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Critical Exponent for the Loop Erased Self-Avoiding Walk by Monte Carlo Methods

A. J. Guttmann[1] and R. J. Bursill[1]

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A Monte Carlo simulation was performed for loop-erased self-avoiding walks (LESAW) to ascertain the exponent ν for the $\mathbf{Z}^2$ and $\mathbf{Z}^3$ lattices. The estimated values were $2\nu = 1.600 \pm 0.006$ in two dimensions and $2\nu = 1.232 \pm 0.008$ in three dimensions, leading to the conjecture $\nu = 4/5$ for the two-dimensional LESAW. These results add to existing evidence that the loop-erased self-avoiding walks are not in the same universality class as self-avoiding walks.

KEY WORDS: Loop-erased SAWS; Monte Carlo; critical exponent; universality class; critical behavior; two dimensional; three dimensional.

1. INTRODUCTION

The problem of self-avoiding walks (SAW) on lattices has been the subject of intense analytical and numerical study over many decades. Despite this, there remains a paucity of rigorous results for the nontrivial case of dimensionality greater than 1. Hammersley[(1)] has proved the existence of a finite, nonzero connective constant μ for the general d-dimensional hypercubic lattice, and Hammersley and Welsh[(2)] have proved that if $c_n(d)$ denotes the number of n-step d-dimensional SAW's then $c_n(d) \sim \mu(d)^n \exp[O(\sqrt{n})]$. For $d = 2, 3$ the existence of a critical exponent has not even been proved {this would correspond to a sharpening of the term $O(\sqrt{n})$ above to $O[\log(n)]$}. The existence of a critical exponent has been proved for d sufficiently large, and much progress has been made for the case $d > 4$ by Brydges and Spencer[(3)] and by Slade,[(4-6)] as discussed below.

A seminal model was proposed by Domb and Joyce,[(7)] which featured a variable interaction in which self-intersections were energetically

[1] Department of Mathematics, University of Melbourne, Parkville, Victoria 3052 Australia.

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unfavorable. The effect of increasing this interaction was then studied. More precisely, the random walk (RW) with repulsive interaction $w\delta_{ij}$ between sites i and j was considered, where δ is the Kronecker δ-function. Each pair of sites in every random walk configuration of N steps is weighted by the factor $(1+w\delta_{ij})$, the weight for the walk being the product of these weights. Then $w=0$ corresponds to a pure random walk, and $w=-1$ to a SAW. As w is varied between 0^- and -1, the walk is believed to be in the SAW universality class, changing discontinuously to the RW universality class at $w=0$. This model has greatly aided our understanding of SAWS, and underlies a number of rigorous calculations, including those of Brydges and Spencer cited above.

For "ordinary" SAWS, if $\langle R_n^2 \rangle$ denotes the mean square end-to-end distance, then we can write $\langle R_n^2 \rangle \sim n^{2\nu}$, where $2\nu=2$ for $d=1$, and Nienhuis[8,9] has shown nonrigorously but apparently exactly that $2\nu=3/2$ for $d=2$, in agreement with the earlier heuristic result of Flory[10] that $2\nu=6/(d+2)$ for $1 \leqslant d \leqslant 4$, with $2\nu=1$ for $d>4$. Remarkably, Flory's result appears to be correct for all dimensionality save $d=3$, where the best series,[11,12] renormalization group,[13] and Monte Carlo work[14] yields $2\nu=1.180 \pm 0.008$, which is less than 2% below the Flory prediction. Renormalization group theory predicts $\langle R_n^2 \rangle \sim n(\log n)^{1/4}$ (despite a number of erroneous statments in the literature to the effect that this exponent is 3/8), whereas for $d>4$ there is no logarithmic confluence (though for odd dimensionality there are nonanalytic correction-to-scaling terms[15]).

Various schemes to study the saw problem have been tried. Fisher and Sykes[16] considered approaching the SAW limit systematically by starting with the random walk problem and forbidding r-gons, and then considering the effect of increasing r. In that approach, the connective constant approaches the SAW limit μ monotonically with r, but the critical exponent remains unchanged, changing discontinuously only in the limit as $r \to \infty$. This reflects the abrupt change from a Markovian to a non-Markovian process. In another study, Klein[17] considered the connective constant of SAWS in a $(d-1)$-dimensional "strip" of width D. One finds, however, that the critical exponent is that of a $(d-1)$-dimensional SAW, with the connective constant monotonically approaching $\mu(d)$ as D increases. Again, the appropriate d-dimensional critical exponent is obtained only in the limit of infinite width, $D \to \infty$.

For the Domb–Joyce model, Brydges and Spencer[3] showed that $\nu=1/2$ for dimensionality $d>4$ and for w sufficiently small. They also prove that the endpoint distribution is Gaussian in that case. Slade[4] has proved that $\nu=1/2$ for the "true" SAW in sufficiently large dimension (that is, the SAW defined without recourse to the Domb–Joyce model). He has also proved[5,6] that under the same conditions, $\gamma = 1$ and the scaling limit of the SAW is Brownian motion.

The SAW (defined in Section 2) has associated with it a particular measure. A different model, the loop-erased SAW (LESAW) was introduced by Lawler.[18] This model (also defined below) has an entirely different associated measure. Informally, it can be most easily appreciated as the erasing of loops in ordinary random walks. If one takes an arbitrary, infinite-length random walk on a lattice and erases all loops (including immediate reversals), one clearly recovers a SAW. As (an infinite number of) different random walks can clearly produce the same SAW, the measure of such loop-erased self-avoiding walks is likely to be different. Additional care is required in two dimensions, where it is known that random walks are infinitely recurrent (but with an infinite recurrence time).

The LESAW is also of interest because of its connection with the Laplacian walk[19,20] and because of the rigorous results obtained by Lawler[21] for the critical properties of the LESAW on $d \geqslant 4$ hypercubic lattices. If it were found that the LESAW and the SAW lay in the same universality class, then these rigorous results would apply to the SAW. In this paper a Monte Carlo simulation is performed to determine the critical exponent ν for the LESAW on the square and simple cubic lattices. The value of ν for the SAW is 3/4 in $2d$ and 0.592 ± 0.003[11,12,14] by Monte Carlo and series work, and 0.588 ± 0.002[13] by renormalization group calculations in $3d$.

The loop-erasing algorithm is defined in Section 2, together with the critical exponent ν. In Section 3 the Monte Carlo simulation is described together with the results of this experiment.

2. DEFINITIONS

Let $\mathbf{N}$ denote the positive integers and zero. Let $\mathbf{Z}^p$ denote the hypercubic integer lattice in p dimensions and let d denote the Euclidean metric on $\mathbf{Z}^p$. The set of n-step random walks on $\mathbf{Z}^p$ for $n \in \mathbf{N}$ is defined as

$$R_n = \{t\colon \{0,..., n\} \to \mathbf{Z}^p\colon t(0) = 0 \;\&\; d(t(i+1), t(i)) = 1\} \tag{1}$$

The set of n-step self-avoiding walks on $\mathbf{Z}^p$ is defined as

$$S_n = \{t \in R_n\colon t(i) = t(j) \Rightarrow i = j\} \tag{2}$$

Let $S = \bigcup_{n \in \mathbf{N}} S_n$ be the set of all saws on $\mathbf{Z}^p$.

In obtaining an $N_n(t)$-step SAW $P_n(t)$ from an n-step random walk t, the loop-erasing algorithm (N_n, P_n) is applied and is inductively defined as follows: $(N_n\colon R_n \to \mathbf{N},\ P_n\colon R_n \to S)$. Let $t \in R_n$ and let $t_0 = t$ and $n_0 = n$. Suppose $n_k \in \mathbf{N}$ and $t_k \in R_{n_k}$ has been defined for some $k \geqslant 0$. If $t_k \in S$, then we are done. Define $P_n(t) = t_k$ and $N_n(t) = n_k$. Then $P_n(t) \in S_{n_k}$. Otherwise, let

$$m = \min\{i \in \{0,..., n_k\}: \exists j \in \{0,..., n_k\}: t_k(i) = t_k(j) \;\&\; i \neq j\}$$

and

$$l = \min\{j \in \{0,..., n_k\} \backslash \{m\}: t(j) = t(m)\}$$

Let $n_{k+1} = n_k - l + m$ and define $t_{k+1}: \{0,..., n_{k+1}\} \to \mathbf{Z}^p$ as follows:

$$\begin{aligned} t_{k+1}(i) &= t_k(i), \qquad & i &= 0,..., m \\ &= t_k(i + l - m), \qquad & i &= m+1,..., n_{k+1} \end{aligned} \tag{3}$$

The induction must terminate after no more than $n/2$ steps for n even or $(n-1)/2$ steps for n odd. Define the average number of steps remaining after loop erasure for n-step random walks as follows:

$$\langle N_n \rangle = (2p)^{-n} \sum_{t \in R_n} N_n(t)$$

as there are $(2p)^n$ n-step random walks on $\mathbf{Z}^p$.

Note that $\langle N_n \rangle \leqslant n$ as $N_n(t) \leqslant n$. Let

$$2v_n = \log n / \log \langle N_n \rangle \geqslant 1, \qquad \forall n > 1 \tag{4}$$

Define the critical exponent v_{LESAW} for the LESAW as lim sup v_n. Then $\langle N_n \rangle \sim n^{1/2v_{\text{LESAW}}}$ as $n \to \infty$ given that lim v_n exists. The critical exponent v for the SAW is defined as follows: The end-to-end squared distance of an n-step random walk t is defined as $r_n^2(t) = [d(t(n), t(0))]^2$. The average end-to-end squared distance of n-step SAWS is defined as

$$\langle r_n^2 \rangle_s = c_n^{-1} \sum_{t \in S_n} r_n^2(t)$$

where c_n is the number of n-step SAWS on $\mathbf{Z}^p$. Now let $2\tilde{v}_n = \log\langle r_n^2 \rangle_s / \log n \; \forall n > 1$. Then $\tilde{v}_n < 1 \; \forall n > 1$ by comparison with linear chains. Define the critical exponent v_{SAW} for the SAW as lim sup $\tilde{v}_n$. Then

$$\langle r_n^2 \rangle_s \sim n^{2v_{\text{SAW}}} \qquad \text{as} \quad n \to \infty \tag{5}$$

given that lim $\tilde{v}_n$ exists. If

$$\langle r_n^2 \rangle_l = (2p)^{-n} \sum_{t \in R_n} r_{N_n(t)}^2(P_n(t)), \qquad \langle r_n^2 \rangle_r = (2p)^{-n} \sum_{t \in R_n} r_n^2(t)$$

we then have the result that $\langle r_n^2 \rangle_l = \langle r_n^2 \rangle_r \sim n$ as $n \to \infty$ by the well-known random walk result, and the fact that $r^2_{N_n(t)}(P_n(t)) = r_n^2(t)$. Hence a qualitative correspondence between ν_{SAW} and ν_{LESAW} may be seen, given that $\lim \nu_n$ exists. Now $\langle N_n \rangle \sim n^{1/2\nu_{\mathrm{SAW}}}$ as $n \to \infty$ and thus $\langle N_n \rangle^{2\nu_{\mathrm{SAW}}} \sim n$ as $n \to \infty$ and hence $\langle r_n^2 \rangle_l \sim \langle N_n \rangle^{2\nu_{\mathrm{SAW}}}$ as $n \to \infty$, which is to be compared with (5).

There are other possible definitions of the critical exponent for LESAWS. Lawler[22] takes infinite LESAWS and considers the mean square distance from the nth point to the origin, $\langle r_n^2 \rangle$, and defines the exponent 2ν by $2\nu = \limsup \ln\langle r_n^2 \rangle / \ln n$. The infinite LESAW is in turn given by two equivalent definitions for $d \geqslant 3$. In the first definition, the loop-erasing algorithm is applied to an infinite random walk to yield an infinite LESAW. In the second definition, Lawler defines the LESAW by the transition probabilities at each step.

The second definition is modified to provide a definition of infinite two-dimensional LESAWS. This definition is not particularly practical as a constructive algorithm. An alternative definition of the LESAW and its exponents is required that does not depend on dimensionality. Such a construction is given by Lyklema and Evertsz, who define the LESAW by generating random walks starting at the origin and ending at the surface of a p-dimensional hypersphere, of radius M, centered at the origin. The loop-erasing algorithm is then applied, resulting in a LESAW of at least M steps. For $n \leqslant M$ a measure $P_{n,M}$ is generated on the n-step SAWS. Lawler[22] proved that $P_{n,n^3}(w) = P_n(w)[1 + O(1/\sqrt{n})]$, where $P_n(w)$ is the measure generated by Lawler's less practical definition, and the subdominant term is uniform over all SAWS w.

3. EXPERIMENT AND RESULTS

A Monte Carlo simulation was performed to monitor the behavior of $\langle N_n \rangle$ in what was hoped to be the asymptotic region and to thus to numerically determine the existence of ν_{LESAW} and its value on the square and simple cubic lattices.

A total of 170,000 random walks, each of 204,800 steps in both two and three dimensions, were generated using a Fortran program which was essentially a linear congruential random number generator with an approximate cycle time of 10^{11}. Loops were erased from the random walks as they occurred. That is, the program noted whether each new point on the walk had been visited before, and if so, erased the loop, constantly keeping track of the number of self-avoiding steps. This is equivalent to performing the loop-erasing algorithm defined in Section 2 after the random walks have been generated. $N_n(t)$ was recorded after n random steps for, $n = 400$, 800, 1600,..., 204, 800 for each random walk t. This is equivalent to individually generating random walks t of $n = 400$, 800, 1600,... steps and noting $N_n(t)$ individually, under the assumption that the random number generator is adequate.

The results so obtained are tabulated in Table I. A plot of $\log\langle N_n\rangle$ verus $\log n$ strongly supported a linear relationship between these two quantities in the asymptotic region. A linear regression was performed to fit $\langle N_n\rangle$ to $n^{1/2\nu}$ for n large. The results are tabulated in Table II, along with the results for SAWS cited above. For $2d$ LESAWS, we find $\nu = 0.800 \pm 0.003$, while for $3d$ LESAWS we find $\nu = 0.616 \pm 0.004$. Both results are different from the corresponding SAW exponents.

Other experiments performed gave less precise estimates of the exponents. In one experiment m-step random walks, with $m = 400$, 800, 1600,..., 204800 steps, were generated and loops erased to yield $N_m(t)$-step LESAWS $P_m(t)$. The squared distance from the origin to the nth point was recorded for all walks for which $N_m(t) \geqslant n$ and the percentage of such

Table I. Results of Monte Carlo Simulations on LESAW of 204,800 Steps

n	$\langle N_n\rangle$	s.d.
Square lattice		
400	52.2	27.8
800	81.0	41.8
1,600	125.4	63.0
3,200	194.2	95.3
6,400	299.8	146.5
12,800	461.7	225.9
25,600	710.7	348.6
51,200	1,095.4	535.1
102,400	1,690.1	825.9
204,800	2,606.6	1,277.5
Simple cubic lattice		
400	125.8	45.3
800	220.5	76.8
1,600	386.4	131.2
3,200	677.6	224.6
6,400	1,186.3	391.7
12,800	2,078.7	683.1
25,600	3,641.4	1,194.8
51,200	6,405.3	2,088.8
102,400	11,242.0	3,652.2
204,800	19,720.8	6,418.3

Table II. Summary of Results Obtained by Monte Carlo Simulations of LESAWS and Exact ($d=2$) and Numerical ($d=3$) Results for SAWS

Lattice	$2\nu_{\mathrm{LESAW}}$	$2\nu_{\mathrm{SAW}}$
Square	1.600 ± 0.006	1.5000
Cubic	1.232 ± 0.008	1.180 ± 0.008

walks was noted. The mean square distance $\langle r_n^2 \rangle_m$ was studied for values of n for which the percentage of LESAWS with $N_m(t) \geqslant n$ was $\geqslant 99.98\,\%$ and $\geqslant 97.77\,\%$ for dimensionality 3 and 2, respectively, and estimates of the critical exponent $2\nu_m = \lim_{n \to \infty} \ln \langle r_n^2 \rangle_m / \ln n$ obtained. These values of ν_m were extrapolated to estimate the exponent that would be obtained by taking infinite LESAWS. We also calculated the mean radius of gyration $\langle s_n^2 \rangle$, and hence we were able to estimate the universal amplitude ratio $\langle r_n^2 \rangle / \langle s_n^2 \rangle$. The results are given in Table III. From this table we estimate that the universal ratio $\langle r_n^2 \rangle / \langle s_n^2 \rangle$ is 8.30 ± 0.02 ($d=2$) and 6.74 ± 0.02 ($d=3$). For "ordinary" saws, the corresponding values are[23] 7.14 ± 0.05 ($d=2$) and 6.45 ± 0.05 ($d=3$). This provides additional evidence that loop-erased SAWS are in a different universality class.

Next, random walks were generated, and loops erased as they occurred, until the number of self-avoiding steps (after loop erasure)

Table III. Estimates of Mean Square End-to-End Distances $\langle R_n^2 \rangle$ and Mean Square Radius of Gyration $\langle S_n^2 \rangle$ for Two- and Three-Dimensional Hypercubic Lattices[a]

	Three Dimensions			Two dimensions		
n	$\langle R_n^2 \rangle$	$\langle S_n^2 \rangle$	$\langle R_n^2 \rangle / \langle S_n^2 \rangle$	$\langle R_n^2 \rangle$	$\langle S_n^2 \rangle$	$\langle R_n^2 \rangle / \langle S_n^2 \rangle$
2	2.420	0.491	4.93	2.729	0.525	5.20
5	7.682	1.294	5.94	10.835	1.622	6.68
10	18.388	2.878	6.39	31.68	4.255	7.45
20	43.965	6.641	6.62	94.1	11.93	7.89
50	138.25	20.530	6.73	403.6	49.24	8.20
100	327.37	48.495	6.75	1217	147.0	8.28
200	774.1	114.76	6.76	3680	444	8.29
300	1279	189.8	6.74	7020	846	8.30
400	1828	271.3	6.74	11200	1350	8.3
500	2410	357.7	6.74			

[a] The entries are believed accurate to at least three significant figures.

reached a preset value n. The mean end-to-end distances $\langle r_n^2 \rangle$ of these n-step SAWS was recorded and an estimate of the critical exponent defined by $\lim_{n \to \infty} \log\langle r_n^2 \rangle / \log n$ was obtained. This procedure roughly corresponds to the measure defined by Lyklema and Evertsz. While not performed on long SAWS, preliminary results yielded $\nu = 0.75 \pm 0.1$ in 2D. Given the relative inaccuracy of this method, we did not pursue it.

4. CONCLUSION

Recently Lawler[22] proved that the above exponent $\nu_{\text{LESAW}} \geqslant \nu_{\text{Flory}}$. Accepting the numerical results for $d = 3$, it immediately follows that the SAW and LESAW models are in different universality clases, as also evidenced by our results above. The rigorous results obtained by Lawler for the LESAW on the four- and higher-dimensional hypercubic lattices do not necessarily apply to the SAW on these lattices.

Given the propensity for two-dimensional lattice models to produce rational critical exponents and the result obtained above, a conjectured result for ν_{LESAW} might be 4/5. Similar results are reported for the two-dimensional case by Lyklema and Evertsz, for their equivalent[19] Laplacian random walk with parameter $\eta = 1$.

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REFERENCES

1. J. M. Hammersley, *Oxford Q. J. Math.* **12**(2):250–256 (1961).
2. J. M. Hammersley and D. J. A. Welsh, *Oxford Q. J. Math.* **13**(2):108–110 (1962).
3. D. Brydges and T. Spencer, *Commun. Math. Phys.* **97**:125–148 (1985).
4. G. Slade, *Commun. Math. Phys.* **110**:661 (1987).
5. G. Slade, *J. Phys. A: Math. Gen.* **21**:L417 (1988).
6. G. Slade, *Ann. Prob.* **17**:91 (1989).
7. C. Domb and G. S. Joyce, *J. Phys. C: Sol. State Phys.* **5**:956–976 (1972).
8. B. Nienhuis, *Phys. Rev. Lett.* **49**:1062–1065 (1982).
9. B. Nienhuis, *J. Stat. Phys.* **34**:731–761 (1984).
10. P. J. Flory, *Statistical Mechanics of Chain Molecules* (Wiley, New York, 1969).
11. A. J. Guttmann, *J. Phys. A: Math. Gen.* **20**:1839–1854 (1987).
12. A. J. Guttmann, *J. Phys. A: Math. Gen.* **22** (1989), to appear.
13. J. C. Le Guillou and J. Zinn-Justin, *Phys. Rev. B* **21**:3976–3998 (1980).

14. N. Madras and A. D. Sokal, *J. Stat. Phys.* **50**:109–186 (1988).
15. A. J. Guttmann, *J. Phys. A: Math. Gen.* **14**:233–239 (1981).
16. M. E. Fisher and M. F. Sykes, *Phys. Rev.* **114**:45–58 (1959).
17. D. Klein, *J. Stat. Phys.* **23**:561–586 (1980).
18. G. F. Lawler, *Duke Math J.* **47**:655–694 (1980).
19. J. W. Lyklema and C. Evertsz, *J. Phys. A: Math. Gen.* **19**:L895–900 (1986).
20. G. F. Lawler, *J. Phys. A: Math. Gen.* **20**:4565–4568 (1987).
21. G. F. Lawler, *Duke Math J.* **53**:249–269 (1986).
22. G. F. Lawler, *J. Stat. Phys.* **50**:91–108 (1988).
23. C. Domb and F. T. Hioe, *J. Chem. Phys.* **51**:1915–1919 (1969).