Analysis of exact enumeration data for self-avoiding walks attached to a surface

K. De'Bell
Department of Physics, Memorial University, Canada A1B 3X7

T. Lookman
Department of Applied Mathematics, University of Western Ontario, Canada N6A 3K7

S. G. Whittington
Department of Chemistry, University of Toronto, Canada M5S 1A1

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An analysis of exact enumeration data for self-avoiding walks attached to a surface is consistent with $\gamma_1=0.694\pm0.004$ and $\gamma_{11}=-0.353\pm0.017$ in three dimensions and consistent with the predictions of conformal invariance theory in two dimensions. Estimates of γ_s are strongly influenced by a confluent term in the generating function. We argue that this confluent term arises from a sum over lattice layers required to construct the generating function. An analysis of the data that allows for this confluent term is consistent with the scaling relation $\gamma_s=\gamma+\nu$.

I. INTRODUCTION

The properties of self-avoiding walks (SAW's) attached to an impenetrable surface have been extensively studied. In particular, it is known[1] that the limits

$$\lim_{N\to\infty}\frac{1}{N}\ln C_N^{11}=\lim_{N\to\infty}\frac{1}{N}\ln C_N^{1}=\lim_{N\to\infty}\frac{1}{N}\ln C_N=\ln\mu \tag{1.1}$$

exist for the number of N-step walks in the bulk C_N, the number of N-step walks attached to the surface by the initial vertex C_N^1, and the number of walks attached to the surface by both initial and finale vertices C_N^{11}. It is generally believed that the asymptotic behavior of these quantities is described by

$$C_N\sim\mu^N N^{\gamma-1}\,, \tag{1.2}$$

$$C_N^1\sim\mu^N N^{\gamma_1-1}\,, \tag{1.3}$$

$$C_N^{11}\sim\mu^N N^{\gamma_{11}-1}\,. \tag{1.4}$$

Scaling arguments lead to the result[2]

$$\gamma+\nu=2\gamma_1-\gamma_{11}\,, \tag{1.5}$$

where ν is the exponent describing the divergence of the root-mean-square (rms) end-to-end distance R of the walks

$$R^2=\sum_r C_N(r)r^2\Big/C_N\sim N^{2\nu}\,, \tag{1.6}$$

where $C_N(r)$ is the number of N-step walks with end-to-end distance r. More generally, if the values of the bulk exponents and any one surface exponent are known, all other surface exponents may be obtained from scaling relations.

Similarly, the expected asymptotic behavior of the (global) function

$$C_N^s=\sum_z[C_N-C_N^1(z)]\,, \tag{1.7}$$

where $C_N^1(z)$ is the number of walks with initial vertex at a point distance z from the impenetrable surface, is

$$C_N^s\sim\mu^N N^{\gamma_s-1}\,, \tag{1.8}$$

and scaling arguments lead to the prediction

$$\gamma_s=\gamma+\nu\,. \tag{1.9}$$

Results for the exponents in two dimensions obtained by conformal invariance[3] and close to four dimensions by renormalization group methods[4] are (inherently) consistent with these scaling predictions. However, although precise estimates of γ_1 have been obtained in three dimensions by exact enumeration techniques,[5] consistency with the scaling relations [especially (1.9)] has been difficult to achieve.

A particular difficulty of exact enumeration techniques is that a knowledge of μ for the lattice considered is, in general, required to obtain the values of individual exponents. However, exact values of μ are not, in general, known. Here we shall consider the elimination of this difficulty by the device of forming the ratios[2,6]

$$C_N/C_N^1\,,$$
$$C_N/C_N^{11}\,,$$
$$C_N^s/C_N\,. \tag{1.10}$$

The generating functions for each of these ratios diverge at unit value of the argument thus eliminating μ as a variational parameter in the analysis. Consequently, the results obtained take the form of differences between a surface exponent and the bulk exponent γ. Both of the scaling relations considered may be expressed in terms of these differences and ν. Since precise estimates of γ are available,[7] we effectively obtain estimates of the surface

exponents. A further advantage of this method is that γ_{11} is expected to be small and negative and such exponents are notoriously difficult to estimate by series analysis techniques; however, the generating function for the ratios C_N/C_N^{11} has an exponent $\gamma-\gamma_{11}+1$ which is expected to be large and positive (≥ 2). In order to provide some feeling for the accuracy obtained when μ is eliminated in this manner, we have also analyzed the ratios

$$\sum_r r^2 C_N(r)/C_N \tag{1.11}$$

for the square and simple cubic lattices[7] to obtain estimates of the exponent ν.

In Sec. II we briefly review the techniques used to analyze the exact enumeration data. Section III describes the results obtained for ν, $\gamma-\gamma_1$, and $\gamma-\gamma_{11}$. The analysis of C_N^s/C_N and reasons for the exceptional behavior of the exponent estimates are discussed in Sec. IV. In the summary in Sec. V we comment on the usefulness and perceived precision of the analysis techniques used.

II. SERIES ANALYSIS

The singular behavior (of interest here) of the generating functions for the ratios described in Sec. I is expected to be of the form

$$G(x)\sim A(1-x)^{-h}[1+B(1-x)^{\Delta_1}+\cdots]\ . \tag{2.1}$$

The confluent term with exponent $(h-\Delta_1)$ represents a possible nonanalytic correction term and the ellipsis indicates analytic and (possible) less singular nonanalytic corrections. Our principal interest here will be the accurate determination of h from the known coefficients in the expansion of $G(x)$

$$G(x)=\sum_N g_N x^N\ . \tag{2.2}$$

In all cases considered the coefficients g_N are known for $N\leq N_{\max}$, where $N_{\max}$ is dependent on the series considered.

A. Neville table analysis

An estimate of the exponent h may be obtained by construction of a Neville table generated by the recursion relations[8]

$$e_N^r=[Ne_N^{r-1}-(N-r)e_{N-1}^{r-1}]/r\ . \tag{2.3}$$

Defining

$$\rho_N=g_N/g_{N-1}\ , \tag{2.4}$$

we construct the sequence

$$e_N^0=N(\rho_N-1)\ . \tag{2.5}$$

The sequence e_N^0 is then zeroth-order estimates which are expected to approach the value of $(h-1)$ as $N\to\infty$. The sequences e_N^1 are linear extrapolants of these estimates and higher values of r give higher-order extrapolations.

This procedure is expected to be effective when the physical singularity at $x_c(=1)$ is the closest to the origin. For loose-packed (bipartite) lattices a singularity also occurs at $x=-x_c$ and in this case the procedure must be modified. For loose-packed lattices we define

$$\rho_N^2=g_N/g_{N-2}\ , \tag{2.6}$$

$$e_N^0=N(\rho_N^2-1)/2\ , \tag{2.7}$$

$$e_N^r=[ne_N^{r-1}-(N-2r)e_{N-2}^{r-1}]/2r\ . \tag{2.8}$$

In general, the columns corresponding to $r=1$ and $r=2$ show the best convergence in the later entries (entries for higher values of r tend to be unstable due to a sensitivity to irregularities in the initial estimates). The central estimates and error bounds quoted in the following sections and tables are based on the later entries in the column of the table which shows the best (apparent) convergence and the stability of neighboring entries in the table. Since the error bounds reflect only a judgment on the stability and convergence of the estimates they are subjective and, indeed, subjectivity in the error estimates is a common feature of the methods we describe.

B. D log Padé approximants

The D log Padé approximant[8,9] method replaces the generating function $G(x)$ by its logarithmic derivative. Since the logarithmic derivative is expected to have a simple pole at x_c it may be approximated by a $[m/n]$ Padé approximant formed by the ratio of two polynomials $P^{(m)}$ and $Q^{(n)}$ of degree m and n respectively chosen to satisfy the equation

$$Q^{(n)}G'(x)=P^{(m)}G(x) \tag{2.9}$$

to $O(N_{\max}-1)$.

The pole of the $[m/n]$ approximants closest to the origin on the positive real axis and the residue at this pole provide an estimate of the x_c and h, respectively. A plot of the pole residue pairs shows a correlation between the exponent and critical point estimates. An estimate of the exponent corresponding to an assumed value of x_c (in particular for the generating functions corresponding to the ratios in Sec. I $x_c=1$) may then be obtained by drawing a smooth curve through the pole residue pairs. The errors quoted for this pole residue method reflect only the uncertainty in the drawn curve.

C. Baker-Hunter confluent singularity method

The above methods do not allow for the presence of confluent singularities and may be adversely affected by the presence of such confluent terms. The Baker-Hunter method[10] attempts to deal with such singularities by forming an auxiliary function χ, such that χ has simple poles at $1/h_1, 1/h_2, \ldots$, where the h_i's are the exponents of the confluent terms. The first $N_{\max}+1$ terms of χ are constructed from the known coefficients of G by making the change of variable to y

$$e^{-y}=(1-x/x_c)\ . \tag{2.10}$$

The kth coefficient of χ is then obtained by multiplying the kth coefficient of $G(y)$ by $k!$. The location of the poles in χ may then be estimated from Padé approximants to this function.

III. TESTS OF THE SCALING RELATION $\gamma+\nu=2\gamma_1-\gamma_{11}$

A. Estimates of ν

Before proceeding to the analysis of the surface series we present in Table I the estimates of the exponent ν obtained by applying the methods described in Sec. II to the generating function $\sum_r C_N(r)r^2/C_N$ for the square and simple cubic lattices.

For the square lattice the Neville table and Baker-Hunter methods give values in good agreement with the expected two-dimensional result $\nu=0.75$. (In view of the subjective nature of the error bounds the small discrepancy with the Neville table results may be neglected.) The estimates obtained by the D log Padé method do not include the expected value of ν within the error bounds. This indicates that the error bounds obtained from "pole-residue" plots should be treated with caution.

The results obtained for the simple cubic lattice by all methods indicate a central value somewhat higher than the value $\nu=0.592\pm0.002$ previously obtained by analysis of exact enumeration data.[7] However, the Neville table and Baker-Hunter methods are both consistent with this if the error bounds are taken into account.

B. Estimates of $\gamma-\gamma_1$ and $\gamma-\gamma_{11}$

The estimates for the exponent differences $\gamma-\gamma_1$ and $\gamma-\gamma_{11}$ are presented in Table II. Results for the two-dimensional lattices may be compared with the predictions of conformal invariance theory

$$\gamma-\gamma_1=0.3906\ldots,$$

$$\gamma-\gamma_{11}=1.5313\ldots$$

In all cases we obtain reasonably good agreement with the conformal invariance results. This indicates that neither a strong background term nor a strong confluent term are influencing the results in these cases. Recently, scaling theory has been extended to more general structures.[11,12] A consequence of this scaling theory is that if we denote the bulk exponent for an f star by $\gamma(f)$ and the exponent for an f star attached to the surface by the end vertex of one arm by $\gamma_1(f)$, then

$$\gamma(f)-\gamma_1(f)$$

is independent of f. Exact enumeration results for $\gamma(f)$ and $\gamma_1(f)$ in two dimensions are available for $f=3$. Combining the results of Refs. 13 and 14 we obtain $\gamma(3)-\gamma_1(3)=0.39\pm0.07$. Despite the wide error bounds, the agreement of the central estimate with the values reported in Table II (for $f=1$) is rather satisfactory.

In three dimensions only numerical results are available for comparison. We note that all methods give reasonable consistency for $\gamma-\gamma_1$ when a comparison of the results for different lattices is made. Based on the overall variation in the estimates in Table II we estimate

$$\gamma-\gamma_1=0.47\pm0.01\ .$$

For the estimates $\gamma-\gamma_{11}$ the best consistency is obtained by the Neville table method. The D log Padé approxi-

TABLE I. Estimates of ν for the square (sq) and simple cubic (sc) lattices from the Neville table (1), D log Padé approximant (2), and Baker-Hunter (3) methods.

Lattice \ Method	1	2	3
sq	0.7490	0.746(5)	0.7500
	±0.0003	±0.001	±0.0013
sc	0.595	0.5975	0.599
	±0.003	±0.0005	±0.007

TABLE II. Estimates of (a) $\gamma-\gamma_1$ and (b) $\gamma-\gamma_{11}$ for the square (sq), triangular (T) diamond (Di), simple cubic (sc), body-centered-cubic (bcc), and face-centered-cubic (fcc) lattices. Methods are labeled as in Table I. The dash indicates that insufficient convergence was obtained.

Lattice \ Method	1	2	3
	(a) $\gamma-\gamma_1$		
sq	0.390	0.3870	0.393
	±0.001	±0.0008	±0.006
T	0.389	0.385	0.397
	±0.002	±0.002	±0.012
Di	0.47	0.464	0.456
	±0.01	±0.001	±0.013
sc	0.4670	0.458	0.47
	±0.0015	±0.006	+0.09
			−0.06
bcc	0.4685	0.460	0.44
	±0.0020	±0.008	+0.12
			−0.06
fcc	0.4674	0.450	0.47
	±0.0003	±0.005	±0.04
	(b) $\gamma-\gamma_{11}$		
sq	1.525	1.538	1.56
	±0.010	±0.002	±0.06
T	1.515	1.530	1.51
	±0.001	±0.005	±0.02
Di	1.50	1.61	1.50
	±0.03	±0.01	±0.025
sc	1.50	–	1.39
	±0.01		±0.06
bcc	1.52	1.47	1.44
	±0.01	±0.05	+0.12
			−0.06
fcc	1.52	1.48	1.47
	±0.03	±0.09	±0.04

mant and Baker-Hunter methods result in somewhat scattered estimates for the simple cubic and diamond lattices. Based on the overall variation in the estimates we obtain

$$\gamma-\gamma_{11}=1.50\pm0.03 .$$

A convenient form for the scaling relation is

$$2(\gamma-\gamma_1)-(\gamma-\gamma_{11})=-\nu .$$

Using the above estimates for the exponent differences, we obtain

$$2(\gamma-\gamma_1)-(\gamma-\gamma_{11})=-0.56\pm0.05 .$$

While this is consistent with[7]

$$\nu=0.592\pm0.002 ,$$

the large error bounds clearly defeat a precise comparison.

It is notable that if we base our estimates on the Neville table results alone we obtain the more precise estimates

$$\gamma-\gamma_1=0.468\pm0.002 ,$$

$$\gamma-\gamma_{11}=1.515\pm0.015 ,$$

and adopting these values we obtain

$$2(\gamma-\gamma_1)-(\gamma-\gamma_{11})=-0.579\pm0.019 .$$

This apparent superiority of the Neville table may indicate that the approximants are being influenced by an analytic background term. (This is perhaps not surprising since the singular part of the generating function for C_N^{11} vanishes at x_c.)

Adopting the Neville table results for the exponent differences and[7]

$$\gamma=1.162\pm0.002 ,$$

we obtain

$$\gamma_1=0.694\pm0.004 ,$$

$$\gamma_{11}=-0.353\pm0.017 .$$

IV. TESTS OF THE SCALING RELATION $\gamma_s-\gamma=\nu$

In two dimensions we may compare our results with the conformal invariance value of $\nu=0.75$. We find that the Baker-Hunter method gives good agreement with this prediction while the other methods give estimates which are too high. This might be assumed to indicate that a confluence with $\Delta_1\leq1$ is present. Inspection of the second pole on the real positive axis of the Baker-Hunter auxilliary function indicated that such a confluent term was present. To ensure that the apparent confluence was not an artifact of analyzing the ratio C_N^S/C_N we repeated the Baker-Hunter analysis for the C_N^s generating function series assuming[7]

$$x_c=0.379\,05$$

and

$$x_c=0.240\,92$$

for the square and triangular lattices, respectively. A second real positive pole corresponding to $\Delta_1\leq1$ was clearly present. To obtain a value for the exponent γ_{s2} of the confluent term [the analog of $(h-\Delta_1)$ in Eq. (2.1)] we plotted the position of the second pole as a function of the first pole position (Fig. 1) and read from this a value of γ_{s2}, assuming $\gamma_s=\gamma+\nu=\frac{67}{32}$, and obtained

$$\gamma_{s2}=1.375\pm0.008 .$$

We note that this is larger than, but numerically close to, γ. In two dimensions the correction to scaling exponent is expected to be $\Delta_1\geq1$.[15] Hence the conventional correction to scaling term does not explain the presence of a confluence with exponent numerically close to γ in two dimensions. An analysis of C_N^s/C_N for the three-dimensional lattices indicates a value of $\gamma_s-\gamma$ significantly higher than $\nu=0.592\pm0.002$ in all cases (Table III). It is noticeable that the analysis for the diamond lattice, for which the longest C_s series in three dimensions is available, results in somewhat lower values of $\gamma_s-\gamma$ than those for other three-dimensional lattices. We repeated the procedure of plotting the first and second real positive pole positions in the Baker-Hunter auxiliary function to the generating function of C_N^s (Fig. 2) for the three-dimensional lattices, assuming $x_c=0.3474$ (diamond), 0.2135 (simple cubic), 0.1531(5) (bcc), and 0.0996 (fcc). The approximants are less well converged than those for the two-dimensional systems; however, assuming that a single line may be used to represent the correlation between the pole positions for all of the three-dimensional lattices, we read from Fig. 2

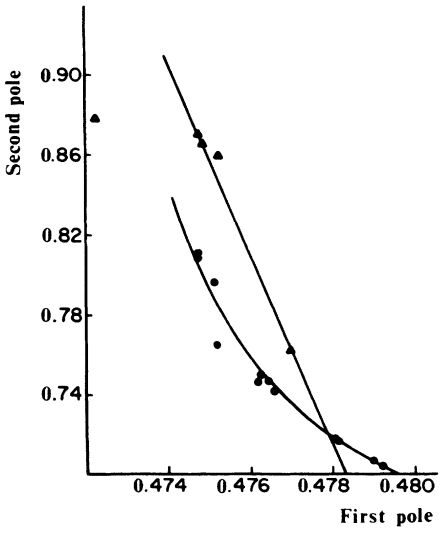

FIG. 1. First (abscissa) and second pole (ordinate) closest to the origin on the real positive axis, of the Baker-Hunter auxilliary function to the series C_s for the square (●) and triangular (▲) lattices.

TABLE III. Estimates of $\gamma_s-\gamma$ from the series C_N^s/C_N. Methods are labeled as in Table I. The dash indicates that insufficient convergence was obtained was obtained.

Lattice \ Method	1	2	3
sq	0.765	0.77	0.743
	±0.004	±0.01	+0.002
			−0.001
T	0.7634	0.78	0.754
	±0.0002	+0.02	+0.007
		−0.01	−0.009
Di	0.615	0.625	0.610
	±0.003	±0.025	+0.025
			−0.020
sc	0.650	0.60	-
	±0.015	±0.05	
bcc	0.65	0.65	0.69
	±0.05	±0.05	+0.09
			−0.08
fcc	0.649	0.740	0.67
	±0.002	±0.02	+0.15
			−0.13

the value of γ_{s2} corresponding to $\gamma_s=\gamma+\nu$ and $\gamma=1.162\pm0.002$ and $\nu=0.592\pm0.002$,

$$\gamma_{s2}=1.21\pm0.02 .$$

This is, as in the two-dimensional case, higher than but numerically close to γ.

The probable source of a confluence with exponent equal to γ is the sum used to construct C_N^s. To understand this consider the argument that leads to the scaling relation $\gamma_s-\gamma=\nu$. For this purpose it is useful to divide C_N^s into three parts

$$C_N^- = \sum_{z=0}^{\xi-\bar{\omega}} [C_N - C_N^1(z)] , \tag{4.1}$$

$$C_N^{\bar{\omega}} = \sum_{\xi-\bar{\omega}}^{\xi+\bar{\omega}} [C_N - C_N^1(z)] , \tag{4.2}$$

$$C_N^+ = \sum_{z=\xi+\bar{\omega}}^{\infty} [C_N - C_N^1(z)] , \tag{4.3}$$

where $\bar{\omega}=o(\xi)$. To evaluate C_N^- we assume the scaling form

$$C_N^1(z) = A\,(z/\xi)^{\gamma-\gamma_1/\nu} N^{\gamma-1}\mu^N$$

(this scaling form has recently been tested numerically[15]); if this form is assumed throughout the range of the sum required to construct C_N^- and we replace the sum by an integral, we obtain

$$C_N^- \sim N^{\gamma+\nu-1}\mu^N . \tag{4.4}$$

The scaling behavior for $z \gg \xi$ has not (to the best of our knowledge) been studied in detail for SAW's. However, by analogy with the Ising model and mean-field theory cases,[16] we assume

$$C_N - C_N^1(z) \propto \exp(-z/\xi) N^{\gamma-1}\mu^N . \tag{4.5}$$

If this form is substituted into the sum for C_N^+, we obtain

$$C_N^+ \propto N^{\gamma+\nu-1}\mu^N . \tag{4.6}$$

The essential point here is that the scaling forms for $C_N^1(z)$ used to evaluate C_N^- and C_N^+ are, in fact, only valid in the regions $z \ll \xi$ and $z \gg \xi$, respectively. Consequently, these scaling forms should not be used in evaluating $C_N^{\bar{\omega}}$. In the region of z used to evaluate $C_N^{\bar{\omega}}$, $C_N(z)$ and $C_N^1(z)$have the same exponent but different amplitudes. After performing the sum we obtain

$$C_N^{\bar{\omega}} \sim \mu^N N^{\gamma-1} , \tag{4.7}$$

if we assume that there is no correction to the N dependence resulting from the variation in the amplitudes, and $\bar{\omega}=\alpha+o(1)$, where α is a constant.

In what follows we shall assume, as a working hypothesis, the presence of a confluent term with exponent γ. In two dimensions we do not expect other confluent terms with similar exponents to be present. However, in three dimensions an additional difficulty is the expected presence of a correction to scaling term with exponent $\gamma+\nu-\Delta_1$. Estimates based on the ϵ expansion predict $\Delta_1\approx0.5$,[17] in which case this term will have an exponent larger than, but very close to, γ. A situation in which two confluent terms with exponents that are numerically very close together is expected to be very difficult to resolve for the methods of analysis described here. The procedure describe in the remainder of this section is expected to be most useful in the simpler case described for two-dimensional systems.

Adopting the hypothesis that the generating function

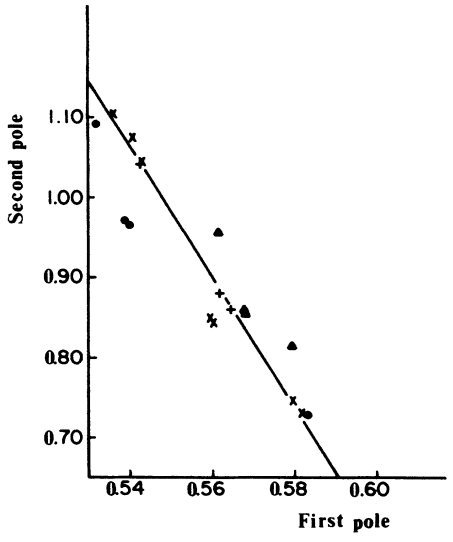

FIG. 2. First (abscissa) and second pole (ordinate) closest to the origin on the real positive axis, of the Baker-Hunter auxilliary function to the series C_s for the diamond (▲), simple cubic (●), body-centered-cubic (×), and face-centered cubic (+) lattices.

of C_N^s is of the form

$$G_s(x) \sim A(x)(1-x/x_c)^{-\gamma_s} + B(x)(1-x/x_c)^{-\gamma}, \quad (4.8)$$

we multiply $G_s(x)$ for each lattice considered by $(1-x/x_c)^{\gamma}$ using the values of x_c given above and $\gamma = 1.162$ for three dimensions and $\gamma = \frac{43}{32} = 1.3438$ for two dimensions. The resulting functions, which are expected to be of the form

$$f(x) \sim A(x)(1-x/x_c)^{\gamma-\gamma_s} + B(x), \quad (4.9)$$

were analyzed by each of the methods described in Sec. II (Table IV). In addition, since the Neville table results for the loose-packed lattices are sensitive to the singularity at $x = -x_c$, we have applied the Euler transform

$$z = (1+x_c)x/(1+x) \quad (4.10)$$

to the generating function [prior to multiplying by $(1-z/x_c)^{\gamma}$] and used the Neville table analysis for the resulting $f(z)$ (Table V). In general, this improves the convergence of the first Neville table column, but the central estimates are not strongly affected. In the Neville table analysis the $r=0$ column is, generally, the best converged and the error bounds for the Neville table method in Tables IV and V reflect only the spread in the last few entries of the $r=0$ column of the Neville table.

In two dimensions the results for the square lattice are in good agreement with $\gamma_s - \gamma = \nu$. In particular, the Neville table method gives excellent agreement with the expected $\gamma_s - \gamma = \frac{3}{4}$. The Baker-Hunter method also gives good agreement with the scaling relation for the triangular lattice.

TABLE IV. Estimates of $\gamma_s - \gamma$ obtained from the series $(1-\mu x)^{\gamma} C_s$. The D log Padé approximant method for the triangular lattice gives exponents close to the expected $\frac{3}{4}$, but values of $x_c \approx 0.2406$ rather than the expected $x_c \approx 0.2409$ (c.f. Refs. 18 and 23). The last few entries in the $r=0$ column of the Neville table for the triangular lattice give estimates of $\gamma_s - \gamma \approx 0.737$, but these have a persistent upward trend. Entries marked by an asterisk required extrapolation from one side in the pole-residue plot. The dash indicates that insufficient convergence was obtained.

Method / Lattice	1	2	3
sq	0.75	0.779	0.77
	±0.03	±0.001	±0.02
T	–	≈0.75	0.746
			+0.017
			−0.015
Di	0.59	0.64*	0.600
	±0.03	±0.02	±0.002
sc	0.605	0.720*	0.53
	±0.005	±0.004	+0.13
			−0.10
bcc	0.58	–	0.59
	±0.03		±0.03
fcc	≈0.6	–	≈0.61

TABLE V. Estimates of $\gamma_s - \gamma$ from the Euler transformed series $(1-\mu z)C_N^s$ using the Neville table method described for open (a) and close-packed (b) lattices.

Method / Lattice	a	b
sq	0.751	0.758
	±0.002	±0.002
Di	0.600	0.60
	±0.001	±0.01
sc	0.62	0.63
	±0.003	±0.01
bcc	0.585	0.60
	±0.015	+0.02
		−0.03

For three-dimensional lattices, the Neville table method gives the most consistent results (between lattices) and the results obtained are in good agreement with the scaling relation. The Baker-Hunter method results are also consistent with this, though spread through a rather wide range. Again we note that the longer diamond lattice series tend to give results closer to the expected value of ν for a given method. We have also repeated the D log Padé approximant analysis for the diamond lattice using the most extreme values for x_c and γ allowed by the published error bounds.[7,18] However, the resulting change in the estimates of $\gamma_s - \gamma$ are small compared with the discrepancy with the expected value of ν.

V. SUMMARY

Our principal aim has been a numerical verification of the scaling laws relating surface and bulk exponents for self-avoiding walks by the analysis of exact enumeration data. In addition to the methods described in Sec. II, we have also used the inhomogeneous partial differential approximant method[19] and the confluent singularity method based on a generalized Roskies transformation.[20] These methods give results consistent with those described above. However, the Adler method did not indicate a confluent term more singular than the first analytic correction term in any of the cases studied.

As a test case we analyzed the ratios $\sum_r C_N(r) r^2 / C_N$ (Sec. II A). Our estimates (Table I) are consistent with the expected values of $\nu = \frac{3}{4}$ for two dimensions and $\nu = 0.592 \pm 0.002$ for three dimensions, though the central estimates in three dimensions favor slightly higher values.

Applying the techniques described in Sec. II to the ratios C_N/C_N^1 and C_N/C_N^{11} (Sec. II B) we obtain estimates of $\gamma - \gamma_1$ and $\gamma - \gamma_{11}$ (Table II). These estimates are consistent with the scaling relation $\gamma - \nu = 2\gamma_1 - \gamma_{11}$ and in two dimensions are consistent with the predictions of conformal invariance theory. Combining our results based on the Neville table analysis with the result[7] $\gamma = 1.162 \pm 0.002$ in three dimensions, we obtain

$$\gamma_1 = 0.694 \pm 0.004,$$

$$\gamma_{11} = -0.353 \pm 0.017.$$

In Sec. IV we have attempted to test the scaling relation $\gamma_s - \gamma = \nu$. With the exception of the Baker-Hunter analysis for the two-dimensional lattices, all methods of analysis applied to the ratio C_N^s/C_N resulted in estimates of $\gamma_s - \gamma$ too high to be consistent with the scaling relation. Further examination of the poles of the Baker-Hunter auxiliary functions to C_N^s/C_N and C_N^s revealed the existence of a confluent term with an exponent numerically close to γ. We have argued that a confluent term in C_N^s with exponent γ arises from the summation over a region $z \approx \xi$ in the formation of C_N^s. To test this hypothesis we multiplied the generating function of C_N^s by $(1-x/x_c)^\gamma$ and analyzed the resulting function. In two dimensions we obtain good agreement with the prediction $\gamma_s - \gamma = \frac{3}{4}$ obtained from the scaling relation and conformal invariance value of ν. In three dimensions the Neville table analysis for the diamond lattice indicates

$$\gamma_s - \gamma = 0.60 \pm 0.01 ,$$

and the results obtained for other lattices are consistent with this but with wider error bounds. This is in good agreement with the scaling relation. It should be recalled that in three dimensions we also expect a correction to scaling confluent term with $\Delta_1 < 1$. The presence of this term would certainly be expected to interfere with the analysis and it is perhaps not surprising that our best behaved results are from the analysis technique which assumes the least about the form of the function, that is, from the $r=0$ column of the Neville table. We conclude that the leading exponent of C_N^s does obey the scaling relation $\gamma_s - \gamma = \nu$, but the analysis of this function is strongly affected by the presence of a confluent term with exponent γ.

Lastly, we comment on the use and perceived precision of the analysis techniques. In general, a comparison of the results for different lattices indicates that the error estimates obtained by considering the results for a single lattice from a single method of analysis may be over optimistic. More importantly, each method of analysis makes assumptions regarding the form of the function being analyzed. As an example, consider the Baker-Hunter analysis which, as we have demonstrated, is useful for identifying and dealing with confluent terms. It is not difficult to see that if the function to be analyzed contains an additive or multiplicative analytic term that can be expanded about x_c and is such that the coefficients in the expansion do not vanish at high orders, the auxiliary function will have a set of poles on the real negative axis close to the origin. In the worst possible case this will be a dense set arbitrarily close to the origin. A Padé approximant analysis of the auxiliary function will certainly be affected by such a set. (Experience with this method shows that, in general, defects on the negative axis and close to the origin will appear in the approximants and it has previously been noted[21,22] that if x_c is used as a variational parameter, the approximants are well converged for values of x_c such that the defects appear on the negative part of the axis only.) On the other hand, an additive analytic term is (expected to be) innocuous in a Neville table analysis.

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