Dynamic algorithm for loop-erased self-avoiding random walks in two and three dimensions

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Monte Carlo simulation of loop-erased self-avoiding random walks in two and three dimensions (2D and 3D) was performed, using an algorithm different from that of Guttmann and Bursill. We obtained $2\nu = 1.571$ in 2D and $2\nu = 1.230$ in 3D. The 3D result compares most favorably with that of Guttmann and Bursill [J. Stat. Phys. **59**, 1 (1990)]. Lawler's conjecture [J. Stat. Phys. **50**, 91 (1988)] that loop-erased self-avoiding random walks are in a different universality class than self-avoiding random walks is strengthened.

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I. INTRODUCTION

There are many simple examples of power laws in physics where the exponent is a rational fraction. However, there is a broad class of phenomena where power law behavior occurs but the exponent is not a simple fraction. Phenomena for which there exists a critical point are just one class of such examples. The study of self-avoiding random walks is one of many examples exhibiting a power law whose exponent is not a simple fraction.

The numerical simulation of the self-avoiding walk (SAW) on a lattice has been the subject of intense study over many decades. This popularity may be attributed to the fact that the SAW provides a useful, simple model for a variety of complex phenomena: in chemistry, the flexible polymer molecule [1,2]; in physics, the $N \to 0$ limit of the N-vector model [3–5]; and in mathematics, a concrete example of a non-Markovian process [6].

Despite many years of effort, there exist few rigorous results when the dimensionality d of the walk is greater than 1.

Consider the usual SAW [7] on the d-dimensional integer lattice. For a walk of m steps, we let R_m denote the end-to-end distance; that is, the Euclidean distance from the initial point to the final point of the walk. If $\langle R_m^2 \rangle$ denotes the mean square end-to-end distance averaged over all SAW's of length m, then we may write the power law as

$$\langle R_m^2 \rangle \sim m^{2\nu}, \tag{1}$$

where ν is the critical exponent. We write $f(m) \sim g(m)$ to mean that $C = \lim_{m\to\infty} f(m)/g(m)$ exists and $0 < C < \infty$. It is believed that this relationship holds for every dimension with the exception of $d = 4$, where it is generally held that the growth rate is $m\,(\log m)^{1/4}$.

Clearly, $2\nu = 2$ for $d = 1$. For $d = 2$ Nienhuis [8,9] has shown that $2\nu = 3/2$, in agreement with the heuristic result of Flory [1] that $2\nu = 6/(d+2)$ for $1 \le d \le 4$ and $2\nu = 1$ for any $d > 4$. Although Flory's argument is flawed, its results appear to be correct for all dimensions except $d = 4$, where the logarithmic correction noted above is needed, and $d = 3$, where the best Monte Carlo work [10], the best series solutions [11,12], and the best renormalization group calculations [13] give $2\nu = 1.180 \pm 0.008$. Hara and Slade [14,15] have recently given a rigorous proof that Flory's conjecture is correct when $d > 4$.

More recently Lawler [16] introduced another type of self-avoiding walk called the loop-erased self-avoiding walk (LESAW). To generate a LESAW, one performs a classical random walk of n steps, which we call a *generating* random walk, and scans the list of nodes visited, searching for self-intersections. Wherever a self-intersection occurs, the intervening "loop" is erased. After all such loops have been erased, including immediate reversals, the result is a self-avoiding walk which we call the *derived* SAW. We denote the number of steps in this derived walk by N_n. See [17] for a rigorous discussion of this construction. We note that distinct random walks can produce the same LESAW.

Evidence is accumulating which suggests that LESAW's and SAW's are in different universality classes, and the results of this paper provide further evidence. Lawler [18] has shown that $\langle R_m^2 \rangle$ for LESAW's grows as fast as $m^{6/5}$ for $d = 3$ and probably faster. Guttmann and Bursill [17] have performed Monte Carlo simulations of LESAW's in $d = 2$ and $d = 3$. Their estimated values were $2\nu = 1.600 \pm 0.006$ in $d = 2$ and $2\nu = 1.232 \pm 0.008$ in $d = 3$; this contrasts with 1.500 and 1.180 ± 0.008, respectively, for SAW's (see Table III below).

II. BATCH AND DYNAMIC ERASURE

Monte Carlo estimates of ν for LESAW's can be obtained in at least two distinct ways. On the one hand,

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one may fit data to the model

$$\langle N_n \rangle \sim n^{1/2\nu}, \tag{2}$$

although the connection between this model and the relation (1) may not be immediately evident. We call such a scheme a *batch-erasing* algorithm because the programmer knows *a priori* how many steps n of a generating classical random walk must be simulated in order to obtain the derived SAW.

Guttman and Bursill used the batch algorithm in [17]. They generated 170 000 classical random walks, each of 204 800 steps, in both $d = 2$ and $d = 3$. In each walk loops were erased as they occurred and the number of self-avoiding steps N_n was recorded for the ten values of n between 400 and 204 800, geometrically distibuted with a common ratio of 2. The mean values $\langle N_n \rangle$ were determined and a regression was run for $\log \langle N_n \rangle$ versus $\log n$, yielding the the values of ν quoted in the previous section.

Relation (2) is equivalent to the relation $\langle N_n \rangle^{2\nu} \sim n$. Furthermore, it is well known that $\langle R_n^2 \rangle \sim n$ for the classical random walk. Finally, R_n^2 for a classical random walk has the same value as $R_{N_n}^2$ for the derived SAW, since the endpoints of the walks are the same. Combining these observations yields

$$\langle R_{N_n}^2 \rangle \sim \langle N_n \rangle^{2\nu}. \tag{3}$$

This relation is similar in form to model (1) but suggests that, unlike model (2), the independent variable should be the length of the walk *after* loop erasure. That is, $m = N_n$ for some unpredictable value $n \geq m$. It seems reasonable to conjecture that fitting experimental data concerning LESAW's to the relation (1) with m so defined would give rise to the estimates of 2ν similar to those yielded up by the batch-erased algorithm. To test this, one should generate classical random walks, erasing loops as they occur, until the derived SAW reaches a predetermined length m. Since the length of the generating random walk cannot be predicted in advance, but only by monitoring the evolving SAW, we call this algorithm *dynamic* loop erasing.

Guttmann and Bursill performed dynamic loop-erasing experiments in [17], but report that preliminary results were relatively inaccurate and so they did not pursue this avenue any further. They cite results for $d = 2$ only, and the experimental error given (± 0.1) makes it impossible to distinguish between the conjectured exact figure of $2\nu = 3/2$ for SAW's and their experimental result of $2\nu = 1.600$ for LESAW's.

The motivation for this work is twofold. First, we wished to investigate the dynamic model for $d = 2$ and $d = 3$ for its own sake and determine numerically the values of its critical exponents. As well, we hoped to lend empirical evidence to justify the conjecture enunciated above relating models (1) and (2).

III. EXPERIMENT AND RESULTS

Using the dynamic algorithm we generated 100 000 LESAW's of 3000 steps each on a square lattice ($d = 2$) and on a cubic lattice ($d = 3$). We measured R_m^2 for a variety of values of m, the number of steps in the derived SAW. The results are summarized in Tables I and II. A plot of $\log \langle R_m^2 \rangle$ versus $\log m$ establishes a linear relation, the coefficents of determination being 0.9995 and 0.9998, respectively, in dimensions 2 and 3. We then performed a weighted linear regression, weighting with the estimated variance of $\log \langle R_m^2 \rangle$ [19]. We used the propogation of error method and estimated the variance as

$$\sigma^2_{\log \langle R_m^2 \rangle} \approx \frac{\sigma^2_{\langle R_m^2 \rangle}}{\langle R_m^2 \rangle^2}.$$

Using this technique we estimate 2ν to be 1.571 with a standard error of 0.006 for $d = 2$. For $d = 3$, the figure is $2\nu = 1.230$ with a standard error of 0.003. In Table III, these are compared to Guttman and Bursill's figures (1.600 and 1.232) and those for SAW's.

Our experiments were performed on a DEC Alpha3000 workstation purchased by Adelphi University. The CPU times were 22.5 days and 3.9 days, respectively, for $d = 2$ and $d = 3$.

TABLE I. Mean square end-to-end distances for dynamic loop-erased SAW's in two dimensions.

m	$\langle R_m^2 \rangle$	Std. Dev.
10	31.40	16.01
20	94.00	49.13
50	400.3	211.2
100	1206	642.4
200	3663	1943
300	6942	3700
400	11050	5896
500	15690	8430
600	21010	11440
700	26790	14660
800	33170	18160
900	40100	22060
1000	47300	25990
1100	54840	30070
1200	62890	34480
1300	71370	39160
1400	79880	43700
1500	88760	48940
1600	98000	54110
1700	107700	59390
1800	117400	64860
1900	127000	70400
2000	136800	76370
2100	146800	82200
2200	156700	88270
2300	166300	94660
2400	175900	101700
2500	184900	108200
2600	193900	114900
2700	202000	121600
2800	208800	128200
2900	214300	133700
3000	217500	137500

TABLE II. Mean square end-to-end distances for dynamic loop-erased SAW's in three dimensions.

m	$\langle R_m^2 \rangle$	Std. Dev.
10	18.35	10.45
20	43.85	26.47
50	138.1	87.19
100	326.5	210.5
200	773.0	501.2
300	1277	832.5
400	1820	1189
500	2405	1572
600	3008	1967
700	3643	2387
800	4288	2814
900	4963	3258
1000	5638	3706
1100	6335	4172
1200	7037	4645
1300	7751	5120
1400	8483	5610
1500	9237	6114
1600	10000	6625
1700	10750	7123
1800	11500	7625
1900	12250	8125
2000	13000	8653
2100	13760	9177
2200	14510	9689
2300	15240	10210
2400	15980	10740
2500	16700	11280
2600	17380	11800
2700	18040	12320
2800	18660	12800
2900	19220	13280
3000	19650	13650

IV. CONCLUSIONS

Our results strongly suggest that the critical exponent for the three-dimensional LESAW is estimated equally well by the batch-erased and dynamic-erased algorithms. The estimate of Guttmann and Bursill falls less than one standard error from our figure and our estimate falls well within the bounds they quote. In two dimensions, there is evidently some disagreement between the batch-erased and dynamic-erased estimates.

Our initial run of this experiment involved 50 000 LESAW's, each 2000 steps long after loop erasure. We were surprised to find the results were not in agreement with those in [17], and so we first increased the number of LESAW's to 100 000 and we then increased the length of the walks to 3000 steps. We found the estimates of the critical exponent to be surprisingly insensitive to these increases in run size. Our estimate of 2ν based on 50 000 walks of length 2000 was 1.570 with a standard error of 0.007. Increasing the number of LESAW's to 100 000 had the effect of decreasing 2ν by 1 in the fourth decimal place and the standard error by 1 in the sixth decimal place. The results of subsequently increasing the length of the walk to 3000 steps are those reported in this paper, and were significant only in the third decimal place.

TABLE III. A comparison of the critical constants for LESAW's using the dynamic algorithm of this work, the batch algorithm of Guttmann and Bursill, and the critical constants for SAW's.

	Dynamic	Batch	SAW
2D	1.571 ± 0.006	1.600 ± 0.006	1.500
3D	1.230 ± 0.003	1.232 ± 0.008	1.18 ± 0.008

TABLE IV. Guttmann and Bursill's data set for two dimensions.

n	$\langle N_n \rangle$
400	52.2
800	81.0
1600	125.4
3200	194.2
6400	299.8
12800	461.7
25600	710.7
51200	1095.4
102400	1690.1
204800	2606.6

Both our two-dimensional and our three-dimensional results were generated by the same C program, which was coded to take the dimension of the lattice as a parameter. This appears to eliminate the possibility that the difference in our two- and three-dimensional results when contrasted to the corresponding batch-erased estimates is due to a difference in programming logic or pseudorandom number generation. This, along with the robustness of our two-dimensional estimates with respect to sample size, leads us to suggest that the differences in the estimates may be due to differences in the algorithms. The two procedures clearly generate different sample spaces, and this may result in different estimates of 2ν, differences which are negligible in three dimensions but measurable in two dimensions.

We performed an additional piece of statistical analysis on the data in Table I. In [17], ten values of $\langle N_n \rangle$ are tabulated, corresponding to values of n distributed geometrically between 400 and 204 800; see Table IV. We chose the nine data points in our Table I for which the value of m most closely match a reported value of $\langle N_n \rangle$ (since both 81.0 and 125.4 round to 100, we have one fewer data point). Using this reduced data set—the lines in Table I corresponding to $m = 50$, 100, 200, 300, 500, 700, 1100, 1700, and 2600—we performed a weighted least squares analysis in the manner described in Sec. III. This yielded an estimate of 1.577 for 2ν with a standard error of 0.008. We note that this estimate of 2ν is within one standard error of the result using the full data set.

Using this data, we see that a 95% confidence interval for 2ν falls short of the figure 1.600 given in [17], but a 99% confidence interval for 2ν is (1.549, 1.606), which includes the entire range given by Guttmann and Bursill and still comfortably excludes the value 1.500, believed to be the critical exponent for the SAW.

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[1] P. J. Flory, *Statistical Mechanics of Chain Molecules* (Wiley, New York, 1969).
[2] C. Domb, Adv. Chem. Phys. **15**, 229 (1969).
[3] P. G. de Gennes, Phys. Lett. **38A**, 339 (1972).
[4] P. G. de Gennes, *Scaling Concepts in Polymer Physics* (Cornell University Press, Ithaca, 1979).
[5] J. des Cloizeaux, J. Phys. (Paris) **38**, 281 (1975).
[6] W. Feller, *An Introduction to Probability Theory*, 3rd ed. (Wiley, New York, 1968), Vol. 1.
[7] S. Windwer, *Markov Chains and Monte Carlo Simulations in Polymer Science* (Dekker, New York, 1970), Chap. 5.
[8] B. Nienhuis, Phys. Rev. Lett. **49**, 1062 (1982).
[9] B. Nienhuis, J. Stat. Phys. **34**, 731 (1984).
[10] N. Madras and A. D. Sokal, J. Stat. Phys. **50**, 109 (1988).
[11] A. J. Guttmann, J. Phys. A **20**, 1839 (1987).
[12] A. J. Guttmann, J. Phys. A **22**, 2807 (1989).
[13] J. C. Le Guillou and J. Zinn-Justin, Phys. Rev. B **21**, 3976 (1980).
[14] T. Hara and G. Slade, Commun. Math. Phys. **147**, 101 (1992).
[15] T. Hara and G. Slade, Rev. Math. Phys. **4**, 235 (1992).
[16] C. F. Lawler, Duke Math. J. **47**, 655 (1980).
[17] A. J. Guttmann and R. Bursill, J. Stat. Phys. **59**, 1 (1990).
[18] C. F. Lawler, J. Stat. Phys. **50**, 91 (1988).
[19] S. Weisberg, *Applied Linear Regression*, 2nd ed. (Wiley, New York, 1985).