Square Lattice Self-Avoiding Walks and Corrections to Scaling

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New data and analysis of a 51-term series for self-avoiding walks on the (anisotropic) square lattice is given. Analysis of the series provides compelling evidence that the generating function for walks cannot be written as an algebraic or D-finite function and that the correction-to-scaling exponent is $\Delta = \frac{3}{2}$. [S0031-9007(96)02026-1]

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The enumeration of self-avoiding walks (SAWs) and polygons has for a quarter of a century been arguably the most powerful method for studying the critical (long-chain) behavior of polymer molecules in a good solvent [1,2]. Its connection with the N-vector model of phase transitions and related problems of physics is elucidated in [1,2]. It has also become a paradigm of algorithm design for other graph-enumeration problems arising in statistical mechanics. In this Letter we present a radical extension of the square lattice SAW series, from 39 steps to 51 steps, and we use it to provide compelling evidence that the correction-to-scaling exponent is $\Delta = \frac{3}{2}$ as predicted by Nienhuis [3]. This provides important validation of the Coulomb gas methods pioneered in [3]. We also find the corresponding exponent at the antiferromagnetic critical point to be 1, implying an analytic correction-to-scaling term.

Until 1993, all SAW enumerations were based on algorithms of exponential complexity, with the time taken growing asymptotically as λ^n, where $\lambda \approx 2.638$, the connective constant for SAWs on the square lattice. In 1993 we [4] introduced a new algebraic technique based on enumerations on a finite lattice coupled with transfer matrices. This algorithm is challenging to implement efficiently, and requires large amounts of physical memory, but affords the advantage of an exponential increase in efficiency over previous algorithms, being of complexity κ^n, where $\kappa = 3^{\frac{1}{4}} \approx 1.316$. We obtained 39-step SAWs from this algorithm, using an IBM 3090 with more than 500 MB of memory.

In the present study, we have parallelized the algorithm in order to run it on a 1024 processor Intel Paragon XP/S 150 supercomputer. While the parallelization is not, in principle, too difficult, an efficient implementation that balances the load across all processors is more demanding. The underlying algorithm is as described in [4], and the details of the parallelization scheme will be published elsewhere [5].

The present calculation took about 12 h, required about 10 GB of memory, and was performed modulo different primes (seven times), with the final results being reconstituted using the Chinese remainder theorem. The scale of the calculation can be gauged by the fact that something like 5 TB of data is moved between processors on each run. Additional processing was required to construct the final series.

The SAW generating function is written $C(x) = \sum c_n x^n$, where c_n denotes the number of n-step SAWs modulo translation. The 12 new series coefficients, being the coefficients $c_{40} \cdots c_{51}$ are given in Table I. (The previous 40 coefficients can be found in [4].)

Analysis of series.—We have studied the SAW generating function by the usual method of differential approximants [6], following the same procedure as in [4]. We find the following unbiased estimates of the critical parameters from both first- and second-order differential approximants:

$$x_c = 0.379\,052\,2(3), \qquad \gamma = 1.343\,67(10) \text{ 1st order,}$$

$$x_c = 0.379\,052\,3(3), \qquad \gamma = 1.343\,72(10) \text{ 2nd order.}$$

These are in perfect agreement with, though more precise than, the estimates given previously [4]. They are also in very good agreement with the believed exact (but

TABLE I. Coefficients $c_{40} \cdots c_{51}$ of the walk generating function of square lattice SAWs.

n	c_n	n	c_n
40	300 798 249 248 474 268	41	800 381 032 599 158 340
42	2 127 870 238 872 271 828	43	5 659 667 057 165 209 612
44	15 041 631 638 016 155 884	45	39 992 704 986 620 915 140
46	106 255 762 193 816 523 332	47	282 417 882 500 511 560 972
48	750 139 547 395 987 948 108	49	1 993 185 460 468 062 845 836
50	5 292 794 668 724 837 206 644	51	14 059 415 980 606 050 644 844

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nonrigorous) value [3] $\gamma = \frac{43}{32} = 1.34375$. Assuming this value for γ then leads to our biased critcal point estimate $x_c = 0.37905227(12)$.

In [7] the estimate $x_c = 0.37905228(14)$ based on a 56-term square lattice polygon series was given. In unpublished work based on a 70-term polygon series [8] we find the central estimate unchanged, and the error reduced by almost 2 orders of magnitude. As noted in [4], this value is indistinguishable from a zero of $581x^4 + 7x^2 - 13 = 0$, which gives $x_c = 0.37905227776\ldots$, and we will use this value in our subsequent analysis.

In [7] we pointed out that there was no numerical evidence for a nonanalytic correction-to-scaling term for polygons. Since the polygon generating function exponent $2 - \alpha$ equals $\frac{3}{2}$, this result is perfectly consistent with the prediction [3] that the correction exponent is $\Delta = \frac{3}{2}$. That is to say, if one writes the polygon generating function as

$$\begin{aligned} P(x) = \sum_{n\geq 0} p_n x^n &\sim A(x) + B(x)(1 - x/x_c)^{2-\alpha}[1 + (1 - x/x_c)^{\Delta} + \cdots] \\ &= A(x) + B(x)(1 - x/x_c)^{\frac{3}{2}}[1 + (1 - x/x_c)^{\frac{3}{2}} + \cdots] = \tilde{A}(x) + B(x)(1 - x/x_c)^{\frac{3}{2}}[1 + \cdots], \end{aligned}$$

one sees that because $2 - \alpha + \Delta$ is an integer, the nonanalytic correction-to-scaling term "folds into" the analytic background term $A(x)$. On the other hand, since $-\gamma + \Delta$ is not an integer, a nonanalytic correction-to-scaling term is implied in the *walk* generating function.

Subsequently, however, Saleur [9] investigated the correction exponents by studying the transfer matrix spectrum. He found two such exponents, corresponding to $\Delta = \frac{1}{2}$ and $\Delta = \frac{11}{16}$. The first operator was dismissed on technical grounds, but the second exponent is more problematical. In the Coulomb gas formulation [10], this exponent arises from four-polymer vertices. It can therefore be argued that this exponent does not contribute to SAWs, but should contribute to lattice trails. For trails we [11] estimated this exponent to be in the range $\frac{1}{2} < \Delta < \frac{3}{4}$, and more recently in [12] the value $\Delta = \frac{11}{16}$ was found. However, in [12] it is argued that the near collisions that a SAW can have with itself also correspond to four-polymer vertices, and so the term may be present. We show below that the amplitude of this term appears to be vanishingly small in the case of SAWs.

We have analyzed the series for the correction-to-scaling exponent by a wide variety of methods. The most convincing, and arguably simplest method is a direct fit of the data to the assumed asymptotic form.

As proved in [13], the SAW generating function $C(x)$ has, in addition to the "ferromagnetic" singularity at $x = x_c$, an "antiferromagnetic" singularity at $x = -x_c$. The exponent at the antiferromagnetic singularity is believed to be equal to the internal energy exponent $2 - \alpha = \frac{3}{2}$.

We therefore expect the generating function for walks to behave like

$$\begin{aligned} C(x) = \sum c_n x^n \sim A(x)(1 - x/x_c)^{-\frac{43}{32}}&[1 + B(x)(1 - x/x_c)^{\Delta} + \cdots] \\ + D(x)(1 + x/x_c)^{\frac{1}{2}}&[1 + E(x)(1 + x/x_c)^{\Lambda} + \cdots], \end{aligned}$$

where A, B, C, D, E are smooth functions.

Hence the asymptotic form of the coefficients is given by

$$\begin{aligned} c_n x_c^n \sim n^{\frac{11}{32}}&[a_1 + a_2 n^{-1} + a_3 n^{-\Delta} + a_4 n^{-2}] \\ &+ (-1)^n n^{-\frac{3}{2}}[b_1 + b_2 n^{-\Lambda} + b_3 n^{-1} + b_4 n^{-2}]. \end{aligned}$$

The correction-to-scaling exponent Λ, associated with the antiferromagnetic singularity, is one about which we have no *a priori* knowledge. Two obvious candidates are $\Lambda = 1$ and 1.5, corresponding, respectively, to an analytic correction and to the same correction as expected for the ferromagnetic singularity. A third possibility is $\Lambda = 0.5$, given that square roots are already present in the antiferromagnetic singularity. We have investigated all three possibilities (as well as others), and the evidence is strongly in favor of only an analytic correction, that is, $\Lambda = 1$.

A fit to the data of the above form with $\Delta = \frac{3}{2}$ and $\Lambda = 1$ (which we believe to be the correct values) is shown in Table II. The coefficient b_3 is redundant since $\Lambda = 1$.

Convergence is seen to be excellent (and quite comparable to a corresponding analysis of the 54-term square lattice Ising susceptibility series [6], where both Δ and Λ are known to be 1). We estimate $a_1 = 1.177043$, $a_2 = 0.5500$, $a_3 = -0.140$, $a_4 = -0.12$, $b_1 = -0.1899$, $b_2 = 0.175$, and $b_3 = -1.51$. We expect errors to be confined to the last quoted digit.

A corresponding fit with $\Delta = \frac{3}{2}$ and $\Lambda = 0.5$ was made (not shown) and the fit to the antiferromagnetic singularity amplitudes was significantly worse than with the above exponent set. More significantly, the amplitude b_2 of the term associated with the assumed correction-to-scaling exponent was small in magnitude, and tending towards zero as n grows: this is a sign of its absence. A similar analysis (not shown) was made with $\Lambda = 1.5$, and again a poorer fit was observed, with the amplitude of

TABLE II. A fit to the asymptotic form with $\Delta = 1.5$ and $\Lambda = 1$.

n	a_1	a_2	a_3	a_4	b_1	b_2	b_4
40	1.177 042 1	0.550 21	−0.141 18	−0.118 16	−0.189 84	0.174 11	−1.495 11
41	1.177 042 2	0.550 18	−0.141 00	−0.118 57	−0.189 84	0.174 22	−1.497 25
42	1.177 042 1	0.550 19	−0.141 04	−0.118 48	−0.189 84	0.174 24	−1.497 70
43	1.177 042 2	0.550 16	−0.140 82	−0.118 99	−0.189 84	0.174 39	−1.500 54
44	1.177 042 2	0.550 17	−0.140 89	−0.118 84	−0.189 84	0.174 43	−1.501 42
45	1.177 042 3	0.550 15	−0.140 71	−0.119 27	−0.189 85	0.174 55	−1.503 89
46	1.177 042 3	0.550 15	−0.140 73	−0.119 22	−0.189 85	0.174 56	−1.504 14
47	1.177 042 3	0.550 14	−0.140 61	−0.119 51	−0.189 85	0.174 64	−1.505 85
48	1.177 042 3	0.550 14	−0.140 60	−0.119 54	−0.189 85	0.174 63	−1.505 66
49	1.177 042 4	0.550 13	−0.140 51	−0.119 76	−0.189 85	0.174 69	−1.507 03
50	1.177 042 4	0.550 13	−0.140 49	−0.119 80	−0.189 85	0.174 68	−1.506 74
51	1.177 042 4	0.550 12	−0.140 42	−0.119 98	−0.189 85	0.174 73	−1.507 91

the assumed correction term decreasing rapidly. Thus we conclude that there is no numerical evidence for a nonanalytic correction at the antiferromagnetic singularity.

Returning to the physical singularity, if we now set $\Delta = \frac{11}{16}$, and also allow for a second correction-to-scaling exponent $\Delta_1 = \frac{3}{2}$, the asymptotic form of the coefficients becomes

$$c_n x_c^n \sim n^{\frac{11}{32}}[a_1 + a_2 n^{-\Delta} + a_3 n^{-1} + a_4 n^{-2\Delta} + a_5 n^{-\Delta_1}] + (-1)^n n^{-\frac{3}{2}}[b_1 + b_2 n^{-1} + b_3 n^{-2}].$$

The results of this fit are shown in Table III. The extremely small values of the estimated a_2 strongly suggest that this term is in fact absent. (Including higher order terms in the above equation strengthens this conclusion.) Furthermore, the values of the other amplitudes are consistent with the values of the corresponding terms in Table II.

A variety of other combinations of values for Δ and Λ were tried, with equally persuasive numerical evidence in favor of just one correction-to-scaling exponent, given originally [3] as $\Delta = 1.5$, and only analytic corrections at the antiferromagnetic singularity, a result we believe to be new. The estimate of Δ is in agreement with a recent finite-size scaling analysis [12], and in disagreement with a recent numerical study [14]. The fact that two independent methods yield an identical estimate for Δ considerably strengthens our confidence in that estimate. It similarly lends support to the Coulomb gas methods that first led to the prediction of that same value, and underpins the application of both methods to other models of phase transitions.

Anisotropic lattice and exact solutions.—Recently [15] a numerical procedure was given that indicates whether a given statistical-mechanical system is solvable, in the sense of being expressible in terms of D-finite functions (one which may be expressed as the solution of a linear ordinary differential equation of finite order with polynomial coefficients). As discussed in [15], most of the solved models in statistical mechanics fall into this class. We can show, on the basis of the behavior of the SAW generating function on the *anisotropic* square lattice, that it is almost surely not D finite.

We first write the walk generating function as

$$C(x,y) = \sum_{m,n=0}^{\infty} c_{m,n} x^m y^n = \sum_{n=0}^{\infty} H_n(x) y^n.$$

Here $c_{m,n}$ is the number of SAWs with m steps in the x direction and n steps in the y direction. From our enumerations we can calculate the first 11 values $H_n(x), n = 0, \ldots, 10$.

TABLE III. A fit to the asymptotic form with $\Delta = \frac{11}{16}$, $\Delta_1 = \frac{3}{2}$, and $\Lambda = 1$. Note that the amplitude a_2 is small, and consistent with a limit of zero.

n	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3
40	1.177 015 9	0.005 55	0.504 39	0.372 07	−0.564 79	−0.189 84	0.174 10	−1.494 95
41	1.177 025 3	0.004 23	0.512 80	0.329 02	−0.525 46	−0.189 84	0.174 17	−1.496 24
42	1.177 017 4	0.005 36	0.505 56	0.366 44	−0.559 76	−0.189 84	0.174 23	−1.497 38
43	1.177 029 3	0.003 62	0.516 76	0.307 99	−0.506 01	−0.189 84	0.174 32	−1.499 18
44	1.177 018 5	0.005 23	0.506 33	0.362 97	−0.556 73	−0.189 84	0.174 40	−1.500 89
45	1.177 029 5	0.003 56	0.517 24	0.304 92	−0.503 01	−0.189 85	0.174 49	−1.502 71
46	1.177 022 5	0.004 64	0.510 10	0.343 25	−0.538 59	−0.189 85	0.174 55	−1.503 93
47	1.177 028 6	0.003 68	0.516 51	0.308 50	−0.506 24	−0.189 85	0.174 60	−1.505 05
48	1.177 025 3	0.004 20	0.513 01	0.327 64	−0.524 11	−0.189 85	0.174 63	−1.505 68
49	1.177 029 0	0.003 61	0.517 01	0.305 58	−0.503 46	−0.189 85	0.174 66	−1.506 40
50	1.177 027 0	0.003 93	0.514 79	0.317 96	−0.515 08	−0.189 85	0.174 68	−1.506 81
51	1.177 029 7	0.003 49	0.517 83	0.300 93	−0.499 05	−0.189 85	0.174 71	−1.507 39

The first few values are

$$H_0(x) = \frac{1 + x}{1 - x},$$
$$H_1(x) = \frac{2(1 + x)^2}{(1 - x)^2},$$
$$H_2(x) = \frac{2(1 + 7x + 14x^2 + 16x^3 + 9x^4 + 3x^5)}{(1 - x)^3(1 + x)^2},$$
$$H_3(x) = \frac{2(1 + 10x + 29x^2 + 44x^3 + 41x^4 + 22x^5 + 7x^6)}{(1 - x)^4(1 + x)^2};$$

the rest will be given elsewhere [5].

The rational functions $H_n(x)$ are observed to have unimodal asymmetric (for $n > 1$) numerators with positive coefficients, and denominators of the same degree as the numerator. The denominators appear to form a regular pattern, though we cannot be certain that this pattern persists. However, if we define $t_{n-1} = \frac{1-x^n}{1-x}$ and $s_n = (1 + x^n)$ then the denominator of $H_n(x)$ appears to be given by

$$(1 - x)^{n+1} s_1^n t_2^{n-4} s_2^{n-7} t_4^{n-9} s_4^{n-10} t_6^{n-14} s_6^{n-17} t_8^{n-19} s_8^{n-20} t_{10}^{n-24} \cdots, \qquad n \text{ even},$$
$$(1 - x)^{n+1} s_1^{n-1} t_2^{n-4} s_2^{n-6} t_4^{n-9} s_4^{n-11} t_6^{n-14} s_6^{n-16} t_8^{n-19} s_8^{n-21} t_{10}^{n-24} \cdots, \qquad n \text{ odd}.$$

In the above expressions, any negative exponents should be replaced by zero. If this is indeed the pattern of the denominators, this regularity must say something profound about the analytic structure of the generating function. While more denominators would be needed to be quite sure that the pattern persists, it clear is that, as n increases, the zeros of the denominator appear to be becoming dense on the unit circle in the complex x plane. As previously discussed [15], this implies that $C(x, y)$ has a natural boundary at $|x| = 1$. This then excludes all algebraic functions, all D-finite functions, and a large class of functions that are common in mathematical physics. [Just what it implies for $C(x, x)$ is less clear.] Regrettably, no obvious regularity has been observed in the numerators, nor does evaluating the numerator polynomials at $x = 1$ lead to any recognizable sequence, which is sometimes the case with simpler problems. There is no feature that suggests the existence of an inversion relation for this problem, unlike the analogous case of the Ising model susceptibility [15], where the numerator polynomials are symmetric, as well as unimodal.

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