# Correction-to-Scaling Exponents for Two-Dimensional Self-Avoiding Walks

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We study the correction-to-scaling exponents for the two-dimensional self-avoiding walk, using a combination of series-extrapolation and Monte Carlo methods. We enumerate all self-avoiding walks up to 59 steps on the square lattice, and up to 40 steps on the triangular lattice, measuring the mean-square endto-end distance, the mean-square radius of gyration and the mean-square distance of a monomer from the endpoints. The complete endpoint distribution is also calculated for self-avoiding walks up to 32 steps (square) and up to 22 steps (triangular). We also generate self-avoiding walks on the square lattice by Monte Carlo, using the pivot algorithm, obtaining the mean-square radii to  $\approx 0.01\%$  accuracy up to N = 4000. We give compelling evidence that the first non-analytic correction term for two-dimensional self-avoiding walks is  $\Delta_1 =$ 3/2. We compute several moments of the endpoint distribution function, finding good agreement with the field-theoretic predictions. Finally, we study a particular invariant ratio that can be shown, by conformal-field-theory arguments, to vanish asymptotically, and we find the cancellation of the leading analytic correction.

**KEY WORDS**: Self-avoiding walk; polymer; exact enumeration; series expansion; Monte Carlo; pivot algorithm; corrections to scaling; critical exponents; conformal invariance.

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# **1. INTRODUCTION**

The study of the universal properties of self-avoiding walks (SAWs) in the long-chain limit has been a central problem in both statistical mechanics and polymer physics for more than three decades.<sup>(1-3)</sup> In an *N*-step chain, the mean value of any global observable  $\mathcal{O}$  typically has an asymptotic expansion as  $N \to \infty$  of the form

$$\langle \mathcal{O} \rangle_N = A N^{p_{\mathcal{O}}} \left[ 1 + \frac{a_1}{N} + \frac{a_2}{N^2} + \dots + \frac{b_0}{N^{\Delta_1}} + \frac{b_1}{N^{\Delta_1 + 1}} + \frac{b_2}{N^{\Delta_1 + 2}} + \dots + \frac{c_0}{N^{\Delta_2}} + \frac{c_1}{N^{\Delta_2 + 1}} + \frac{c_2}{N^{\Delta_2 + 2}} + \dots \right],$$
(1.1)

where the leading exponent  $p_{\mathcal{O}}$  and the correction-to-scaling exponents  $\Delta_1 < \Delta_2 < \cdots$  are *universal*, i.e. they depend on the spatial dimension *d* but not on the microscopic details of the interactions (provided that the interactions are short-ranged and primarily repulsive). This universality justifies the intense efforts that have been devoted to determining these universal exponents, using a variety of analytical and numerical approaches.

In this paper we will address the problem of determining the leading non-analytic correction-to-scaling exponent  $\Delta_1$  for the two-dimensional self-avoiding walk and for the closely related problem of self-avoiding polygons (SAPs). At least two different theoretical predictions have been made for the purportedly exact value of this exponent:  $\Delta_1 = 3/2$  based on Coulomb-gas arguments,<sup>(4,5)</sup> and  $\Delta_1 = 11/16$  based on conformalinvariance methods.<sup>(6)</sup> In addition, several numerical methods have been employed to estimate  $\Delta_1$ , notably exact enumeration and extrapolation (series analysis)<sup>(7-19)</sup> and Monte Carlo.<sup>(18,20-23)</sup> The estimates of  $\Delta_1$  resulting from these numerical works are, for the most part, wildly contradictory: even when one compares estimates produced by a single method, such as series analysis, they range from  $\approx 0.5^{(18)}$  to  $\approx 0.65^{(8,10,13,14)}$  to  $\approx 0.85^{(15)}$  to  $\approx 1^{(7,14)}$  to  $1.5.^{(16,17,19)}$  Similar variation can be found in estimates of  $\Delta_1$  obtained from Monte Carlo studies, ranging from  $\approx 0.5^{(18)}$  to  $\approx 0.6^{(23)}$  to  $\approx 0.84^{(21)}$  to  $\approx 1.1^{(23)}$  to  $\approx 1.2.^{(20)}$ 

Other models in the same universality class have also been considered, yielding results in contrast with those for the SAW. For instance, for lattice trails (connected paths where the self-avoidance constraint is applied only to bonds, not vertices) it was shown by a transfer-matrix study<sup>(24)</sup> that the correction-to-scaling exponent is indeed  $\approx 11/16$ , confirming an earlier result based on series analysis.<sup>(25)</sup> This same transfer-matrix study also found  $\Delta_1 \approx 3/2$  for SAWs. What remains to be understood is why the contribution with  $\Delta_1 = 11/16$  seems to be absent for square- and triangular-lattice SAWs, yet present for trails.

To further confuse the subject, we should mention the recent results of Jensen<sup>(26)</sup> for osculating SAPs on the square lattice: these are a superset of SAPs in which bonds may touch at a vertex but not cross. In a sense they interpolate between SAPs, in which intersections are strictly forbidden, and closed trails, in which crossing at a vertex is allowed. A careful analysis of the corresponding series<sup>(26)</sup> shows very convincingly that  $\Delta_1 =$ 3/2 and finds no correction corresponding to  $\Delta_1 = 11/16$ .

To add to our list of unexplained phenomena, we remark on a recent Monte Carlo study of SAWs on the Manhattan lattice,<sup>(27)</sup> where it was found that the critical exponent  $\gamma$  has the same value 43/32 as for SAWs on regular lattices *provided* that the value  $\Delta_1 = 11/16$  is used in the analysis. It is quite unclear why a different value of  $\Delta_1$  should arise for the Manhattan lattice than is found for the square lattice.

Returning now to the simplest case of SAWs and SAPs on regular lattices, the gross disparities among the extant estimates of the correction-to-scaling exponent might lead one to suspect that different methods are computing different quantities. For example, it might be that some methods are measuring (or predicting) the leading correction exponent  $\Delta_1$ , while others are measuring (or predicting) a subleading correction exponent  $\Delta_2$  or  $\Delta_3$ , and still others are measuring some sort of "effective" exponent  $\Delta_{\text{eff}}$  that represents phenomenologically the observed corrections to scaling in some specified interval of walk length N (and arising in reality from the sum of two or more correction-to-scaling terms).

Moreover, it may even be true that different observables produce different patterns of nonvanishing corrections to scaling. For instance, the  $\Delta_1 = 3/2$  correction term appears to be present for SAWs but absent for SAPs. While this may at first sight be considered a violation of universality, we show below that it is not.

Two recent analyses<sup>(17,19)</sup> based on very long series for square-lattice SAWs and SAPs have, however, yielded a consistent and convincing picture of the corrections to scaling: the first non-analytic correction-to-scaling exponent is indeed just  $\Delta_1 = 3/2$ , as predicted by Nienhuis;<sup>(4,5)</sup> but there are also analytic corrections to scaling proportional to integer powers of 1/N, the first of which dominates asymptotically. More precisely, a careful numerical study based on a 51-term SAW series<sup>(17)</sup> found that the number of *N*-step SAWs on the square lattice is given asymptotically by

$$c_N \sim \mu^N N^{11/32} [1.177043 + 0.5500/N - 0.140/N^{3/2} - 0.12/N^2 + \cdots] + (-\mu)^N N^{-3/2} [-0.1899 + 0.175/N - 1.51/N^2 + \cdots].$$
(1.2)

It is likely that previous studies identified some sort of effective exponent that reflects a combination of the effects of the 1/N and  $1/N^{3/2}$ 

correction-to-scaling terms (see Section 2.2 for further discussion of this point). Similarly, a careful numerical study based on a 90-term SAP series<sup>(19)</sup> found that the number of 2*N*-step SAPs on the square lattice is given asymptotically by

$$p_{2N} \sim \mu^{2N} N^{-5/2} [0.0994018 - 0.02751/N + 0.0255/N^2 + 0.12/N^3 + \cdots];$$
  
(1.3)

note that here there is *no*  $N^{-3/2}$  (or  $N^{-5/2}$ ) correction term. Finally, a recent transfer-matrix analysis<sup>(24)</sup> of SAWs on the square lattice also found compelling numerical evidence in favour of the value  $\Delta_1 = 3/2$ , and against all values  $\Delta_1$  significantly less than 3/2.

One possible cause of some confusion is that, because the value of the leading critical exponent of the SAP generating function is  $2-\alpha = 3/2$ , any correction-to-scaling term with  $\Delta =$  half-integer "folds into" the analytic background term and is therefore undetectable! In other words, no corrections proportional to  $N^{-\Delta}$  appear in the coefficients  $p_N$ . In order to understand this point, let us recall that the critical exponent  $\alpha$  is defined by the leading asymptotic behavior  $p_N \propto \mu^N N^{\alpha-3}$  of the polygon counts, corresponding to a leading behavior  $P(x) \equiv \sum_{N \ge 0} p_N x^N \sim \text{const} \times (1 - x/x_c)^{2-\alpha}$  as  $x \uparrow x_c = 1/\mu$  for the polygon generating function. If we now include both analytic and non-analytic corrections to scaling, the polygon generating function can be written generically as

$$P(x) = \sum_{N \ge 0} p_N x^N \sim A(x) + B(x)(1 - x/x_c)^{2-\alpha} [1 + c(1 - x/x_c)^{\Delta_1} + \cdots]$$
(1.4)

with A(x) and B(x) analytic in the neighbourhood of the critical point  $x_c = 1/\mu$ . Since  $\alpha = 1/2$  for two-dimensional SAPs,<sup>(4,5,19)</sup> if  $\Delta_1$  = half-integer the above equation may be rewritten as

$$P(x) = \sum_{N \ge 0} p_{2N} x^N \sim \widehat{A}(x) + \widehat{B}(x)(1 - x/x_c)^{3/2} [1 + \cdots], \qquad (1.5)$$

with the  $(1 - x/x_c)^{\Delta_1}$  correction term absorbed into the analytic background term  $\widehat{A}(x)$ . Therefore, if (1.4) holds, no correction of the form  $N^{-\Delta_1}$  is present. On the other hand, if the polygon counts were to exhibit a behaviour of the form  $p_N \propto \mu^N N^{\alpha-3} [1 + \dots + a/N^{\Delta_1} + \dots]$  with  $\alpha = 1/2$ and  $\Delta_1 = 3/2$ —and hence include a term  $\propto \mu^N N^{-4}$ —then the generating function P(x) would exhibit, on top of the  $(1 - x/x_c)^{3/2}$  leading behaviour, a non-analytic confluent term of the form  $(1 - x/x_c)^3 \log(1 - x/x_c)$  in addition to the analytic term  $(1 - x/x_c)^3$ . However, as discussed in some detail in ref. 19, there is no evidence for a term of the form  $a/N^{3/2}$  in the analysis of the SAP count series, and indeed there is considerable evidence for the absence of such a term. There is, however, abundant evidence of such a term in the radius-of-gyration series of SAPs.<sup>(28)</sup>

In the present paper we make some further progress in supporting the assertion that  $\Delta_1 = 3/2$  for SAWs on regular two-dimensional lattices (here square and triangular). First, we make a conventional analysis of corrections to scaling in the standard observables  $\langle R_e^2 \rangle$ ,  $\langle R_e^2 \rangle$  and  $\langle R_m^2 \rangle$ ; our contribution here is to present and use extended series expansions and a more efficient Monte Carlo algorithm. The results of this analysis are consistent with other recent work in supporting the conclusion that  $\Delta_1 = 3/2$ . In the course of this analysis we point out that, for certain observables, pairs of correction terms of opposite sign can (and do) conspire to give an effective exponent that is smaller than both of the individual exponents; this explains the apparent exponents  $\Delta < 1$  observed in some earlier work. Second—and this is perhaps our main contribution—we point out several observables in which a correction-to-scaling term becomes the leading *term.* These include: (a) the combination  $\frac{246}{91}\langle R_g^2 \rangle - 2\langle R_m^2 \rangle + \frac{1}{2}\langle R_e^2 \rangle$ , which arises in the conformal-invariance theory;<sup>(29,30)</sup> and (b) quantities related to the breaking of Euclidean invariance down to the lattice symmetry group, the simplest of which is (on the square lattice) the fourth-order moment  $\langle r^4 \cos 4\theta \rangle = \langle x^4 - 6x^2y^2 + y^4 \rangle$ . Analysis of these quantities by Monte Carlo methods yields only a modest improvement over the analysis of conventional quantities—the trouble is that the new quantities exhibit a low "signal-to-noise ratio"—but the series analysis is quite precise.

The plan of this paper is as follows. In Section 2 we define the quantities to be studied and collect some theoretical results that will be used or tested in the following sections. Section 3 reports the results of our series analysis: first, we analyze the SAW counts (Section 3.3); then, we analyze the radius of gyration, the end-to-end distance and the average distance of a monomer from the endpoints, along with their invariant ratios (Section 3.4); finally, we analyze the higher-order rotationally-invariant moments of the endpoint distribution function (Section 3.5) and the corresponding non-rotationally invariant moments (Section 3.6). For each of them, we determine the asymptotic behaviour as  $N \rightarrow \infty$ , focusing in particular on the correction-to-scaling exponent  $\Delta_1$  and on the behaviour at the antiferromagnetic singularity (in the case of the square lattice). In Section 4 we report the analyses of our Monte Carlo data, confirming the absence of a correction-to-scaling exponent  $\Delta_1 = 11/16$ . Finally, in Section 5 we draw our conclusions.

#### 2. DEFINITIONS AND THEORETICAL BACKGROUND

In this section we review briefly the basic facts and conjectures about the SAW that will be used (or tested) in the remainder of the paper.

## 2.1. Definitions and Notation

Let  $\mathcal{L}$  be some regular *d*-dimensional lattice. Then an *N*-step selfavoiding walk (SAW)  $\omega$  on  $\mathcal{L}$  is a sequence of distinct points  $\omega_0, \omega_1, \ldots, \omega_N$ in  $\mathcal{L}$  such that each point is a nearest neighbour of its predecessor. We assume all walks to begin at the origin ( $\omega_0 = 0$ ) unless stated otherwise.

First we define the quantities relating to the *number* (or "entropy") of SAWs. Let  $c_N$  [resp.  $c_N(\mathbf{x})$ ] be the number of *N*-step SAWs on  $\mathcal{L}$  starting at the origin and ending anywhere [resp. ending at  $\mathbf{x}$ ]. Then  $c_N$  and  $c_N(\mathbf{x})$  are believed to have the asymptotic behaviour

$$c_N \sim \text{const} \times \mu^N N^{\gamma - 1} \tag{2.1}$$

$$c_N(\mathbf{x}) \sim \operatorname{const} \times \mu^N N^{\alpha - 2}$$
 (**x** fixed  $\neq 0$ ) (2.2)

as  $N \to \infty$ ; here  $\mu$  is called the connective constant of the lattice, and  $\gamma$ and  $\alpha$  are *critical exponents*. The critical exponents are believed to be universal among lattices of a given dimension d. For rigorous results concerning the asymptotic behaviour of  $c_N$  and  $c_N(\mathbf{x})$ , see refs. 31–34

Next we define several measures of the size of an N-step SAW:

• The squared end-to-end distance

$$R_{\rm e}^2 = \omega_N^2. \tag{2.3}$$

• The squared radius of gyration

$$R_{\rm g}^2 = \frac{1}{2(N+1)^2} \sum_{i,j=0}^{N} (\omega_i - \omega_j)^2 \,. \tag{2.4}$$

• The mean-square distance of a monomer from the endpoints

$$R_{\rm m}^2 = \frac{1}{2(N+1)} \sum_{i=0}^{N} \left[ \omega_i^2 + (\omega_i - \omega_N)^2 \right].$$
(2.5)

We then consider the mean values  $\langle R_e^2 \rangle_N$ ,  $\langle R_g^2 \rangle_N$  and  $\langle R_m^2 \rangle_N$  in the probability distribution that gives equal weight to each *N*-step SAW. Very little has been proven rigorously about these mean values, but they are believed to have the leading asymptotic behaviour

$$\langle R_{\rm e}^2 \rangle_N, \, \langle R_{\rm g}^2 \rangle_N, \, \langle R_{\rm m}^2 \rangle_N \sim {\rm const} \times N^{2\nu}$$
 (2.6)

as  $N \to \infty$ , where  $\nu$  is another (universal) critical exponent. Hyperscaling<sup>(35)</sup> predicts that

$$d\nu = 2 - \alpha \,. \tag{2.7}$$

For SAWs in two dimensions, Coulomb-gas arguments<sup>(4,5)</sup> as well as arguments based on stochastic Loewner evolution (SLE)<sup>(36)</sup> predict that  $\nu = 3/4$ ,  $\alpha = 1/2$  and  $\gamma = 43/32$ . Prior numerical studies have confirmed these values to high precision;<sup>(17,19,37)</sup> in this paper we take them for granted.

The amplitude ratios

$$A_N = \frac{\langle R_g^2 \rangle_N}{\langle R_e^2 \rangle_N} \tag{2.8}$$

$$B_N = \frac{\langle R_{\rm m}^2 \rangle_N}{\langle R_{\rm e}^2 \rangle_N} \tag{2.9}$$

are expected to approach universal values in the limit  $N \rightarrow \infty$ , which we call A and B; one of our goals is to estimate these limiting amplitude ratios. Many other universal amplitude combinations (notably involving SAPs) are discussed in ref. 38, 39.

Of particular interest is the linear combination<sup>(29,30)</sup>

$$F_N \equiv \left(2 + \frac{y_{\rm t}}{y_{\rm h}}\right) A_N - 2B_N + \frac{1}{2} \tag{2.10}$$

and the corresponding unnormalized quantity

$$f_N \equiv F_N \langle R_e^2 \rangle_N \equiv \left(2 + \frac{y_t}{y_h}\right) \langle R_g^2 \rangle_N - 2 \langle R_m^2 \rangle_N + \frac{1}{2} \langle R_e^2 \rangle_N, \quad (2.11)$$

where  $y_t = 1/\nu$  and  $y_h = 1 + \gamma/(2\nu)$  are the thermal and magnetic renormalization-group eigenvalues, respectively, of the *n*-vector model at n = 0. In two dimensions—where  $y_t = 4/3$  and  $y_h = 91/48$ , hence  $2 + y_t/y_h = 246/91$ —Cardy and Saleur<sup>(29)</sup> (as corrected by Caracciolo, Pelissetto and Sokal<sup>(30)</sup>) have predicted, using conformal field theory, that  $\lim_{N\to\infty} F_N = 0$ . We shall henceforth refer to this relation as the CSCPS relation. This conclusion has been confirmed by previous high-precision Monte Carlo work<sup>(30)</sup> as well as by series extrapolations.<sup>(40)</sup> It is therefore of interest to examine the *rate* at which  $F_N$  tends to zero, as this gives information on the correction-to-scaling terms. We will discuss this from a theoretical point of view near the end of Section 2.2, and from a numerical point of view in Sections 3.4.2 and 4.2.

It turns out that  $\lim_{N\to\infty} F_N = 0$  holds not only for the ordinary square-lattice SAW, but also for SAWs with nearest-neighbour interactions, right up to (but not at) the theta point.<sup>(41)</sup> Moreover, the relation appears to hold *at* the theta point if  $2 + y_t/y_h$  is given its theta-point value 23/8 instead of 246/91. This observation is used in ref. 41 to locate the theta point more precisely.

We shall also consider higher moments of the end-to-end distance. Limiting ourselves to two-dimensional lattices, let us write

$$\omega_N \equiv (x, y) \equiv (r \cos \theta, r \sin \theta). \qquad (2.12)$$

The Euclidean-invariant moments  $\langle r^k \rangle_N$  are of course expected to behave as

$$\langle r^k \rangle_N \sim \operatorname{const} \times N^{k\nu}$$
 (2.13)

as  $N \rightarrow \infty$ . One can consider the dimensionless ratios

$$M_{2k,N} = \frac{\langle r^{2k} \rangle_N}{\langle r^2 \rangle_N^k}, \qquad (2.14)$$

which approach finite limits for  $N \to \infty$ ; these limiting ratios  $M_{2k,\infty}$  are universal quantities that characterize the end-to-end distribution function. Estimates of  $M_{2k,\infty}$  have been obtained in ref. 42 using field theory and the Laplace-deGennes transform method. It turns  $\operatorname{out}^{(43,44)}$  that the 2-point function is very nearly equal to that of a free field, so that when the rescaled inverse propagator in momentum space<sup>5</sup> is written as

 $<sup>{}^{5}\</sup>widetilde{D}(q)$  is the Fourier transform of the two-point correlation function, rescaled so that the first two terms at small q are  $1-q^2+O(q^4)$ .

$$\widetilde{D}(q)^{-1} = 1 + q^2 + \sum_{n=2}^{\infty} b_n q^{2n},$$
 (2.15)

one has  $1 \gg |b_2| \gg |b_3| \gg |b_4| \gg \dots$  One obtains<sup>(42)</sup>

$$M_{2k,\infty} = \frac{\Gamma(\gamma + 2\nu)^k}{\Gamma(\gamma + 2k\nu)\Gamma(\gamma)^{k-1}} \left[1 - b_2(k-1) + R_k\right] k! \prod_{j=0}^{k-1} \left(1 + \frac{2j}{d}\right), \quad (2.16)$$

where  $R_k$  is a very small correction (unless k is very large) that involves the constants  $b_3$ ,  $b_4$ , ... as well as higher powers  $b_i b_j$ ,  $b_i b_j b_k$ , .... Explicitly,

$$R_k = \sum_{n=3}^{k} (-1)^{n+1} (k+1-n) b_n + \frac{1}{2} (k-2) (k-3) b_2^2 + \cdots$$
 (2.17)

Note that  $R_2=0$  exactly. The universal nonperturbative constants  $b_2, b_3, \ldots$  have been obtained from the analysis of exact-enumeration series on the square, triangular and hexagonal lattices.<sup>(44)</sup> Numerically, it is found<sup>(44)</sup> that  $b_2$  is extremely small,  $b_2 = 0.00015(20)$ , and that  $b_3$  is even smaller,  $|b_3| \leq 3 \times 10^{-5}$ . Using the estimate of  $b_2$  in (2.16) and neglecting  $R_k$ , we obtain for the lowest values of k:

$$M_{4,\infty} = 1.44574(28) \tag{2.18}$$

$$M_{6,\infty} = 2.5876(10) \tag{2.19}$$

$$M_{8,\infty} = 5.3805(32) \tag{2.20}$$

$$M_{10,\infty} = 12.557(10). \tag{2.21}$$

A second class of interesting observables are moments that are invariant under the symmetry group of the lattice but *not* under the full Euclidean group: examples are the moments  $\langle r^k \cos n\theta \rangle$  with  $n \neq 0$ , where for the square (resp. triangular) lattice *n* must be a multiple of 4 (resp. 6). We expect these non-Euclidean-invariant moments to behave as

$$\langle r^k \cos n\theta \rangle \sim \operatorname{const} \times N^{k\nu - \Delta_{\operatorname{nr}}},$$
 (2.22)

where  $\Delta_{nr} > 0$  is a new correction-to-scaling exponent<sup>(43)</sup> associated with the breaking of full rotation invariance down to the lattice rotation group: it thus depends on the lattice in question (e.g., square or triangular) and

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is in general different from the leading correction-to-scaling exponent  $\Delta_1$  (which corresponds to a Euclidean-invariant irrelevant operator).

For Gaussian models—and thus also for *n*-vector models (including the SAW case n=0) in dimension  $d \ge 4$ —we have  $\Delta_{nr} = 2\nu = 1$  on any hypercubic lattice. For *n*-vector models in dimension  $d=4-\epsilon$ , this relation is modified at order  $\epsilon^2$ :<sup>(43)</sup>

$$\Delta_{\rm nr} = \nu \left[ 2 + \frac{7}{20} \frac{n+2}{(n+8)^2} \epsilon^2 + O(\epsilon^3) \right].$$
 (2.23)

In dimension d = 3, several alternative methods—field theory and exactenumeration analysis—show that  $\Delta_{nr}$  is very close to  $2\nu$ , though not exactly equal.<sup>(43)</sup> In two dimensions on the square lattice,  $\Delta_{nr} = 2\nu$  exactly for the Ising model and for the *n*-vector model with  $n \ge 3$  (in the latter case with logarithmic corrections).<sup>(43)</sup> For the triangular lattice, similar arguments<sup>(43)</sup> predict  $\Delta_{nr} = 4\nu$ .<sup>6</sup> For the Ising model, these predictions can be obtained using conformal field theory (see ref. 45, 46 for the classification of the subleading operators appearing in the Ising model); they can be checked explicitly<sup>(43)</sup> for at least one specific observable, using the analytic expression for the mass gap.<sup>(47,48,44)7</sup> It is therefore suggestive to conjecture that the same relations between  $\Delta_{nr}$  and  $\nu$  are valid for the SAW. This would predict  $\Delta_{nr} = 3/2$  on the square lattice, and  $\Delta_{nr} = 3$  on the triangular lattice. In Section 3.6 we will test (and confirm) this conjecture, by series analysis, for both square-lattice and triangular-lattice SAWs.

# 2.2. Corrections to Scaling

Let us now make some general remarks concerning corrections to scaling. Clearly, (2.1)/(2.2)/(2.6) are only the leading term in a large-N

<sup>6</sup>For the hexagonal lattice,  $\Delta_{nr} = 4\nu$  for observables that break rotational invariance but are invariant under interchange of the two sublattices, while  $\Delta_{nr} = 3\nu$  for observables that distinguish the two sublattices.<sup>(43)</sup>

<sup>7</sup>For instance, consider on a square lattice the mass gap  $m(\hat{n})$  in the direction  $\hat{n}$  defined as

$$m(\hat{n}) = -\lim_{r \to \infty} \frac{1}{|r|} \log \left( \sum_{\vec{x} \cdot \hat{n} = r} G(\vec{x}) \right),$$

where  $\hat{n} = (\cos \theta, \sin \theta)$  is a unit vector and the summation runs over all  $\vec{x}$  such that  $\vec{x} \cdot \hat{n} = r$ . From the exact solution,<sup>(47)</sup> one can easily see that, for  $\beta \to \beta_c$ ,

$$m(\hat{n}) = m_0(\beta_c - \beta)^{-1} \left[ 1 + (\beta_c - \beta)^2 (a_0 + b_0 \cos 4\theta) + \cdots \right]$$

with  $b_0 \neq 0$ . This result shows explicitly that  $\Delta_{nr} = 2 = 2\nu$ .

asymptotic expansion. According to renormalization-group theory,<sup>(49)</sup> the mean value of any global observable O behaves as  $N \to \infty$  as

$$\langle \mathcal{O} \rangle_{N} = A N^{p_{\mathcal{O}}} \left[ 1 + \frac{a_{1}}{N} + \frac{a_{2}}{N^{2}} + \dots + \frac{b_{0}}{N^{\Delta_{1}}} + \frac{b_{1}}{N^{\Delta_{1}+1}} + \frac{b_{2}}{N^{\Delta_{1}+2}} + \dots + \frac{c_{0}}{N^{\Delta_{2}}} + \frac{c_{1}}{N^{\Delta_{2}+1}} + \frac{c_{2}}{N^{\Delta_{2}+2}} + \dots \right].$$

$$(2.24)$$

Thus, in addition to "analytic" corrections to scaling of the form  $a_k/N^k$ , there are "non-analytic" corrections to scaling of the form  $b_k/N^{\Delta_1+k}$ ,  $c_k/N^{\Delta_2+k}$  and so forth, as well as more complicated terms [not shown in (2.24)] which have the general form  $const/N^{k_1\Delta_1+k_2\Delta_2+\cdots+l}$  where  $k_1, k_2, \ldots$ and l are non-negative integers. The leading exponent  $p_{\mathcal{O}}$  and the correction-to-scaling exponents  $\Delta_1 < \Delta_2 < \cdots$  are universal;  $p_{\mathcal{O}}$  of course depends on the observable  $\mathcal{O}$  in question, but the  $\Delta_i$  do not. The various amplitudes (both leading and subleading) are all nonuniversal (and of course also depend on the observable<sup>8</sup>). However, *ratios* of the corresponding amplitudes A,  $b_0$  and  $c_0$  (but not  $a_k$  or the higher  $b_k, c_k$ ) for different observables are universal.<sup>(50,51)</sup>

In fact, (2.24) is incomplete, as there are "mixing" terms arising from the fact that the temperature deviation from criticality is a smooth but *nonlinear* function of the nonlinear scaling fields  $g_t$  and  $g_h$ . This has the consequence<sup>(35, 52-55)</sup> that the susceptibility (or SAW generating function), which has a leading singularity  $(x_c - x)^{-\gamma}$ , also contains an additive term proportional to the energy, of order  $(x_c - x)^{1-\alpha}$ . In the case of the twodimensional Ising model, we have  $\alpha = 0$ , and this term is responsible for the logarithmic terms in the susceptibility, as was recently exhaustively studied in ref 56. For the two-dimensional SAW, we have  $\alpha = 1/2$ , and so one would expect a term  $\widetilde{A}(x)(x_c - x)^{1/2}$  in the SAW generating function. To incorporate this term requires that the naively expected asymptotic form

$$c_N \sim \mu^N N^{11/32} [a_0 + a_1/N + a_2/N^{3/2} + a_3/N^2 + a_4/N^{5/2} + \cdots]$$
 (2.25)

be modified to read

$$c_N \sim \mu^N N^{11/32} [a_0 + a_1/N + a_2/N^{3/2} + a_3/N^2 + a_4/N^{5/2} + \cdots] + \mu^N N^{-3/2} [\widetilde{a}_0 + \widetilde{a}_1/N + \cdots].$$
(2.26)

<sup>&</sup>lt;sup>8</sup>Sometimes a particular correction-to-scaling amplitude will vanish for some observables but not for others (e.g. for symmetry reasons).

For loose-packed (i.e., bipartite) lattices, such as the square and simplecubic lattices, there is an additional set of terms arising from the antiferromagnetic singularity, of the form

$$(-1)^{N} N^{q} \left[ d_{0} + \frac{d_{1}}{N} + \frac{d_{2}}{N^{2}} + \dots + \frac{e_{0}}{N^{\Delta_{1}^{AF}}} + \frac{e_{1}}{N^{\Delta_{1}^{AF}+1}} + \frac{e_{2}}{N^{\Delta_{1}^{AF}+2}} + \dots \right],$$
(2.27)

where the exponent q of course depends on the observable. We know of no theoretical argument that predicts the value of the exponent  $\Delta_1^{AF}$ . For the exponent q, in the closely related problem of the Ising-model susceptibility in two and three dimensions, Sykes<sup>(57)</sup> has given a configurational "counting theorem" that enables one to guess that the antiferromagnetic susceptibility behaves as the internal energy. This reasoning is discussed in greater detail in ref. 58, 59.<sup>9</sup> It follows that there should be a term in the susceptibility of the form  $D(x)(1 + x/x_c)^{1-\alpha}$  [where D(x) is analytic in a neighbourhood of the antiferromagnetic critical point  $x = -x_c$ ] and thus a term  $(-x_c)^{-N}N^{\alpha-2}$  in the high-temperature-series coefficients. This result can be put on more solid ground<sup>(60)</sup> by noting that at the antiferromagnetic critical point the (unstaggered) magnetic field is an irrelevant variable, so that the leading contribution to the free energy is

$$F(x,h) = ag_{t}(x,h)^{2-\alpha} + F_{reg}(x,h), \qquad (2.28)$$

where x is the inverse temperature and  $g_t(x, h)$  is the nonlinear scaling field associated with the temperature at the antiferromagnetic critical point. Since

$$g_t(x,h) = (1+x/x_c) + a_t h^2 + \cdots,$$
 (2.29)

by performing the appropriate derivatives we obtain the result reported above (provided of course that  $a_t \neq 0$ ). This argument is very general and applies to any *n*-vector model; in particular, it applies for n=0, i.e. to the SAW. Thus, for the SAW counts  $c_N$  we expect a term  $(-\mu)^N N^{\alpha-2}$ , so that  $q = \alpha - 2$  for this observable.<sup>(61)</sup>

The argument of Sykes can be generalized to higher moments of the two-point function, i.e.,  $\sum_{r} |r|^{2k} G(r)$ . Also in this case one can identify

<sup>&</sup>lt;sup>9</sup>The basic idea is that the susceptibility can be rewritten as the sum of two terms: one proportional to the energy, and a second one which can be argued (by series analysis) to give an algebraically small contribution near the antiferromagnetic critical point.

two terms: one is proportional to the energy, while the other is conjectured to give an algebraically small (i.e., noncritical) correction at the antiferromagnetic critical point. Such a conjecture was numerically verified in ref. 62 for the three-dimensional Ising model. As for the susceptibility, this implies that asymptotically the moments have the form  $D(x)(1+x/x_c)^{1-\alpha}$ , with D(x) analytic, for any k. Therefore, a term  $(-\mu)^N N^{\alpha-2}$  should be present in their high-temperature-series coefficients. Extending this conjecture to the *n*-vector model and in particular to the SAW (n=0), we predict

$$c_N \sim \mu^N N^{\gamma-1}[a_0 + \cdots] + (-\mu)^N N^{\alpha-2}[d_0 + \cdots],$$
 (2.30)

$$c_N \langle r^{2k} \rangle_N \sim \mu^N N^{2k\nu+\gamma-1} [a'_0 + \cdots] + (-\mu)^N N^{\alpha-2} [d'_0 + \cdots].$$
 (2.31)

For k = 1, (2.31) gives the behaviour of  $c_N \langle R_e^2 \rangle_N$ . It may seem natural to generalize the expression (2.31) to the other metric quantities, namely  $R_m^2$  and  $R_g^2$ . Surprisingly (to us), our subsequent analysis (see Section 3.4.2) shows that, while the unnormalized second-moment series of the end-toend distance series behaves precisely as expected in (2.31), the unnormalized series corresponding to both the radius of gyration and the mean monomer-endpoint distance behave a little differently. We find

$$c_N \langle R_{g,m}^2 \rangle_N \sim \mu^N N^{2\nu+\gamma-1} [a'_0 + \cdots] + (-\mu)^N [d'_0 + \cdots].$$
 (2.32)

That is to say, the antiferromagnetic exponent is different in the latter cases, namely 0 instead of  $\alpha - 2 = -3/2$ . Nevertheless, by taking the quotient of either (2.31) or (2.32) by (2.30), we obtain in all cases

$$\langle R^2 \rangle_N \sim N^{2\nu} [a_0'' + \cdots] + (-1)^N N^q [d_0'' + \cdots]$$
 (2.33)

with  $q = 2\nu + \alpha - 1 - \gamma$ . [For the end-to-end distance, the *dominant* antiferromagnetic correction always comes only from (2.30); for the other two metric quantities, it comes from both (2.30) and (2.32).] For the end-toend distance only, we have the additional relation

$$\frac{a_0''}{d_0''} = -\frac{a_0}{d_0}.$$
(2.34)

Similarly, the rotationally-invariant higher moments  $\langle r^{2k} \rangle_N$  are expected to behave as

$$\langle r^{2k} \rangle_N \sim N^{2k\nu} [a_0^{\prime\prime\prime} + \cdots] + (-1)^N N^{q_k} [d_0^{\prime\prime\prime} + \cdots]$$
 (2.35)

with  $q_k = 2k\nu + \alpha - 1 - \gamma$ . The coefficients  $a_0'''$  and  $d_0'''$  also satisfy a relation analogous to (2.34). Our numerical analysis, described below, provides supporting evidence that the corresponding exponents are indeed  $q_k = 3k/2 - 59/32$  in two dimensions (see Sections 3.4.2 and 3.5).

Finally, the non-analytic correction-to-scaling exponent  $\Delta_1^{AF}$  was found numerically, in the case of the square-lattice SAW counts, to be  $1.^{(17)}$  It would seem likely that this value should also hold for other properties, such as the metric quantities  $\langle R^2 \rangle_N$ . Our numerical studies, discussed below, are consistent with this conjecture—or, put another way, they are insufficiently sensitive to refute this obvious first guess.

Let us now return to the question of the corrections to the CSCPS relation  $\lim_{N\to\infty} F_N = 0$  [cf. (2.10)]. Series analysis and Monte Carlo simulations (see Sections 3.4.2 and 4.2 below) indicate that  $F_N \propto N^{-3/2}$ , i.e. that the leading analytic correction cancels. Such a cancellation may seem surprising, but it can be understood by means of a standard renormalization-group argument. Consider the continuum O(n) model with Hamiltonian

$$\mathcal{H} = \mathcal{H}^* + \int d^2 r \left[ t E(r) + h s^1(r) \right], \qquad (2.36)$$

where  $\mathcal{H}^*$  is the fixed-point Hamiltonian, and E(r) and  $s^i(r)$  are the energy and spin operators, respectively. The CSCPS relation<sup>(29,30)</sup> is a consequence of the sum rule

$$\int d^2 r \left\langle \Theta(0)^{\text{cont}} \Theta(r)^{\text{cont}} \right\rangle = 0, \qquad (2.37)$$

where  $\Theta(r)^{\text{cont}}$  is the trace of the continuum stress-energy tensor, and of course we must set n = 0 to obtain SAWs. In order to translate this continuum relation into a lattice one, we must relate the continuum operator to its lattice counterpart. It is natural to assume that the trace of the lattice stress-energy tensor,  $\Theta(r)^{\text{latt}}$ , whose explicit form is given in ref. 29, behaves as

$$\Theta(r)^{\text{latt}} = Z(t, h)\Theta(r)^{\text{cont}} + \cdots, \qquad (2.38)$$

where Z(t, h) is a smooth function of t and h, and the dots represent the contributions of the subleading operators. As a consequence of (2.38) we have

$$\int d^2 r \left\langle \Theta(0)^{\text{latt}} \Theta(r)^{\text{latt}} \right\rangle = \mathcal{O}(t^{\Delta_1}, h^{(y_t/y_h)\Delta_1}).$$
(2.39)

No corrections of order *t* appear in the previous relation. Equation (2.39) therefore implies the absence of the analytic corrections in the CSCPS relation  $\lim_{N\to\infty} F_N = 0$ .

The observation that  $F_N \propto N^{-3/2}$  implies a constraint on the subdominant amplitudes. More precisely, if we write

$$\langle R_{\rm e}^2 \rangle_N \sim a_{\rm e} N^{3/2} + b_{\rm e} N^{1/2} + c_{\rm e} + \mathcal{O}(1/\sqrt{N})$$
 (2.40)

$$\langle R_{\rm g}^2 \rangle_N \sim a_{\rm g} N^{3/2} + b_{\rm g} N^{1/2} + c_{\rm g} + \mathcal{O}(1/\sqrt{N})$$
 (2.41)

$$\langle R_{\rm m}^2 \rangle_N \sim a_{\rm m} N^{3/2} + b_{\rm m} N^{1/2} + c_{\rm m} + {\rm O}(1/\sqrt{N}),$$
 (2.42)

then the original CSCPS relation  $F_N \rightarrow 0$  implies

$$91a_{\rm e} = 364a_{\rm m} - 492a_{\rm g}\,,\tag{2.43}$$

while the absence of a 1/N term in  $F_N$  means that the leading subdominant terms also satisfy an amplitude relationship analogous to (2.43), namely

$$91b_{\rm e} = 364b_{\rm m} - 492b_{\rm g} \,. \tag{2.44}$$

Note too from (2.11) that

$$f \equiv \lim_{N \to \infty} f_N = (2 + y_T / y_H)c_e - 2c_m + c_g/2.$$
 (2.45)

Let us conclude by discussing briefly the behaviour of "effective exponents". Given a function f(N), let us define  $\Delta_{\text{eff}}(N)$  by fitting locally to the Ansatz  $f(N) = a + b/N^{\Delta}$ : this gives

$$\Delta_{\rm eff}(N) \equiv -\frac{d\log f'(N)}{d\log N} - 1.$$
(2.46)

Applying this to  $f(N) = a_0 + a_1/N^{\Delta_1} + a_2/N^{\Delta_2}$ , we obtain

$$\Delta_{\rm eff}(N) = \frac{a_1 \Delta_1^2 N^{-\Delta_1} + a_2 \Delta_2^2 N^{-\Delta_2}}{a_1 \Delta_1 N^{-\Delta_1} + a_2 \Delta_2 N^{-\Delta_2}}.$$
(2.47)

Thus, if  $a_1$  and  $a_2$  have the same sign, the "effective" exponent  $\Delta_{\text{eff}}(N)$  lies between  $\Delta_1$  and  $\Delta_2$  for all N, and decreases monotonically to  $\Delta_1$  as  $N \to \infty$ . (This is the behaviour one would expect intuitively for an

"effective exponent".) By contrast, if  $a_1$  and  $a_2$  have opposite signs, then  $\Delta_{\text{eff}}(N)$  starts *above*  $\Delta_2$  for small N, *increases* monotonically and reaches  $+\infty$  at some finite value of N; it then jumps to  $-\infty$ , after which it continues to increase monotonically, tending asymptotically to  $\Delta_1$  from below as  $N \to \infty$ . Thus, the qualitative behaviour of the effective exponents depends crucially on the sign (and magnitude) of  $a_1/a_2$ , which can vary from one observable to another. We shall see this phenomenon quite clearly in the two-dimensional SAW.

# 3. SERIES ANALYSIS

## 3.1. Summary of Our Data

We have previously reported enumerations of square-lattice SAWs up to 29 steps for  $c_N$ ,  $\langle R_e^2 \rangle_N$ ,  $\langle R_g^2 \rangle_N$  and  $\langle R_m^2 \rangle_N$ ,<sup>(63,64)</sup> and of triangular-lattice SAWs up to 22 steps for  $c_N$  and  $\langle R_e^2 \rangle_N$ <sup>(63)</sup> and up to 19 steps for  $\langle R_g^2 \rangle_N$  and  $\langle R_m^2 \rangle_N$ .<sup>(64)</sup> Analysis of these series can be found in refs. 63, 64. We have also previously presented the square-lattice SAW counts  $c_N$  up to 51 steps<sup>(17)</sup> and the square-lattice polygon counts  $p_{2N}$  up to 90 steps.<sup>(19)</sup> Analysis of these SAW series<sup>(17,19)</sup> provided good evidence that the non-analytic correctionto-scaling exponent is exactly  $\Delta_1 = 3/2$  as predicted by Nienhuis,<sup>(4,5)</sup> and that there is also the expected analytic term of leading order 1/N (as well as  $1/N^2$ ,  $1/N^3$ ,...). For SAPs we found compelling evidence for purely analytic correction-to-scaling terms. We have thus far found no numerical evidence of a second non-analytic correction-to-scaling exponent  $\Delta_2$ , although it is reasonable to expect that one exists.

In the present paper, we have extended the previous work by enumerating all SAWs on the square lattice up to 59 steps, and on the triangular lattice up to 40 steps, using refinements of the finite-lattice method (FLM) due to Rogers (unpublished) and Jensen.<sup>(65)</sup> The results for  $c_N$ ,  $\langle R_e^2 \rangle_N$ ,  $\langle R_g^2 \rangle_N$  and  $\langle R_m^2 \rangle_N$  are collected in Tables I and II.

For square-lattice SAPs, the counts are now known up to 110 steps,<sup>(66)</sup> and the radii of gyration up to 100 steps.<sup>(66)</sup> For triangular-lattice SAPs, the counts  $p_N$  were previously known up to N = 35;<sup>(67)</sup> in as-yet-unpublished work, one of us (ANR) has extended them up to N = 40,<sup>(68)</sup> while even more recently another of us (IJ) has extended the series to N = 60 steps.<sup>(69)</sup>

As the FLM does not enable us to record the full end-point distribution, nor higher moments (at least not with the amount of memory available to us), we also programmed a conventional backtracking algorithm and recorded the full end-point distribution  $c_N(\mathbf{x})$  for  $N \leq 32$  (square lattice) and for  $N \leq 22$  (triangular lattice). As a result, we are able to study

Ν	$c_N$	$rac{1}{4} c_N \langle R_{ m c}^2  angle_N$	$rac{1}{4}(N+1)^2 c_N \langle R_{\rm g}^2 \rangle_N$	$\frac{1}{4}(N+1)c_N\langle R_m^2\rangle_N$
1	4	1	1	1
2	12	8	14	11
3	36	41	116	74
4	100	176	722	390
5	284	679	3887	1801
9	780	2452	18508	7537
7	2172	8447	82160	29684
8	5916	28120	340180	110796
6	16268	91147	1351555	399375
10	44100	289324	5136194	1391809
11	120292	902721	18989580	4741466
12	324932	2777112	68082102	15783154
13	881500	8441319	239338055	51704949
14	2374444	25398500	822629240	166550157
15	6416596	75744301	2786064872	530165200
16	17245332	224156984	9274487688	1666083296
17	46466676	658855781	30521878637	5188200085
18	124658732	1924932324	99086541810	15993447527
19	335116620	5593580859	318742922236	48946213794
20	897697164	16175728584	1014076260686	148574713674
21	2408806028	46572304083	3202213457395	448343690109
22	6444560484	133556779740	10019907413348	1343838723819
23	17266613812	381611332725	31158181454688	4008314601988
24	46146397316	1086759598120	96149048417484	11888228627772
25	123481354908	3085406711831	295142819123871	35114454662483
26	329712786220	8735073410100	900066956153270	103219276329251

(Continued)
<u>_</u> :
Table

N	$c_N$	$rac{1}{4}c_N\langle R_{ m e}^2 angle_N$	$rac{1}{4}(N+1)^2c_N\langle R_{ m g}^2 angle_N$	$rac{1}{4}(N+1)c_N\langle R_m^2 angle_N$
27	881317491628	24665061125667	2732505731274220	302350533278086
28	2351378582244	69477665745896	8248829001382526	881974673999634
29	6279396229332	195265123427301	24804499283684685	2564984750250567
30	16741957935348	547633156505396	74221205928683512	7432620540208579
31	44673816630956	1532838884952299	221333034486502552	21480821587356344
32	119034997913020	4282540754311160	657175409080839632	61884062343185928
33	317406598267076	11944032183124129	1945418024966109721	177867529730724713
34	845279074648708	33257656763184556	5736868444918797822	509789937527302533
35	2252534077759844	92461749453584977	16872515769277148908	1458110752331771118
36	5995740499124412	256685581589089720	49453169481202211510	4160050173516616850
37	15968852281708724	711610318376609453	144602103638139094373	11846978451964635723
38	42486750758210044	1970232464253179804	421517897111033526836	33661784893928852621
39	113101676587853932	5448222121256407587	1226106614925695416296	95488104372916704748
40	300798249248474268	15048127109659424048	3556566126265101309980	270319420601198687276
41	800381032599158340	41516822124396623905	10296602201097594942225	764112980773483151309
42	2127870238872271828	114420546244580495788	29734383555237595018738	2155935506456910539997
43	5659667057165209612	315023293116319316107	85715948159939093661428	6074721940189140309702
4	15041631638016155884	866485020069260644664	246526159900360427960866	17087792773773847037390
45	39992704986620915140	2381096560500892770793	707895621958240811004041	48007613778509804802835
46	106255762193816523332	6537456672967882139948	2028423176500049998353720	134668241475007682635679
47	282417882500511560972	17933790994378821974707	5803786650111498416967400	377337842568931343367952
48	750139547395987948108	49156721156019804756024	16573780740476629162797384	1055798043293664579046904
49	1993185460468062845836	134634067180094086612595	47265785843405796903827851	2951082969829519054855011
50	5292794668724837206644	368470259697878846546356	134553477427137032959671590	8237877051162727078333841
51	14059415980606050644844	1007714451664000011164731	382563667789601278749936172	22973891188237620817265778
52	37325046962536847970116	2754055291248183384820416	1085908845295037795117686914	63992592137176740914658486
53	99121668912462180162908	7521747594983831934039415	3078819835262093742193456615	178090816717561120403807465

1054

542630902982460504898047082052996173170669487082516871581154464247987484601766849507063499523912311272388355698501700277581954674604559998896785424609197906672464726729955982881811954815213751098664697184193120545085618535891517894742538305001526612002743138403216072069599920787167645242434336340381553453453458884215297244856457492014607531300086059614041593055845867119231180569919634437713356751604991430637110578959386509767813477708087581305388464151657277815504411325891115670681806342384365531576270202955197194444931382930777594007396431477709022415813053884641516572778155044113258911156706818063423843655315762702029551971944449313829302775940073964314777090224159346427926345908244996721963082415161154176613766926049155696265758461941079587831015681108542428478523911668978514	Ν	сN	$rac{1}{4}c_N \langle R_{ m e}^2 \rangle_N$	$rac{1}{4}(N+1)^2 c_N (R_{ m g}^2)_N$	$rac{1}{4}(N+1)c_N\langle R_m^2 angle_N$
55698501700277581954674604559998596785424609197906672464726729955982881811954815213751056185358915178947425383050015266120027431384038216072069599920787167645242434336340381551574920146075313000860596140415930558458671192311805699196344377133567516049914306371105789158130538846415165727781550441132589111567068180634238436553157627020295519719444493138293027759346427926345908244996721963082411541766137669260491556962657584619410795878310156811085-	54	263090298246050489804708	20529906173170669487082516		495070634995239123112723883
56       1853589151789474253830500       152661200274313840382160720       69599920787167645242434336340       38155         57       4920146075313000860596140       415930558458671192311805699       196344377133567516049914306371       105789:         58       13053884641516572778155044       1132589111567068180634238436       553157627020295519719444493138       293027         59       34642792634590824499672196       3082415161154176613766926049       15569622657584619410795878310156       811085-	55	698501700277581954674604		24647267299559828818119548152	1375109866469718419312054508
<ul> <li>4920146075313000860596140</li> <li>415930558458671192311805699</li> <li>196344377133567516049914306371</li> <li>1057892</li> <li>13053884641516572778155044</li> <li>1132589111567068180634238436</li> <li>553157627020295519719444493138</li> <li>293027</li> <li>34642792634590824499672196</li> <li>3082415161154176613766926049</li> <li>1556962657584619410795878310156</li> <li>811085-</li> </ul>	56	1853589151789474253830500			3815534534588842152972448564
58 1305388464151657278155044 1132589111567068180634238436 5531576270295519719444493138 2930277 59 34642792634590824499672196 3082415161154176613766926049 1556962657584619410795878310156 811085-	57	4920146075313000860596140	415930558458671192311805699		10578959386509767813473708087
59 34642792634590824499672196 3082415161154176613766926049 1556962657584619410795878310156 811085 <sup>c</sup>	58	13053884641516572778155044	1132589111567068180634238436	553157627020295519719444493138	29302775940073964314770902241
	59	34642792634590824499672196	3082415161154176613766926049	1556962657584619410795878310156	81108542428478523911668978514

Table I. (Continued)

1     6       2     30       3     138       4     618       5     618       6     11946       6     11946       7     51882       8     224130       9     964134       10     4133166		6 (1 1 1) CIV (1 8/11)	$\hat{\overline{6}}(N+1)c_N \langle K_{\mathrm{m}}^z \rangle_N$
2 30 3 138 5 138 6 618 7 2730 6 11946 7 51882 8 224130 9 964134 10 41334 10 4133166	1	Ι	1
3     138       4     618       5     2730       6     11946       7     51882       8     224130       9     964134       10     4133166	12	22	17
4     618       5     2730       6     11946       7     51882       8     224130       9     964134       10     4133166	67	282	178
5     2730       6     11946       7     51882       8     224130       9     964134       10     4133166	654	2778	1476
6 11946 7 51882 8 224130 9 964134 10 4133166	3977	23305	10667
7 51882 8 224130 9 964134 10 4133166	22624	175194	70359
8 224130 9 964134 10 4133166	122821	1215740	434708
9 964134 10 4133166 11 17260000	644082	7939156	2557166
10 4133166 11 17660020	3288739	49422491	14477823
11 17660030	16440648	295993366	79492861
11 1 / 008938	80783857	1717056604	425633898
12 75355206	391310240	9697408184	2231674940
13 320734686	1872763387	53533130211	11494836257
14 1362791250	8870963422	289769871988	58310378811
15 5781765582	41647686501	1541876281342	291901836462
16 24497330322	194014270964	8081886977224	1444405248178
17 103673967882	897639074623	41801262603145	7074419785415
18 438296739594	4127904278590	213650877117460	34334678700977
19 1851231376374	18879838654237	1080407596025856	165283451747722
20 7812439620678	85930246593928	5411153165106856	789827267540498
21 32944292555934	389382874004291	26865804448156781	3749241090582031
22 138825972053046	1757383045067340	132328831054383256	17689855417349797
23 584633909268402	7902553525660965	647064413113509344	83004601828121876
24 2460608873366142	35417121500633314	3142945284616515512	387503899136724032
25 10350620543447034	158241760294727837	15172247917136636793	1800616777561080887

Table II. Exact enumeration data for SAWs on the triangular lattice

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N	$c_N$	$rac{1}{6}c_N \langle R_{ m c}^2  angle_N$	$rac{1}{6}(N+1)^2 c_N \langle R_g^2  angle_N$	$rac{1}{6}(N+1)c_N \langle R_{ m m}^2  angle_N$
26	43518414461742966	705008848574456242	72826367061554681960	8330920471773661365
27	182885110185537558	3132749279518281223	347722481262776946768	38390978707292879316
28	768238944740191374	13886614514918779812	1652126117509776447678	176259763248055992656
29	3225816257263972170	61415827107198652263	7813839241496101017943	806446563482615080995
30	13540031558144097474	271046328280157919578	36798230598686798952874	3677867046530479086571
31	56812878384768195282	1193838903060544883615	172603075240086498030932	16722626138383080469074
32	238303459915216614558	5248569464050058190772	806559315077883801952302	75819788411079420147060
33	999260857527692075370	23034474248167644819305	3755672941408238341746325	342850281196290726391195
34	4188901721505679738374	100925879660029490332616	17429779928912903943728776	1546457563237807336247617
35	17555021735786491637790	441524252843364233569911	80636231608943399450377104	6958970268567678359172166
36	73551075748132902085986	1928731794198995523104424	371943975622752362856339418	31245121332848941331142166
37	308084020607224317094182	8413734243045682304542891	1710813401690158618688146075	139991577634597301110308061
38	1290171266649477440877690	36655327788277288494374240	7848181414990001769700643892	625968026891459936611240307
39	5401678666643658402327390	159494618902280757690831541	35911648943670829119431170002	2793684462154188994667777314
40	22610911672575426510653226	693174559672551318610401776	163929038497681452701025717812	12445679176337664122926617782

Table II. (Continued)

arbitrary moments. We refrain here from inundating the reader with the complete tables of  $c_N(\mathbf{x})$ ; they are available on www.ms.unimelb.edu.au/ ~iwan. However, we do list here most of those series that we subsequently analyse. For the square lattice, we give in Table III the rotationally invariant moments  $\langle r^4 \rangle_N$ ,  $\langle r^6 \rangle_N$  and  $\langle r^8 \rangle_N$ , and in Table IV the corresponding non-rotationally-invariant moments  $\langle r^4 \cos 4\theta \rangle_N$ ,  $\langle r^6 \cos 4\theta \rangle_N$  and  $\langle r^8 \cos 4\theta \rangle_N$ . For the triangular lattice, we give in Table V the rotationally invariant

Ν	$rac{1}{4}c_N\langle r^4 angle_N$	$\frac{1}{4}c_N\langle r^6\rangle_N$	$\frac{1}{4}c_N\langle r^8\rangle_N$
1	1	1	1
2	24	80	288
3	233	1481	10313
4	1552	15584	171712
5	8261	118741	1876421
6	40128	761824	15997248
7	174687	4216895	113009823
8	711744	21139264	699292800
9	2756691	98246971	3911019843
10	10258032	430155712	20197992960
11	36953225	1794576465	97801373081
12	129595552	7194227712	449049597184
13	444358551	27891276903	1971835847895
14	1494601312	105092615072	8336039677888
15	4944384005	386372087101	34107295967573
16	16121969312	1390424839040	135635987698688
17	51903980173	4910490964373	526075527334141
18	165229382704	17055786755328	1995781800318592
19	520720306083	58367380590987	7423576318235379
20	1626289219696	197097871552608	27128806075092160
21	5037880731363	657614956490835	97570424122840995
22	15491105783776	2170327643009376	345877992391828288
23	47313566966717	7091919679833573	1210056084152236397
24	143616941038800	22964364302956192	4182680502669028416
25	433471181567175	73742760159367607	14298788347356195303
26	1301492251611088	234986541658461504	48385725874370354944
27	3888842767461723	743493757302422163	162197418768856363467
28	11567743361677920	2336936884325400320	538986352207098913536
29	34265929488742837	7300504880342236965	1776583932652252100533
30	101107717070386128	22676475755899170368	5811758654106692557056
31	297251719690114411	70061223151862034731	18878148082088838145579
32	870928677714199072	215380608263460514688	60916738136365328424448

Table III. Exact enumeration data for SAWs on the square lattice

Rotationally invariant moments.

Ν	$\frac{1}{4}c_N\langle r^4\cos 4\theta\rangle_N$	$\frac{1}{4}c_N \langle r^6 \cos 4\theta \rangle_N$	$\frac{1}{4}c_N\langle r^8\cos 4\theta\rangle_N$
1	1	1	1
2	8	48	224
3	41	521	5513
4	176	3616	64832
5	517	18581	515461
6	2464	96672	3460288
7	8543	424767	19559327
8	28672	1744320	99520384
9	93715	6804987	467838211
10	300016	25497024	2067530752
11	943881	92462801	8694947865
12	2927136	326371072	35106653952
13	8966103	1126120359	136996603671
14	27176192	3810903520	519344946752
15	81614149	12681966461	1920357610645
16	243136160	41589494144	6948572721152
17	719161805	134640733141	24668510505533
18	2113740144	430916393344	86113474737024
19	6177297699	1365089628939	296122738362483
20	17960659728	4284776312224	1004647110417216
21	51978553251	13337579454483	3367181961982563
22	149793700032	41203857605920	11161461862577856
23	430013901309	126414733312805	36627023206822344
24	1230085625008	385396000445280	119090886021960640
25	3507275950151	1168118922135351	383951817561778304
26	9970080369360	3521536905190720	1228239234255697152
27	28262765992155	10563701297658387	3900781003385081163
28	79911109071584	31542297194620416	12305781139629052160
29	225398486017269	93778343662150501	38579685692175173877
30	634334283147728	277695329500224576	120249249844158963968
31	1781434024153067	819226661598869419	372773226138821611691
32	4993035148467488	2408303159048790400	1149726544611189212672

Table IV. Exact enumeration data for SAWs on the square lattice

Non-rotationally-invariant moments.

moments  $\langle r^4 \rangle_N$ ,  $\langle r^6 \rangle_N$  and  $\langle r^8 \rangle_N$ , and in Table VI the corresponding non-rotationally invariant moments  $\langle r^6 \cos 6\theta \rangle_N$  and  $\langle r^8 \cos 6\theta \rangle_N$ .

# 3.2. Method of Analysis

In this subsection we explain in detail the method we used to analyse the data, the results of which are reported in subsequent subsections. For the triangular lattice, we expect the series coefficients of any generic

Ν	$rac{1}{6}c_N\langle r^4 angle_N$	$\frac{1}{6}c_N\langle r^6\rangle_N$	$\frac{1}{6}c_N\langle r^8\rangle_N$
1	1	1	1
2	36	120	420
3	529	3337	22993
4	5454	53358	579918
5	46169	633185	9725849
6	344428	6221884	126456796
7	2352769	53647549	1380311377
8	15060090	420194610	13256099610
9	91701871	3057404227	115436446639
10	536695548	20985811596	930424151244
11	3041620465	137386509145	7043622904369
12	16784388968	864860517248	50628426215432
13	90564392107	5267777416675	348381660817291
14	479388030946	31195330864090	2309752803978322
15	2495911050345	180302936975925	14829889785198921
16	12808562012852	1020273312831596	92588968138883348
17	64901247920059	5666785971562159	564018088195524619
18	325170745810666	30958613694252346	3361656410695492858
19	1612871078099977	166655904211475269	19649810153900928217
20	7927964773508104	885333404431705216	112867935343523712424
21	38652473796950531	4647266177110051355	638156051853903239891
22	187056802703356296	24130876287242419704	3556820174217345377400

Table V. Exact enumeration data for SAWs on the triangular lattice

Rotationally invariant moments.

quantity, such as the SAW generating function, to have an asymptotic expansion of the form

$$\mu^N N^{\gamma-1} \left( a_0 + \sum_{i=1}^k \frac{a_i}{N^{\Delta_i}} \right), \tag{3.1}$$

where  $\mu$  is the connective constant and  $\gamma$  is the critical exponent. Likewise, we expect the square-lattice series coefficients to have an asymptotic expansion of the form

$$\mu^{N} N^{\gamma - 1} \left( a_0 + \sum_{i=1}^{k} \frac{a_i}{N^{\Delta_i}} \right) + (-\mu)^{N} N^{\alpha - 2} \left( b_0 + \sum_{i=1}^{m} \frac{b_i}{N^{\Delta_i^{AF}}} \right), \quad (3.2)$$

where  $\alpha$  is the critical exponent occurring in the polygon generating function. Similar expansions hold for metric quantities, and involve also the

Ν	$\frac{1}{6}c_N\langle r^6\cos 6\theta\rangle_N$	$\frac{1}{6}c_N\langle r^8\cos 6\theta\rangle_N$
1	1	1
2	12	96
3	97	1609
4	654	17454
5	3977	151649
6	22684	1149148
7	123721	7935829
8	652842	51236610
9	3357439	314319571
10	16914348	1852261068
11	83777857	10566164665
12	409089560	58677117008
13	1973505067	318573263587
14	9421326322	1696583222746
15	44567944521	8885936605365
16	209144745044	45868003547852
17	974497840243	233746526628199
18	4511869867210	1177691322037546
19	20770914530257	5873419831448317
20	95130303643048	29024633960838784
21	433664585252891	142245181072370291
22	1968525488778840	691879404495232056

Table VI. Exact enumeration data for SAWs on the triangular lattice

Non-rotationally-invariant moments.

critical exponent v. Since the exact values  $\gamma = 43/32$ ,  $\alpha = 1/2$  and  $\nu = 3/4$  are well established, we shall use them throughout this paper.

Given the calculated terms of the series up to some order  $N_{\text{max}}$ , we proceed as follows: First we decide how many correction terms  $\{a_i\}$  and  $\{b_i\}$  we wish to include (i.e., we fix the numbers k and m); then we make some assumption for the values of  $\mu$ ,  $\Delta_i$  and  $\Delta_i^{\text{AF}}$ ; finally, we fit the data to (3.1) or (3.2) by taking (k+m+2)-tuples of successive values of N and solving for  $\{a_i\}$  and  $\{b_i\}$ . This can be done by solving a system of linear equations.

By using (k+m+2)-tuples at steadily larger values of N, many estimates for the  $\{a_i\}$  and  $\{b_i\}$  are found. If the different estimates seem stable as N grows, we presume that they provide an acceptably accurate estimate of the actual asymptotic coefficients.

A noteworthy feature of the method is that, if a blatantly-too-low correction-to-scaling exponent is given as input (for example, specifying  $\Delta_1 = 1/2$  for the two-dimensional SAW), the sequence of amplitude estimates for the term corresponding to that exponent will converge

rapidly to zero, giving a very strong signal that the exponent in question is absent. (Of course, if such a term were to occur with an amplitude several orders of magnitude smaller than the amplitudes of the other terms, one could be fooled into thinking such a term is absent. Our analysis assumes the absence of such pathologies.)

Another point to bear in mind is that even if one knows the precise asymptotic form, with a limited number of series coefficients one can fit only to a small number of asymptotic terms (i.e., k and m cannot be taken too large). Beyond a certain number of terms in the asymptotic form, the quality of the fit visibly deteriorates. The more series coefficients are available, the more terms can be included in the Ansatz (provided that sufficient numerical precision is retained during the analysis).

A universally observed feature of the method is that the apparent accuracy of the amplitude estimates decreases rapidly as we move to higher-order terms in the asymptotic expansions. That is to say, the apparent accuracy of the estimate of amplitude  $a_{i+1}$  is significantly less than that of  $a_i$ . Moreover, adding further terms in the assumed asymptotic form (i.e., increasing k and m) improves convergence of the low-order amplitudes  $a_i$  provided that k+m does not get too large, but after a certain point actually slows the convergence. In the case at hand, allowing more than 2–5 terms (these being the values of k + 1 and m + 1 separately) in the assumed asymptotic form led to a deteriorating (i.e., less stable) fit.

As the series data at very small N are probably not reflective of asymptotic behaviour, and we have here the luxury of access to many terms (i.e., quite large  $N_{\text{max}}$ ), the first 19 - k - m terms of the series will not be used in any of our analyses here.

Our analysis thus comprises two phases. In the first phase, we determine the correct connective constant  $\mu$  and the correct exponents  $\Delta_i$  and  $\Delta_i^{AF}$  for the asymptotic expansion, as just described. In the second phase, we determine how many terms in the asymptotic expansion we can reliably use. We now describe our procedure for the second phase of the analysis.

We begin by fitting for only one correction coefficient,  $a_1$ . Then we add further asymptotic terms until the estimates obtained do not appear to be converging as  $N \to \infty$  to a value that is consistent with the previous estimates given by fits with one fewer asymptotic term. We define "consistent" by the requirement that estimates of all included asymptotic coefficients be well-converged and of the same sign and within a factor F = 2.4 of the previous estimates. More specifically, we invoke this requirement as follows: setting k = K gives estimates of  $a_0, \ldots, a_K$ ; repeating the analysis with k = K + 1 yields estimates

of  $a_0, \ldots, a_{K+1}$ . We require that the coefficients  $a_0, \ldots, a_K$  from the two fits agree in sign and in magnitude within a factor of F; otherwise, we reject the fit with k = K + 1 and stop at k = K. Note that the choice of the value of F is somewhat arbitrary. Realistically, one can reasonably make any choice in the range  $1.5 \leq F \leq 3$ , the lower value being more conservative. We chose a value in this range that included most data sets with small values of k and m, and excluded those with higher values.

Please note that the convergence (as N grows) of each fit is here judged by traditional intuitive (and thus somewhat subjective) methods. It would be an interesting project to find a precise definition of "wellconverged" (or its synonym, "stable") that accords satisfactorily with our intuitive judgments and gives good results on test series; this would allow the series analysis to be converted into a precise algorithm. But we do not purport to carry out such a project here.

For the triangular lattice, this procedure is thus relatively simple to implement. We compute fits initially with k=0, incrementing k by 1 until a non-stable or inconsistent estimate (as defined in the preceding paragraph) is found; we then revert to the previous group of stable and consistent estimates. The final entries (i.e., those corresponding to the maximum N) in the largest stable group are taken as our final estimates.

For the square lattice, the procedure is more complicated, as it is not clear *a priori* whether terms involving  $\Delta_i$  or  $\Delta_i^{AF}$  should be added to a given group. Empirically we have found that groups containing approximately equal numbers of  $\Delta_i$  and  $\Delta_i^{AF}$  terms, or slightly more  $\Delta_i$  terms, are more stable than estimates with significantly different values of k and m. Hence we begin by exploring groups with equal numbers of  $\Delta_i$  and  $\Delta_i^{AF}$  terms, that is with k = m, adding one coefficient to each group at every stage. Next we try groups with one more  $\Delta_i$  term than  $\Delta_i^{AF}$  terms, so that k = m + 1; and finally we try groups with two more  $\Delta_i$  terms, so that k = m + 2. Again, the largest group that provides stable and consistent estimates is selected. As always, the given estimates are taken from the fits to the largest available value of N, which is  $N_{\text{max}}$ , since these should best reflect the asymptotic regime.

The estimated error is calculated as the change between the estimate given by the longest series and the series ten terms shorter, multiplied by a factor reflective of the expected rate of convergence of the estimates. This latter factor is determined by assuming that the error in the estimates is principally given by the first omitted  $\Delta_i$  or  $\Delta_i^{AF}$  term. The difference in the exponents between the term in question and the first omitted term is then used to predict the value of the estimate on a fit to an infinite series.

To illustrate these procedures, we show below the output from fitting the triangular-lattice series for  $c_N \langle R_g^2 \rangle_N$  with increasing numbers of correction-to-scaling terms. We make the Ansatz

$$(N+1)^{2}c_{N}\langle R_{g}^{2}\rangle_{N}/6 \sim \mu^{N}N^{123/32} \times [a_{0}+a_{1}/N+a_{2}/N^{3/2}+a_{3}/N^{2}+a_{4}/N^{5/2}+\cdots]$$
(3.3)

and obtain fits as follows:

Ν	$a_0$	$a_1$
21	0.01929438	0.08276963
22	0.01932692	0.08208623
23	0.01935556	0.08145624
24	0.01938091	0.08087327
25	0.01940346	0.08033194
26	0.01942363	0.07982768
27	0.01944175	0.07935660
28	0.01945809	0.07891535
29	0.01947289	0.07850104
30	0.01948633	0.07811114
31	0.01949859	0.07774345
32	0.01950980	0.07739603
33	0.01952007	0.07706717
34	0.01952952	0.07675536
35	0.01953823	0.07645924
36	0.01954628	0.07617761
37	0.01955373	0.07590938
38	0.01956064	0.07565359
39	0.01956707	0.07540935
40	0.01957306	0.07517587

Ν	$a_0$	$a_1$	$a_2$
22	0.01976614	0.05375917	0.08754307
23	0.01976114	0.05408172	0.08654625
24	0.01975680	0.05437453	0.08562049
25	0.01975301	0.05464205	0.08475611
26	0.01974966	0.05488785	0.08394517
27	0.01974669	0.05511490	0.08318096
28	0.01974404	0.05532562	0.08245789
29	0.01974166	0.05552207	0.08177122
30	0.01973951	0.05570593	0.08111693
31	0.01973756	0.05587867	0.08049156

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32	0.01973578	0.05604149	0.07989215		
33	0.01973415	0.05619545	0.07931614		
34	0.01973265	0.05634145	0.07876131		
35	0.01973127	0.05648027	0.07822571		
36	0.01972999	0.05661259	0.07770765		
37	0.01972881	0.05673898	0.07720563		
38	0.01972770	0.05685998	0.07671833		
39	0.01972667	0.05697603	0.07624459		
40	0.01972571	0.05708754	0.07578337		
N	$a_0$	<i>a</i> <sub>1</sub>	<i>a</i> <sub>2</sub>	<i>a</i> <sub>3</sub>	
23	0.01970992	0.06084150	0.04428770	0.07428718	
24	0.01971020	0.06080458	0.04451851	0.07388144	
25 26	0.01971034	0.06078451 0.06077784	0.04464682 0.04469036	0.07365079 0.07357085	
20 27	0.01971039 0.01971036	0.06077784	0.04469036	0.07363327	
27	0.01971036	0.06078284	0.04465705	0.07382009	
28 29	0.01971020	0.06081948	0.04440510	0.07382009	
29 30	0.01971013	0.06084830	0.04440310	0.07452360	
31	0.01970995	0.06084830	0.04420187	0.07432300	
32	0.01970970	0.06092130	0.04367303	0.07560099	
33	0.01970931	0.06096380	0.04335757	0.07625946	
34	0.01970908	0.06100940	0.04301375	0.07698862	
35	0.01970883	0.06105753	0.04264515	0.07778247	
36	0.01970859	0.06110773	0.04225488	0.07863562	
37	0.01970834	0.06115962	0.04184568	0.07954324	
38	0.01970809	0.06121284	0.04141995	0.08050094	
39	0.01970785	0.06126712	0.04097980	0.08150474	
40	0.01970761	0.06132220	0.04052709	0.08255105	
Ν	$a_0$	$a_1$	$a_2$	$a_3$	$a_4$
24	0.01971252	0.06028314	0.04946255	0.05630611	0.02220967
25	0.01971161	0.06048759	0.04752405	0.06319720	0.01350151
26	0.01971081	0.06067477	0.04571025	0.06978710	0.00499021
27	0.01971004	0.06086343	0.04384348	0.07671271	-0.00414364
28	0.01970935	0.06103877	0.04207338	0.08341263	-0.01315896
29	0.01970871	0.06120830	0.04032868	0.09014499	-0.02239437
30	0.01970812	0.06137074	0.03862565	0.09683963	-0.03175015
31	0.01970757	0.06152632	0.03696505	0.10348538	-0.04120539
32	0.01970707	0.06167592	0.03534052	0.11010004	-0.05078048
33	0.01970660	0.06181962	0.03375373	0.11666979	-0.06045075
34	0.01970616	0.06195787	0.03220232	0.12319772	-0.07021604
35	0.01970575	0.06209097	0.03068515	0.12968223	-0.08006943
36 37	0.01970536	0.06221921	0.02920108	0.13612229	-0.09000497 0.10001832
51	0.01970501	0.06234286	0.02774880	0.14251786	-0.10001832

38	0.01970467	0.06246219	0.02632719	0.14886860	-0.11010477
39	0.01970435	0.06257743	0.02493510	0.15517452	-0.12026033
40	0.01970406	0.06268879	0.02357145	0.16143576	-0.13048133

We observe in these fits the following behaviour: As N increases, the estimates of the amplitudes  $a_i$  appear to be converging in each set, until we reach the set with five asymptotic coefficients  $(a_0, \ldots, a_4)$ . In this latter fit, we see that the estimate of  $a_4$  appears to be diverging. Further, the estimates of  $a_1$ ,  $a_2$  and  $a_3$  have deteriorating apparent convergence as we go from a four-term to a five-term fit. By contrast, going from a two-term to a three-term fit, and from a three-term to a four-term fit, improved the apparent convergence of the amplitude sequences. Thus we reject the five-term fit, and base our estimates on the four-term fit.

Finally, the estimated error from a series of length N is taken to be the appropriately scaled difference between the values obtained from this series and those obtained from the series of length N - 10. This difference is scaled by a factor dependent on the difference between the exponent in question and the first omitted exponent. The scaling factor follows from our assumption that the error is given principally by the first neglected term,  $c/N^{\Delta_{k+1}}$  (or similarly with  $\Delta_{m+1}^{AF}$ ). Hence, if the actual value of the coefficient in question is  $a_i$  and the two estimates are  $a_i^{(N)}$  and  $a_i^{(N-10)}$ , we expect that

$$\frac{a_i^{(N)}}{N^{\Delta_i}} = \frac{a_i}{N^{\Delta_i}} + \frac{c}{N^{\Delta_{k+1}}}$$
(3.4a)

$$\frac{a_i^{(N-10)}}{(N-10)^{\Delta_i}} = \frac{a_i}{(N-10)^{\Delta_i}} + \frac{c}{(N-10)^{\Delta_{k+1}}}$$
(3.4b)

Simple algebra then yields

$$a_i^{(N)} - a_i = -\frac{a_i^{(N)} - a_i^{(N-10)}}{\left(\frac{N}{N-10}\right)^{\Delta_{k+1} - \Delta_i} - 1}.$$
(3.5)

Therefore,  $a_i$  is estimated by  $a_i^{(N)}$  with error quoted as

$$2\left|a_{i}^{(N)}-a_{i}^{(N-10)}\right| / \left[\left(\frac{N}{N-10}\right)^{\Delta_{k+1}-\Delta_{i}}-1\right].$$
(3.6)

The factor of 2 is included to make our errors more conservative. More adventurous readers may choose to reduce this factor.

In the above example, the first omitted term is  $O(N^{-5/2})$ . The difference in the estimate of  $a_0$  from the N = 40 series with four asymptotic coefficients (0.019707611) and that from a N = 30 series (0.019709959) is 2.348 ×10<sup>-6</sup>. Thus the error is quoted as  $2 \times 2.348 \times 10^{-6}/((40/30)^{2.5} - 1) = 4.5 \times 10^{-6}$ . Our amplitude estimate is then  $a_0 = 0.019708 \pm 0.000005$ . Similarly,  $a_1 = 0.0613 \pm 0.0018$ , where the error is given by  $2 \times 0.0004739/((40/30)^{1.5} - 1)$ . Likewise,  $a_2 = 0.04 \pm 0.02$ , and  $a_3 = 0.08 \pm 0.1$ .

# 3.3. SAW Counts

In this subsection we discuss the analysis of the newly extended series for SAW counts on the square and triangular lattices. Here we give only a brief analysis, as fuller details will be published elsewhere,<sup>(65)</sup> along with a discussion of the series derivation.

Let us begin with the triangular lattice. We first analysed the extended SAP series using biased differential approximants using the known exponent  $\alpha = 1/2$  (see ref. 19 for the method). We obtained

$$x_c = 1/\mu = 0.240\,917\,574 \pm 0.000\,000\,004\,,\tag{3.7}$$

which we will use in subsequent analyses.

We also performed a similar analysis using the extended SAW series, biasing the estimate with the known exponent  $\gamma = 43/32$ . We obtained the estimate  $x_c = 1/\mu = 0.240917579 \pm 0.00000008$ , in agreement with the SAP result but less precise.

Using the estimate (3.7) of  $x_c$ , we proceeded as described in Section 3.2 to fit the series coefficients to various asymptotic forms. For triangular-lattice SAWs, we expect, based on earlier investigations of the corresponding square-lattice series,<sup>(17)</sup> that

$$c_N \sim \mu^N N^{11/32} [a_0 + a_1/N + a_2/N^{3/2} + a_3/N^2 + a_4/N^{5/2} + a_5/N^3 + \cdots].$$
  
(3.8)

However, as discussed in Section 2.2, renormalization-group theory predicts an additional "energy-like" term arising from the mixing between nonlinear scaling fields. For the two-dimensional SAW ( $\alpha = 1/2$ ), incorporating this term requires that (3.8) be modified to read

$$c_N \sim \mu^N N^{11/32} [a_0 + a_1/N + a_2/N^{3/2} + \tilde{a}_0/N^{59/32} + a_3/N^2 + a_4/N^{5/2} + \cdots]$$
  
(3.9)

[cf. (2.26)].

In our analysis, we tried both the asymptotic forms (3.8) and (3.9). Since the exponents associated with amplitudes  $\tilde{a}_0$  and  $a_3$  are numerically close (1.84375 and 2, respectively), we expect that it will be very difficult to distinguish numerically between the Ansätze (3.8) and (3.9). This is indeed the case. Under the assumption (3.8), we found that the sequences corresponding to the amplitudes are well converged up to k = 4 for triangular-lattice SAW and we estimate  $a_0 = 1.183966(1)$ ,  $a_1 = 0.5960(4)$ ,  $a_2 = -0.274(6)$ ,  $a_3 = -0.14(4)$ , and  $a_4 = 0.09(10)$ . Our errors are calculated as described in Section 3.2 and are given, in parentheses, as the uncertainty in the last quoted digit(s). Under the alternative Ansatz (3.9), we find that the fit is neither better nor worse. We observed that the sequences of estimates of the corresponding amplitudes  $\tilde{a}_0$  and  $a_3$  appear to be correlated: they are monotonically increasing in magnitude but are of opposite sign, the sum  $\tilde{a}_0 + a_3$  being almost constant.

To investigate this point further, we constructed a test series, with known asymptotic behaviour, similar to that in (3.9), namely

$$d_N = N^{11/32} \left[ 1 + 1/N + 0.7/N^{3/2} + 1.25/N^{59/32} + 3/N^2 - 4/N^{5/2} + 5/N^3 - 6/N^{7/2} \right] + (0.5)^N.$$
(3.10)

The last term is included to incorporate the fact that there are other singularities in the complex plane, beyond  $x_c$ , which will make an exponentially decaying contribution to the asymptotics. We generated the first 1000 terms of this sequence and analysed them as above, including either a term  $N^{-59/32}$  or a term  $N^{-2}$  or both. The analyses using either one of these two terms behaved similarly. The analysis using both terms gave *inferior* estimates of the first three amplitudes, and the *wrong sign* for the amplitude of the  $N^{-2}$  term, when  $N \leq 240$ . Only beyond this point does the analysis using both terms give superior estimates of the first three amplitudes, along with the right sign for the  $N^{-2}$  term (the two issues clearly go together). We conclude that using series of the length available to us  $(N \leq 40)$ , it is unfeasible to determine whether a term  $N^{-59/32}$  is present or absent.

In conclusion, our analysis is unable to resolve the question of whether the "energy-like" term  $N^{-59/32}$  is present or not. Therefore, for the subsequent analysis of the metric quantities, reported in the next subsection, we have assumed for simplicity the absence of this term, and just assumed the asymptotic form (2.24) with one correction-to-scaling exponent  $\Delta_1 = 3/2$ .

On the square lattice, the situation is complicated by the presence of an "antiferromagnetic" singularity at  $x = -1/\mu$ . From (2.27) ff. we recall

that the asymptotic form of the coefficients given in (3.8) and (3.9) is modified by the additional term

$$(-1)^{N} \mu^{N} N^{-3/2} [d_0 + d_1/N + d_2/N^2 + d_3/N^3 + \cdots].$$
(3.11)

Analysing the square-lattice SAW data using as our estimate of  $x_c$  the positive real root of

$$581x^4 + 7x^2 - 13 = 0, (3.12)$$

which is a useful mnemonic for the current best estimate  $x_c^2 = 0.143680$ 62927(1),<sup>(19)</sup> we obtain a very convincing fit with k=3 and m=2, enabling the following amplitude estimates to be made:  $a_0 = 1.1770425(7)$ ,  $a_1 = 0.5501(2)$ ,  $a_2 = -0.1402(3)$  and  $a_3 = -0.12(2)$  for the "ferromagnetic" amplitudes, and  $d_0 = -0.189848(3)$ ,  $d_1 = 0.17473(9)$  and  $d_2 = -1.51(1)$ for the "antiferromagnetic" amplitudes. This is in close agreement with the earlier estimates (1.2) based on slightly shorter series; here we have obtained a slight improvement in the precision of the estimates for the leading amplitudes  $a_0$ ,  $d_0$  and  $d_1$ .

If instead we assume the asymptotic form (3.9) for the "ferromagnetic" term, we find that estimates of  $a_3$  are small (less than 0.03 in magnitude) and tending toward zero. Estimates of  $a_4$  are tending toward the estimate for this term obtained in the absence of the additional term with amplitude  $a_3$ . Once again, we are unable to distinguish (3.8) from (3.9).

# 3.4. Metric Quantities $\langle R_e^2 \rangle$ , $\langle R_g^2 \rangle$ and $\langle R_m^2 \rangle$

In this subsection we shall analyse the metric quantities  $\langle R_e^2 \rangle_N$ ,  $\langle R_g^2 \rangle_N$ and  $\langle R_m^2 \rangle_N$ , any one of which we shall generically denote by  $\langle R^2 \rangle_N$ . As discussed in Section 2.2 [cf. (2.24)/(2.27)], their asymptotic behaviour is expected in the first instance to be

$$\langle R^2 \rangle_N \sim N^{2\nu} [a_0 + a_1/N + a_2/N^{\Delta_1} + a_3/N^2 + \cdots]$$
 (3.13)

for the triangular lattice, and

$$\langle R^2 \rangle_N \sim N^{2\nu} [a_0 + a_1/N + a_2/N^{\Delta_1} + a_3/N^2 + \cdots]$$
  
+  $(-1)^N N^q [b_0 + b_1/N^{\Delta_1^{AF}} + b_2/N + \cdots]$  (3.14)

for the square lattice. As mentioned earlier, there is overwhelming numerical evidence<sup>(37,17)</sup> that the leading exponent  $2\nu$  equals 3/2 exactly, as predicted by Coulomb-gas arguments;<sup>(4,5)</sup> we shall henceforth take this fact for granted. We also expect  $\Delta_1 = 3/2$ , as predicted by Nienhuis<sup>(4)</sup> and confirmed numerically for the SAW counts. Furthermore, for the square lattice we predict q = -11/32 [cf. (2.33)]. Finally, in Section 2.2 we pointed out that renormalization-group theory predicts an additional "energy-like" term in the susceptibility [cf. (3.9)], though alas we were unable to distinguish it numerically (see Section 3.3); it is reasonable to guess that there may be a corresponding term also in the series for the unnormalized second moments  $c_N \langle R^2 \rangle_N$ . Whether or not the latter term is present, the existence of an "energy-like" term in  $c_N$  will induce in  $\langle R^2 \rangle_N$  additional correction-to-scaling terms  $N^{-59/32}$ ,  $N^{-91/32}$ , ... beyond those included in (3.13)/(3.14).

In addition to the normalized metric quantities  $\langle R^2 \rangle_N$ , we also studied the corresponding unnormalized quantities  $c_N \langle R^2 \rangle_N$ , whose expected asymptotic form is

$$c_N \langle R^2 \rangle_N \sim \mu^N N^{2\nu+\gamma-1} [b_0 + b_1/N + b_2/N^{\Delta_1} + b_3/N^2 + \cdots],$$
 (3.15)

with appropriate additional antiferromagnetic terms (2.31) when analysing the square-lattice data. The latter quantities have the disadvantage that the analysis depends sensitively on an input estimate of  $\mu$ ; but, for loosepacked lattices and for  $\langle R_e^2 \rangle_N$  only, they have the advantage that the effect of the antiferromagnetic singularity is weaker. To see this, compare (2.30)– (2.33): the antiferromagnetic contribution in  $c_N \langle R_e^2 \rangle_N$  is relatively weaker than that in  $c_N$ ; but the antiferromagnetic contribution in  $\langle R_e^2 \rangle_N$  is dominated by that in  $c_N$ . Therefore, the antiferromagnetic contribution is relatively weaker in  $c_N \langle R_e^2 \rangle_N$  than in  $\langle R_e^2 \rangle_N$ .

Our method of analysis is based on directly fitting  $\langle R^2 \rangle_N$  and  $c_N \langle R^2 \rangle_N$  to the assumed asymptotic form (3.13)/(3.14)/(3.15), as described in Section 3.2. The values of the exponents v, q,  $\Delta_1$  and  $\Delta_1^{AF}$  are assumed, and the appropriate system of linear equations is solved to give estimates of the amplitudes  $\{a_i\}$  and  $\{b_i\}$ . In applying the method to metric quantities (see, for example, the table in Section 3.2), the fit to the leading amplitude is rather stable, that to the first analytic correction term is moderately stable, while the fit to the amplitude of the assumed correction-to-scaling term  $N^{-3/2}$  converges less impressively for both the normalized and unnormalized metric quantities. As already noted, adding further terms in the assumed asymptotic form beyond the first initially improved convergence, but this improvement is not sustained. That

is to say, allowing more than between two and five terms in the assumed asymptotic form led to an apparently deteriorating fit.

#### 3.4.1. Triangular Lattice

With our 40-term triangular-lattice series we found that we could fit to  $a_0$ ,  $a_1$ ,  $a_2$  and sometimes  $a_3$ . For the normalized and unnormalized metric quantities, the estimate of  $a_0$  could usually be made to four-digit precision, while the estimate of  $a_1$  could be made only to one or two significant digits, and the estimate of  $a_2$  is accurate only to at best one significant digit. For  $a_3$  the error is comparable to or greater than the estimate.

We have applied this analysis method to the triangular-lattice data, using a 40-term series for all metric quantities. Because the triangular lattice is close-packed, there is only one singularity on the circle of convergence, which makes the analysis simpler than for the square lattice [compare (3.13)-(3.14)].

The tables of estimates for the metric quantities obtained according to the procedure described in Section 3.2 are shown in Table VII. The results are:

$$\langle R_e^2 \rangle_N \sim N^{3/2} [0.71174(32) + 0.95(12)/N - 2.6(1.6)/N^{3/2} + 3(7)/N^2 + O(1/N^{5/2})]$$

$$\langle R_g^2 \rangle_N \sim N^{3/2} [0.09989(4) + 0.056(16)/N + 0.3(2)/N^{3/2} 0.2(1.0)/N^2 + O(1/N^{5/2})]$$

$$(3.16)$$

$$-0.2(1.0)/N^{2} + O(1/N^{3/2})]$$
(3.17)  
$$\langle R_{m}^{2} \rangle_{N} \sim N^{3/2} [0.3133(4) + 0.24(12)/N - 0.2(1.0)/N^{3/2} + O(1/N^{2})]$$
(3.18)

These were obtained with k=3, k=3, and k=2 respectively. Unfortunately the uncertainties in the coefficients of the  $O(1/N^{3/2})$  are so great as to be comparable to (or, in the case of  $\langle R_m^2 \rangle$ , larger than) the coefficient itself. Further, the analysis of the  $\langle R_g^2 \rangle_N$  series violates the convergence criterion we have set, in that the coefficient of  $a_1$  differs by nearly a factor of 3 in going from a two-term fit (k=1) to a three-term fit (k=2). We have nevertheless presented results for k=3. Our justification for this is twofold. Firstly, the estimate of  $a_1$  stabilises if we then go to a four-term fit. Secondly, as we have already seen, the data for the essentially equivalent series  $(N + 1)^2 c_N \langle R_g^2 \rangle_N / 6$  supports a four-term fit. For the reader unconvinced by these arguments, the corresponding analysis with k=0 (a one-term fit, as would be justified by strict adherence to the convergence criteria we have set), gives  $a_0 = 0.106 \pm 0.012$ .

triangular lattice							
Ν	$a_0$	<i>a</i> <sub>1</sub>	<i>a</i> <sub>2</sub>	<i>a</i> <sub>3</sub>			
19	0.712401	0.847374	-1.932382	1.872489			
20	0.712338	0.854132	-1.970591	1.933229			
21	0.712262	0.862841	-2.021181	2.015860			
22	0.712207	0.869360	-2.060036	2.080978			
23	0.712154	0.876015	-2.100682	2.150783			
24	0.712108	0.882131	-2.138917	2.217997			
25	0.712067	0.887809	-2.175211	2.283237			
26	0.712030	0.893200	-2.210408	2.347867			
27	0.711996	0.898252	-2.244079	2.410972			
28	0.711965	0.903032	-2.276568	2.473071			
29	0.711937	0.907558	-2.307916	2.534132			
30	0.711912	0.911851	-2.338197	2.594197			
31	0.711888	0.915933	-2.367500	2.653354			
32	0.711867	0.919820	-2.395884	2.711636			
33	0.711847	0.923529	-2.423411	2.769094			
34	0.711828	0.927073	-2.450135	2.825769			
35	0.711811	0.930464	-2.476105	2.881700			
36	0.711795	0.933713	-2.501366	2.936922			
37	0.711780	0.936831	-2.525957	2.991468			
38	0.711766	0.939827	-2.549918	3.045367			
39	0.711753	0.942708	-2.573280	3.098647			
40	0.711741	0.945482	-2.596077	3.151335			
19	0.099915	0.050034	0.335467	-0.323304			
20	0.099919	0.049550	0.338206	-0.327657			
21	0.099919	0.049529	0.338324	-0.327850			
22	0.099920	0.049454	0.338770	-0.328598			
23	0.099919	0.049539	0.338252	-0.327708			
24	0.099918	0.049696	0.337275	-0.325990			
25	0.099917	0.049907	0.335921	-0.323556			
26	0.099915	0.050176	0.334165	-0.320333			
27	0.099913	0.050482	0.332124	-0.316508			
28	0.099911	0.050822	0.329820	-0.312103			
29	0.099908	0.051186	0.327296	-0.307186			
30	0.099906	0.051570	0.324587	-0.301813			
31	0.099904	0.051969	0.321720	-0.296026			
32	0.099901	0.052380	0.318722	-0.289869			
33	0.099899	0.052799	0.315611	-0.283376			
34	0.099897	0.053224	0.312408	-0.276582			
35	0.099895	0.053652	0.309126	-0.269516			
36	0.099893	0.054083	0.305781	-0.262203			
37	0.099891	0.054513	0.302384	-0.254667			
38	0.099889	0.054943	0.298944	-0.246930			
39 40	0.099887	0.055372	0.295472	-0.239010			
40	0.099885	0.055797	0.291974	-0.230925			

Table VII. Fit to  $\langle R^2 \rangle = N^{3/2} (a_0 + a_1 N^{-1} + a_2 N^{-3/2} + a_3 N^{-2})$  for SAWs on the triangular lattice

Ν	$a_0$	$a_1$	<i>a</i> <sub>2</sub>	<i>a</i> <sub>3</sub>
19	0.313864	0.190168	-0.037972	
20	0.313817	0.192786	-0.045478	
21	0.313772	0.195399	-0.053166	
22	0.313731	0.197964	-0.060906	
23	0.313691	0.200488	-0.068707	
24	0.313655	0.202966	-0.076542	
25	0.313620	0.205394	-0.084387	
26	0.313588	0.207772	-0.092232	
27	0.313558	0.210098	-0.100063	
28	0.313529	0.212373	-0.107868	
29	0.313502	0.214597	-0.115640	
30	0.313477	0.216769	-0.123371	
31	0.313453	0.218892	-0.131055	
32	0.313430	0.220965	-0.138688	
33	0.313409	0.222990	-0.146266	
34	0.313388	0.224969	-0.153785	
35	0.313369	0.226902	-0.161244	
36	0.313351	0.228791	-0.168639	
37	0.313333	0.230637	-0.175971	
38	0.313317	0.232441	-0.183237	
39	0.313301	0.234205	-0.190437	
40	0.313286	0.235930	-0.197570	

Table VII. (Continued)

Data are for  $\langle R_e^2 \rangle_N$  at top, then  $\langle R_g^2 \rangle_N$  at middle, then  $\langle R_m^2 \rangle_N$  at bottom. The fit for  $\langle R_m^2 \rangle_N$  includes only terms up to order  $(N^{-3/2})$ .

We can do somewhat better from a similar analysis of the unnormalized metric quantities, using the estimate  $\mu = 4.15079723$  from (3.7), which gave

$$c_N \langle R_e^2 \rangle_N / 6 \sim \mu^N N^{59/32} [0.14045(6) + 0.256(26)/N - 0.53(32)/N^{3/2} + 0.6(1.6)/N^2 + O(1/N^{5/2})]$$
(3.19)

$$(N+1)^2 c_N \langle R_g^2 \rangle_N / 6 \sim \mu^N N^{123/32} [0.019708(5) + 0.0613(18)/N + 0.04(2)/N^{3/2} + 0.08(10)/N^2 + O(1/N^{5/2})]$$
(3.20)

$$(N+1)c_N \langle R_m^2 \rangle_N / 6 \sim \mu^N N^{91/32} [0.06183(12) + 0.136(28)/N -0.02(24)/N^{3/2} + O(1/N^2)].$$
(3.21)

These estimates were also obtained with k = 3, k = 3 and k = 2, respectively. From these we can estimate the amplitudes of the metric quantities by dividing through by the asymptotic form (3.8) for  $c_N$ , and accounting for the factor of 6 and appropriate factors of (N + 1). In this way we obtain a second set of amplitude estimates,

$$\langle R_e^2 \rangle_N \sim N^{3/2} [0.71176(15) + 0.94(7)/N - 2.5(8)/N^{3/2} + 3(3)/N^2 + O(1/N^{5/2})]$$
 (3.22)

$$\langle R_g^2 \rangle_N \sim N^{3/2} [0.09987(2) + 0.061(5)/N + 0.23(5)/N^{3/2} - 0.5(5)/N^2 + O(1/N^{5/2})]$$
 (3.23)

$$\langle R_m^2 \rangle_N \sim N^{3/2} [0.3133(3) + 0.22(7)/N - 0.03(60)/N^{3/2} + O(1/N^2)].$$
 (3.24)

These differ from the directly measured amplitudes only within the quoted errors for each amplitude, consistent with our claimed errors.

One immediate observation is that for  $\langle R_e^2 \rangle_N$  and  $\langle R_m^2 \rangle_N$  the correction-to-scaling amplitudes corresponding to the 1/N and  $1/N^{3/2}$  terms are of *opposite* sign, while for  $\langle R_g^2 \rangle_N$  they are of the the same sign (though the errors associated with the estimates of the amplitude of the  $1/N^{3/2}$  term are rather large). Note too that for both  $\langle R_e^2 \rangle_N$  and  $\langle R_g^2 \rangle_N$  the amplitude of the  $1/N^{3/2}$  term is larger (in magnitude) than the amplitudes of both the leading term and first analytic correction; for  $\langle R_m^2 \rangle$ , by contrast, the error in the  $1/N^{3/2}$  term is too great to comment on the relative size of this term.

As a consequence, the "effective" exponent  $\Delta_{\text{eff}}$  based on fitting to a given range of N behaves differently as a function of N for the different observables. For  $\langle R_g^2 \rangle_N$ ,  $\Delta_{\text{eff}}$  lies between 1 and 3/2 for all N, and decreases monotonically to 1 as  $N \to \infty$ . For  $\langle R_e^2 \rangle_N$  and  $\langle R_m^2 \rangle_N$ , by contrast,  $\Delta_{\text{eff}}$  starts *above* 3/2 for very small N, then *increases* monotonically, reaching  $+\infty$  at some finite value of N (here  $\approx 15$ ); then it jumps to  $-\infty$ , after which it continues to increase monotonically, tending asymptotically to 1 as  $N \to \infty$ . These observations are in accordance with previous studies. Most studies of  $\langle R_e^2 \rangle_N$  resulted in estimates for  $\Delta$  of  $\approx 0.65$ ,<sup>(8,10,13,14,23)</sup> while most studies of  $\langle R_g^2 \rangle_N$  resulted in estimates for  $\Delta$  in the range 1.05–1.2.<sup>(13,14,20,23)</sup> (There have been few previous studies of  $\langle R_m^2 \rangle_N$ .) This is clearly a source—indeed, probably the major source of the long-standing difficulty in the analysis of these quantities for the correction-to-scaling term.

The amplitude ratios A and B [defined as the  $N \rightarrow \infty$  limit of (2.8)] follow immediately from (3.22)–(3.24) as A = 0.14031 and B = 0.4398, and from (3.16)–(3.18) as A = 0.14033 and B = 0.4402.

We also estimated the ratios A and B by direct extrapolation of the appropriate coefficient quotients, using the following method:<sup>(41)</sup> Given a sequence  $\{a_n\}$  defined for  $n \ge 1$ , which is known or assumed to converge to a limit  $a_{\infty}$  with corrections of the form  $a_n \sim a_{\infty}(1 + b/n + \cdots)$ , we first construct a new sequence  $\{h_n\}$  defined by  $h_n = \prod_{m=1}^n a_m$ . Then the generating function  $\sum h_n x^n \sim (1 - a_{\infty} x)^{-(1+b)}$ . We obtain estimates of the required limit  $a_{\infty}$  and parameter b by analysing this generating function by the standard method of differential approximants. (The value of the parameter b can also be obtained numerically from the amplitude estimates given in (3.22)–(3.24) above.) In this way, we obtain the estimates

$$A = 0.140296(6) \tag{3.25}$$

$$B = 0.439649(9) \,. \tag{3.26}$$

## 3.4.2. Square Lattice

Let us now consider the square-lattice data. We first analysed the three metric quantities  $\langle R_e^2 \rangle_N$ ,  $\langle R_g^2 \rangle_N$  and  $\langle R_m^2 \rangle_N$  by a method similar to that leading to (3.16)–(3.18), but including the contribution of the antiferromagnetic singularity. We imposed the exponent values v = 3/4,  $\Delta_1 = 3/2$ , q = -11/32 and  $\Delta_1^{AF} = 1$ ; the justification for these choices has already been given above. The sequences of amplitude estimates are shown in Tables VIII–X. In this way, we obtain the following results: As discussed in Section (3.2), some experimentation was needed to determine the maximum values of the parameters *m* and *k* in (3.2). The results given below are given by m = 4, k = 2 for  $\langle R_e^2 \rangle_N$ , by m = 2, k = 1 for  $\langle R_g^2 \rangle_N$ , and by m = 3, k = 1 for  $\langle R_m^2 \rangle_N$ . We find

$$\langle R_e^2 \rangle_N \sim N^{3/2} [0.77124(5) + 1.159(38)/N - 3.13(74)/N^{3/2} + 6(6)/N^2 - 6(24)/N^{5/2} + 0.4(4.0)/N^3 + O(1/N^{7/2})] + (-1)^N N^{-11/32} [0.12451(17) - 0.027(24)/N + O(1/N^2)] (3.27)$$

$$\langle R_g^2 \rangle_N \sim N^{3/2} [0.108230(1) + 0.1019(1)/N + 0.1082(4)/N^{3/2} - O(1/N^2)]$$
  
+  $(-1)^N N^{-11/32} [0.008364(19) + 0.0031(21)/N + O(1/N^2)]$  (3.28)

$$\langle R_m^2 \rangle_N \sim N^{3/2} [0.33913(8) + 0.426(17)/N - 1.1(1.1)/N^{3/2} + 2(4)/N^2 + O(1/N^{5/2})] + (-1)^N N^{-11/32} [0.03652(11) + 0.015(12)/N + O(1/N^2)].$$
(3.29)

Table VIII.		= N <sup>3/2</sup> (a <sub>0,e</sub> + a <sub>1,e</sub>	$, N^{-1} + a_{2,e} N^{-3/2}$	+ <i>a<sub>3,e</sub>N</i> <sup>-2</sup> + <i>a<sub>4,e</sub>N</i> <sup>-</sup> square lattice	Fit $\langle R_e^2 \rangle_N = N^{3/2} (a_{0,e} + a_{1,e} N^{-1} + a_{2,e} N^{-3/2} + a_{3,e} N^{-2/2} + a_{4,e} N^{-5/2} + (-1)^N N^{-11/32} (b_{0,e} + b_{1,e}/N + b_{2,e}/N^2)$ for SAWs on the square lattice	$^{11/32}(b_{0,e}+b_{1,e})$	<i>N</i> + <i>b</i> <sub>2,e</sub> / <i>N</i> 2) for	SAWs on the
Ν	$a_{0,e}$	$a_{1,e}$	$a_{2,e}$	$a_{3,e}$	$a_{4,e}$	$b_{0,e}$	$b_{1,e}$	$b_{2,e}$
33	0.771324	1.127229	-2.737952	3.927648	-2.772841	0.124654	-0.037820	0.655979
34	0.771291	1.137155	-2.846606	4.373539	-3.423234	0.124636	-0.036728	0.639632
35	0.771305	1.132833	-2.798505	4.172870	-3.125666	0.124628	-0.036255	0.632312
36	0.771288	1.138263	-2.859903	4.433123	-3.517795	0.124619	-0.035663	0.622865
37	0.771293	1.136612	-2.840943	4.351507	-3.392907	0.124616	-0.035484	0.619916
38	0.771279	1.141331	-2.895949	4.591870	-3.766261	0.124609	-0.034975	0.611270
39	0.771286	1.138877	-2.866927	4.463195	-3.563461	0.124605	-0.034711	0.606663
40	0.771271	1.144437	-2.933613	4.763067	-4.042810	0.124596	-0.034116	0.595971
41	0.771280	1.141243	-2.894778	4.586020	-3.755880	0.124592	-0.033776	0.589685
42	0.771265	1.146886	-2.964317	4.907314	-4.283596	0.124584	-0.033177	0.578325
43	0.771273	1.143785	-2.925602	4.726095	-3.982046	0.124580	-0.032849	0.571943
4	0.771260	1.149042	-2.992074	5.041219	-4.513116	0.124573	-0.032296	0.560888
45	0.771267	1.146099	-2.954406	4.860421	-4.204625	0.124569	-0.031987	0.554570
46	0.771255	1.151169	-3.020088	5.179507	-4.755692	0.124563	-0.031458	0.543460
47	0.771262	1.148199	-2.981150	4.988102	-4.421211	0.124559	-0.031148	0.536820
48	0.771250	1.153164	-3.047007	5.315582	-5.000119	0.124553	-0.030633	0.525499
49	0.771257	1.150204	-3.007298	5.115889	-4.643109	0.124550	-0.030327	0.518620
50	0.771246	1.155004	-3.072388	5.446844	-5.241340	0.124545	-0.029833	0.507257
51	0.771253	1.152113	-3.032759	5.243165	-4.869182	0.124541	-0.029536	0.500287
52	0.771243	1.156733	-3.096758	5.575580	-5.483004	0.124536	-0.029063	0.488950
53	0.771249	1.153911	-3.057261	5.368299	-5.096275	0.124534	-0.028775	0.481902
54	0.771240	1.158369	-3.120296	5.702470	-5.726090	0.124529	-0.028322	0.470577
55	0.771245	1.155612	-3.080928	5.491689	-5.324869	0.124526	-0.028042	0.463455
56	0.771237	1.159915	-3.142971	5.827124	-5.969610	0.124522	-0.027607	0.452155
57	0.771242	1.157229	-3.103869	5.613694	-5.555442	0.124520	-0.027337	0.444986
58	0.771234	1.161379	-3.164847	5.949657	-6.213520	0.124516	-0.026920	0.433734
59	0.771239	1.158766	-3.126105	5.734233	-5.787657	0.124513	-0.026658	0.426540

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Ν	$a_{0,g}$	$a_{1,g}$	$a_{2,g}$	$b_{0,g}$	$b_{1,g}$
33	0.108213	0.103702	0.100792	0.008333	0.004174
34	0.108216	0.103450	0.101736	0.008370	0.003016
35	0.108218	0.103242	0.102526	0.008339	0.003994
36	0.108220	0.103040	0.103306	0.008369	0.003017
37	0.108221	0.102873	0.103959	0.008345	0.003842
38	0.108223	0.102712	0.104599	0.008368	0.003025
39	0.108224	0.102579	0.105134	0.008349	0.003715
40	0.108225	0.102452	0.105653	0.008367	0.003039
41	0.108226	0.102347	0.106085	0.008352	0.003607
42	0.108227	0.102249	0.106500	0.008366	0.003058
43	0.108228	0.102168	0.106842	0.008355	0.003515
44	0.108228	0.102092	0.107166	0.008365	0.003078
45	0.108229	0.102032	0.107429	0.008357	0.003436
46	0.108229	0.101976	0.107674	0.008365	0.003100
47	0.108230	0.101933	0.107867	0.008359	0.003367
48	0.108230	0.101894	0.108043	0.008364	0.003122
49	0.108230	0.101865	0.108175	0.008360	0.003307
50	0.108230	0.101840	0.108290	0.008363	0.003145
51	0.108230	0.101823	0.108367	0.008361	0.003254
52	0.108230	0.101810	0.108428	0.008363	0.003166
53	0.108230	0.101804	0.108456	0.008362	0.003207
54	0.108230	0.101801	0.108470	0.008363	0.003187
55	0.108230	0.101804	0.108455	0.008363	0.003165
56	0.108230	0.101810	0.108427	0.008362	0.003207
57	0.108230	0.101821	0.108373	0.008364	0.003128
58	0.108230	0.101834	0.108307	0.008362	0.003226
59	0.108230	0.101852	0.108219	0.008364	0.003094

Table IX. Fit  $\langle R_g^2 \rangle_N = N^{3/2} (a_{0,g} + a_{1,g}N^{-1} + a_{2,g}N^{-3/2}) + (-1)^N N^{-11/32} (b_{0,g} + b_{1,g}/N)$  for SAWs on the square lattice

A similar analysis of the unnormalized quantities, using the estimate  $\mu = 2.63815853034174086843$  from (3.12), was made. The results below are given by m = 4, k = 2 for the first two quantities, and m = 3, k = 1 for the third. For the first two quantities we have not given our estimate of  $a_4$  as the associated error is significantly bigger than the estimate. We find

$$c_N \langle R_e^2 \rangle_N / 4 \sim N^{59/32} [0.226945(14) + 0.4471(11)/N - 0.95(22)/N^{3/2} + 2(2)/N^2 + O(1/N^{5/2})] + (-1)^N N^{-3/2} [0.019098(1) + 0.0415(41)/N - 0.08(45)/N^2 + O(1/N^3)]$$
(3.30)

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	1 ( 1) /	( <i>b</i> 0, <i>m</i> ¬			square lat	
Ν	$a_{0,m}$	$a_{1,m}$	<i>a</i> <sub>2,<i>m</i></sub>	<i>a</i> <sub>3,<i>m</i></sub>	$b_{0,m}$	$b_{1,m}$
33	0.339223	0.401114	-0.849196	1.011789	0.036366	0.020608
34	0.339252	0.395837	-0.810037	0.930082	0.036379	0.020222
35	0.339210	0.403819	-0.870217	1.057665	0.036397	0.019642
36	0.339233	0.399343	-0.835945	0.983880	0.036407	0.019318
37	0.339198	0.406364	-0.890517	1.103143	0.036422	0.018812
38	0.339216	0.402541	-0.860364	1.036281	0.036430	0.018538
39	0.339188	0.408723	-0.909807	1.147474	0.036442	0.018096
40	0.339202	0.405479	-0.883503	1.087501	0.036448	0.017866
41	0.339178	0.410928	-0.928281	1.190967	0.036458	0.017480
42	0.339190	0.408177	-0.905379	1.137357	0.036463	0.017286
43	0.339170	0.413005	-0.946085	1.233861	0.036472	0.016947
44	0.339180	0.410665	-0.926109	1.185914	0.036476	0.016783
45	0.339163	0.414963	-0.963242	1.276125	0.036483	0.016483
46	0.339170	0.412973	-0.945843	1.233355	0.036486	0.016345
47	0.339156	0.416811	-0.979781	1.317746	0.036492	0.016080
48	0.339162	0.415122	-0.964678	1.279766	0.036495	0.015963
49	0.339150	0.418559	-0.995753	1.358778	0.036500	0.015727
50	0.339155	0.417130	-0.982689	1.325201	0.036502	0.015629
51	0.339144	0.420217	-1.011200	1.399256	0.036506	0.015418
52	0.339148	0.419011	-0.999949	1.369730	0.036508	0.015336
53	0.339139	0.421791	-1.026155	1.439200	0.036512	0.015148
54	0.339142	0.420779	-1.016525	1.413417	0.036513	0.015079
55	0.339134	0.423289	-1.040647	1.478633	0.036516	0.014910
56	0.339137	0.422446	-1.032471	1.456316	0.036517	0.014854
57	0.339130	0.424716	-1.054707	1.517578	0.036520	0.014702
58	0.339132	0.424021	-1.047836	1.498474	0.036521	0.014655
59	0.339126	0.426078	-1.068359	1.556056	0.036523	0.014518

Table X. Fit  $\langle R_m^2 \rangle_N = N^{3/2} (a_{0,m} + a_{1,m}N^{-1} + a_{2,m}N^{-3/2} + a_{3,m}N^{-2}) + (-1)^N N^{-11/32} (b_{0,m} + b_{1,m}/N)$  for SAWs on the square lattice

$$c_N \langle R_g^2 \rangle_N \sim N^{59/32} [0.127388(31) + 0.181(17)/N + 0.10(26)/N^{3/2} + 0.1(1.0)/N^2 + O(1/N^{5/2})] + (-1)^N [-0.010688(15) + 0.0047(17)/N - 0.20(5)/N^2 + O(1/N^3)]$$
(3.31)  
$$c_N \langle R_m^2 \rangle_N \sim N^{59/32} [0.39917(11) + 0.686(44)/N - 1.3(6)/N^{3/2} + 2(2)/N^2$$

$$C_N \langle R_m^2 \rangle_N \sim N^{35/32} [0.39917(11) + 0.686(44)/N - 1.3(6)/N^{3/2} + 2(2)/N^2 + O(1/N^{5/2})] + (-1)^N [-0.021383(45) + 0.028(5)/N + O(1/N^2)].$$
(3.32)

From these we can estimate the amplitudes of the normalized metric quantities by dividing through by the asymptotic form (2.30) for  $c_N$ . In this

way we obtain a second set of amplitude estimates,

$$\langle R_{\rm e}^2 \rangle_N \sim N^{3/2} [0.77124(5) + 1.1593(38)/N - 3.13(75)/N^{3/2} + 6(8)/N^2 + O(1/N^{5/2})] + (-1)^N N^{-11/32} [0.12439(4) - 0.0144(9)/N + O(1/N^2)]$$
(3.33)

$$\langle R_{g}^{2} \rangle_{N} \sim N^{3/2} [0.108227(50) + 0.103(17)/N + 0.098(160)/N^{3/2} - O(1/N^{2})]$$
  
+  $(-1)^{N} N^{-11/32} [0.008376(20) + 0.0006(30)/N + O(1/N^{2})]$  (3.34)

$$\langle R_{\rm m}^2 \rangle_N \sim N^{3/2} [0.33913(8) + 0.424(19)/N - 1(1)/N^{3/2} + O(1/N^2)]$$
  
+  $(-1)^N N^{-11/32} [0.03654(7) + 0.027(8)/N + O(1/N^2)].$  (3.35)

These differ from the directly analysed amplitudes only in the last quoted digits for all but the least significant amplitudes, and are consistent with our quoted errors in all cases. In the notation of (2.34), from (3.33) we have  $a_0'/d_0'' = 6.200(3)$ , while from the amplitudes quoted below (3.12) we have  $a_0/d_0 = 6.1999(1)$ , in complete agreement.

The amplitude ratios A and B follow immediately from (3.27)–(3.29) as A = 0.14033 and B = 0.43971. From (3.33)–(3.35) we obtain the almost identical values, A = 0.14033 and B = 0.43972.

We also analysed these amplitude ratios directly, using the same method as discussed above for the analysis of the triangular-lattice data. We obtained

$$A = 0.140299(6) \tag{3.36}$$

$$B = 0.439647(6) \,. \tag{3.37}$$

Comparison with the corresponding estimates (3.25)–(3.26) for the triangular lattice is entirely consistent with the belief that these ratios are lattice-independent.<sup>(25)</sup>

These amplitude ratios are also consistent with the CSCPS relation (2.10): using our best estimates (3.36)–(3.37), we find  $F \equiv \lim_{N\to\infty} F_N = -0.000024 \pm 0.000025$  for the square lattice; and using (3.25)–(3.26), we find  $F \equiv \lim_{N\to\infty} F_N = -0.000036 \pm 0.000036$  for the triangular lattice. A direct analysis of the sequence  $\{F_N\}$  was also undertaken, but that sequence was found difficult to extrapolate; and our estimate of the limit, while entirely consistent with zero, was a factor of 10 less precise than the one just quoted.

If it is in fact true (as certainly seems to be the case) that  $F_N \rightarrow 0$ as  $N \rightarrow \infty$ , then it is of interest to investigate the *rate* at which  $F_N \rightarrow 0$ . If  $F_N \propto N^{-\delta}$ , then  $f_N \equiv F_N \langle R_e^2 \rangle_N \propto N^{3/2-\delta}$ . For both square and triangular lattices, we find that  $\delta = 3/2$ , i.e. that  $f_N$  approaches a nonzero constant  $f \equiv \lim_{N\to\infty} f_N$  as  $N \to \infty$ . This behaviour was initially surprising to us, because it implies that there is no analytic correction-to-scaling term 1/N in  $f_N$ , even though such terms are manifestly present in each of the three individual metric quantities  $\langle R^2 \rangle$ . Moreover, this remarkable result appears to hold for both lattices.<sup>10</sup> However, we were subsequently able to provide a renormalization-group argument for this cancellation (see Section 2.2 above). Our estimates of the amplitude are  $f = 0.78 \pm 0.03^{(64)}$  for the square lattice and  $f = 0.96 \pm 0.04$  for the triangular lattice. These estimates are based on extrapolation of the sequences  $f_N$  using a variety of extrapolation algorithms, including Levin's *u* transform, Brezinski's  $\theta$  algorithm, Neville-Aitken extrapolation and Wynn's  $\epsilon$  algorithm. Details of these and other algorithms, as well as programs for their implementation, can be found in ref. 70.

As noted in Section 2.2, the observation that  $\delta = 3/2$  implies the constraint (2.44) on the subdominant amplitudes arising in (2.40)–(2.42). Our series estimates (3.22)–(3.24) and (3.27)–(3.29) are consistent with this prediction, as are our Monte Carlo estimates (4.3)–(4.11). Furthermore, our series and Monte Carlo estimates of f are consistent with the relation (2.45); but the associated error bars are very large, so this is not a stringent test.

Finally, we note the fact that  $\delta = 3/2$  is another indicator that the correction-to-scaling exponent is indeed 3/2. If it were less than this, then the leading non-analytic correction-to-scaling term would have to cancel miraculously (as the 1/N term does) in the combination (2.11) for  $f_N$ . This seems a priori unlikely.

# 3.5. Euclidean-Invariant Moments of the Distribution Function

We have also analysed the series for rotationally-invariant and nonrotationally-invariant moments of the endpoint distribution function, given in Tables III–VI, using methods similar to those just described for the analysis of  $\langle R^2 \rangle$ . Let us start with the rotationally-invariant moments  $\langle r^{2k} \rangle_N$ , for which we expect an asymptotic behaviour of the form

$$\langle r^{2k} \rangle_N \sim N^{2k\nu} [c_{0,k} + c_{1,k}/N + c_{2,k}/N^{\Delta_1} + c_{3,k}/N^2 + \cdots]$$
 (3.38)

<sup>&</sup>lt;sup>10</sup>Indeed, as shown in ref. 41 it appears to hold even in the case of *interacting* SAWs within the good-solvent regime (i.e., above the theta temperature). Of course, the limiting constant f depends on the interaction. For repulsive nearest-neighbour interactions, f increases from 0.78 to an asymptotic value of about 1.6 as the repulsion gets very strong.

for the triangular lattice, and

$$\langle r^{2k} \rangle_N \sim N^{2k\nu} [c_{0,k} + c_{1,k}/N + c_{2,k}/N^{\Delta_1} + c_{3,k}/N^2 + \cdots] + (-1)^N N^{q_k} [d_{0,k} + d_{1,k}/N^{\Delta_1^{\rm AF}} + d_{2,k}/N + \cdots]$$
(3.39)

for the square lattice. In Section 2.2, we gave arguments predicting that  $q_k = 2k\nu + \alpha - 1 - \gamma = 3k/2 - 59/32$ . Furthermore, it is reasonable to expect  $\Delta_1^{AF} = 1$  as was already observed for the SAW counts<sup>(17)</sup> and for the metric quantities  $\langle R^2 \rangle$ . Our numerical results are consistent with these predictions.

We began by analysing the moments  $\langle r^{2k} \rangle_N$  using the method of differential approximants,<sup>(71,70)</sup> with the aim of confirming the predicted leading exponents 2kv = 3k/2 and  $q_k = 3k/2 - 59/32$ . It is a previously observed feature of the method of differential approximants (DA) that its application to the analysis of SAW moment series is less accurate than might be expected.<sup>(71)</sup> For example, DA analysis of a 27-term squarelattice  $\langle R_e^2 \rangle_N$  series, biased at a critical point of 1, produces estimates of  $2\nu$  in the range 1.495–1.497,<sup>(71)</sup> whereas an *unbiased* analysis of a 27term SAW series on the same lattice yields exponent estimates of  $\gamma =$  $1.34364 \pm 0.00088$ , which is rather more accurate, as well as more precise. This behaviour is most likely connected to the fact that the method of differential approximants tacitly assumes that the function is well approximated by a differentially finite (D-finite) function, i.e. the solution of a linear ordinary differential equation with polynomial coefficients.<sup>(72)</sup> While there is strong evidence that neither SAWs nor SAPs are D-finite,<sup>(72)</sup> it nevertheless appears that the SAW and SAP counts are well approximated by a D-finite function, while the generating functions for SAW and SAP metric properties (such as  $\langle R_e^2 \rangle_N$ ) appear not to be. Evidence for this remark includes the telling fact that most of the differential approximants for  $\langle R^2 \rangle$  (for both SAWs and SAPs) are *defective*,<sup>(71)</sup> which is usually a signal that the function being approximated is not of the type tacitly assumed by the analysis. For this reason, our DA analysis gives only moderately accurate estimates of the leading exponents, both ferromagnetic and antiferromagnetic, but no reliable information as to the value of the subleading exponents.

Our DA analysis confirmed the expected leading behaviour  $\langle r^{2k} \rangle_N \propto N^{3k/2}$ , the exponents being identified as 1.4997(5), 2.998(6), 4.496(9), 5.996(12), and 7.496(12) for k = 1, 2, 3, 4, 5 on the square lattice, and 1.4997(5), 2.996(7), 4.495(9), 5.997(12), and 7.500(10) for k = 1, 2, 3, 4, 5 on the triangular lattice. DA analysis also gave reasonable estimates of the

leading antiferromagnetic exponent on the square lattice: we found  $q_k = 3k/2 - 59/32$  to an accuracy of approximately 0.01, 0.04, 0.05, 0.05, 0.06 for k = 1, 2, 3, 4, 5, respectively. It is possible that higher moments (k > 1)may have non-analytic correction-to-scaling terms with exponent  $\Delta_1 < 1.5$ which would then be more prominent than the leading correction-to-scaling term of the second-moment quantities  $\langle R^2 \rangle$ . A more prominent such singularity would also explain the relatively poor accuracy of the DA analysis. We allow for this possibility in our analysis, described immediately below, but find no evidence for such a term.

We next proceeded to fit  $\langle r^{2k} \rangle_N$  to the asymptotic forms (3.38) and (3.39), setting  $\nu = 3/2$  and  $q_k = 3k/2 - 59/32$  and investigating the quality of the fit for a variety of possible values of  $\Delta_1$  and  $\Delta_1^{AF}$ . Among other things, we considered the possibility that  $\Delta_1 < 1$ , even though no such term is observed in the metric quantities  $\langle R^2 \rangle_N$ .

We first fitted the available series to the above forms with  $\Delta_1 = 1/2$ . Estimates of the associated amplitude were, in all cases, monotonically decreasing toward zero. Furthermore, as we increased the number of subdominant terms included in the fit, this amplitude approached zero more and more closely. The data are insufficient to judge whether the rate of approach to zero increased, but the entries were numerically smaller. Also, estimates of the leading amplitude  $c_{0,k}$  did not display the sort of convergence we found in the analysis of  $\langle R^2 \rangle_N$ ; rather, the convergence deteriorated as we increased the number of subdominant terms included in the fit. Both of these observations suggest that there is no term  $c_{2k}/N^{\Delta_1}$ with  $\Delta_1 \approx 1/2$ . Similar behaviour was observed with  $\Delta_1 = 11/16$ , though we cannot say whether the effect was stronger or weaker. That is to say, the analysis is insensitive to this level of exponent change for these series. This is consistent with the situation found in the analysis of  $\langle R^2 \rangle$ . We conclude that there is no evidence of a correction term  $c_{2,k}/N^{\Delta_1}$ with  $\Delta_1 < 1$ .

We then reanalysed the data assuming that the only correction-toscaling term, other than integer powers of 1/N, was that with exponent  $\Delta_1 = 3/2$ , exactly as found for the second-moment series. As for the second-moment series, we retained only analytic correction terms to the antiferromagnetic singularity. As we increased the order of the fit, the leading amplitudes  $c_{0,k}$  and  $d_{0,k}$  displayed improved convergence. This is usually an indicator that the guessed asymptotic form is correct. The higher-order amplitudes displayed less convincing convergence, but we ascribe this to a lack of adequate data. For the second moment, we have a 59-term series, which converged rather well, as can be seen from Table VIII. But the convergence is much less impressive after only 32 terms—which is all we have available for the higher moments.

In order to test the conclusion that the leading correction term in all these series is the 1/N term, we used the method of differential approximants on a modified series obtained by subtracting the estimated leading-order term from the original series: that is, we analysed  $\langle r^{2k} \rangle_N - c_{0,k} N^{2k\nu}$ . We found that the series coefficients behave like  $N^{2k\nu-1}$ , consistent with the conclusion that the leading correction term is 1/N and that the non-analytic correction-to-scaling term(s), have exponent  $\Delta_1 > 1$ , consistent with our view that  $\Delta_1 = 3/2$ .

With the foregoing observations in mind, we obtained the following estimates for the corresponding amplitudes for the square-lattice moments  $\langle r^{2k} \rangle_N$ , where we have assumed a single correction-to-scaling exponent  $\Delta_1 = 3/2$  associated with the ferromagnetic singularity, and otherwise only analytic corrections to both the ferromagnetic and antiferromagnetic singularities:

$$k=2: c_{0,2}=0.860(2), c_{1,2}=1.9(2), d_{0,2}=0.139(5), d_{1,2}=-0.03(2),$$
(3.40)

$$k = 3: \ c_{0,3} = 1.184(5), \ c_{1,3} = 3(1), d_{0,3} = 0.193(5), \ d_{1,3} = -2(1),$$
(3.41)

$$k=4: c_{0,4}=1.907(10), c_{1,4}=2.5(5), d_{0,4}=0.310(3), d_{1,4}=-0.46(5),$$
(3.42)

$$k = 5: \ c_{0,5} = 3.434(10), \ c_{1,5} = -3(1), \\ d_{0,5} = 0.551(3), \ d_{1,5} = -1.6(2).$$
(3.43)

As a check we verify relation (2.34). Our results for  $c_N$  predict  $d_{0,k}/c_{0,k} = 0.161292(2)$ , a relation that is well satisfied by our results for  $c_{0,k}$  and  $d_{0,k}$ .

We can now provide a direct estimate of the invariant ratios  $M_{2k,N} = \langle r^{2k} \rangle_N / \langle r^2 \rangle_N^k$  in the limit  $N \to \infty$ . From the above amplitude estimates, we have, for the square lattice,

$$M_{4,\infty} = 1.446(3) \tag{3.44}$$

$$M_{6,\infty} = 2.581(11) \tag{3.45}$$

$$M_{8,\infty} = 5.391(28) \tag{3.46}$$

$$M_{10,\infty} = 12.59(4). \tag{3.47}$$

These estimates agree well with the estimates (2.18)–(2.21) obtained previously,<sup>(42)</sup> but are a factor 5–10 less precise.

For the triangular lattice, there is of course no "antiferromagnetic" singularity, so that the terms corresponding to the amplitudes  $d_{j,k}$  are absent. We find from the triangular lattice data:

$$k=2: c_{0,2}=0.7330(9), c_{1,2}=1.2(2), c_{2,2}=-5(1),$$
 (3.48)

$$k=3: c_{0,3}=0.934(2), c_{1,3}=1.5(5),$$
 (3.49)

$$k = 4$$
:  $c_{0,4} = 1.383(3), c_{1,4} = 2(1),$  (3.50)

$$k=5: c_{0,5}=2.31(3), c_{1,5}=-8.4(5).$$
 (3.51)

From the above amplitude estimates, we have, for the triangular lattice,

$$M_{4,\infty} = 1.446(2) \tag{3.52}$$

$$M_{6,\infty} = 2.588(5) \tag{3.53}$$

$$M_{8,\infty} = 5.381(12) \tag{3.54}$$

$$M_{10,\infty} = 12.64(15). \tag{3.55}$$

These estimates agree well with those found for the square lattice, confirming the expected universality. Therefore they are also in agreement with the field-theory estimates (2.18)–(2.21), though less precise.

# 3.6. Non-Euclidean-Invariant Moments of the Distribution Function

In this section we discuss the behaviour of the non-rotationally-invariant moments:  $\langle r^{2k} \cos 4\theta \rangle_N$  with k = 2, 3, 4 and  $\langle r^8 \cos 8\theta \rangle_N$  for the square lattice, and  $\langle r^{2k} \cos 6\theta \rangle_N$  with k = 3, 4 for the triangular lattice.

Let us first consider the triangular lattice. We began by analysing the series using the method of differential approximants, with the aim of determining the leading exponent. For the triangular lattice we write

$$\langle r^{2k}\cos 6\theta \rangle_N \sim N^{2k\nu - \Delta_{\rm nr}} [a_{0,k} + a_{1,k}/N^{\Delta} + a_{2,k}/N + \cdots].$$
 (3.56)

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Using first- and second-order differential approximants, we found  $\Delta_{nr} = 3.00 \pm 0.10$  for k = 3 and  $\Delta_{nr} = 2.95 \pm 0.10$  for k = 4, from which we conjecture that  $\Delta_{nr} = 4\nu = 3$  exactly, as predicted in Section 2.1.

Fitting the triangular-lattice data to the asymptotic form (3.56), we found good convergence only if we set the correction-to-scaling exponent to a value  $\Delta \approx 1/2$ —in sharp contrast to situation for the corresponding rotationally invariant moments, where we found  $\Delta = 3/2$ . To test the conjecture that the leading correction is  $N^{-1/2}$ , we subtracted the estimated leading term  $a_{0,k}N^{2k\nu-\Delta_{nr}}$  from  $\langle r^{2k}\cos \theta \rangle_N$  and analysed the resulting series. It was found to behave as  $a_{1,k}N^{2k\nu-\Delta_{nr}-0.50\pm0.10}$ , implying that  $\Delta = 0.5\pm0.10$ . At this stage, we have no theoretical explanation for this numerical observation. Setting  $\Delta_{nr} = 3$  and  $\Delta = 1/2$  and assuming subsequent half-integer terms in the asymptotic expansion (3.56), we obtained the following estimates for the triangular-lattice amplitudes:

$$k=3: a_{0,3}=1.120(3), a_{1,3}=-1.95(5), a_{2,3}=1.7(4)$$
 (3.57)

$$k = 4$$
:  $a_{0,4} = 4.05(5), a_{1,4} = -9(1), a_{2,4} = 20(4).$  (3.58)

For the square lattice, equation (3.56) needs to be modified by the addition of a term representing the antiferromagnetic singularity, so we write

$$\langle r^{2k} \cos 4\theta \rangle_N \sim N^{2k\nu - \Delta_{\rm nr}} [a_{0,k} + a_{1,k}/N^{\Delta} + a_{2,k}/N + \cdots] + (-1)^N N^{\psi} [b_{0,k} + b_{1,k}/N^1 + b_2/N^2 + \cdots].$$
(3.59)

From first- and second-order differential approximants applied to the square-lattice data, we found  $\Delta_{nr} = 1.46 \pm 0.03$ ,  $\Delta_{nr} = 1.45 \pm 0.06$ and  $\Delta_{nr} = 1.44 \pm 0.09$  for k = 2, 3, 4, respectively. From these results we conjecture that  $\Delta_{nr} = 2\nu = 3/2$  exactly, as predicted in Section 2.1. Differential-approximant analysis also gave reasonable estimates of the leading antiferromagnetic exponent: we found  $\psi = 2k\nu - \Delta_{nr} - 3 + \gamma = 2k\nu - 101/32$ , accurate to  $\pm 0.013$  for  $k = 2, \pm 0.05$  for k = 3, and  $\pm 0.15$  for k = 4. This expression for  $\psi$  is different from the one which is the natural generalization of the result for the Euclidean-invariant moments,  $2k\nu - \Delta_{nr} + \alpha - 1 - \gamma = 2k\nu - 107/32$ , which is excluded from the analysis: the difference is 6/32 = 0.1875, much larger than the errors.

Fitting the data to the above asymptotic form (3.59) with  $\Delta_{nr} = 3/2$ and  $\psi = 2k\nu - 101/32$ , and assuming only analytic corrections to scaling at the antiferromagnetic critical point, as found for all the other series, we again found good convergence only if we set the ferromagnetic correction-to-scaling exponent  $\Delta$  to approximately 1/2, just as was found in the analysis of the triangular-lattice data. As in the triangular-lattice analysis, we verified this conjecture by subtracting the estimated leading term  $a_{0,k}N^{2k\nu-\Delta_{nr}}$  from  $\langle r^{2k}\cos 4\theta \rangle_N$  and analysing the resulting series, which was found to behave as  $a_{1,k}N^{2k\nu-\Delta_{nr}-0.497\pm0.005}$ . This is strong support for an  $N^{-1/2}$  correction.

Setting  $\Delta_{nr} = 3/2$ ,  $\psi = 2k\nu - 101/32$  and  $\Delta = 1/2$  and assuming subsequent half-integer terms in the asymptotic expansion of the ferro-magnetic singularity (3.59), we obtained the following estimates for the square-lattice amplitudes:

$$k=2: \ a_{0,2}=1.148(6), \ a_{1,2}=-1.70(5), \ a_{2,2}=2.7(3), \\ b_{0,2}=0.060(5), \ b_{1,2}=0.6(2),$$
(3.60)

$$k = 3: \ a_{0,3} = 3.200(10), \ a_{1,3} = -6.25(10), \ a_{2,3} = 12.0(5), b_{0,3} = 0.175(10), \ b_{1,3} = 1.2(4),$$
(3.61)

$$k = 4: \ a_{0,4} = 8.90(10), \ a_{1,4} = -20(2), \ a_{2,4} = 50(8), b_{0,4} = 0.47(5), \ b_{1,4} = 3(1).$$
(3.62)

Finally, we analyzed the series  $\langle r^8 \cos 8\theta \rangle_N$  on the square lattice. A differential-approximant analysis gave  $\langle r^8 \cos 8\theta \rangle_N \propto N^{3.07\pm0.1}$ . We conjecture that the exponent is exactly 3, consistent with the behaviour  $\langle r^8 \cos 8\theta \rangle_N \propto N^{8\nu-\Delta_{nr,8}}$  with  $\Delta_{nr,8}=3$ . This is exact at the mean-field level and also for the two-dimensional Ising model. In the same spirit that we previously conjectured that  $\Delta_{nr}=2\nu$ , we now conjecture that  $\Delta_{nr,8}=4\nu$ . The antiferromagnetic exponent in  $\langle r^8 \cos 8\theta \rangle_N$  was estimated to be  $\psi = 1.35 \pm 0.05$ , which, by analogy with the antiferromagnetic exponents for  $\langle r^{2k} \cos 4\theta \rangle_N$ , we conjecture is exactly  $8\nu - \Delta_{nr,8} - 3 + \gamma = 43/32$ . We found the subsequent analysis consistent with only analytic corrections at the antiferromagnetic critical point. At the ferromagnetic critical point, the data were again consistent with a leading  $N^{-1/2}$  correction-to-scaling term. In an identical notation to that used above, we find the amplitudes to be:

$$a_0 = 135(2), a_1 = -540(10), a_2 = 1440(50),$$
  
 $b_0 = 6.5(1), b_1 = -11(3).$  (3.63)

# 4. MONTE CARLO ANALYSIS

## 4.1. Summary of Our Data

We have also generated extensive Monte Carlo data, using the pivot algorithm,<sup>(37,73–75)</sup> for SAWs on the square lattice at selected values of N in the range  $40 \le N \le 4000$ , measuring the observables  $\langle R_e^2 \rangle$ ,  $\langle R_g^2 \rangle$  and  $\langle R_m^2 \rangle$ . The results are collected in Tables XI and XII. Unfortunately, in some runs we did not measure all observables: in particular, for larger values of N, the statistics available for  $\langle R_m^2 \rangle$  are much smaller than for the other radii. The statistics range from 10<sup>9</sup> to 10<sup>10</sup> pivot iterations per point, or approximately  $10^7$ – $10^9$  times the integrated autocorrelation time  $\tau_{int,A}$  for these observables.<sup>11</sup>

We begin by analyzing the Monte Carlo data in an unbiased way, in order to extract the leading amplitudes and the correction-to-scaling exponents and amplitudes (Section 4.2). Then we compare the Monte Carlo

Ν	$\langle R_e^2 \rangle_N$	$\langle R_g^2 \rangle_N$	$\langle R_m^2 \rangle_N$	$F_N \langle R_e^2 \rangle_N$
40	$200.106 \pm 0.011$			
60	$364.977 \pm 0.012$	$51.2026 \pm 0.0031$	$160.10 \pm 0.04$	$0.71 \pm 0.08$
80	$559.656 \pm 0.033$	$78.4660 \pm 0.0051$	$245.51 \pm 0.06$	$0.91 \pm 0.13$
100	$780.245 \pm 0.028$	$109.351 \pm 0.007$	$342.34 \pm 0.09$	$1.06 \pm 0.18$
120	$1023.812 \pm 0.064$	$143.488 \pm 0.010$	$449.39 \pm 0.12$	$1.02 \pm 0.24$
140	$1288.631 \pm 0.064$	$180.599 \pm 0.013$	$565.93 \pm 0.16$	$0.67 \pm 0.32$
150	$1428.367 \pm 0.035$	$200.185 \pm 0.015$	$627.51 \pm 0.18$	$0.32 \pm 0.36$
180	$1875.399 \pm 0.081$	$262.858 \pm 0.020$	$823.95 \pm 0.13$	$0.38 \pm 0.26$
200	$2195.00 \pm 0.11$	$307.676 \pm 0.024$	$964.36 \pm 0.13$	$0.52 \pm 0.27$
250	$3064.11 \pm 0.11$	$429.499 \pm 0.024$	$1346.26 \pm 0.19$	$0.59 \pm 0.39$
300	$4024.66 \pm 0.17$	$564.226 \pm 0.021$	$1768.44 \pm 0.07$	$0.71 \pm 0.18$
400	$6190.01 \pm 0.26$	$867.890 \pm 0.033$	$2720.27 \pm 0.12$	$0.62 \pm 0.28$
500	$8645.61 \pm 0.31$	$1212.26 \pm 0.07$	$3799.66 \pm 0.25$	$0.57 \pm 0.57$
700	$14311.70 \pm 0.57$	$2007.10 \pm 0.11$		
1000	$24421.12 \pm 0.85$	$3425.28 \pm 0.11$	$10734.5 \pm 0.53$	$1.15 \pm 1.20$
1400	40439.29 ± 2.11	$5671.95 \pm 0.42$		
2000	$69028.33 \pm 3.82$	$9684.17 \pm 0.79$	$30347.0 \pm 3.5$	$-0.6 \pm 7.5$
3000	$126789.4 \pm 7.9$	$17790.3 \pm 2.1$		
4000	$195162.3 \pm 12.2$	$27376.1 \pm 2.7$	$85773.6 \pm 13.$	$40 \pm 27$

Table XI. Our Monte Carlo data for radii  $\langle R^2 \rangle_N$  as a function of walk length *N*. Errors (one standard deviation) are shown in parentheses

<sup>11</sup>High-precision Monte Carlo data for  $\langle R_e^2 \rangle_N$  have been kindly provided by Peter Grassberger. His results have been merged with ours and appear in Tables XI and XII.

		longth		
Ν	$A_N$	$B_N$	$C_N$	$F_N$
60	0.140290 (10)	0.438644 (100)	0.319826 (76)	0.001957 (200)
80	0.140204 (12)	0.438689 (120)	0.319598 (85)	0.001635 (230)
100	0.140149 (11)	0.438756 (120)	0.319425 (88)	0.001354 (240)
120	0.140150 (13)	0.438938 (120)	0.319294 (88)	0.000992 (240)
140	0.140148 (12)	0.439171 (130)	0.319118 (93)	0.000518 (250)
150	0.140149 (11)	0.439320 (130)	0.319014 (94)	0.000225 (250)
180	0.140161 (12)	0.439347 (71)	0.319022 (55)	0.000204 (140)
200	0.140171 (13)	0.439344 (63)	0.319047 (49)	0.000236 (120)
250	0.140171 (9)	0.439365 (64)	0.319030 (48)	0.000193 (130)
300	0.140192 (8)	0.439402 (26)	0.319052 (18)	0.000177 (45)
400	0.140208 (8)	0.439462 (26)	0.319045 (18)	0.000101 (46)
500	0.140216 (10)	0.439490 (33)	0.319043 (29)	0.000066 (66)
700	0.140242 (10)	. /		. /
1000	0.140259 (7)	0.439557 (27)	0.319091 (19)	0.000047 (48)
1400	0.140258 (13)	. /		. /
2000	0.140293 (14)	0.439630 (56)	0.319115 (45)	-0.000008 (110)
3000	0.140314 (19)	. /		
4000	0.140274 (16)	0.439499 (71)	0.319167 (57)	0.000204 (140)

 
 Table XII. Our Monte Carlo data for amplitude ratios as a function of walk length

Errors (one standard deviation) are shown in parentheses.

data, which lie at relatively high N but are afflicted by statistical errors, with the formulae (3.27)–(3.29) obtained by extrapolating the series data, which lie at much smaller N but are exact (Section 4.3).

## 4.2. Data Analysis

In order to determine the leading amplitudes and the correction-toscaling exponent(s) and amplitude(s), we have analysed the three quantities  $\langle R_e^2 \rangle$ ,  $\langle R_g^2 \rangle$  and  $\langle R_m^2 \rangle$ . We first tried nonlinear least-squares fits of the form<sup>12</sup>

$$\langle R^2 \rangle_N / N^{2\nu} = a + b(N/N_0)^{-\Delta},$$
(4.1)

<sup>&</sup>lt;sup>12</sup>Note that we have rescaled the length *N* by a fixed parameter  $N_0$  that has always been taken equal to  $N_0 = 750$ . The purpose of this rescaling is to minimize the covariance between the estimates of *b* and  $\Delta$ . (The optimal choice is to take  $N_0$  equal to the weighted geometric mean of the *N* values occurring as data points.) As a consequence, the relative error on *b* is a factor of 3–4 smaller than in fits with  $N_0 = 1$ . The error on  $\Delta$  does not depend on the choice of  $N_0$ .

in which  $\nu$  has been fixed equal to 3/4 and the parameters  $a, b, \Delta$  are free. In these fits we use only the data with  $N \ge$  some cutoff value  $N_{\min}$ ; we then vary  $N_{\min}$  systematically and investigate the quality of the fit (see Tables XIII–XV). For  $N_{\min} \gtrsim 60$  the  $\chi^2$  values are reasonable. The fits are

N <sub>min</sub>	ae	be	Δ	$\chi^2$	DF	CL
40	0.770998(23)	0.001644(16)	0.855(3)	40.9	16	0.1%
60	0.771054(25)	0.001589(19)	0.869(4)	14.9	15	46.2%
80	0.771081(30)	0.001559(26)	0.878(7)	12.2	14	59.0%
100	0.771106(32)	0.001532(29)	0.887(8)	8.4	13	82.0%
120	0.771122(37)	0.001512(36)	0.894(12)	7.6	12	81.8%
140	0.771140(38)	0.001491(38)	0.902(13)	4.8	11	93.9%
150	0.771140(39)	0.001492(39)	0.902(13)	4.8	10	90.2%
180	0.771160(45)	0.001467(47)	0.914(19)	4.1	9	90.7%
200	0.771148(49)	0.001481(54)	0.906(23)	3.7	8	88.1%
250	0.771155(55)	0.001472(62)	0.911(29)	3.6	7	82.0%
300	0.771148(64)	0.001481(73)	0.905(39)	3.6	6	73.2%
400	0.771136(82)	0.001495(94)	0.895(58)	3.5	5	61.8%
500	0.771161(93)	0.001469(104)	0.921(80)	3.3	4	51.0%
700	0.771249(110)	0.001396(109)	1.051(156)	2.3	3	51.1%
1000	0.770975(410)	0.001571(344)	0.692(332)	0.9	2	62.4%

Table XIII. Fit  $\langle \boldsymbol{R}_{e}^{2} \rangle = N^{2\nu} [\boldsymbol{a}_{e} + \boldsymbol{b}_{e} (N/750)^{\Delta}]$ 

N <sub>min</sub>	$a_g$	$b_g$	Δ	$\chi^2$	DF	CL
60	0.108213(4)	0.000142(3)	1.037(8)	19.9	15	17.5%
80	0.108209(5)	0.000146(4)	1.023(11)	16.8	14	26.7%
100	0.108205(5)	0.000151(5)	1.007(15)	14.2	13	35.9%
120	0.108205(6)	0.000150(5)	1.008(18)	14.2	12	28.8%
140	0.108207(6)	0.000148(6)	1.018(22)	13.5	11	25.9%
150	0.108207(7)	0.000148(7)	1.019(26)	13.5	10	19.5%
180	0.108210(8)	0.000145(8)	1.033(34)	13.1	9	15.7%
200	0.108208(9)	0.000147(9)	1.023(41)	12.9	8	11.4%
250	0.108205(10)	0.000151(11)	1.000(53)	12.5	7	8.5%
300	0.108208(11)	0.000147(13)	1.025(66)	12.1	6	6.0%
400	0.108201(15)	0.000155(17)	0.966(100)	11.5	5	4.2%
500	0.108198(19)	0.000158(21)	0.937(146)	11.5	4	2.2%
700	0.108213(20)	0.000146(19)	1.161(286)	10.6	3	1.4%
1000	0.107954(1213)	0.000384(1200)	0.206(779)	8.8	2	1.3%

Table XIV. Fit  $\langle R_g^2 \rangle = N^{2\nu} [a_g + b_g (N/750)^{\Delta}]$ 

DF is the number of degrees of freedom and CL is the confidence level of the fit.

N <sub>min</sub>	a <sub>m</sub>	$b_{ m m}$	Δ	$\chi^2$	DF	CL
60	0.338957(32)	0.000635(27)	0.850(17)	15.4	12	21.9%
80	0.338932(38)	0.000661(33)	0.828(23)	13.3	11	27.1%
100	0.338940(41)	0.000652(38)	0.836(29)	13.1	10	21.7%
120	0.338971(43)	0.000618(41)	0.871(36)	10.2	9	33.6%
140	0.339008(44)	0.000577(42)	0.917(42)	5.7	8	68.1%
150	0.339018(45)	0.000566(44)	0.930(47)	5.3	7	62.7%
180	0.339013(48)	0.000571(48)	0.923(52)	5.2	6	52.1%
200	0.338990(56)	0.000598(58)	0.890(62)	4.2	5	51.7%
250	0.338962(71)	0.000630(75)	0.852(79)	3.7	4	45.3%
300	0.338955(75)	0.000638(81)	0.842(84)	3.6	3	31.3%
400	0.338915(115)	0.000683(126)	0.784(136)	3.3	2	19.2%
500	0.338896(146)	0.000702(155)	0.752(186)	3.2	1	7.2%

Table XV. Fit  $(R_m^2) = N^{2\nu} [a_m + b_m (N/750)^{\Delta}]$ 

DF is the number of degrees of freedom and CL is the confidence level of the fit.

stable and the error bars reasonable up to  $N_{\min} \approx 700$ ; after this, the error bars increase drastically and the estimates should be considered unreliable.

Let us consider first  $\langle R_e^2 \rangle$  and  $\langle R_g^2 \rangle$ , the radii for which we have the best statistics. The fit for the radius of gyration is extremely stable<sup>13</sup> and clearly suggests  $\Delta = 1$ . No subleading exponent with  $\Delta < 1$  appears to be present; in particular, this excludes  $\Delta = 11/16 = 0.6875$  unless the corresponding amplitude is extremely small. By contrast, the fit of  $\langle R_a^2 \rangle$  gives estimates that vary with  $N_{\min}$ : the estimate of  $\Delta$  at first increases with  $N_{\rm min}$ , then flattens off at  $\Delta \approx 0.9$ . The theoretical prediction  $\Delta = 11/16$  is again excluded, but in this case a non-analytic correction  $\Delta_1 < 1$  is still possible *a priori*. However, we believe that a subleading exponent  $\Delta_1 \approx 0.9$ is unlikely: after all, it does not agree with any theoretical prediction; and the observed behaviour can be explained equally well, as noted earlier, by the competition between two correction terms of opposite sign, provided that both terms are still sizable in the range of N that we are considering. The fact that a range  $500 \le N \le 4000$  is insufficient to see clearly that  $\Delta = 1$  shows how difficult is the determination of  $\Delta$  and explains the wide range of contradictory results found in previous work.

<sup>&</sup>lt;sup>13</sup>The  $\chi^2$  of the fit is somewhat large, and the corresponding confidence level too small. Since the confidence level actually gets *worse* as  $N_{\min}$  grows, the cause does not seem to be corrections to scaling. The most likely interpretation is that our error bars are, for some unknown reason, somewhat underestimated for large values of *N*. (Perhaps we have underestimated the integrated autocorrelation time by failing to include a sufficient amount of the tail of the autocorrelation function.)

We can also consider  $\langle R_m^2 \rangle$ . The behaviour is similar to that observed for  $\langle R_e^2 \rangle$ , although the errors are larger. Again, the data are compatible with  $\Delta \approx 0.9$ , but, as before, we believe that what we are observing is simply an effective exponent arising from the competition between two correction terms of opposite sign. Moreover, we are here probing shorter walks than in the case of  $\langle R_e^2 \rangle$ , because of the lack of statistics for larger N: the fit is effectively dominated by the data in the range  $300 \leq N \leq 1000$ .

Since we have little evidence that  $\Delta_1 = 11/16$ , the most likely possibility is that  $\Delta_1 = 3/2$ . We have therefore checked whether our data can be fitted by the simple Ansatz

$$\langle R^2 \rangle_N = N^{2\nu} (a + bN^{-1} + cN^{-3/2}),$$
(4.2)

with a, b, c free parameters. As before, we perform several fits using only data with  $N \ge N_{\min}$ , varying  $N_{\min}$  systematically. The results are reported in Tables XVI–XVIII. The fit quality is good even for the lowest value of  $N_{\min}$ : additional corrections do not play much role for  $N \ge 60$ . Notice that for  $\langle R_g^2 \rangle$  the constant *c* is very small, explaining why the previous fit gave  $\Delta = 1$  essentially without corrections. For  $\langle R_e^2 \rangle$  and  $\langle R_m^2 \rangle$ , *c* is instead sizable and of opposite sign with respect to *b*, giving in fit (4.1) an effective exponent  $\Delta < 1$ .

N <sub>min</sub>	a <sub>e</sub>	be	Ce	$\chi^2$	DF	CL
40	0.771261(16)	1.093(7)	-1.93(4)	15.4	16	49.4%
60	0.771247(18)	1.104(9)	-2.03(7)	12.1	15	67.1%
80	0.771224(20)	1.131(15)	-2.30(14)	6.7	14	94.6%
100	0.771224(22)	1.131(18)	-2.30(18)	6.7	13	91.7%
120	0.771211(25)	1.150(26)	-2.52(29)	5.7	12	93.0%
140	0.771218(27)	1.139(29)	-2.39(32)	5.0	11	93.1%
150	0.771216(27)	1.143(30)	-2.44(34)	4.8	10	90.1%
180	0.771218(31)	1.137(42)	-2.36(54)	4.8	9	85.0%
200	0.771206(33)	1.165(52)	-2.79(70)	3.9	8	86.6%
250	0.771204(37)	1.170(65)	-2.86(95)	3.9	7	79.3%
300	0.771194(42)	1.199(87)	-3.38(1.41)	3.6	6	72.6%
400	0.771177(53)	1.257(136)	-4.50(2.46)	3.3	5	64.9%
500	0.771187(62)	1.218(186)	-3.68(3.65)	3.2	4	51.9%
700	0.771244(85)	0.936(340)	3.16(7.80)	2.3	3	52.2%
1000	0.771118(142)	1.680(755)	-16.96(19.82)	1.0	2	59.7%

Table XVI. Fit  $(R_e^2) = N^{2\nu} (a_e + b_e N^{-1} + c_e N^{-3/2})$ 

DF is the number of degrees of freedom and CL is the confidence level of the fit.

N <sub>min</sub>	$a_{\mathrm{g}}$	$b_{ m g}$	Cg	$\chi^2$	DF	CL
60	0.108209(3)	0.107(2)	0.08(2)	17.8	15	27.5%
80	0.108207(4)	0.109(3)	0.06(3)	16.3	14	29.3%
100	0.108204(4)	0.113(4)	0.02(4)	14.3	13	35.6%
120	0.108204(5)	0.113(5)	0.02(5)	14.3	12	28.5%
140	0.108206(5)	0.110(6)	0.05(6)	13.5	11	25.9%
150	0.108206(5)	0.110(6)	0.06(8)	13.5	10	19.6%
180	0.108208(6)	0.106(8)	0.11(11)	13.0	9	16.4%
200	0.108207(7)	0.108(10)	0.08(14)	12.9	8	11.7%
250	0.108205(8)	0.113(13)	0.00(19)	12.5	7	8.5%
300	0.108208(9)	0.106(17)	0.12(25)	12.0	6	6.1%
400	0.108203(11)	0.120(26)	-0.14(45)	11.5	5	4.2%
500	0.108201(13)	0.128(37)	-0.30(72)	11.5	4	2.2%
700	0.108212(17)	0.076(64)	0.95(1.46)	10.5	3	1.5%
1000	0.108185(30)	0.227(156)	-3.03(4.03)	9.4	2	0.9%

Table XVII. Fit  $(R_g^2) = N^{2\nu} (a_g + b_g N^{-1} + c_g N^{-3/2})$ 

DF is the number of degrees of freedom and CL is the confidence level of the fit.

N <sub>min</sub>	a <sub>m</sub>	$b_{\rm m}$	c <sub>m</sub>	$\chi^2$	DF	CL
60	0.339040(21)	0.447(14)	-0.99(12)	18.6	12	9.9%
80	0.339013(23)	0.479(18)	-1.37(18)	11.3	11	41.7%
100	0.339008(25)	0.487(23)	-1.47(26)	11.0	10	35.7%
120	0.339019(27)	0.469(28)	-1.23(34)	9.8	9	36.4%
140	0.339038(29)	0.436(33)	-0.76(42)	6.3	8	61.7%
150	0.339044(30)	0.426(37)	-0.61(48)	5.9	7	55.6%
180	0.339041(32)	0.431(41)	-0.69(55)	5.8	6	44.8%
200	0.339028(34)	0.457(49)	-1.09(69)	4.9	5	43.1%
250	0.339010(41)	0.496(68)	-1.69(1.01)	4.2	4	38.0%
300	0.339005(43)	0.508(75)	-1.88(1.13)	4.1	3	25.5%
400	0.338976(62)	0.583(140)	-3.21(2.37)	3.6	2	16.1%
500	0.338964(74)	0.623(194)	-4.04(3.62)	3.6	1	5.9%

Table XVIII. Fit  $(R_m^2) = N^{2\nu}(a_m + b_m N^{-1} + c_m N^{-3/2})$ 

DF is the number of degrees of freedom and CL is the confidence level of the fit.

The leading amplitudes are extremely stable and, using the data with  $N_{\min} = 200$ , we can estimate

$$a_{\rm e} = 0.77121 \pm 0.00004 \tag{4.3}$$

$$b_{\rm e} = 1.17 \pm 0.05 \tag{4.4}$$

$$c_{\rm e} = -2.8 \pm 0.7,\tag{4.5}$$

$$a_{\rm g} = 0.108207 \pm 0.000007 \tag{4.6}$$

$$b_{\rm g} = 0.108 \pm 0.010 \tag{4.7}$$

$$c_{\rm g} = 0.0 \pm 0.2,$$
 (4.8)

$$a_{\rm m} = 0.33903 \pm 0.00004 \tag{4.9}$$

$$b_{\rm m} = 0.46 \pm 0.05 \tag{4.10}$$

$$c_{\rm m} = -1.1 \pm 0.7. \tag{4.11}$$

where the error bars are 68% confidence limits. We can compare these results with the series estimates (3.27)–(3.29), and note that they agree well within quoted errors with one exception:  $a_g$  differs by three error bars from one set of the corresponding series estimate. We consider the stated errors of this series estimate to be anomalously low, compared to all other error estimates, and thus not to be taken literally.

We have also considered the universal amplitude ratios  $A_N$  and  $B_N$ . The most notable feature of the raw data for  $A_N$  (Table XII) is its nonmonotonicity: at first  $A_N$  decreases, reaching a minimum at  $N \approx 130$ ; then it increases. This immediately suggests the presence of two correction-to-scaling terms of opposite sign, in agreement with the analysis presented above. We have therefore analysed the ratios  $A_N$  and  $B_N$  by performing a fit of the form

$$\mathcal{O}_N = a + bN^{-1} + cN^{-3/2} \,. \tag{4.12}$$

The results are reported in Tables XIX and XX. Again the quality of the fits is quite good, and we obtain the final estimates (again we use conservatively the data for  $N_{\min} = 200$ )

 $A = 0.140310 \pm 0.000011 \tag{4.13}$ 

$$B = 0.439614 \pm 0.000050, \tag{4.14}$$

where the error bars are 68% confidence limits.<sup>14</sup>

Next we analysed the CSCPS combination (2.11). Conformal-invariance theory<sup>(29,30)</sup> predicts that  $\lim_{N\to\infty} F_N = 0$ , and we confirm this prediction numerically to very high precision: see Table XXI. Therefore,  $f_N$ 

<sup>&</sup>lt;sup>14</sup>Cardy and Mussardo<sup>(39)</sup> have used the form-factor method, applied to the exact S-matrix of the massive O(n) model, to derive the estimates  $A \approx 0.126$  and  $B \approx 0.420$ . This is impressive accuracy for a first-principles theoretical calculation; the approximately 5% error is about what one expects from the one-particle approximation used in this computation.

N <sub>min</sub>	$a_A$	$b_A$	$\mathcal{C}_A$	$\chi^2$	DF	CL
60	0.140305(6)	-0.062(3)	0.47(2)	8.4	15	90.7%
80	0.140306(6)	-0.064(5)	0.49(4)	8.1	14	88.2%
100	0.140303(7)	-0.060(6)	0.45(6)	7.1	13	89.6%
120	0.140306(8)	-0.064(8)	0.49(9)	6.6	12	88.2%
140	0.140306(8)	-0.064(9)	0.50(10)	6.6	11	83.0%
150	0.140307(9)	-0.065(10)	0.52(12)	6.5	10	77.0%
180	0.140309(10)	-0.071(13)	0.59(17)	6.2	9	72.5%
200	0.140310(11)	-0.072(16)	0.62(22)	6.1	8	63.4%
250	0.140307(12)	-0.065(21)	0.51(31)	5.9	7	55.7%
300	0.140312(14)	-0.078(27)	0.72(42)	5.3	6	50.3%
400	0.140310(18)	-0.072(42)	0.61(74)	5.3	5	38.2%
500	0.140304(21)	-0.049(59)	0.12(1.15)	5.0	4	28.9%
700	0.140306(27)	-0.060(104)	0.39(2.38)	5.0	3	17.4%
1000	0.140297(47)	-0.007(244)	-1.03(6.34)	4.9	2	8.6%

Table XIX. Fit  $A_N = a_A + b_A N^{-1} + c_A N^{-3/2}$ 

DF is the number of degrees of freedom and CL is the confidence level of the fit.

N <sub>min</sub>	$a_B$	$b_B$	c <sub>B</sub>	$\chi^2$	DF	CL
60	0.439619(31)	-0.062(21)	-0.02(17)	12.8	12	38.1%
80	0.439587(34)	-0.024(27)	-0.45(27)	8.3	11	68.3%
100	0.439578(38)	-0.012(34)	-0.61(37)	8.0	10	63.2%
120	0.439596(41)	-0.040(42)	-0.24(49)	6.6	9	67.5%
140	0.439620(43)	-0.082(49)	0.34(61)	4.0	8	85.6%
150	0.439629(45)	-0.098(55)	0.59(70)	3.5	7	83.4%
180	0.439626(48)	-0.091(61)	0.48(80)	3.4	6	75.2%
200	0.439614(51)	-0.068(73)	0.12(1.01)	3.1	5	68.5%
250	0.439590(61)	-0.014(102)	-0.72(1.52)	2.5	4	63.6%
300	0.439583(65)	0.004(118)	-1.02(1.79)	2.4	3	48.5%
400	0.439558(89)	0.073(207)	-2.27(3.55)	2.3	2	31.9%
500	0.439528(106)	0.174(284)	-4.35(5.35)	2.0	1	15.6%

Table XX. Fit  $B_N = a_B + b_B N^{-1} + c_B N^{-3/2}$ 

DF is the number of degrees of freedom and CL is the confidence level of the fit.

is expected to scale as  $N^{2\nu-\delta}$  where  $\delta$  is some subleading exponent. Our data are consistent with  $\delta = 3/2$ , although not so accurate as to establish it unambiguously; in other words,  $f_N$  appears to approach a nonzero constant as  $N \to \infty$ . This means, as noted earlier, that the 1/N correction is absent within our errors. A fit to a constant gives the results reported in Table XXII. The results show an initial downward trend with  $N_{\min}$  and

N <sub>min</sub>	$a_F$	$b_F$	$c_F$	$\chi^2$	DF	CL
60	0.000043(59)	-0.039(39)	1.30(33)	11.5	12	49.0%
80	0.000105(65)	-0.112(52)	2.14(51)	6.7	11	81.9%
100	0.000117(71)	-0.129(65)	2.36(71)	6.5	10	76.8%
120	0.000087(77)	-0.082(79)	1.72(94)	5.4	9	79.4%
140	0.000041(82)	-0.004(93)	0.64(1.17)	3.0	8	93.5%
150	0.000026(86)	0.023(104)	0.24(1.34)	2.6	7	91.7%
180	0.000037(90)	0.002(116)	0.54(1.54)	2.5	6	87.2%
200	0.000064(98)	-0.052(139)	1.38(1.94)	2.0	5	85.3%
250	0.000110(116)	-0.153(195)	2.95(2.89)	1.4	4	83.9%
300	0.000133(124)	-0.205(220)	3.80(3.32)	1.2	3	76.2%
400	0.000167(174)	-0.298(398)	5.45(6.75)	1.1	2	58.1%
500	0.000189(206)	-0.372(545)	6.98(10.23)	1.0	1	30.7%

Table XXI. Fit  $F_N = a_F + b_F N^{-1} + c_F N^{-3/2}$ 

DF is the number of degrees of freedom and CL is the confidence level of the fit.

N <sub>min</sub>	f	$\chi^2$	DF	CL
60	0.75(5)	12.7	14	55.4%
80	0.79(7)	12.2	13	51.3%
100	0.73(8)	10.7	12	55.4%
120	0.65(9)	6.7	11	82.0%
140	0.58(10)	4.1	10	94.5%
150	0.57(11)	4.0	9	91.2%
180	0.60(11)	3.5	8	90.3%
200	0.64(12)	2.7	7	91.5%
250	0.68(14)	2.4	6	88.1%
300	0.69(15)	2.3	5	80.2%
400	0.64(25)	2.3	4	68.6%
500	0.69(51)	2.3	3	52.0%
1000	1.18(1.17)	2.0	2	36.1%

Table XXII. Fit  $F_N < R_e^2 > N = f$ 

DF is the number of degrees of freedom and CL is the confidence level of the fit.

then increase again. A stable region may be identified for  $N_{\min} \ge 250$ . For  $N_{\min} = 250$  we have

$$f = 0.68 \pm 0.14. \tag{4.15}$$

This is in agreement with, but less precise than, the result  $f = 0.79 \pm 0.03$  obtained from series analysis.

Finally, we have tried to see whether our estimated values of A and B are consistent with simple rational values that satisfy the CSCPS formula. If we require the denominators to be  $\leq 1000$ , then the only possible values anywhere near our estimates are

$$A = \frac{23}{164} \approx 0.1402439, \qquad B = \frac{40}{91} \approx 0.4395604 \tag{4.16}$$

and

$$A = \frac{91}{648} \approx 0.1404321, \qquad B = \frac{95}{216} \approx 0.4398148. \tag{4.17}$$

Our data are, however, precise enough to clearly exclude both guesses. We therefore conjecture that *A* and *B* do *not* take simple rational values, even though one particular linear combination of them does.

# 4.3. Comparison to Series-Extrapolation Predictions

We can also directly compare our raw Monte Carlo data to the extrapolation formulas (3.27)–(3.29). For this purpose we compute

$$\chi^{2} = \sum_{\text{MC data}} \frac{(R_{MC}^{2} - R_{\text{series}}^{2})^{2}}{\sigma_{MC}^{2}},$$
(4.18)

where  $R_{MC}^2$  is the Monte Carlo estimate,  $\sigma_{MC}$  the corresponding error, and  $R_{\text{series}}^2$  the prediction of the extrapolations (3.27)–(3.29). For  $\langle R_e^2 \rangle$  we find that (3.27) describes the numerical data rather well. Indeed,  $\chi^2 = 29$  for 19 data points. The small remaining discrepancy is mainly due to the error on the coefficients. Indeed, if we use for the ferromagnetic part the results of the Monte Carlo fit with  $N_{\min} = 40$  reported in Table XVI—these estimates are compatible with the exact-enumeration ones reported in (3.27)—the  $\chi^2$  drops to 15. Analogous discussion applies to  $\langle R_m^2 \rangle$ . If we use (3.29) we obtain  $\chi^2 = 55$  with 15 data points. But again it is enough to replace the ferromagnetic coefficients obtained using exact enumeration with those obtained in the Monte Carlo fit, see Table XVIIII—they are fully compatible—to have  $\chi^2 = 19$  with 15 points. The situation is worse for  $\langle R_g^2 \rangle$ . Using all data we obtain  $\chi^2 = 80$  with 18 data points. Such a result does not improve significantly if we change the coefficients in (3.28) within error bars. This is related to the fact we have already noticed that the leading amplitude for  $\langle R_g^2 \rangle_N$  reported in (3.28) significantly differs from the Monte Carlo estimate obtained for any value of  $N_{\min}$ .

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# 5. CONCLUSIONS AND OPEN QUESTIONS

In this study of the SAW correction-to-scaling exponents, we have seen a consistent picture emerging, given independent support by both Monte Carlo and series analysis. We have presented compelling evidence that the first non-analytic correction term in the generating function for both SAWs and SAPs, as well as in several Euclidean-invariant metric properties, is  $\Delta_1 = 3/2$ , as predicted by Nienhuis some 20 years ago.<sup>(4,5)</sup> We find no evidence for the presence of an exponent  $\Delta_1 = 11/16$  in SAWs and SAPs on the square and triangular lattices. Our analysis of the interplay between dominant and subdominant correction-to-scaling terms also enables us to explain quantitatively why many earlier analyses gave incorrect conclusions, predicting exponents  $\Delta_1 < 1$ . For certain observables, we find pairs of correction terms of opposite sign that conspire to give effective exponents that are smaller than both of the individual exponents. Thus, corrections behaving as  $a/N + b/N^{3/2}$  with ab < 0 were incorrectly identified with a single correction term  $c/N^{\Delta_1}$  with  $\Delta_1 < 1$ .

Monte Carlo and series analysis turn out to complement each other well. Series provide a basis for calculating the amplitudes of several subdominant asymptotic terms, while the Monte Carlo data frequently provide greater accuracy for the estimate of the leading amplitudes.

We have also studied the asymptotic behaviour of several non-Euclidean-invariant quantities. Their leading behaviour is characterized by a new exponent  $\Delta_{nr}$ . We find compelling evidence that  $\Delta_{nr} = 2\nu$  on the square lattice and  $\Delta_{nr} = 4\nu$  on the triangular lattice, confirming the conjecture of.<sup>(44,43)</sup> We also computed the leading correction-to-scaling exponent in these observables, finding  $\Delta_1 \approx 0.5$ . We are unaware of any theoretical prediction for this quantity.

We have also determined the dominant and subdominant exponents characterizing the "antiferromagnetic singularity" of the square lattice. These exponent predictions are for the most part new.

We also tested the CSCPS relation  $\lim_{N\to\infty} F_N = 0$  [cf. (2.10)], which arises from conformal field theory.<sup>(29,30)</sup> Both our Monte Carlo and series work are completely consistent with the CSCPS relation. Further, we find that the 1/N correction term in  $F_N$  is absent, so that  $F_N \sim \text{const} \times N^{-\Delta_1}$ with  $\Delta_1 = 3/2$ . The absence of this analytic correction-to-scaling term implies a new amplitude relation (2.44).

Finally, we remark that our numerical estimates for the universal amplitude ratios A and B are now so precise as to allow us to rule out the possibility that these are rational numbers with small integer denominators. Some other universal amplitude ratios include powers of  $\pi$ ,<sup>(38)</sup> so it is possible that A and B are combinations of  $\pi$  and rational numbers; but

there is no *a priori* reason why powers of  $\pi$  should enter into the amplitude ratios A and B.

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