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High-Precision Monte Carlo Test of the Conformal-Invariance Predictions for Two-Dimensional Mutually Avoiding Walks

Bin Li[1] **and Alan D. Sokal**[1]

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Let ζ_l be the critical exponent associated with the probability that l independent N-step ordinary random walks, starting at nearby points, are mutually avoiding. Using Monte Carlo methods combined with a maximum-likelihood data analysis, we find that in two dimensions $\zeta_2 = 0.6240 \pm 0.0005 \pm 0.0011$ and $\zeta_3 = 1.4575 \pm 0.0030 \pm 0.0052$, where the first error bar represents systematic error due to corrections to scaling (subjective 95% confidence limits) and the second error bar represents statistical error (classical 95% confidence limits). These results are in good agreement with the conformal-invariance predictions $\zeta_2 = 5/8$ and $\zeta_3 = 35/24$.

KEY WORDS: Monte Carlo; conformal invariance; random walk; mutually-avoiding walks; self-avoiding walk; maximum-likelihood estimation.

1. INTRODUCTION

The intersection properties of ordinary random walks have long been of interest in probability theory.[1-8] In recent years they have served as a valuable test problem for critical phenomena and quantum field theory, analogous to but simpler than self-avoiding walks, Ising models, and φ^4 field theories.[9-13] In addition, they provide a simple model of diffusion near an absorbing fractal,[14] and they may describe interacting polymer chains of different chemical species in a θ solvent.[15]

In this paper we consider the following problem: Let $p_l(N)$ be the probability that l ($\geqslant 2$) independent N-step ordinary random walks, start-

[1] Department of Physics, New York University, New York, New York 10003.

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ing at some specified points $x_1, x_2, \ldots, x_l$ in a d-dimensional regular lattice, are *mutually avoiding*. How does $p_l(N)$ behave as $N \to \infty$?[2]

It is known rigorously[2,16] that

$$\lim_{N \to \infty} p_l(N) = \begin{cases} c_l(x_1, \ldots, x_l; d) > 0 & \text{for} \quad d > 4 \\ 0 & \text{for} \quad d \leqslant 4 \end{cases} \tag{1.1}$$

In the borderline dimension $d = 4$, it has been proven[3-5] that[3]

$$p_2(N) \sim (\log N)^{-1/2} \times \text{possible log log corrections} \tag{1.2}$$

and nonrigorous renormalization-group calculations[17] predict that $p_l(N) \sim (\log N)^{-l(l-1)/4}$. For dimension $d < 4$, one expects a nontrivial scaling

$$p_l(N) \sim N^{-\zeta_l} \tag{1.3}$$

and for $l = 2$ this behavior has recently been proven[7] modulo possible logarithmic corrections.[4] The *critical exponents* $\zeta_l(d)$ are expected to be *universal*, in the sense that they depend only on l and d (and not on the specific lattice or on the starting points $x_1, x_2, \ldots, x_l$). The best available rigorous bounds on ζ_2 are

$$d = 1^{(18)}: \qquad \zeta_2 = 1 \tag{1.4}$$

$$d = 2^{(6,8)}: \qquad \frac{1}{2} + \frac{1}{8\pi} \leqslant \zeta_2 < \frac{3}{4} \tag{1.5}$$

$$d = 3^{(3,8)}: \qquad \frac{1}{4} \leqslant \zeta_2 < \frac{1}{2} \tag{1.6}$$

Also, some rather weak bounds are known on ζ_l for $l \geqslant 3$. Nonrigorous renormalization-group calculations in dimension $d = 4 - \varepsilon$ yield the prediction[17]

$$\zeta_l = \frac{l(l-1)}{8}\varepsilon - \frac{l(l-1)(2l-5)}{32}\varepsilon^2 + O(\varepsilon^3) \tag{1.7}$$

[2] To avoid trivial cases, we assume henceforth that $x_1, x_2, \ldots, x_l$ are "sufficiently separated." Alternatively, we could modify the definition of $p_l(N)$ so as to ignore intersections arising from "early" parts of both intersecting walks.

[3] More precisely, what has been proven is that $\lim_{N \to \infty} [\log p_2(N)/\log \log N] = -1/2$.

[4] More precisely, what has been proven is that $\zeta_2 \equiv \lim_{N \to \infty} [-\log p_2(N)/\log N]$ exists. Also, this exponent ζ_2 equals the exponent for the corresponding continuum (Brownian-motion) problem.

Since Brownian motion (the scaling limit of ordinary random walk) is known to be conformal-invariant,[19] it is natural to suppose that the scaling limit of mutually avoiding walks (MAWs) would also be conformal-invariant. Indeed, Duplantier and Kwon[20] have recently used a combination of conformal-invariance arguments and Monte Carlo computations to deduce (nonrigorously) the *exact* critical exponents ζ_l in dimension $d=2$: they predict

$$\zeta_l = \frac{4l^2 - 1}{24} \tag{1.8}$$

In Section 2 we briefly recapitulate their argument.

The principal purpose of this paper is to make a high-precision Monte Carlo measurement of the exponents ζ_2 and ζ_3 for two-dimensional MAWs, in order to test the conformal-invariance prediction (1.8). In Section 3 we explain our methodology; in particular, we explain how the problem can be cast in a form allowing the use of maximum-likelihood estimation. In Section 4 we present our numerical results: using MAWs of length up to $N_{\max} = 50000$, we find

$$\zeta_2 = 0.6240 \pm 0.0005 \pm 0.0011 \tag{1.9}$$

$$\zeta_3 = 1.4575 \pm 0.0030 \pm 0.0052 \tag{1.10}$$

where the first error bar represents systematic error due to corrections to scaling (subjective 95% confidence limits) and the second error bar represents statistical error (classical 95% confidence limits). We find unexpectedly large corrections to scaling in $p_2(N)$, *possibly* corresponding to a correction-to-scaling exponent Δ in the range ≈ 0.4–0.5. In Section 5 we discuss briefly our results, and compare them to previous work.[6,20]

2. THE CONFORMAL-INVARIANCE ARGUMENT

Let $\mathscr{G}$ be a connected finite graph containing n_l vertices of order l ($l \geqslant 1$); such a graph has $\mathscr{E}$ edges and $\mathscr{L}$ loops, where

$$\mathscr{E} = \sum_{l \geqslant 1} \tfrac{1}{2} l n_l \tag{2.1}$$

$$\mathscr{L} = 1 + \sum_{l \geqslant 1} (\tfrac{1}{2} l - 1) n_l \tag{2.2}$$

A *$\mathscr{G}$-net of N-step mutually avoiding walks* (MAWs) is, by definition, a mapping that assigns a site in $\mathbf{Z}^d$ to each vertex of $\mathscr{G}$ and an N-step walk in $\mathbf{Z}^d$ (with the appropriate endpoints) to each edge in $\mathscr{G}$, such that distinct walks have no intersections except where required at their endpoints.[5] Let $Z_N(\mathscr{G})$ be the number of distinct such nets (modulo translation).[6] Then $Z_N(\mathscr{G})$ is expected to have the scaling behavior

$$Z_N(\mathscr{G}) \sim \mu^{N\mathscr{E}} N^{\gamma_{\mathscr{G}}-1} \tag{2.3}$$

as $N \to \infty$, where $\mu = 2d$ is the coordination number of $\mathbf{Z}^d$ and $\gamma_{\mathscr{G}}$ is a critical exponent. Moreover, Duplantier has argued[17,21] (see also ref. 22) that $\gamma_{\mathscr{G}}$ for a general graph can be decomposed into contributions from loops and vertices:

$$\gamma_{\mathscr{G}} - 1 = -d\nu\mathscr{L} + \sum_{l \geq 1} n_l \sigma_l \tag{2.4}$$

where $\nu = 1/2$ is the size exponent for ordinary random walks, and $\{\sigma_l\}_{l \geq 1}$ is a new family of critical exponents; this is a kind of generalized hyperscaling relation.[7] Applying this formula to the l-leg star $\mathscr{S}_l$ and the l-leg "watermelon" (or "fuseau")[23,24,21,20] $\mathscr{W}_l$, we obtain

$$-\zeta_l \equiv \gamma_{\mathscr{S}_l} - 1 = \sigma_l + l\sigma_1 \tag{2.5}$$

$$\gamma_{\mathscr{W}_l} - 1 = -d\nu(l-1) + 2\sigma_l \tag{2.6}$$

Let us now consider l-leg MAW watermelons in which the edges have *variable numbers of steps* $N_1, N_2, \ldots, N_l$ and *fixed endpoints* $X, Y \in \mathbf{Z}^d$. Let $\mathscr{Z}_{N_1,\ldots,N_l}(X-Y)$ be the number of such MAWs, and let $G_l(X-Y;\beta)$ be the generating function with respect to the fluctuating total length:

$$G_l(X-Y;\beta) = \sum_{N_1,\ldots,N_l=0}^{\infty} \beta^{N_1+N_2+\cdots+N_l} \mathscr{Z}_{N_1,\ldots,N_l}(X-Y) \tag{2.7}$$

This correlation function has a critical point $\beta_c = 1/\mu$, at which the mean length diverges. Now, MAWs can be represented by a lattice field theory (see below), and the generating function G_l is the two-point correlation function at inverse temperature β of a scalar field operator ϕ_l that creates l-leg vertices:

$$G_l(X-Y;\beta) = \langle \phi_l(X)\, \phi_l(Y) \rangle_\beta \tag{2.8}$$

[5] Alternatively, we could "split" each vertex into a cluster of nearby points, and then impose *strict* mutual avoidance. Indeed, such a modification is *required* if the graph $\mathscr{G}$ has any vertices of order $> 2d$. The critical exponents should be unchanged by any such "local" modification.

[6] In dimension $d = 2$ we consider only *planar* graphs $\mathscr{G}$, since otherwise $Z_N(\mathscr{G}) = 0$ for all N.

[7] Identical reasoning holds for nets of walks that are *self-avoiding* as well as mutually avoiding, but μ, ν, and $\{\sigma_l\}_{l \geq 1}$ of course take different values.[21,22]

At criticality, this correlation function decays asymptotically as

$$\langle \phi_l(X)\, \phi_l(Y) \rangle_{\beta_c} \sim |X-Y|^{-2x_l} \tag{2.9}$$

where x_l is the scaling dimension of ϕ_l. Then $\gamma_{\mathscr{W}_l}$ can be related to x_l by the scaling law

$$\gamma_{\mathscr{W}_l} = (d - 2x_l)\nu - (l-1) \tag{2.10}$$

[This is a generalization of the well-known scaling law $\gamma = (2-\eta)\nu$. The term $l-1$ arises from the fact that G_l has *variable* numbers of steps on each edge, while $Z_N(\mathscr{W}_l)$ is built from walks of *fixed* length N.] Combining (2.6) and (2.10), we find

$$\sigma_l = -\nu x_l + \frac{l}{2}(d\nu - 1) \tag{2.11}$$

Inserting this into (2.5), we conclude that

$$\zeta_l = (x_l + l x_1)\nu - l(d\nu - 1) \tag{2.12}$$

It suffices, therefore, to compute the anomalous dimensions x_l.

One exponent is easy: for MAWs we have $\zeta_1 = 0$, hence $\sigma_1 = 0$ and $x_1 = \frac{1}{2}(d-2)$. It follows that $\zeta_l = \frac{1}{2}x_l - \frac{1}{4}l(d-2)$.

To proceed further, we restrict attention to $d = 2$, and assume that MAWs are described by a conformal field theory[25-27] with central charge c. We then argue as follows:

(a) We *guess* that the scalar field ϕ_l is a *primary* conformal field of weight h_l. Then the anomalous dimension x_l equals $2h_l$. [If ϕ_l were instead a *secondary* field descended from a primary field of weight h_l, we would have $x_l = 2(h_l + \text{positive integer})$.]

(b) MAWs can be represented[9,10,13] by a theory of l n-component fields φ_i $(1 \leqslant i \leqslant l)$ with quartic interaction $\sum_{i \neq j} |\varphi_i|^2\, |\varphi_j|^2$, analytically continued to $n = 0$. For such a zero-component model, the free energy is identically zero; and since the finite-size corrections to the free energy in a strip of width L are proportional to the central charge c,[28-30] we conclude that $c = 0$.

(c) The pair (c, h_l) labels a highest-weight representation of the Virasoro algebra.[31-34] At certain special values of the weight h, namely

$$h_{r,s}^{(c)} = \frac{1}{24}(c-1) + \frac{1}{96}(r\beta_+ - s\beta_-)^2 \tag{2.13}$$

with

$$\beta_{\pm} = (25 - c)^{1/2} \pm (1 - c)^{1/2} \tag{2.14}$$

$$r, s \text{ integers} \geqslant 1 \tag{2.15}$$

the representation of the Virasoro algebra is *degenerate.*[31-34] In this case the correlation functions of the corresponding primary field ϕ satisfy linear differential equations.[25] If, in addition, β_-/β_+ is a rational number—say, $\beta_-/\beta_+ = m/m'$, where $m' \geqslant m \geqslant 1$ are relatively prime integers—then there exists a closed operator algebra involving only a finite number of conformal families, namely those given by (2.13) with

$$1 \leqslant r \leqslant m-1, \qquad 1 \leqslant s \leqslant m'-1 \tag{2.16}$$

(see ref. 25). Theories satisfying these two conditions are said to be *minimal* conformal field theories; they can be parametrized by

$$c = 1 - \frac{6(m-m')^2}{mm'} \tag{2.17}$$

where m and m' are as above. The minimal models appear to play a special role (not yet completely understood[35,36]) in two-dimensional critical phenomena.

(d) Motivated by the above, Duplantier and Kwon[20] *guess* that the MAW exponents can be obtained from the Kac table (2.13) with $c = 0$ and suitable choices of r, s. However, r and s must in general be chosen *outside* the "minimal block" (2.16). [For two-dimensional *self-avoiding* walks, an Ansatz of this type gives exponents agreeing with those obtained by Coulomb-gas methods, in both the dilute $(c = 0)$[23,21,37] and dense $(c = -2)$[24,38] regimes, but in this case one must allow also *half-integer* values of r, s. Fractional values of r, s have been encountered also in refs. 39 and 30.]

(e) It remains to identify the (r, s) pair corresponding to each MAW exponent h_l. To do this, Duplantier and Kwon[20] carry out a Monte Carlo study of l-star MAWs for $l = 2$, 3, 4, 5, thereby obtaining an estimate of ζ_l; since the possible exponents $h_{r,s}^{(c=0)}$ are rather widely spaced, even modest accuracy suffices to determine (r, s) and hence ζ_l *exactly.*[8] Duplantier and Kwon find that $\zeta_l = h_{0,l}^{(c=0)} = (4l^2 - 1)/24$ for the four l values that they

[8] In fact, for $l = 2$ there is a *unique* value in the $c = 0$ Kac table (with r, s integer or half-integer) that is consistent with the rigorous bound (1.5): it is $\zeta_2 = 5/8$. Therefore, for $l = 2$ the Monte Carlo study is not even necessary, if the conformal-invariance guess is correct.

studied, and they make the plausible guess that this formula is correct for *all* $l \geq 2$.

Remarks. 1. Many important statistical mechanical models (Ising, Potts, etc.) correspond to conformal field theories satisfying *reflection positivity.*[40–42] In such cases the representation of the Virasoro algebra must be *unitary.* These representations have been completely classified[43–46]; they are given by

$$\left.\begin{cases} c = 1 - \dfrac{6}{m(m+1)} & m \text{ integer} \geq 2 \\ h = h_{r,s}^{(c)} \equiv \dfrac{[(m+1)r - ms]^2 - 1}{4m(m+1)} & r, s \text{ integers}, \\ & 1 \leqslant s \leqslant r \leqslant m-1 \end{cases}\right\} \quad \text{or} \quad \begin{Bmatrix} c \geq 1 \\ h \geq 0 \end{Bmatrix} \tag{2.18}$$

In particular, for $c = 0$ the only unitary representation is the trivial one ($h = 0$). But the MAW and SAW are *not* reflection positive, so there is no contradiction with the Duplantier–Saleur–Kwon Ansatz.

2. The argument presented above is in fact a slight variant of the one given by Duplantier and Kwon.[20] We relate the Duplantier–Saleur–Kwon Ansatz to the degenerate representations (2.13) [possibly extended *ad hoc* to allow r, s half-integer], while Duplantier and Kwon describe their Ansatz as an *ad hoc* extension of the discrete unitary series (2.18a). We suspect that the former description may give better insight into why the Ansatz works.

3. THE MONTE CARLO METHOD

The most obvious Monte Carlo method for the MAW problem is:

1. Generate many l-tuples of N-step ordinary random walks (ORWs), and test each l-tuple for intersection. The fraction of cases that are nonintersecting constitutes an estimate of $p_l(N)$.
2. Repeat step 1 for many values of N. Fit the results to (1.3) to obtain an estimate of ζ_l.

This method works; it was employed by Duplantier and Kwon[20] with $N \leqslant 70$ to estimate ζ_2, ζ_3, ζ_4, ζ_5 in $d = 2$. The disadvantage of this method is that it is necessary to make many separate simulations, one for each value of N.

A more efficient Monte Carlo method can be based on the observation that the equal-weight probability distributions on N-step ORWs for different values of N are *consistent*: that is, if $N < N'$, then the restriction to the first N steps of the equal-weight distribution on N'-step ORWs gives equal weight to each N-step walk. (The corresponding statement for self-avoiding walks is *false*.) It follows that there exists a probability measure on the space of *infinite*-length walks whose restriction to the first N steps gives equal weight to each N-step walk, for each N. In other words, ordinary random walk is a *stochastic process*. Moreover, this stochastic process has the following property[(2)]: if ω_1 and ω_2 are independent infinite-length ORWs in $\mathbf{Z}^d$ ($d \leqslant 4$), then with probability 1, ω_1 and ω_2 have a nonempty intersection (in fact, they have infinitely many intersections).

We can therefore study the MAW problem for all N *simultaneously*, as follows:

1. Initialize $\omega_1, \ldots, \omega_l$ to empty walks (with initial points $x_1, \ldots, x_l$, respectively). Initialize $\mathcal{N} \leftarrow 0$.
2. Independently extend $\omega_1, \ldots, \omega_l$ by one random step each. Increment $\mathcal{N}$ by 1.
3. Test whether $\omega_1, \ldots, \omega_l$ are mutually avoiding. If so, go to step 2. If not, output the *death time* $\mathcal{N}$ and halt.

For $d \leqslant 4$, this algorithm is guaranteed to halt (with probability 1), and the probability distribution of the death time $\mathcal{N}$ is given by

$$P(\mathcal{N} > N) = p_l(N) \tag{3.1}$$

and hence

$$P(\mathcal{N} = N) = q_l(N) \equiv p_l(N-1) - p_l(N) \tag{3.2}$$

From (1.3), we have

$$q_l(N) \sim N^{-(1+\zeta_l)} \qquad \text{as} \quad N \to \infty \tag{3.3}$$

In other words, the large-N behavior of the probability distribution of $\mathcal{N}$ is determined *exactly* (modulo corrections to scaling) in terms of the single exponent ζ_l. We have, therefore, a parametric-estimation problem for which we can use the method of maximum likelihood[(47,48)], as described below, to estimate ζ_l.

There is one slight snag: If $\zeta_l \leqslant 1$ (as we know to be the case for $l = 2$ in all dimensions), then the death time $\mathcal{N}$, though finite with probability 1, has infinite mean:

$$\langle \mathcal{N} \rangle = \sum_{N=1}^{\infty} N q_l(N) = \infty \tag{3.4}$$

This would imply that the mean CPU time per iteration is also infinite—a rather unpleasant situation! We therefore modify step 3 of the algorithm to impose a cutoff $N_{\max}$:

3′. Test whether $\omega_1, \ldots, \omega_l$ are mutually avoiding. If so:

a. If $\mathcal{N} < N_{\max}$, go to step 2.
b. If $\mathcal{N} = N_{\max}$, output the message "Death time $> N_{\max}$" and halt.

If $\omega_1, \ldots, \omega_l$ are not mutually avoiding, output the death time $\mathcal{N}$ and halt.

This algorithm has a mean running time that behaves as

$$\langle \text{CPU time} \rangle \sim \langle \mathcal{N} \rangle \sim \begin{cases} O(N_{\max}^{1-\zeta_l}) & \text{if } 0 < \zeta_l < 1 \\ O(\log N_{\max}) & \text{if } \zeta_l = 1 \\ O(1) & \text{if } \zeta_l > 1 \end{cases} \tag{3.5}$$

as $N_{\max} \to \infty$. The cutoff $N_{\max}$ can be chosen to optimize the statistical efficiency (see the Appendix). If $\zeta_l > 1$, we are free to take $N_{\max} = \infty$.

The maximum-likelihood method is defined as follows[9]: Let us assume temporarily that the asymptotic form (3.3) is *exact* for $N \geqslant N_{\min}$. Then the probability distribution of the death time $\mathcal{N}$, *conditional on it being between* $N_{\min}$ *and* $N_{\max}$, is

$$P(\mathcal{N} = N \mid N_{\min} \leqslant \mathcal{N} \leqslant N_{\max}) = Z(\zeta_l, N_{\min}, N_{\max})^{-1} \times N^{-(1+\zeta_l)} \tag{3.6}$$

where

$$Z(\zeta_l, N_{\min}, N_{\max}) \equiv \sum_{N=N_{\min}}^{N_{\max}} N^{-(1+\zeta_l)} \tag{3.7}$$

Successive samples $\mathcal{N}_1, \mathcal{N}_2, \ldots$ are independent; the probability of observing any particular set $\{\mathcal{N}_1, \ldots, \mathcal{N}_n\}$ is therefore

$$\text{likelihood} = \prod_{\substack{1 \leqslant i \leqslant n \\ N_{\min} \leqslant \mathcal{N}_i \leqslant N_{\max}}} Z(\zeta_l, N_{\min}, N_{\max})^{-1} \times \mathcal{N}_i^{-(1+\zeta_l)} \tag{3.8}$$

(Here the product is taken over only those i for which $N_{\min} \leqslant \mathcal{N}_i \leqslant N_{\max}$; the walks that die before time $N_{\min}$ or after time $N_{\max}$ play no role in this analysis.) The maximum-likelihood estimate $\hat{\zeta}_l = \hat{\zeta}_l(\mathcal{N}_1, \ldots, \mathcal{N}_n)$ is, by defini-

[9] The maximum-likelihood method was used for similar purposes in a study of self-avoiding walks.[49]

tion, the value of ζ_l that maximizes the likelihood (3.8). In other words, it is the value of ζ_l that maximizes the probability of observing the particular data set $\{\mathcal{N}_1,..., \mathcal{N}_n\}$ that was in fact observed. Since (3.8) is an "exponential family,"[47,48] $\hat{\zeta}_l$ is determined by the simple condition

$$\langle \log \mathcal{N} \rangle_{\hat{\zeta}_l} = \langle \log \mathcal{N} \rangle_{\text{obs}} \tag{3.9}$$

where we have defined the theoretical mean value

$$\langle f(\mathcal{N}) \rangle_{\zeta_l} \equiv \sum_{N=N_{\min}}^{N_{\max}} f(N)\, N^{-(1+\zeta_l)} \Bigg/ \sum_{N=N_{\min}}^{N_{\max}} N^{-(1+\zeta_l)} \tag{3.10}$$

and the observed mean value

$$\langle f(\mathcal{N}) \rangle_{\text{obs}} \equiv \sum_{\substack{1 \leqslant i \leqslant n \\ N_{\min} \leqslant \mathcal{N}_i \leqslant N_{\max}}} f(\mathcal{N}_i) \Bigg/ \sum_{\substack{1 \leqslant i \leqslant n \\ N_{\min} \leqslant \mathcal{N}_i \leqslant N_{\max}}} 1 \tag{3.11}$$

The likelihood equation (3.9) is easily solved numerically for $\hat{\zeta}_l$, e.g., by Newton's method. By the general theory of maximum-likelihood estimation,[47,48] the probability distribution of $\hat{\zeta}_l$ is asymptotically Gaussian as the sample size $n \to \infty$, with mean

$$\langle \hat{\zeta}_l \rangle_{\zeta_l} = \zeta_l + O\left(\frac{1}{n'}\right) \tag{3.12}$$

and variance

$$\operatorname{var}_{\zeta_l}(\hat{\zeta}_l) = \frac{1}{n' \operatorname{var}_{\zeta_l}(\log \mathcal{N})} + O\left(\frac{1}{n'^2}\right) \tag{3.13}$$

where

$$n' \equiv n \sum_{N=N_{\min}}^{N_{\max}} q_l(N) = \left\langle \sum_{\substack{1 \leqslant i \leqslant n \\ N_{\min} \leqslant \mathcal{N}_i \leqslant N_{\max}}} 1 \right\rangle \tag{3.14}$$

is the expected censored sample size. Note that $\operatorname{var}(\hat{\zeta}_l)$ depends on the unknown "true" value ζ_l; but since this dependence is rather weak, and since $\hat{\zeta}_l$ will be a fairly close estimate of ζ_l (provided $n' \gg 1$), it suffices for our purposes to replace ζ_l by the estimated value $\hat{\zeta}_l$ when attempting to compute error bars for $\hat{\zeta}_l$.[10] These error bars are computed (for $n' \gg 1$) by

[10] More rigorously, one would limit oneself to some interval $[\zeta_{l,\min}, \zeta_{l,\max}]$ in which the true value ζ_l is *assumed* to lie, compute the *worst* possible error bar subject to that assumption, and thereby derive a rigorous classical confidence interval for ζ_l subject to the assumption that $\zeta_l \in [\zeta_{l,\min}, \zeta_{l,\max}]$.

assuming the distribution of $\hat{\zeta}_l$ to be Gaussian with mean ζ_l and variance given by (3.13).[11] A very important feature of this method is that *the statistical error bars can be estimated prior to performing the Monte Carlo experiment.* Moreover, it can be proven that in the large-sample limit $n \to \infty$ *the maximum-likelihood estimator is the optimal estimator*, in the sense that any other estimator (within a certain very broad class) has larger or equal mean-square error at leading order in $1/n$.[47,48] Thus, the maximum-likelihood method provides an optimal data analysis: it extracts from the Monte Carlo data $\{\mathcal{N}_1,..., \mathcal{N}_n\}$ their full content as regards the parameter ζ_l.

We now return to the problem of corrections to scaling. Clearly, (3.3) is only the leading term in an asymptotic expansion of $q_l(N)$ for large N; the renormalization group predicts[50] that the actual behavior is

$$q_l(N) \sim N^{-(1+\zeta_l)} \left[a_0 + \frac{a_1}{N} + \frac{a_2}{N^2} + \cdots + \frac{b_0}{N^{\Delta_1}} + \frac{b_1}{N^{\Delta_1+1}} + \cdots \right.$$
$$\left. + \frac{c_0}{N^{\Delta_2}} + \frac{c_1}{N^{\Delta_2+1}} + \cdots \right] \tag{3.15}$$

Here $\Delta_1 < \Delta_2 < \cdots$ are correction-to-scaling exponents, and there is an infinite spectrum of correction terms of the form $1/N^{m_1\Delta_1 + m_2\Delta_2 + \cdots + m_k\Delta_k + n}$, where $m_1, m_2,..., m_k, n$ are nonnegative integers. The exponents $\Delta_1, \Delta_2,...$ are believed to be universal among lattices of a given dimension d; the amplitudes $a_0, a_1,..., b_0, b_1,..., c_0, c_1,...$ depend on the lattice and on the initial points $x_1, x_2,..., x_l$.

The maximum-likelihood analysis described above is based on the assumption that (3.3) is exact for $N \geqslant N_{\min}$; if (3.15) is correct, then this assumption is in error by an amount of order $1/N_{\min}^{\Delta}$, where $\Delta \equiv \min(\Delta_1, 1)$. Thus, we expect that the estimates of ζ_l derived using (3.3) likewise have a systematic error of this order (as well as higher-order corrections). A useful procedure would then be to perform the analysis for a variety of values of $N_{\min}$; to plot $\hat{\zeta}_l$, together with its purely statistical error bars, as a function of $N_{\min}$ (or of $1/N_{\min}^{\Delta}$ for some guessed Δ); and finally to attempt an extrapolation to $N_{\min} = \infty$. Unfortunately, such an extrapolation is extremely difficult: as a matter of principle, one must go to large enough values of $N_{\min}$ so that the subleading corrections to scaling are negligible compared to the leading correction; but it is precisely in this region that the data become very "noisy" (the statistical error bars grow

[11] For $n' \gg 1$ we can neglect the bias (which is of order $1/n'$), since it is much smaller than the standard deviation [which is of order $1/(n')^{1/2}$].

rapidly with $N_{\min}$), making reliable extrapolation almost impossible. A similar difficulty arises if we attempt to make a two-parameter maximum-likelihood fit, for example, to the form

$$q_l(N) \sim N^{-(1+\zeta_l)} \exp(a/N^{\Delta}) \tag{3.16}$$

with Δ fixed. (A fit to three or more parameters, such as allowing Δ to be variable, is even more difficult.) We therefore adopt the most primitive method (which might be called "zeroth-order extrapolation"): we plot $\hat{\zeta}_l$ and its statistical error bars as a function of $N_{\min}$, and note the $N_{\min}$ value at which $\hat{\zeta}_l$ becomes roughly constant within error bars. The error bars at this $N_{\min}$ value are declared to be the *statistical* error bars on $\hat{\zeta}_l$ (classical confidence limits); and a subjective estimate of the uncertainty in extrapolating to $N_{\min}=\infty$ is reported as a *systematic* error induced by corrections to scaling.

4. NUMERICAL RESULTS

We have implemented the algorithm described in the previous section, taking $d=2$ and $l=2, 3$, with $N_{\max}=50000$. The only nonobvious part of the program is the test for intersection, which we wish to perform in a time of order 1 (i.e., independent of N). To do this, we store the current state of the walks $\omega_1, \omega_2,..., \omega_l$ in hash tables[51] $H_1, H_2,..., H_l$, which are updated at each step. We also maintain linear lists of the occupied locations in the hash tables; this allows us to clean the tables rapidly at the end.[12] For $l=2$, for example, the logic is as follows:

```
last1 ← x1; insert x1 in H1
last2 ← x2; insert x2 in H2
𝒩 ← 0
while 𝒩 < Nmax do
    𝒩 ← 𝒩 + 1
    last1 ← last1 + random step
    if last1 ∈ H2 then goto finish
    insert last1 in H1
    last2 ← last2 + random step
    if last2 ∈ H1 then goto finish
    insert last2 in H2
endwhile
print "Death time > Nmax"; clean H1 and H2; halt

finish: print 𝒩; clean H1 and H2; halt
```

[12] For a similar use of hash tables, see ref. 52, Section 3.4.

Table I. Parameters of Our Runs with $l = 2$[a]

Machine	Number of pairs ($\times 10^6$)	PRNG	CPU time/pair
Astronautics ZS-2	310	II	8.5 msec
Convex C-1	484	III	5.5 msec
Cyber 205	20	II	3.0 msec
Elxsi 6400	161	II	19 msec
VAX 11/785	24	I	55 msec

[a] In all cases we took $x_1 = x_2 = 0$ and $N_{\max} = 50{,}000$. Note that the mean CPU time per pair is strongly dependent on $N_{\max}$ [Eq. (3.5)].

Note that we ignore possible intersections at time $(0, 0)$ [which occur if $x_1 = x_2$], but not intersections at time $(t_1, 0)$ or $(0, t_2)$. The hash-table size M should be at least several times $N_{\max}$; we used $M = 247{,}879$.

The parameters of our $l = 2$ runs are shown in Table I; in all cases we took $x_1 = x_2 = 0$ and $N_{\max} = 50000$. In total we generated slightly less than 10^9 pairs of walks. As a precaution, we did our runs with three different pseudo-random-number generators (PRNGs): all were linear congruential generators[(53)] of the form

$$X_{n+1} = (aX_n + c) \bmod m \tag{4.1}$$

with the following parameters:

PRNG I:	$m = 2^{48}$,	$a = 31167285$,	$c = 1$
PRNG II:	$m = 2^{48}$,	$a = 3581664053$,	$c = 1$
PRNG III:	$m = 2^{64}$,	$a = 31026 \times 2^{32} + 21597$,	$c = 1$

These generators were chosen on the basis of their excellent scores on the spectral test[(53)]: see ref. 53, p. 102 for generator I, and ref. 54 for generators II and III. As a check for subtle defects of these PRNGs (or compiler bugs or gross programming errors), we analyzed each set of runs separately, and compared the results. All pairs of runs agree within at most 2 standard deviations for all values of $N_{\min}$, except that generators II and III disagree by 2.1–2.3 standard deviations for $N_{\min} = 1500$, 1600, 1700. We are therefore satisfied that none of our runs suffer from a statistically significant bias due to a defective PRNG. The results presented below are based on the merged data from all of our runs.

In Table II we give our raw data for $\langle \log \mathcal{N} \rangle_{\mathrm{obs}}$ as a function of $N_{\min}$, along with the corresponding estimates $\hat{\zeta}_2$. We also report how many

Table II. Raw Data for $l = 2$ as a Function of N_{min} [a]

N_{min}	Number of pairs survived ($\times 10^6$)	$\langle \log \mathcal{N} \rangle_{obs}$	ζ_2
0	999.0		
102	39.9	6.0969	0.62026 (0.00012)
200	26.0	6.7214	0.62091 (0.00016)
300	20.0	7.0893	0.62144 (0.00019)
400	16.6	7.3461	0.62192 (0.00022)
500	14.3	7.5430	0.62198 (0.00024)
600	12.7	7.7020	0.62221 (0.00026)
700	11.5	7.8349	0.62253 (0.00028)
800	10.5	7.9492	0.62259 (0.00030)
900	9.7	8.0494	0.62255 (0.00032)
1000	9.0	8.1383	0.62247 (0.00034)
1100	8.4	8.2181	0.62246 (0.00036)
1200	7.9	8.2903	0.62268 (0.00037)
1300	7.5	8.3564	0.62282 (0.00039)
1400	7.1	8.4172	0.62284 (0.00041)
1500	6.8	8.4736	0.62288 (0.00042)
1600	6.5	8.5261	0.62281 (0.00044)
1700	6.2	8.5749	0.62313 (0.00046)
1800	6.0	8.6208	0.62327 (0.00047)
1900	5.8	8.6639	0.62347 (0.00049)
2000	5.5	8.7048	0.62349 (0.00050)
2100	5.4	8.7434	0.62365 (0.00052)
2200	5.2	8.7802	0.62363 (0.00053)
2300	5.0	8.8151	0.62382 (0.00055)
2400	4.9	8.8484	0.62380 (0.00056)
2500	4.7	8.8802	0.62400 (0.00058)
2600	4.6	8.9107	0.62399 (0.00059)
2700	4.5	8.9400	0.62398 (0.00061)
2800	4.3	8.9680	0.62410 (0.00062)
2900	4.2	8.9949	0.62424 (0.00064)
3000	4.1	9.0210	0.62414 (0.00065)
3100	4.0	9.0460	0.62421 (0.00067)
3200	3.9	9.0703	0.62403 (0.00068)
3300	3.8	9.0938	0.62383 (0.00070)
3400	3.7	9.1164	0.62373 (0.00071)
3500	3.7	9.1382	0.62385 (0.00073)
3600	3.6	9.1596	0.62352 (0.00074)
3700	3.5	9.1801	0.62354 (0.00076)
3800	3.4	9.2001	0.62361 (0.00077)

[a] Error bar on ζ_2 is $\pm$ one standard deviation. Conformal-invariance prediction is $\zeta_2 = 5/8 = 0.625$.

Table continued

Table II. (*Continued*)

$N_{\min}$	Number of pairs survived ($\times 10^6$)	$\langle \log \mathcal{N} \rangle_{\text{obs}}$	$\hat{\zeta}_2$
3900	3.4	9.2193	0.62387 (0.00079)
4000	3.3	9.2381	0.62388 (0.00080)
4100	3.2	9.2564	0.62401 (0.00082)
4200	3.2	9.2741	0.62424 (0.00083)
4300	3.1	9.2916	0.62393 (0.00085)
4400	3.1	9.3085	0.62404 (0.00086)
4500	3.0	9.3251	0.62372 (0.00088)
4600	2.9	9.3411	0.62386 (0.00089)
4700	2.9	9.3568	0.62408 (0.00091)
4800	2.8	9.3721	0.62413 (0.00092)
4900	2.8	9.3871	0.62400 (0.00094)
5000	2.8	9.4017	0.62412 (0.00095)
5100	2.7	9.4161	0.62395 (0.00097)
5200	2.7	9.4301	0.62398 (0.00098)
5300	2.6	9.4437	0.62440 (0.00100)
5400	2.6	9.4571	0.62451 (0.00101)
5500	2.5	9.4703	0.62439 (0.00103)
5600	2.5	9.4832	0.62423 (0.00105)
5700	2.5	9.4959	0.62396 (0.00106)
5800	2.4	9.5083	0.62410 (0.00108)
5900	2.4	9.5204	0.62422 (0.00109)
6000	2.4	9.5323	0.62421 (0.00111)

of the 999×10^6 initial pairs of walks survived to the given length. These raw data may be of use to researchers who wish to do runs of their own, or who wish to reanalyze our runs (e.g., using other methods to handle corrections to scaling).

In Fig. 1 we plot $\hat{\zeta}_2$, together with its one-standard-deviation error bar, as a function of $N_{\min}$. Statistically significant corrections to scaling are observed until at least $N_{\min} = 2000$. For $N_{\min} \gtrsim 2500$, $\hat{\zeta}_2$ is constant within error bars. We therefore take $\hat{\zeta}_2(N_{\min} = 2500)$ as our "best estimate" of ζ_2, and set the systematic error bars (95% subjective confidence limits) so as to encompass the central value at any $N_{\min}$ between 2000 and 5000. The statistical error bar (classical 95% confidence limits) is taken to be 1.96 times the standard deviation at $N_{\min} = 2500$. The result is

$$\zeta_2 = 0.6240 \pm 0.0005 \pm 0.0011 \tag{4.2}$$

where the first error bar represents systematic error and the second error

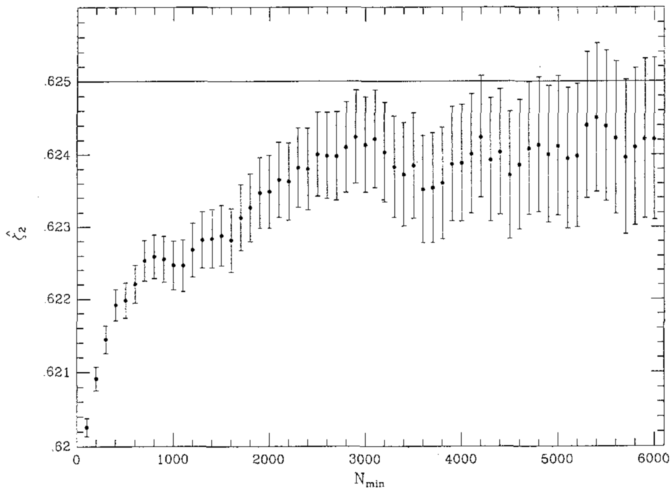

Fig. 1. Estimator $\hat{\zeta}_2$ versus N_{min}. Error bar is $\pm$ one standard deviation. The predicted exact value $\zeta_2 = 5/8$ is indicated by the horizontal line.

bar represents statistical error. This result is in good agreement with the conformal-invariance prediction $\zeta_2 = 5/8 = 0.625$.

A closer analysis shows that the corrections to scaling for $100 \leqslant N_{min} \lesssim 1500$ are very roughly proportional to $1/N_{min}^{0.4}$. We therefore tried fits to the form (3.16), using the *one*-parameter maximum-likelihood method with a variety of *fixed* values of Δ and a. For $(\Delta, a) = (0.4, -0.15)$ and $(0.5, -0.2)$ we obtained estimates $\hat{\zeta}_2$ that are reasonably flat as a function of N_{min} in the range $100 \leqslant N_{min} \leqslant 1600$: these estimates are ≈ 0.6246 and ≈ 0.6240, respectively. We wish to emphasize that these pairs (Δ, a) should *not* be considered to be estimates of the correction-to-scaling exponent Δ_1 and its amplitude b_0/a_0 as defined in (3.15). Rather, they define only an empirical *effective* exponent and amplitude that fit the data reasonably well in a particular nonasymptotic range of N; they do this quite possibly by mimicking a *combination* of correction-to-scaling terms as shown in (3.15). For the same reason, we do not consider these "corrected" estimates of ζ_2 to be any more accurate or reliable than the "primitive" estimate (4.2). All we can say is that the data appear to require at least one correction-to-scaling exponent $\Delta \approx 0.4$–0.5 or smaller.

The parameters of our $l = 3$ runs are shown in Table III; in all cases we took $x_1 = (0, 1)$, $x_2 = (-1, 0)$, $x_3 = (1, -1)$, and $N_{max} = 50{,}000$. In total we generated slightly more than 4×10^9 triplets of walks. The CPU time per iteration is much smaller for $l = 3$ than for $l = 2$, because the $l = 3$ walks die much sooner. Separate analyses of the runs showed no statistically

Table III. Parameters of Our Runs with $l = 3$[a]

Machine	Number of triplets ($\times 10^6$)	PRNG	CPU time/triplet
Astronautics ZS-2	1592	II	1.15 msec
Convex C-1	870	III	0.86 msec
Convex C-210	1748	III	0.32 msec

[a] In all cases we took $x_1 = (0, 1)$, $x_2 = (-1, 0)$, $x_3 = (1, -1)$, and $N_{max} = 50000$. Note that the mean CPU time per triplet is rather weakly dependent on N_{max}, because $\zeta_3 > 1$ [Eq. (3.5)].

significant differences; the results presented below are based on the merged data from all runs.

In Table IV we give our raw data for $\langle \log \mathcal{N} \rangle_{obs}$ as a function of N_{min}, along with the corresponding estimates $\hat{\zeta}_3$. We also report how many of the 4210×10^6 initial triplets of walks survived to the given length (note that very few did!). In Fig. 2 we plot $\hat{\zeta}_3$, together with its one-standard-deviation error bar, as a function of N_{min}. Statistically significant corrections to scaling are observed until about $N_{min} = 1000$, after which $\hat{\zeta}_3$ is essentially constant within error bars. The value at $N_{min} = 1000$ is almost exactly equal to the predicted value 35/24, but this is pure coincidence. A fairer choice is to select our "best estimate" and systematic error bars (95% subjective confidence limits) so as to encompass the central value at any

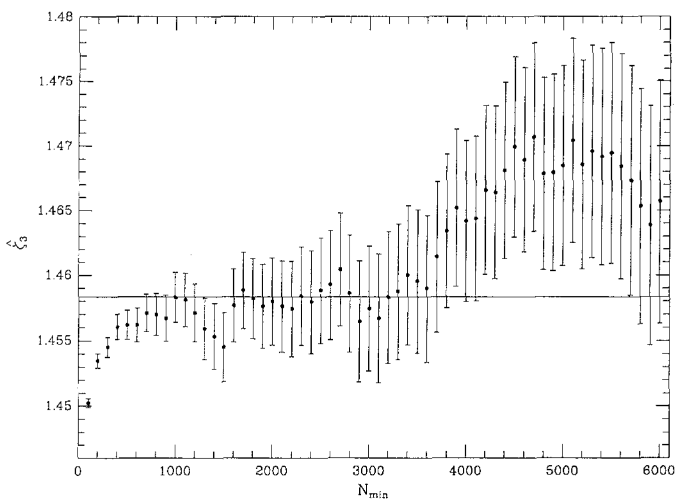

Fig. 2. Estimator $\hat{\zeta}_3$ versus N_{min}. Error bar is $\pm$ one standard deviation. The predicted exact value $\zeta_3 = 35/24$ is indicated by the horizontal line.

Table IV. Raw Data for $l = 3$ as a Function of N_{min} [a]

N_{min}	Number of triplets survived ($\times 10^6$)	$\langle \log \mathcal{N} \rangle_{obs}$	ζ_3
0	4210.000		
102	18.381	5.3088	1.45023 (0.00034)
200	6.904	5.9820	1.45347 (0.00056)
300	3.827	6.3866	1.45451 (0.00076)
400	2.518	6.6727	1.45606 (0.00094)
500	1.818	6.8947	1.45619 (0.00111)
600	1.393	7.0758	1.45620 (0.00128)
700	1.113	7.2282	1.45710 (0.00144)
800	0.916	7.3603	1.45700 (0.00160)
900	0.771	7.4767	1.45671 (0.00175)
1000	0.661	7.5799	1.45830 (0.00190)
1100	0.575	7.6738	1.45812 (0.00205)
1200	0.506	7.7596	1.45713 (0.00220)
1300	0.450	7.8385	1.45590 (0.00234)
1400	0.403	7.9112	1.45533 (0.00249)
1500	0.364	7.9789	1.45451 (0.00264)
1600	0.332	8.0405	1.45768 (0.00278)
1700	0.304	8.0990	1.45883 (0.00292)
1800	0.279	8.1547	1.45821 (0.00306)
1900	0.258	8.2073	1.45761 (0.00321)
2000	0.239	8.2568	1.45799 (0.00335)
2100	0.223	8.3040	1.45761 (0.00349)
2200	0.208	8.3489	1.45743 (0.00363)
2300	0.195	8.3912	1.45839 (0.00377)
2400	0.183	8.4322	1.45796 (0.00392)
2500	0.172	8.4710	1.45885 (0.00406)
2600	0.163	8.5083	1.45925 (0.00420)
2700	0.154	8.5439	1.46045 (0.00434)
2800	0.146	8.5791	1.45862 (0.00449)
2900	0.138	8.6132	1.45647 (0.00464)
3000	0.131	8.6449	1.45745 (0.00478)
3100	0.125	8.6762	1.45670 (0.00492)
3200	0.119	8.7057	1.45831 (0.00507)
3300	0.114	8.7345	1.45876 (0.00521)
3400	0.109	8.7622	1.46002 (0.00536)
3500	0.105	8.7895	1.45956 (0.00550)
3600	0.100	8.8161	1.45898 (0.00565)
3700	0.096	8.8410	1.46142 (0.00579)
3800	0.093	8.8652	1.46343 (0.00594)

[a] Error bar on ζ_3 is $\pm$ one standard deviation. Conformal-invariance prediction is $\zeta_3 = 35/24 = 1.458333\ldots$.

Table continued

Table IV. (*Continued*)

$N_{\min}$	Number of triplets survived ($\times 10^6$)	$\langle \log \mathcal{N} \rangle_{\text{obs}}$	ζ_3
3900	0.089	8.8889	1.46520 (0.00608)
4000	0.086	8.9128	1.46420 (0.00624)
4100	0.083	8.9356	1.46439 (0.00639)
4200	0.080	8.9573	1.46659 (0.00653)
4300	0.077	8.9791	1.46640 (0.00668)
4400	0.075	8.9999	1.46811 (0.00683)
4500	0.072	9.0200	1.46993 (0.00698)
4600	0.070	9.0405	1.46895 (0.00714)
4700	0.068	9.0598	1.47070 (0.00729)
4800	0.065	9.0799	1.46785 (0.00745)
4900	0.063	9.0987	1.46794 (0.00760)
5000	0.061	9.1170	1.46847 (0.00776)
5100	0.060	9.1346	1.47043 (0.00791)
5200	0.058	9.1527	1.46856 (0.00807)
5300	0.056	9.1697	1.46959 (0.00823)
5400	0.055	9.1868	1.46919 (0.00839)
5500	0.053	9.2033	1.46946 (0.00855)
5600	0.052	9.2198	1.46842 (0.00871)
5700	0.050	9.2361	1.46734 (0.00888)
5800	0.049	9.2522	1.46535 (0.00905)
5900	0.048	9.2679	1.46388 (0.00922)
6000	0.046	9.2825	1.46573 (0.00938)

$N_{\min}$ between 1000 and 3500. The statistical error bar (classical 95% confidence limits) is taken to be 1.96 times the standard deviation at $N_{\min} = 1500$. The result is

$$\zeta_3 = 1.4575 \pm 0.0030 \pm 0.0052 \tag{4.3}$$

where the format is as before. This result is in good agreement with the conformal-invariance prediction $\zeta_3 = 35/24 = 1.458333...$.

Our error bars for ζ_3 are five times as large as those for ζ_2, in spite of a sample four times as large; this is because very few triplets of walks survive to $N_{\min} = 1000$. In particular, the statistical errors appear to be too large to permit a meaningful analysis of corrections to scaling.

5. DISCUSSION

In summary, our Monte Carlo data agree well with the conformal-invariance predictions $\zeta_2 = 5/8$ and $\zeta_3 = 35/24$, *provided* that one considers only walks of length $\gtrsim 1000$–2000. Shorter walks are subject to strong corrections to scaling, leading to *apparent* exponents $\zeta_{2,\mathrm{eff}}$ and $\zeta_{3,\mathrm{eff}}$ that differ from the predicted exact values by 20–40 standard deviations. In part these large discrepancies are due to the (apparently) small value of the correction-to-scaling exponent $\Delta \approx 0.4$–0.5, which induces a very slow convergence to the $N \to \infty$ limit; and in part they are due to the extraordinary statistical precision with which we are able to measure critical exponents (standard deviation of 0.0001 for ζ_2 at $N_{\min} = 102$).

It is worth comparing these results to the earlier Monte Carlo work of Duplantier and Kwon[20] and Burdzy *et al.*[6] Duplantier and Kwon measured $p_l(N)$ by making separate simulations for various values of N up to about 70, generating about 6×10^5 samples per run. They then estimated ζ_l from the ratios $p_l(N)/p_l(N-20)$ for $40 \leqslant N \leqslant 70$. For $l = 2, 3$ they found

$$\zeta_2 = 0.622 \pm 0.004$$

$$\zeta_3 = 1.457 \pm 0.003$$

where no distinction is made between systematic and statistical error, and the error bars are presumably intended to be *one* standard deviation. This result for ζ_2 is at least roughly consistent with our estimate for $N_{\min} = 102$, and possibly also with the extrapolation of our estimates to $N_{\min} \approx 25$–50.[13] The estimate for ζ_3 is, however, only barely consistent with our estimate for $N_{\min} = 102$, and inconsistent with the extrapolation of our estimates to $N_{\min} \approx 25$–50. It seems that Duplantier and Kwon were very lucky in that the statistical errors happened in both cases to be opposite in sign (and comparable in magnitude) to the systematic error induced by corrections to scaling.

Burdzy *et al.* generated 3×10^6 pairs of random walks of length 500, from which they deduced $p_2(N)$ for $N \leqslant 500$. They then estimated ζ_2 from the ratios $p_2(N_2)/p_2(N_1)$ for various pairs (N_1, N_2) ranging from (50, 70) [in order to compare with Duplantier–Kwon] to (450, 499). They found

$$N_1 = 50,\quad N_2 = 70: \qquad \zeta_2 = 0.610 \pm 0.008$$

$$N_1 = 70,\quad N_2 = 100: \qquad \zeta_2 = 0.613 \pm 0.008$$

$$N_1 = 100,\quad N_2 = 150: \qquad \zeta_2 = 0.613 \pm 0.009$$

[13] Note that our estimate for $N_{\min} = 102$ is based on walks of *all lengths from* 102 *to* 50,000. In fact, as can be seen from Table II, half of these walks survived to $N = 300$, and a quarter survived to $N = 800$. Therefore, this estimate should *not* be compared with a Duplantier–Kwon-type estimate for $N = 100$; rather, it corresponds to something more like $N \approx 300$. Alternatively, a Duplantier–Kwon-type estimate for $N = 70$ might correspond to an estimate by our method with $N_{\min} \approx 25$–50.

$$N_1 = 150,\ N_2 = 200: \qquad \zeta_2 = 0.612 \pm 0.011$$
$$N_1 = 200,\ N_2 = 250: \qquad \zeta_2 = 0.617 \pm 0.014$$
$$N_1 = 250,\ N_2 = 300: \qquad \zeta_2 = 0.623 \pm 0.016$$
$$N_1 = 300,\ N_2 = 350: \qquad \zeta_2 = 0.635 \pm 0.018$$
$$N_1 = 350,\ N_2 = 400: \qquad \zeta_2 = 0.613 \pm 0.019$$
$$N_1 = 400,\ N_2 = 450: \qquad \zeta_2 = 0.591 \pm 0.021$$
$$N_1 = 450,\ N_2 = 499: \qquad \zeta_2 = 0.615 \pm 0.024$$

where the error bars are classical 95% confidence intervals (statistical error only) derived from the binomial distribution. These results are qualitatively and quantitatively consistent with ours, though the error bars are about 30–50 times bigger.[14] In particular, they show a rough trend toward increasing estimates of ζ_2 with increasing (N_1, N_2). The result for $(N_1, N_2) = (50, 70)$ is barely consistent with that of Duplantier and Kwon, but without the fortuitous cancellation of systematic and statistical errors.

With the very high statistical precision of the present study, one can now see clearly the corrections to scaling for $N_{\min} \lesssim 2000$, and the approach toward the conformal-invariance predictions for $N_{\min} \gtrsim 2000$. While we cannot assert definitively that the conformal-invariance predictions are correct, our results are most definitely consistent with those predictions, to a numerical accuracy of better than 0.002 for ζ_2 and about 0.008 for ζ_3. Since conformal-invariance predictions are supposed to be either *exact* or else *grossly wrong*—they cannot give answers that are *approximately* correct, except by mere coincidence—such a close numerical correspondence is in fact strong evidence that the conformal-invariance prediction (1.8) is *exact*.

But many aspects of the Duplantier–Saleur–Kwon Ansatz are still very mysterious. What is the meaning of exponents taken from the Kac table (2.13) with r, s *outside* the minimal block (2.16)? What is the meaning of the *half-integer* values of r, s that arise in the corresponding problem for self-avoiding walks? And can the observed correction-to-scaling exponent $\Delta \approx 0.4$–0.5 be explained by conformal-invariance methods? We do not feel qualified to answer these questions, but we do think that their resolution is likely to lead to new insights into two-dimensional conformal invariance in statistical mechanics.

[14] Our smaller error bars are due partly to the fact that we generated about 330 times as many walks as Burdzy *et al.* (this accounts for a factor ≈ 18 in the error bars), and partly to our use of the maximum-likelihood method with a large $N_{\max}$ (which corresponds in the Burdzy *et al.* method to a much larger value of N_2/N_1 than they took).

APPENDIX. OPTIMAL CHOICE OF $N_{\max}$

In this Appendix we work out the optimal choice of $N_{\max}$, assuming that $\zeta_l < 1$. (If $\zeta_l > 1$, there is little harm in taking $N_{\max} = \infty$.) We take the following point of view: First $N_{\min}$ is chosen so that the correction-to-scaling terms in (3.15) are adequately small for $N \geqslant N_{\min}$. (How small is "adequately small" depends on a somewhat subjective tradeoff of systematic error versus statistical error.) Then, with $N_{\min}$ fixed, we choose $N_{\max}$ so as to optimize the statistical efficiency of the algorithm, that is, to minimize the variance–time product

$$\operatorname{var}(\hat{\zeta}_l) \times \langle \text{CPU time} \rangle$$
$$\sim \frac{\langle \mathcal{N} \rangle}{(n'/n)\operatorname{var}(\log \mathcal{N})} \frac{\sum_{N=1}^{\infty} \min(N, N_{\max})\, q_l(N)}{\left(\sum_{N=N_{\min}}^{N_{\max}} q_l(N)\right)\left(\frac{d^2}{d\zeta^2} \log \sum_{N=N_{\min}}^{N_{\max}} N^{-(1+\zeta)}\right)^{-1}} \tag{A.1}$$

[see (3.4), (3.5), (3.10), (3.13), and (3.14)], where to lighten the notation we write ζ in place of ζ_l. Let us first work on the numerator, splitting it as

$$\sum_{N=1}^{\infty} \min(N, N_{\max})\, q_l(N)$$
$$= \sum_{N=1}^{N_{\text{submin}}-1} N q_l(N) + \sum_{N=N_{\text{submin}}}^{N_{\max}} N q_l(N) + \sum_{N=N_{\max}+1}^{\infty} N_{\max} q_l(N) \tag{A.2}$$

where N_{submin} is chosen so that $q_l(N) \sim N^{-(1+\zeta)}$ holds *at least very roughly* for $N \geqslant N_{\text{submin}}$. In general N_{submin} can be much smaller than $N_{\min}$; in practice, $N_{\text{submin}} \approx 10$ is probably fine. (The point is that we want very small systematic error in our estimates of *critical exponents*, but we are prepared to tolerate a much larger error, say of order 10%, in our estimates of *computer time*!) Typically N_{submin} is so small that the first term on the right side of (A.2) is negligible compared to the other two terms. We therefore find

$$\sum_{N=1}^{\infty} \min(N, N_{\max})\, q_l(N) \approx \text{const} \times \left[\frac{N_{\max}^{1-\zeta} - N_{\text{submin}}^{1-\zeta}}{1-\zeta} + \frac{N_{\max}^{1-\zeta}}{\zeta}\right]$$
$$\approx \text{const} \times N_{\max}^{1-\zeta}$$
$$= \text{const} \times \alpha^{1-\zeta} \tag{A.3}$$

where we have first taken the liberty of approximating a sum by an integral (which is obviously valid, since $N_{\text{submin}} \gg 1$), next assumed that

$(N_{\text{submin}}/N_{\max})^{1-\zeta} \ll 1$ (which is valid provided that ζ is not too near 1), and finally introduced the definition $\alpha = N_{\max}/N_{\min}$. Next we work on the denominator of (A.1):

$$\sum_{N=N_{\min}}^{N_{\max}} q_l(N) \approx \text{const} \times (N_{\min}^{-\zeta} - N_{\max}^{-\zeta}) \\ = \text{const} \times (1 - \alpha^{-\zeta}) \tag{A.4}$$

while

$$\frac{d^2}{d\zeta^2} \log \sum_{N=N_{\min}}^{N_{\max}} N^{-(1+\zeta)} \approx \frac{d^2}{d\zeta^2} \log \left[\frac{N_{\min}^{-\zeta} - N_{\max}^{-\zeta}}{\zeta} \right] \\ = \frac{1}{\zeta^2} - (\log^2 \alpha) \frac{\alpha^\zeta}{(\alpha^\zeta - 1)^2} \tag{A.5}$$

Putting everything together, we need to minimize

$$\text{var}(\hat{\zeta}_l) \times \langle \text{CPU time} \rangle \sim \frac{\alpha^{1-\zeta}}{(1-\alpha^{-\zeta})\{1/\zeta^2 - (\log^2 \alpha)[\alpha^\zeta/(\alpha^\zeta - 1)^2]\}} \\ \sim \frac{\beta^{1/\zeta}(\beta - 1)}{(\beta-1)^2 - \beta \log^2 \beta} \tag{A.6}$$

where $\beta \equiv \alpha^\zeta$. For $\zeta \to 0$ the optimal β is near 1; expanding the denominator of (A.6) in powers of $\beta - 1$, we find

$$\beta_{\text{opt}} = 1 + 3\zeta + O(\zeta^2) \Rightarrow \alpha_{\text{opt}} = e^3 + O(\zeta) \tag{A.7}$$

For $\zeta \to 1$ the optimal β is near ∞; expanding the denominator of (A.6) for large β, we find

$$\beta_{\text{opt}} = \frac{\log^2 \varepsilon}{\varepsilon} \left[1 + O\left(\frac{\log\log \varepsilon}{\log \varepsilon} \right) \right] \Rightarrow \alpha_{\text{opt}} = \frac{\log^2 \varepsilon}{\varepsilon} \left[1 + O\left(\frac{\log\log \varepsilon}{\log \varepsilon} \right) \right] \tag{A.8}$$

where $\varepsilon \equiv 1 - \zeta$. For general ζ, (A.6) must be evaluated numerically; the results are shown in Fig. 3. It is pleasant to note that in the range $8 \lesssim \alpha \lesssim 250$, the variance–time product depends only very weakly on α: any value in this range leads to an efficiency that is within a factor of 2 of optimal. So one need not lose sleep over the choice of $N_{\max}$.

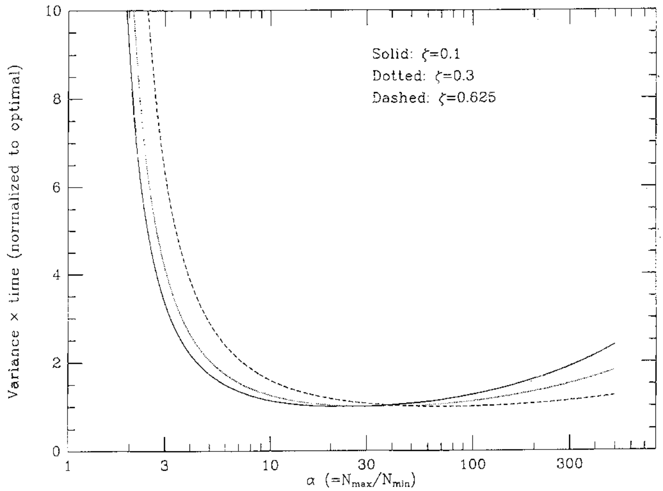

Fig. 3. Variance–time product (A.6), normalized to its minimum value, versus $\alpha \equiv N_{\max}/N_{\min}$.

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