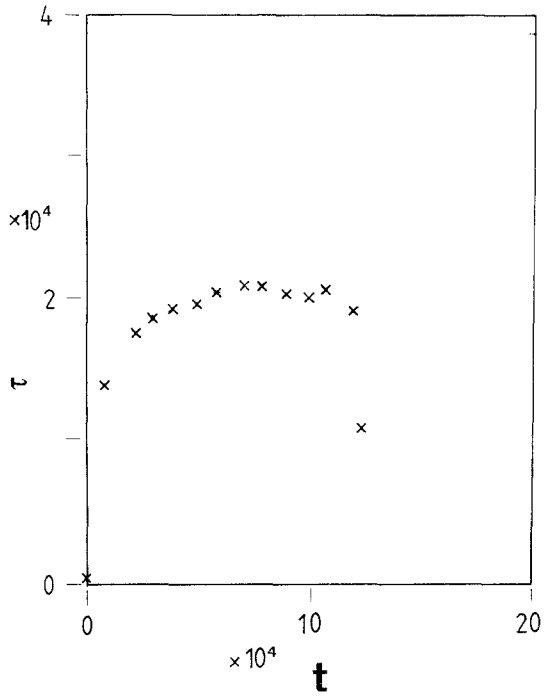

Fig. 1. Plot of τ as a function of t. The reach of the asymptotic plateau is evident. (See Ref. 8.)

In practice the numerically evaluated τ is an increasing function of t that is expected to attain asymptotically a constant value before it disappears in the statistical noise. In Fig. 1 we present τ as a function of t for the random variable N.

Typically we get for the autocorrelation time τ the value $\tau \sim 2 \times 10^4$.

It is expected that $\tau \sim \kappa \langle N \rangle^2$; hence $\kappa \sim 4$, and the information about the walk of length N will be lost after $2\tau \sim 8\langle N \rangle^2$ steps.

3.1. Computing μ and Exponents γ and ν

For determining μ and the exponents γ and ν we used the standard method.[7] Recall that relation (1) is used to determine two parameters, μ and γ; the most efficient method to compute them is a maximum likelihood fit. It is worth noting that it is possible to use a three-parameter least square fit; although it may give a more or less reliable estimate for μ, the value of γ can be completely wrong. For a discussion of this effect, occurring in a similar situation, see Ref. 1. Hence we use a maximum likelihood fit on relation (1) to get μ and γ and a least square fit on relation (3) to compute ν. We get

$$\mu = 4.68323 \pm 0.00099 \pm 0.00017$$

$$\gamma = 1.1756 \pm 0.0062 \pm 0.0080$$

$$\nu = 0.5745 \pm 0.0087 \pm 0.0056$$

(The format of these results is: parameter = central value $\pm$ systematic error $\pm$ statistical error. The total error provides 67% confidence intervals.)

The systematic error is due to corrections to scaling, formulas (1) and (3) being only asymptotically true for $N \to \infty$. The fact that we use finite walks introduces corrections that are taken into account phenomenologically as explained in Refs. 7 and 14. The statisticl error is given by the standard theory of maximum likelihood fit. However, this naive error is multiplied by a factor $(2\tau)^{1/2}$ in the above results to take into account the correlation of the data.

The reader can judge the asymptotic behavior in Fig. 2, which plots $\ln c_N - N \ln(\beta\mu)$ as a function of $\ln N$, and Fig. 3, which gives $\ln\langle r_N \rangle$ versus $\ln N$.

3.2. Computing α

The algorithm used for the simulation is not the most appropriate for the computation of the exponent α, since it does not keep the end of the

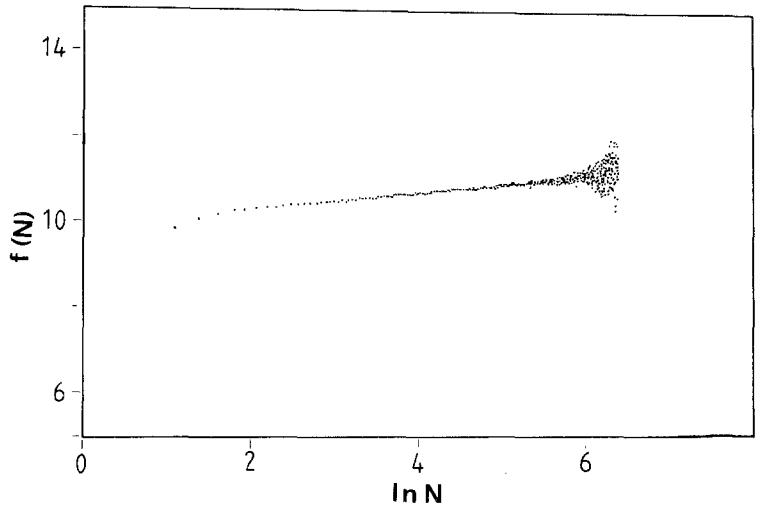

Fig. 2. Plot of $f(N) = \ln c_N - N \ln(\beta\mu)$ as a function of N.

walk fixed. A better algorithm for that particular exponent is the one introduced in Ref. 4. However, the algorithm of Ref. 4 has a much greater autocorrelation time; hence it is desirable to extract even some poor information contained in our data. In the following we explain how the information is extracted from our data. We are aware that an independent simulation using another algorithm is needed for the determination of α.

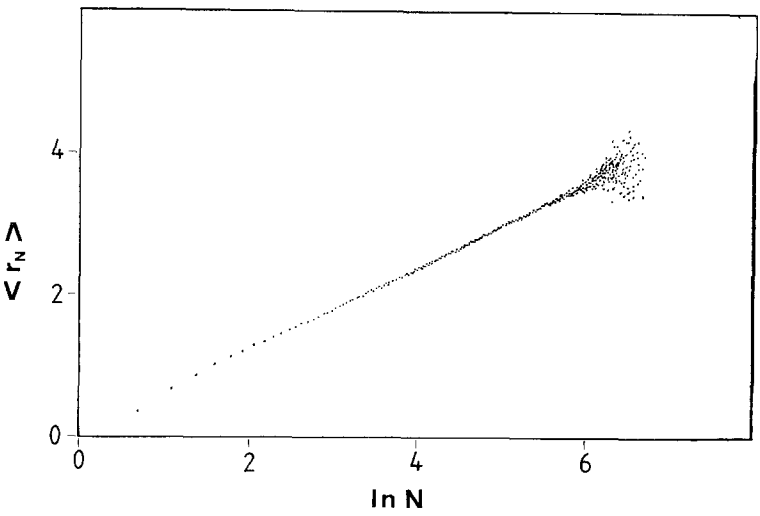

Fig. 3. Plot of $\ln\langle r_N \rangle$ versus $\ln N$.

The computation of the exponent α is simpler in the present case than that encountered in our previous two-dimensional case[14] since the statistics is better here and data are more independent.

We only use the rotational symmetry of the problem to integrate over spheres of given radius. Namely, asymptotically for large N, $c_N(\mathbf{x})$ does not depend on $\mathbf{x}$, but only on $x = |\mathbf{x}|$. Hence, the data are sorted according to the Euclidean end-to-end distance into $c_N(x)$. We use the value of μ determined by the maximum likelihood fit in relation (1) to extract by a least square fit the value of α from (2). Moreover, we impose a lower cutoff on the value of N to be sure that the asymptotic regime is attained. The fit is done for various values of x ranging from 1 to 10 and the mean is taken on the different α's computed. The most difficult part of this fit is the determination of the lower cutoff for N. We did various least square fits for different values of the cutoff. We chose, for each value of x, the fit that minimizes the least square function divided by the population of the sample after cutoff. Figure 4 provides the plot of $\ln c_N(x) - N \ln(\beta\mu)$ versus $\ln N$ for $x = 3$. We get (in the usual format)

$$\alpha = 0.275 \pm 0.010 \pm 0.005$$

For the analysis of α it would be possible to integrate our data over x between $x_{\min}$ and $x_{\max}$. This precedure does not affect the central value of α very significantly, provided one correctly chooses the lower cutoff; however, this choice becomes more and more subjective; so the total error does not improve.

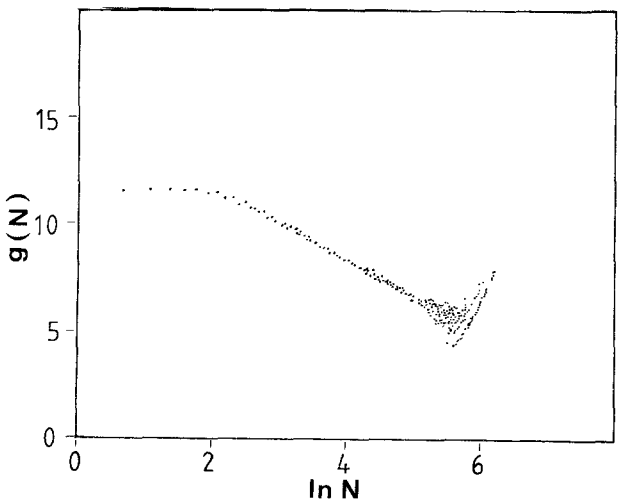

Fig. 4. Plot of $g(N) = \ln c_N(x) - N \ln(\beta\mu)$ versus $\ln N$ for $x = 3$.

3.3. Computation of Δ_4

The computation of Δ_4 was sketched in Ref. 15. It goes as follows. Walks of equal length (stored in separate files for each length) are compared pairwise and the distinct translations of one walk with respet to the other that lead to an intersecting pair are counted exhaustively. (This procedure is carried out for walks of many different lengths.) One can easily see by combining relations (1) and (4) that the average number of translates of one walk that overlap with the other walk behaves as

$$I_N \sim N^{2\Delta_4 - \gamma} \tag{9}$$

In order for the intersections in (9) to be meaningful, it is crucial to ensure the independence of walks in each file of given length. Some evidence of independence can be found in Fig. 5, where we plot the mean distance between reappearances of the same length, as a function of length. It turns out that this distance is of the order of 10^6 Monte Carlo steps. (This is because we sample once every 10^4 Monte Carlo steps. Hence it is very improbable to obtain two walks of exactly the same length in successive data points.) A least square fit on relation (9) (remark that I_N is *independent* of μ) gives

$$2\Delta_4 - \gamma = 1.7317 \pm 0.0074 \pm 0.0074$$

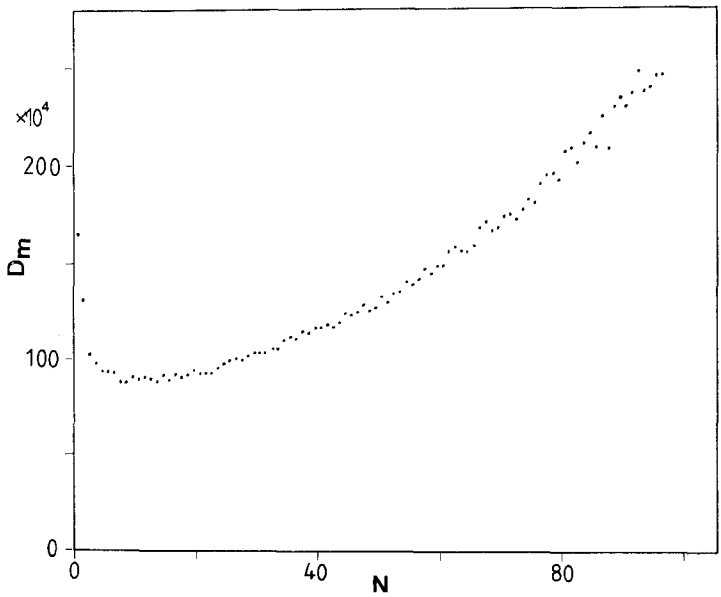

Fig. 5. Plot of the mean distance D_m of reappearance of walks of length N as a function of N.

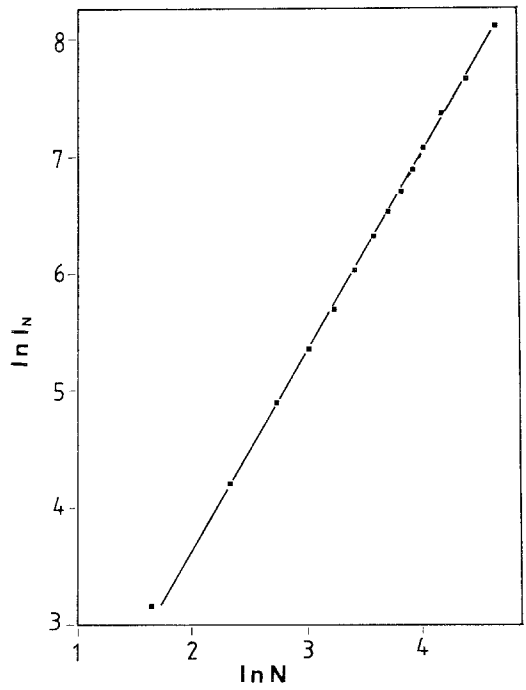

Fig. 6. Plot of $\ln I_N$ as a function of $\ln N$. The straight line corresponds to the case where hyperscaling is assumed correct.

In Fig. 6 we exhibit the values of $\ln I_N$ versus $\ln N$ for the different lengths where intersections are tested. The straight line is the expected one if hyperscaling is valid.

4. CONCLUSION

Table I compares the results of the present work with previous ones found in the literature. Our error bars are larger than the ones quoted in the literature. In order to lower them,simulations of much longer walks are needed, but, then, to get rid of the increase in the autocorrelation time, one has to perform much more Monte Carlo steps. We hope our results shed light on the long controversy about hyperscaling relations in three dimensions. Both of them are satisfied with good accuracy.

For the first hyperscaling relation we find

$$d\nu - 2 + \alpha = -0.0015 \pm 0.028 \pm 0.017$$

However, our value for α lies three standard deviations away from other quoted values for this parameter. We do not claim that our method to

Table I. Comparison of Our Results with Literature

Parameter	Series extrapolation	Previous MC	Field-theoretic RG	Present work
μ	4.68391 ± 0.00022[a]			$4.68323 \pm 0.00099 \pm 0.00017$
γ	1.162 ± 0.002[18]		1.1615 ± 0.0015[23]	$1.1756 \pm 0.0062 \pm 0.0080$
ν	0.592 ± 0.002[18]	0.592 ± 0.001[28]	0.588 ± 0.001[23]	$0.5745 \pm 0.0087 \pm 0.0056$
α	0.224 ± 0.006[a]		0.236 ± 0.003[23]	$0.275 \pm 0.010 \pm 0.005$
Δ_4	1.469 ± 0.003[a]		1.463 ± 0.002[23,b]	$1.4537 \pm 0.0048 \pm 0.0037$

[a] If hyperscaling is assumed valid.

[b] Hyperscaling is *implicit* in the field-theoretic renormalization group.

compute α is the best one; the algorithm of Ref. 4 is much more appropriate. In order to judge if the validity found for the first hyperscaling relation is a matter of chance, a more accurate determination of ν is needed, since the error bars of ν are multiplied by the dimensionality of the space ($d=3$ in our case).

For the second hyperscaling relation we find

$$d\nu - 2\Delta_4 + \gamma = -0.0082 \pm 0.027 \pm 0.018$$

The value 0 lies within less than a standard deviation of the statistical or systematic error from our central value. We think that the famous result of Baker[5] for the Ising model, which was at the origin of this controversy ($d\nu - 2\Delta_4 + \gamma = 0.038 \pm 0.012$), has very optimistic error bars.

Moreover, the computation of $2\Delta_4 - \gamma$ provides an indirect measurement of Δ_4, which has never been done.

ACKNOWLEDGMENTS

We wish to thank Alan Sokal for useful discussions and correspondence and for his interest in our work. D.P. was supported by the Swiss National Science Foundation.

REFERENCES

1. J. Ambjørn, Ph. de Forcrand, F. Koukiou, and D. Petritis, *Monte Carlo simulations of triangulated random surfaces*, Preprint, Lausanne University (1987).
2. M. Aizenman, *Commun. Math. Phys.* **86**:1–48 (1982).
3. M. Aizenman, *Commun. Math. Phys.* **97**:91–110 (1985).
4. C. Aragão de Carvalho, S. Caracciolo, and J. Fröhlich, *Nucl. Phys. B* **215**:209–248 (1983).
5. G. A. Baker, Jr., *Phys. Rev. B* **15**:1552–1559 (1975).
6. B. Baumann, *Noncanonical path and surface simulation*, DESY Preprint 86–134 (1986).
7. A. Berretti and A. D. Sokal, *J. Stat. Phys.* **40**:483–531 (1985).
8. D. C. Brydges, J. Fröhlich, and T. Spencer, *Commun. Math. Phys.* **83**:123–150 (1982).
9. D. C. Brydges, J. Fröhlich, and A. D. Sokal, *Commun. Math. Phys.* **91**:141–186 (1983).
10. D. C. Brydges and T. Spencer, *Commun. Math. Phys.* **97**:125–148 (1985).
11. Des Cloizeaux, private communivation, cited by E. Brézin, in *Order and Fluctuations in Equilibrium and Noneequilibrium Statistical Mechanics* (17th Solvay Conference 1978), G. Nicolis, G. Dewel, and J. W. Turner, eds. (Wiley-Interscience, New York, 1981).
12. B. Derrida, *J. Phys. A: Math. Gen.* **14**:L5–L9 (1981).
13. M. E. Fisher and Jing-Huei Chen, *J. Phys. (Paris)* **46**:1645–1654 (1985).
14. Ph. de Forcrand, F. Koukiou, and D. Petritis, *J. Stat. Phys.* **45**:459–470 (1986).
15. Ph. de Forcrand, F. Koukiou, and D. Petritis, *Phys. Lett. B* **189**:341–342 (1987).
16. P. G. de Gennes, *Phys. Lett.* **38A**:339–340 (1972); *Scaling Concepts in Polymer Physics* (Cornell University Press, Ithaca, New York, 1979).
17. A. J. Guttmann, *J. Phys. A: Math. Gen.* **17**:455–468 (1980).
18. A. J. Guttmann, *Phys. Rev. B* **33**:5089–5092 (1986).

19. A. J. Guttmann, *On the critical behaviour of self-avoiding walks*, University of Melbourne preprint (1986).
20. G. F. Lawler, *Duke Math. J.* **47**:655–693 (1980).
21. G. F. Lawler, *Commun. Math. Phys.* **86**:539–554 (1982).
22. G. F. Lawler, *Commun. Math. Phys.* **97**:583–594 (1985).
23. J. C. LeGuillou and J. Zinn-Justin, *Phys. Rev. B* **21**:3976–3998 (1980).
24. B. Nienhuis, *Phys. Rev. Lett.* **49**:1062–1064 (1982).
25. B. G. Nickel and B. Sharpe, *J. Phys. A: Math. Gen.* **12**:1819–1834 (1979).
26. G. Parisi and N. Sourlas, *J. Phys. Lett. (Paris)* **41**:L403–L406 (1980).
27. J. J. Rehr, *J. Phys. A: Math. Gen.* **12**:L179–L183 (1979).
28. D. C. Rapaport, *J. Phys. A: Math. Gen.* **18**:113–126 (1985).
29. A. D. Sokal, unpublished result.
30. G. Slade, The diffusion of self-avoiding walk in high dimensions, University of Virginia preprint (1986).
31. S. R. S. Varadhan, Appendix to the course by K. Symanzik, *Euclidean Quantum Field Theory* (Academic Press, New York, 1969).
32. M. J. Westwater, *Commun. Math. Phys.* **72**:131–174 (1980).
33. J. Zinn-Justin, *J. Phys. (Paris)* **40**:969–975 (1979).