Reassessment of critical exponents and corrections to scaling for self-avoiding walks

T. Ishinabe
Faculty of Engineering, Yamagata University, Yonezawa 992, Japan
(Received 6 April 1988)

The exact enumeration series of the radius of gyration S_N for self-avoiding walks are analyzed for various lattices in three and two dimensions (3D and 2D) in addition to those of the end-to-end distance R_N and the number of walks C_N using a method newly developed. The estimates of ν for R_N and γ for C_N are in good agreement with the renormalization-group calculations in 3D and Nienhuis's analytical results in 2D; the estimates of ν for S_N in both 3D and 2D are somewhat greater than those for R_N. The average estimates of the correction-to-scaling exponent Δ_1 are $\Delta_1=0.48$ (3D) and 0.65 (2D) for R_N, and $\Delta_1=1.19$ (3D) and 1.06 (2D) for S_N, while $\Delta_1=0.99$ (3D) and 0.97 (2D) for C_N.

I. INTRODUCTION

The self-avoiding walk (SAW) on a lattice serves not only as a model of a single polymer chain in dilute solution but also as a test case in the theory of critical phenomena through its identity[1] with the $O(n)$ model in the $n=0$ limit. The mean-square end-to-end distance R_N^2 and the number of N-step walks C_N can be written as[2]

$$R_N^2=AN^{2\nu}(1+BN^{-\Delta_1}+CN^{-\Delta_2}+\cdots) \tag{1}$$

and

$$C_N=A'\mu^N N^{\gamma-1}(1+B'N^{-\Delta_1}+C'N^{-\Delta_2}+\cdots)\,, \tag{2}$$

respectively. Here ν and γ are leading scaling exponents, and the Δ_i terms are the ith correction terms, which also contain analytic ones; μ is the connective constant (i.e., effective coordination number) of a lattice, and A, B, and C (A', B', C') are critical amplitudes.

A mean-field theory[1] leads to the Flory formula $\nu=3/(d+2)$ for d-dimensional space. Early numerical estimates[3] of ν for SAW's in two and three dimensions (2D and 3D) are almost reconciled with the formula. The renormalization-group (RG) calculations[4,5] suggest, however, somewhat different values: $\nu=0.588$ (3D) and 0.77 (2D), while Nienhuis's analytical argument[6] for the $O(n)$ model gives $\nu=\frac{3}{4}$ for $d=2$, which coincides exactly with the Flory value. The assessment of ν, γ, and μ from numerical data may be affected by the presence of Δ_i terms, especially the leading correction-to-scaling exponent Δ_1. Recent series analyses for SAW's in 3D (Refs. 7–11) and 2D (Refs. 8 and 11–16) taking account of Δ_1, and Monte Carlo techniques[9,17,18] for larger N have confirmed that $\nu=0.588$ (3D) and 0.75 (2D). The estimates of γ from similar series analyses for C_N in 3D (Refs. 9 and 11) and 2D (Refs. 11 and 19–21) are consistent with the RG result[4,5] $\gamma=1.1615$ (3D) and Nienhuis's[6] $\gamma=\frac{43}{32}$ (2D). The value of Δ_1 is, however, still controversial and there is no consensus on it although RG arguments[4,5] predict $\Delta_1=0.47$ (3D) and 1.18 (2D). Majid, Djordjevic, and Stanley[7] and McKenzie[22] have estimated Δ_1 in 3D which is in agreement with the RG result by the use of exact series of R_N and C_N, respectively. Almost the same result has been obtained by Havlin and Ben-Avraham[8] and Kelly, Hunter, and Jan[10] by exploiting Monte Carlo data. As for Δ_1 in 2D, Djordjevic, Majid, Stanley, and dos Santos[12] and Privman[13] have estimated the values reconciled with $\Delta_1=\frac{2}{3}$ from the exact series of R_N, whereas Havlin and Ben-Avraham[8] and Lyklema and Kremer[14] have found $\Delta_1=1.2$ and 0.84, respectively, using Monte Carlo techniques. On the other hand, Guttmann[11,21] and Rapaport[9,15,17] have asserted that there is no need to assume the presence of a nonanalytic correction term, i.e., $\Delta_1=1$ for $d=2$ and 3; Adler[20] and Hunter, Jan, and MacDonald[16] have obtained the result in favor of it from the analyses of C_N series and Monte Carlo data of R_N in 2D, respectively.

In a preceding (brief) publication,[23] we have reported a new method to estimate ν and γ together with Δ_1 from R_N and C_N series. The estimates of ν and γ for the triangular (tri) lattice are in excellent agreement with Nienhuis's analytical prediction while Δ_1 is different between R_N and C_N: $\Delta_1=0.63$ (R_N) and 0.95 (C_N). We have also found that $\nu=0.755\pm0.001$ and $\Delta_1=1.04$ by applying this method to the series of the radius of gyration S_N; the Δ_1 value is in favor of the presence of the analytic correction term in contrast to the case of R_N. The estimate of ν for S_N is a little but evidently larger than Nienhuis's value; it seems to contradict the commonly believed relation $\nu_S=\nu_R$, which is supported by other numerical work[9,17,18,24–26] and RG calculations.[27–30] In the present paper we reexamine these results using the exact enumeration series data of S_N newly obtained in addition to the extant ones of R_N, S_N, and C_N for the face-centered cubic (fcc),[7,9,22] body-centered cubic (bcc),[25,31–33] simple cubic (sc),[11,25] tetrahedral (tet),[34] and square (sq) (Refs. 11 and 25) lattices; much attention is focused on ν and Δ_1 for S_N. We have added S_N terms for the bcc ($N=9-13$), tet ($N\le21$), sc ($N=11-14$), and sq ($N=16-21$) lattices and the R_N term of $N=13$ for the bcc lattice to the existing series.[35] These series are reproduced in Tables IX–XIII; S_N series for the tri lattice and R_N series for some lattices are also given for the sake of convenience. Note that these tables quote the values divided by q, the coordination number of a lattice; the step length is taken as unity.

II. SERIES ANALYSIS

A. Method

Our method to estimate ν and Δ_1 is based on the conventional technique of series analysis combined with the finite-size scaling idea of Privman and Fisher[36] employing the cancellation of the leading correction term. First we evaluate the two types of ratios:

$$\nu^{\mathrm{I}}_{N,k}=\tfrac{1}{2}N(\rho_{N+K}/\rho_N-1)/k \tag{3}$$

and[8,37]

$$\nu^{\mathrm{II}}_{N,k}=\tfrac{1}{2}\ln(\rho_N/\rho_{N-k})/\ln[N/(N-k)] \tag{4}$$

for $k=1$ or 2, where $\rho_N\equiv R_N^2$ (or S_N^2). The ratios ($k=1$) of adjacent terms are used for close-packed lattices while the alternate ratios ($k=2$) are used for loose-packed lattices owing to the characteristic odd-even oscillation. After forming these ratios, we construct the Neville table for linear, quadratic, and cubic extrapolants of them:

$$\nu^{(r)}_{N,k}=[N\nu^{(r-1)}_{N,k}-(N-kr)\nu^{(r-1)}_{N-k,k}]/kr \tag{5}$$

for $r=1-3$, with $\nu_N^{(0)}\equiv\nu_N^{\mathrm{I}}$ or ν_N^{II}. We determine the first trial value of ν by plotting these extrapolants against N^{-1} and extrapolate to $N\to\infty$ having in mind the curvature of convergence as a whole together with damping oscillations. Then the estimators[38]

$$B_{N,k}(\Delta_1)=\frac{(N-k)^{2\nu}\rho_N-N^{2\nu}\rho_{N-k}}{N^{2\nu-\Delta_1}\rho_{N-k}-(N-k)^{2\nu-\Delta_1}\rho_N}$$
$$=B+(\Delta_2/\Delta_1)CN^{\Delta_1-\Delta_2}+\cdots \tag{6}$$

are constructed; the second equality follows from substitution of Eq. (1). The curves $B_{N,k}(\Delta_1)$ as a function of Δ_1 for different N intersect at a point close to correct Δ_1 if ν is known and $|C|$ is small enough compared with $|B|$;[36] approximate values of Δ_1 and B can be estimated simultaneously for the trial ν. We perform the transformation $\rho_N^*=\rho_N/(1+BN^{-\Delta_1})$ using the result to eliminate the singular term. Similarly, the improved ν is estimated from ρ_N^* series. Thus we get the reliable estimates of ν and Δ_1 by repeating the above procedure several times.

We can also estimate Δ_1 (and A) similarly from the estimators[13]

$$A_{N,k}(\Delta_1)=\frac{N^{\Delta_1-2\nu}\rho_N-(N-k)^{\Delta_1-2\nu}\rho_{N-k}}{N^{\Delta_1}-(N-k)^{\Delta_1}}$$
$$=A+(\Delta_2/\Delta_1-1)ACN^{-\Delta_2}+\cdots \tag{7}$$

if the exact ν is known. We shall rely mainly on Eq. (6) since reliable values of Δ_1 and B are necessary in order to get the accurate ν from R_N and S_N series.

B. End-to-end distance

We will estimate critical quantities for R_N by employing the method described above. Figure 1 illustrates the first plots of $\nu^{(r)}_{N,2}$ ($r=1$ and 2) obtained from the alternate ratios $\nu^{\mathrm{II}}_{N,2}$ against N^{-1} for the tet lattice. We get the estimate $\nu=0.593\pm0.004$ considering the slight downward tendency of convergence for the linear extrapolant as $N^{-1}\to0$ together with damping oscillation with the interval of four successive terms. The similar plots for $\nu^{\mathrm{I}}_{N,2}$ suggest $\nu=0.592\pm0.004$; the estimate of ν will mean the value obtained from $\nu^{\mathrm{II}}_{N,k}$ hereafter unless otherwise stated since in most cases there exists no significant difference between these two schemes. Using the trial value $\nu=0.593$, we have $\Delta_1=0.78$ and $B=-0.244$ from the intersection of $B_{N,2}(\Delta_1)$ curves for different N. The improved estimate of ν is obtained by performing the transformation $\rho_N^*=\rho_N/(1+BN^{-\Delta_1})$; we get $\nu=0.5885\pm0.002$ as our final estimate after repeating such a procedure three times. Some terms in the corresponding Neville table of $\nu^{(r)}_{N,2}$ ($r=1-3$) for ρ_N^* are given in Table I; $\nu^{(1)}_{N,2}$ and $\nu^{(2)}_{N,2}$ converge to a constant value with damping oscillations of period four, from which (mainly from that of $\nu^{(1)}_{N,2}$) the error limit is estimated. Figure 2 shows $B_{N,2}(\Delta_1)$ curves for $N=17-22$ for $\nu=0.5885$; the successive average $\bar{B}_{N,2}=\frac{1}{2}(B_{N-1,2}+B_{N,2})$ is employed in place of $B_{N,2}$ to lessen the odd-even effect for a loose-packed lattice, but we omit the bar in $\bar{B}_{N,2}$ and $\bar{A}_{N,2}$ hereafter. We get $\Delta_1=0.53$ and $B=-0.244$ although the intersection is somewhat dispersed in this case. The corresponding $A_{N,2}(\Delta_1)$ curves are given in Fig. 3; almost the same value of Δ_1 and $A=1.442$ are estimated. We take $\Delta_1=0.53\pm0.06$ as our final estimate; the error limit is determined by taking into account that of ν in addition to uncertainty of the intersection. Similarly, we have $\nu=0.589\pm0.002$ and $\Delta_1=0.50\pm0.1$ for the bcc lattice while $\nu=0.5910\pm0.0006$ and $\Delta_1=0.44\pm0.05$ for the sc lattice.

The first trial value $\nu=0.593\pm0.002$ is estimated for the fcc lattice (see Table 5 in Ref. 9), but the above

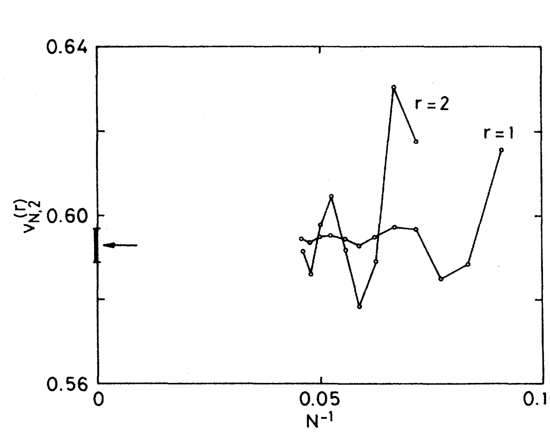

FIG. 1. Ratio estimate of ν for R_N from linear ($r=1$) and quadratic ($r=2$) extrapolants $\nu^{(r)}_{N,2}$ for the tet lattice.

TABLE I. Neville table for estimation of ν from the ratios $\nu_{N,2}^{\mathrm{II}}$ of transformed R_N series for the tet lattice.

N	$\nu_{N,2}^{\mathrm{II}}$	$\nu_{N,2}^{(1)}$	$\nu_{N,2}^{(2)}$	$\nu_{N,2}^{(3)}$
14	0.588 600	0.590 44	0.612 17	0.683 38
15	0.589 580	0.590 90	0.625 16	0.797 11
16	0.588 639	0.588 92	0.584 33	0.537 93
17	0.589 256	0.586 83	0.573 60	0.479 05
18	0.588 635	0.588 60	0.587 51	0.593 87
19	0.589 293	0.589 61	0.600 04	0.657 34
20	0.588 719	0.589 47	0.592 95	0.605 65
21	0.589 182	0.588 13	0.581 85	0.536 36
22	0.588 756	0.589 12	0.587 55	0.573 13

method is unavailable to the estimation of Δ_1 since $B_{N,1}(\Delta_1)$ curves do not intersect; it seems that $|C|$ is too large in this case. We then take another approach using the power-series expressions in Eqs. (6) and (7); respective plots of $A_{N,k}$ and $B_{N,k}$ as a function of $N^{-\Delta_2}$ and $N^{\Delta_1-\Delta_2}$ for larger N are expected to be linear for suitable Δ_1 and Δ_2. If we assume $\Delta_2=1$, the values $\Delta_1=0.5$ and $B=-0.155$ are obtained for the trial value $\nu=0.593$ by examining the linearity of the plots. An improved ν can be estimated recurrently exploiting the transformation $\rho_N^*=\rho_N/(1+BN^{-\Delta_1})$. Figure 4 illustrates the third plots of $A_{N,1}(\Delta_1)$ for $\nu=0.589$ against N^{-1} for several choices of Δ_1; the plots for $\Delta_1=0.4$ and 0.5 display the excellent linear dependence whereas those for $\Delta_1<0.4$ are bowed upwards and those for $\Delta_1>0.5$ are slightly bowed downwards. The analogous plots of $B_{N,1}(\Delta_1)$ against N^{Δ_1-1} for $\Delta_1=0.40$, 0.45, and 0.50 are shown in Fig. 5; excellent linearity is also found, especially for $\Delta_1=0.45$. We then have $\Delta_1=0.45\pm0.05$, $A=1.04$, and $B=-0.24$ for the fcc lattice. The slope of the $B_{N,1}(\Delta_1)$ line for $\Delta_1=0.45$ yields $C\simeq0.21$; it should be noted that $|C|$ is comparable to $|B|$. Some terms in the Neville table of $\nu_{N,1}^{(r)}$ $(r=1-3)$ for the final series are given in Table II; we take

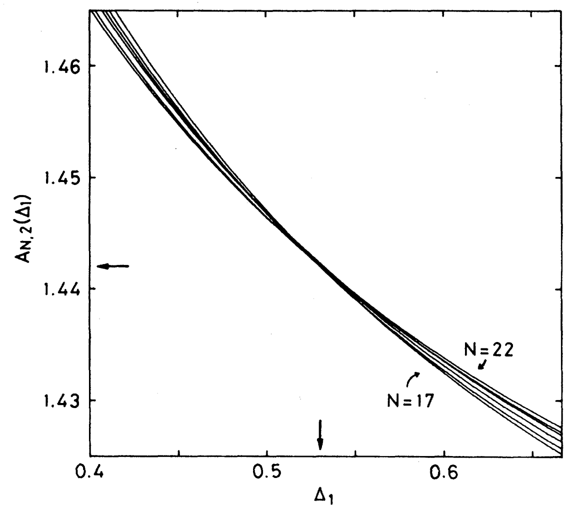

FIG. 3. The same as Fig. 2 but for $A_{N,2}(\Delta_1)$.

$\nu=0.5880\pm0.0006$ as our final estimate bearing in mind the trend of linear decrease in $\nu_{N,1}^{(1)}$ and $\nu_{N,1}^{(2)}$ with increasing N. These results are compatible with the estimates from a different series analysis by Majid *et al.*[7] for the fcc lattice: $\nu=0.5875\pm0.0015$, $\Delta_1=0.47$, $A=1.05$, $B=-0.286$, and $C\simeq0.25$.

As for $d=2$, we get the estimates $\nu=0.750\pm0.001$, $\Delta_1=0.66\pm0.05$, $A=0.766$, and $B=0.37$ from the first plots of $\nu_{N,2}^{(r)}$ $(r=1$ and 2) and the intersection of $A_{N,2}(\Delta_1)$ and $B_{N,2}(\Delta_1)$ curves using ρ_N series $(N\leq27)$ (Ref. 11) for the sq lattice; the transformed ρ_N^* series little improve the error limit of ν, probably because ρ_N series for up to fairly large N are available in this case. The value of Δ_1 is in accord with our previous result for the tri lattice. Hunter

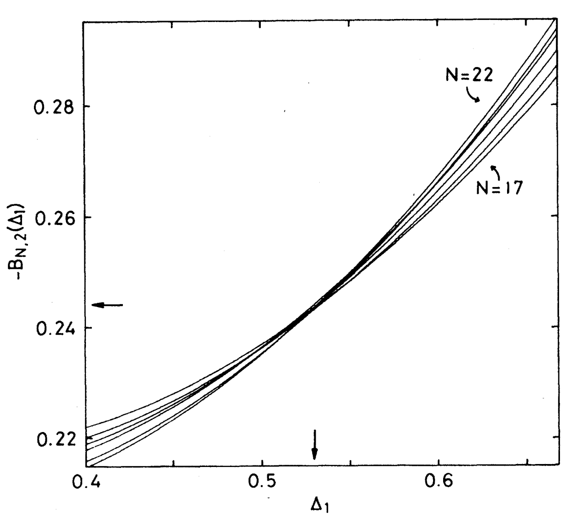

FIG. 2. Curves of $B_{N,2}(\Delta_1)$ for the input $\nu=0.5885$ in the case of R_N for the tet lattice.

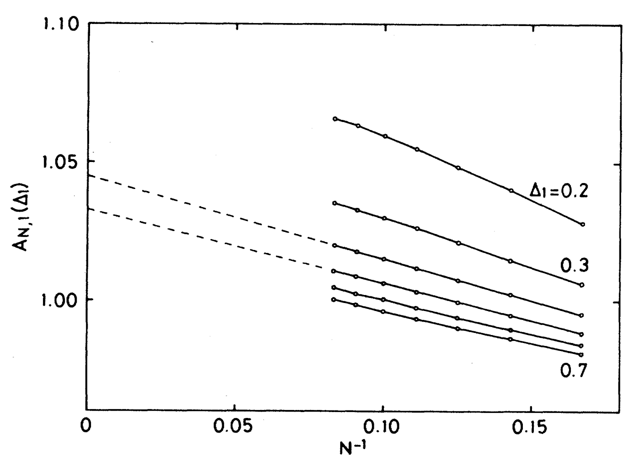

FIG. 4. Plots of $A_{N,1}(\Delta_1)$ vs N^{-1} for the input $\nu=0.5890$ in the case of R_N for the fcc lattice.

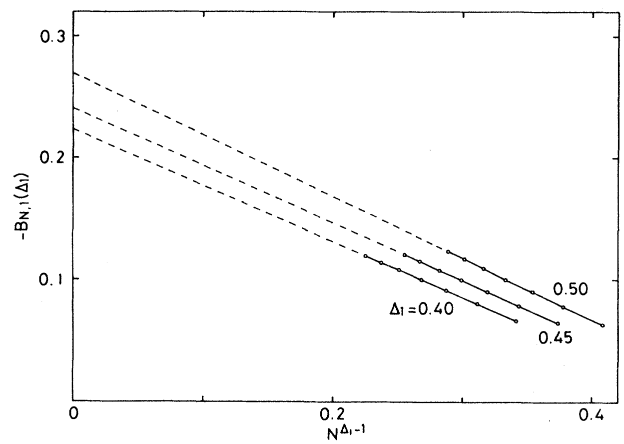

FIG. 5. The same as Fig. 4 but for the plots of $B_{N,1}(\Delta_1)$ vs N^{Δ_1-1}.

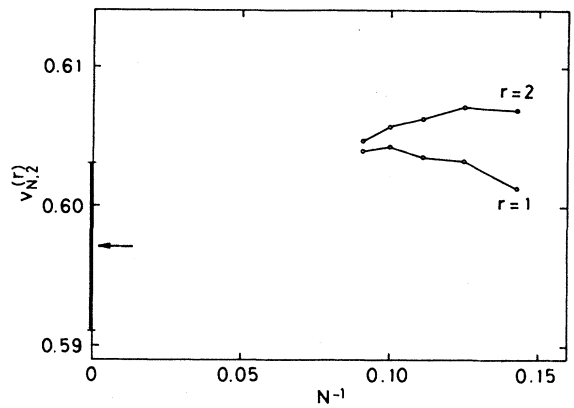

FIG. 6. The same as Fig. 1 but for S_N for the bcc lattice.

et al.[16] have estimated the values $\Delta_1 = 1.0 \pm 0.1$, $A = 0.775$, and $B = 0.79$ from Monte Carlo data for the sq lattice.

C. Radius of gyration

We use S_N series newly obtained for several lattices (see Tables IX–XIII) and the extant series[9] for the fcc lattice. Figure 6 illustrates the plots of $\nu_{N,2}^{(r)}$ ($r=1$ and 2) evaluated from $\nu_{N,2}^{\mathrm{I}}$ ratios against N^{-1} for the bcc lattice; we have $\nu = 0.597 \pm 0.006$ as a first trial value. The $B_{N,2}(\Delta_1)$ curves for $N = 9-13$ are shown in Fig. 7 for the value $\nu = 0.599$, which was estimated by repeating the above procedure twice; the intersection is somewhat dispersive but suggests $\Delta_1 = 1.15$ and $B = 0.89$. Some terms in the appropriate Neville table of $\nu_{N,2}^{(r)}$ ($r = 1-3$) for the transformed series are reproduced in Table III; we get $\nu = 0.599 \pm 0.003$ in view of the trend of $\nu_{N,2}^{(1)}$ and $\nu_{N,2}^{(2)}$ bowed downwards for larger N. The corresponding Neville table for transformed S_N series for the fcc lattice is given in Table IV (cf. Table 6 in Ref. 9); we have $\nu = 0.599 \pm 0.004$ taking account of the increase in $\nu_{N,1}^{(1)}$, but with a tendency somewhat bowed downwards and the decrease in $\nu_{N,1}^{(2)}$ as N increases. The intersection of $B_{N,1}(\Delta_1)$ curves for this value of ν yields $\Delta_1 = 1.15 \pm 0.15$. Analogous estimation gives $\nu = 0.6025 \pm 0.004$ and $\Delta_1 = 1.28 \pm 0.3$ for the sc lattice. For the tet lattice, however, we only have $\nu = 0.593 \pm 0.006$ from the untransformed S_N series since no intersection is found in $B_{N,2}(\Delta_1)$ curves as in the case of R_N for the fcc lattice, and that the method to seek linear dependence of $B_{N,2}(\Delta_1)$ on $N^{-\Delta_2}$ is ineffective due to the odd-even oscillation inherent to a loose-packed lattice.

Figure 8 shows the plots of $\nu_{N,2}^{(r)}$ ($r=1$ and 2) obtained from ρ_N series against N^{-1} for the sq lattice; the estimate $\nu = 0.751 \pm 0.0015$ is obtained in view of the linear decrease in $\nu_{N,2}^{(1)}$ as a whole but with damping odd-even al-

TABLE II. Neville table for estimation of ν from the ratios $\nu_{N,1}^{\mathrm{II}}$ of transformed R_N series for the fcc lattice.

N	$\nu_{N,1}^{\mathrm{II}}$	$\nu_{N,1}^{(1)}$	$\nu_{N,1}^{(2)}$	$\nu_{N,1}^{(3)}$
6	0.567 601	0.593 02	0.584 70	0.577 60
7	0.570 882	0.590 57	0.584 43	0.584 07
8	0.573 315	0.590 35	0.589 70	0.598 46
9	0.575 189	0.590 18	0.589 58	0.589 35
10	0.576 669	0.589 99	0.589 24	0.588 43
11	0.577 866	0.589 83	0.589 12	0.588 82
12	0.578 852	0.589 70	0.589 02	0.588 72

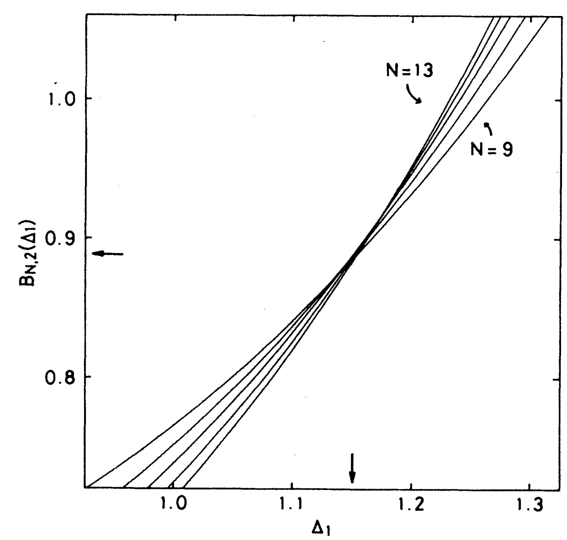

FIG. 7. Curves of $B_{N,2}(\Delta_1)$ for the input $\nu = 0.599$ in the case of S_N for the bcc lattice.

TABLE III. Neville table for estimation of ν from the ratios $\nu^{\mathrm{I}}_{N,2}$ of transformed S_N series for the bcc lattice.

N	$\nu^{\mathrm{I}}_{N,2}$	$\nu^{(1)}_{N,2}$	$\nu^{(2)}_{N,2}$	$\nu^{(3)}_{N,2}$
6	0.617 072	0.595 84	0.600 72	
7	0.615 393	0.597 29	0.601 63	0.578 68
8	0.612 608	0.599 21	0.602 59	0.603 21
9	0.611 873	0.599 55	0.602 39	0.602 77
10	0.610 180	0.600 47	0.602 35	0.602 20
11	0.609 780	0.600 36	0.601 77	0.601 25

ternate oscillation and the somewhat irregular decrease in $\nu^{(2)}_{N,2}$ with the damping oscillation as $N^{-1}\rightarrow 0$. Using the value of ν, we have $\Delta_1=1.07$ and $B=1.51$ from the $B_{N,2}(\Delta_1)$ curves depicted in Fig. 9. Some terms in the Neville table for $\nu^{(r)}_{N,2}$ $(r=1-3)$ obtained from ρ^*_N series using these Δ_1 and B are reproduced in Table V; we get a little improved value $\nu=0.751\pm0.001$ as our final estimate bearing in mind the damping odd-even oscillation of $\nu^{(1)}_{N,2}$ about a constant value together with somewhat irregular damping oscillation of $\nu^{(2)}_{N,2}$, and $\Delta_1=1.07\pm0.04$ is determined. These values are compared with $\nu=0.755\pm0.001$ and $\Delta_1=1.04\pm0.03$ for the tri lattice.

D. Number of walks

We form for C_N series

$$\mu_{N,k}=(C_N/C_{N-k})^{1/k} \tag{8}$$

and

$$\gamma^{(r)}_{N,k}=N(\mu_{N,k}/\mu^{(r)}_{N,k}-1)+1\ , \tag{9}$$

where $\mu^{(r)}_{N,k}$ $(r=1-3)$ are rth extrapolants of $\mu_{N,k}$ defined such as Eq. (5), and determine first trial values of μ and γ by plotting $\mu^{(r)}_{N,k}$ and $\gamma^{(r)}_{N,k}$ against N^{-1}. We then construct the estimators:

$$A'_{N,k}(\Delta_1)=\frac{N^{\Delta_1-\gamma+1}C_N-\mu^k(N-k)^{\Delta_1-\gamma+1}C_{N-k}}{\mu^N[N^{\Delta_1}-(N-k)^{\Delta_1}]} \tag{10}$$

and

$$B'_{N,k}(\Delta_1)=\frac{(N-k)^{\gamma-1}C_N-\mu^kN^{\gamma-1}C_{N-k}}{\mu^kN^{\gamma-\Delta_1-1}C_{N-k}-(N-k)^{\gamma-\Delta_1-1}C_N}\ . \tag{11}$$

Using these μ and γ values, Δ_1 is estimated from the intersection of $A'_{N,k}(\Delta_1)$ or $B'_{N,k}(\Delta_1)$ curves for different N. Improved estimates of μ, γ, and Δ_1 are obtained in the same manner as in R_N and S_N cases with the aid of the transformation $C^*_N=C_N/(1+B'N^{-\Delta_1})$.

The second trial values $\mu=10.0362\pm0.0006$ and $\gamma=1.163\pm0.003$ are estimated from the first values $\mu=10.0368\pm0.0010$ and $\gamma=1.164\pm0.004$ for the fcc lattice. Figure 10 shows $B'_{N,1}(\Delta_1)$ curves $(N=10-14)$ for the second values of μ and γ; the intersection of the

TABLE IV. Neville table for estimation of ν from the ratios $\nu^{\mathrm{II}}_{N,1}$ of transformed S_N series for the fcc lattice.

N	$\nu^{\mathrm{II}}_{N,1}$	$\nu^{(1)}_{N,1}$	$\nu^{(2)}_{N,1}$	$\nu^{(3)}_{N,1}$
6	0.600 345	0.589 65	0.604 96	0.600 81
7	0.599 332	0.593 25	0.602 28	0.598 70
8	0.598 949	0.596 27	0.605 31	0.610 38
9	0.598 863	0.598 17	0.604 82	0.603 84
10	0.598 910	0.599 33	0.603 98	0.602 02
11	0.599 015	0.600 06	0.603 35	0.601 66
12	0.599 139	0.600 51	0.602 72	0.600 83

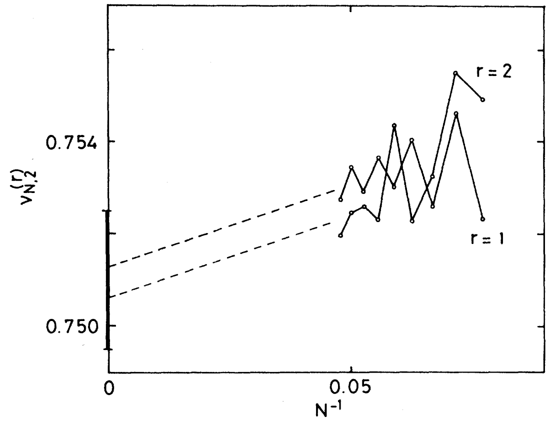

FIG. 8. The same as Fig. 1 but for S_N for the sq lattice.

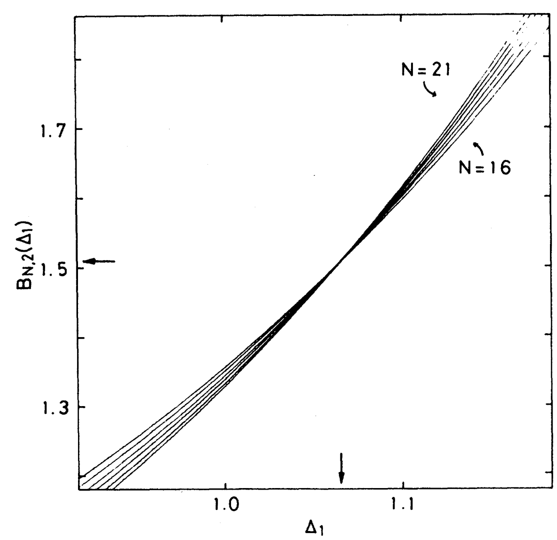

FIG. 9. The same as Fig. 7 but for the input $\nu=0.751$ for the sq lattice.

TABLE V. Neville table for estimation of ν from the ratios $\nu^{II}_{N,2}$ of transformed S_N series for the sq lattice.

N	$\nu^{II}_{N,2}$	$\nu^{(1)}_{N,2}$	$\nu^{(2)}_{N,2}$	$\nu^{(3)}_{N,2}$
13	0.751 705	0.749 22	0.753 03	0.762 68
14	0.750 353	0.751 71	0.753 73	0.748 58
15	0.751 457	0.749 85	0.751 58	0.749 40
16	0.750 493	0.751 47	0.750 73	0.745 74
17	0.751 352	0.750 56	0.752 89	0.755 30
18	0.750 588	0.751 35	0.750 94	0.751 37
19	0.751 286	0.750 72	0.751 32	0.747 90
20	0.750 662	0.751 33	0.751 25	0.751 97
21	0.751 234	0.750 75	0.750 84	0.749 65

TABLE VI. Neville table for estimation of γ from the ratios $\mu_{N,1}$ of transformed C_N series for the fcc lattice.

N	$\mu_{N,1}$	$\gamma^{(1)}_{N,1}$	$\gamma^{(2)}_{N,1}$	$\gamma^{(3)}_{N,1}$
6	10.339 506	1.205 70	1.161 53	1.156 39
7	10.292 955	1.195 25	1.165 09	1.177 13
8	10.258 690	1.191 52	1.178 81	1.207 97
9	10.232 436	1.188 60	1.177 15	1.176 23
10	10.211 703	1.186 14	1.175 22	1.172 98
11	10.194 919	1.184 12	1.174 14	1.173 61
12	10.181 059	1.182 43	1.173 26	1.172 83
13	10.169 421	1.181 02	1.172 61	1.172 57
14	10.159 511	1.179 81	1.172 05	1.172 01

curves yields $\Delta_1 = 1.1$ and $B' = 0.069$. Since the third estimation of μ and γ makes no improvement on the second values, we take these values as our final estimates; $\Delta_1 = 1.1 \pm 0.3$ is determined in view of both error limits of μ and γ. Some terms in the Neville table of the extrapolants $\gamma^{(r)}_{N,1}$ $(r = 1-3)$ for the transformed C^*_N series are reproduced in Table VI. Our value of μ is compatible with $\mu = 10.0346 \pm 0.001$ by Watts[39] and 10.0364 by Rapaport.[9] Similarly, we have $\Delta_1 = 1.02 \pm 0.4$ (bcc), 0.95 ± 0.3 (sc), and 0.9 ± 0.4 (tet) for other lattices in 3D; values of μ, γ, A', and B' estimated are listed in Table VIII.

For the sq lattice, we estimate $\mu = 2.638\,15 \pm 0.000\,15$ and $\gamma = 1.343 \pm 0.003$ from untransformed C_N series, which are our final estimates in this case. Figure 11 illustrates $B'_{N,2}(\Delta_1)$ curves $(N = 21-27)$ for these values; we obtain $\Delta_1 = 0.97 \pm 0.3$, which is consistent with the previous value[23] $\Delta_1 = 0.95 \pm 0.15$ for the tri lattice. Guttmann[11] has estimated $\mu = 2.638\,160 \pm 0.000\,004$ using the same data but a different method.

III. DISCUSSION AND CONCLUSION

Several critical quantities we estimated for various lattices in 3D and 2D are listed in Tables VII and VIII together with the existing estimates from exact series or Monte Carlo data; the values in a preceding paper for the tri lattice are republished there for the sake of convenience. The error limits of Δ_1 are estimated by considering those of ν for R_N and S_N, and μ and γ for C_N. The values of ν for R_N in 3D are entirely reconciled with $\nu = 0.588$ from RG calculations; those in 2D are in good

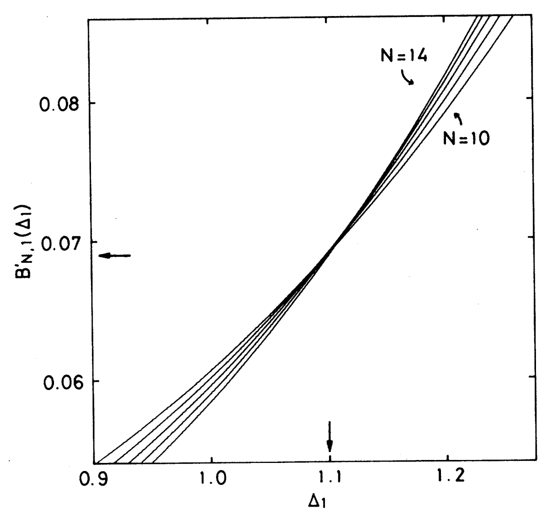

FIG. 10. Curves of $B'_{N,1}(\Delta_1)$ for the inputs $\mu = 10.0362$ and $\gamma = 1.163$ in the case of C_N for the fcc lattice.

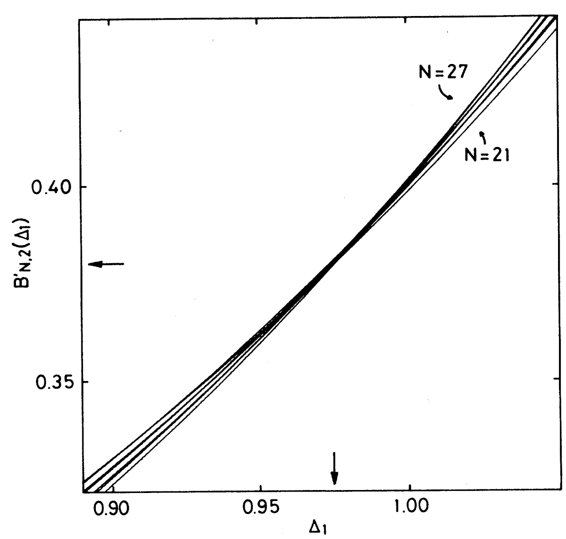

FIG. 11. Curves of $B'_{N,2}(\Delta_1)$ for the inputs $\mu = 2.63815$ and $\gamma = 1.343$ in the case of C_N for the sq lattice.

TABLE VII. Critical values estimated for R_N and S_N for several lattices.

Lattices		ν	Δ_1	A	B
fcc	R_N	0.5880±0.0006	0.45±0.05	1.04	−0.24
		0.5875±0.0015[a]	0.470,[a] 1[b]	1.05[a]	−0.286[a]
	S_N	0.599±0.004	1.15±0.15	0.145	0.96
bcc	R_N	0.589±0.002	0.50±0.10	1.06	−0.22
		0.5909±0.0002[b]	1[b]	1.031[b]	
	S_N	0.599±0.003	1.15±0.10	0.151	0.89
		0.5912±0.0004[b]		0.1633[b]	
sc	R_N	0.5910±0.0006	0.44±0.05	1.212	−0.145
		0.5919±0.0004[b]	1,[b] 0.50 ±0.05[c,d]	1.134[b]	−0.16[c]
	S_N	0.6025±0.0040	1.28±0.30	0.165	0.80
		0.5933±0.0003[b]		0.1772[b]	
tet	R_N	0.5885±0.0020	0.53±0.06	1.442	−0.244
	S_N	0.593±0.006			
tri	R_N	0.7503±0.0004	0.63±0.05	0.7052	0.2935
		0.7500±0.0025[e]	0.66±0.07[e,f]	0.708[e,f]	0.30[e]
		0.7488±0.0010[g]	1[g,h]	0.7145[g]	0.761[h]
	S_N	0.7550±0.0010	1.04±0.03	0.0944	1.710
		0.7489±0.0006[g]		0.1002[g]	
sq	R_N	0.750±0.001	0.66±0.05	0.766	0.37
		0.7479±0.0010[g]	1,[g,h,i] 1.2±0.1[c]	0.774[g]	0.95[h]
		0.75[i,j]	0.84±0.04[j]	0.775[i]	0.79[i]
	S_N	0.751±0.001	1.07±0.04	0.107	1.51
		0.7484±0.0006[g]		0.108[g]	

[a]Reference 7.
[b]Reference 9 [Monte Carlo data (MC)].
[c]Reference 8 (MC).
[d]Reference 10 (MC).
[e]Reference 12.
[f]Reference 13.
[g]Reference 17 (MC).
[h]Reference 15.
[i]Reference 16 (MC).
[j]Reference 14 (MC).

agreement with Nienhuis's analytical prediction (or the Flory value) $\frac{3}{4}$ and $\nu=0.7503\pm0.0002$ from the transfer-matrix method by Derrida.[40] The mean value of Δ_1 for R_N is $\Delta_1=0.48$ in 3D, and $\Delta_1=0.65$ in 2D. The former is in accord with $\Delta_1=0.47$ obtained from RG calculations and exact series analysis by Majid *et al.*[7] for the fcc lattice, and it is compared with $\Delta_1=0.5$ from Monte Carlo approaches by Havlin and Ben-Avraham[8] and Kelly *et al.*[10] for the sc lattice; the latter is consistent with the conjecture $\Delta_1=\frac{2}{3}$ from exact series analyses by Djordjevic *et al.*[12] and Privman[13] for the tri lattice, but inconsistent with $\Delta_1=1.0$ estimated by Hunter *et al.*[16] using

TABLE VIII. Critical values estimated for C_N for several lattices.

Lattices	μ	γ	Δ_1	A'	B'
fcc	10.0362±0.0006	1.163±0.003	1.1±0.3	1.139	0.069
	10.0364±0.0006[a,b]	1.1629±0.0020[a]	1[b], 0.465[c]		
bcc	6.5300±0.0015	1.163±0.005	1.02±0.4	0.143	0.0755
	6.5295±0.0020[d]	1.1650±0.001[d]			
sc	4.6839±0.0004	1.162±0.002	0.95±0.30	1.184	0.076
	4.6839±0.0002[a]	1.1613±0.0021[a]			
tet	2.8790±0.0015	1.162±0.007	0.9±0.4	0.304	0.125
	2.8792±0.0005[d]	1.157±0.003[d]			
tri	4.1507±0.0008	1.344±0.003	0.95±0.15	1.191	0.345
	4.150 82±0.000 08[a]	1.3431±0.0010[a]	1[e]		
sq	2.638 15±0.000 15	1.343±0.003	0.98±0.3	1.181	0.384
	2.638 160±0.000 004[a]	1.3436±0.000 13[a]	1[e]		

[a]Reference 11.
[b]Reference 9.
[c]Reference 22.
[d]Reference 39.
[e]Reference 21.

TABLE IX. Exact series of C_N, R_N, and S_N for the tet lattice.

N	$\frac{1}{4}C_N$	$\frac{1}{4}C_N R_N^2$	$\frac{1}{4}(N+1)^2 C_N S_N^2$
1	1	1	1
2	3	8	14
3	9	41	116
4	27	176	746
5	81	689	4121
6	237	2552	20 300
7	699	9083	93 440
8	2049	31 408	405 636
9	6015	106 239	1 687 383
10	17 547	353 304	6 753 810
11	51 321	1 158 617	26 307 092
12	149 499	3 756 384	99 817 558
13	436 137	12 061 945	371 382 217
14	1 268 475	38 418 328	1 355 404 008
15	3 693 663	121 504 271	4 875 193 600
16	10 730 613	381 942 224	17 280 369 496
17	31 203 621	1 194 166 357	60 563 128 677
18	90 566 913	3 715 993 832	209 818 417 170
19	2 63 067 933	11 514 366 573	720 394 458 228
20	7 62 975 129	35 543 506 848	2 450 455 002 848
21	22 14 262 551	109 342 447 895	8 274 346 083 763
22	64 17 997 005	335 329 803 992	

Monte Carlo data for the sq lattice. Guttmann[11,21] and Rapaport[9,15,17] suggest the presence of the analytic value $\Delta_1=1$ for $d=2$ and 3.

Our estimates of ν for S_N are slightly larger than those for R_N; the difference is conspicuous for lattices in 3D and the values are close to the Flory value $\frac{3}{5}$. This seems to contradict the widely accepted belief that ν is equivalent between R_N and S_N, which is supported by earlier numerical work[24,25] and RG calculations.[27–30] Our result suggesting $\nu_S > \nu_R$ can probably be ascribed, as Rapaport[9] indicated, to the slow rate of convergence of S_N series since it includes contributions from all possible distances between pairs of sites in a walk. Recent Monte Carlo estimates[17,18,26] for SAW's in 2D are consistent with the conjecture $\nu_S=\nu_R$ while those[9,18,26] in 3D seem to give $\nu_S > \nu_R$.

We get $\Delta_1=1.19$ (3D) and 1.06 (2D) as the averages of our estimates of Δ_1 for S_N. They are evidently different from those for R_N and in favor of the presence of the analytic correction of $\Delta_1=1$ as shown in a preceding publication for the tri lattice, but Δ_1 in 3D is a little larger than that in 2D. The estimation of Δ_1 is dependent on a given value of ν, so that the discrepancy may be attributed to the difference in ν between S_N and R_N. However, the discrepancy increases for smaller ν_S; for example, $\Delta_1=1.6$ for the fcc lattice if we choose $\nu_S=0.588$, and $\Delta_1=1.13$ for $\nu_S=0.750$ for the tri lattice.

The estimates of γ in 3D are entirely reconciled with

TABLE X. Exact series of C_N, R_N, and S_N for the bcc lattice.

N	$\frac{1}{8}C_N$	$\frac{1}{8}C_N R_N^2$	$\frac{1}{8}(N+1)^2 C_N S_N^2$
1	1	1	1
2	7	16	30
3	49	177	548
4	331	1696	7766
5	2245	14 917	95 581
6	15 007	124 468	1 059 212
7	100 603	999 995	10 958 400
8	668 965	7 819 224	107 000 732
9	4 456 585	59 853 953	1 002 919 433
10	29 536 387	450 672 532	9 061 897 542
11	196 006 195	3 347 481 963	79 685 665 460
12	1 296 083 749	24 590 339 689	683 195 865 502
13	8 578 330 951	178 939 306 279	5 745 246 546 465

TABLE XI. Exact series of C_N and S_N for the sc lattice.

N	$\frac{1}{6}C_N$	$\frac{1}{6}(N+1)^2C_NS_N^2$
1	1	1
2	5	22
3	25	292
4	121	2994
5	589	26 613
6	2821	212 532
7	13 565	1 583 808
8	64 661	11 126 940
9	308 981	75 021 053
10	1 468 313	487 286 330
11	6 989 025	3 079 847 364
12	33 140 457	18 971 359 374
13	157 329 085	114 611 086 221
14	744 818 613	679 491 899 320

TABLE XIII. Exact series of C_N and S_N for the tri lattice.

N	$\frac{1}{6}C_N$	$\frac{1}{6}(N+1)^2C_NS_N^2$
1	1	1
2	5	22
3	23	282
4	103	2778
5	455	23 305
6	1991	175 194
7	8647	1 215 740
8	37 355	7 939 156
9	160 689	49 422 491
10	688 861	295 993 366
11	2 944 823	1 717 056 604
12	12 559 201	9 697 408 184
13	53 455 781	53 533 130 211
14	227 131 875	289 769 871 988
15	963 627 597	1 541 876 281 342

the RG value[4] $\gamma = 1.1615$; almost the same results are obtained from exact series analyses by Rapaport[9] and Guttmann.[11] Those in 2D are in good agreement with Nienhuis's prediction $\gamma = \frac{43}{32}$, which is supported by other numerical attempts.[11,20,21] The average values of Δ_1 for C_N are $\Delta_1 = 0.99$ (3D) and 0.97 (2D), which confirm the presence of the analytic correction $\Delta_1 = 1$ both in 3D and 2D. The value in 2D is compatible with $\Delta_1 = 0.93$ estimated by Adler[20] from the series analysis for the honeycomb lattice whereas $\Delta_1 = 0.465$ is given by McKenzie[22] for the fcc lattice. Recently, Guttmann and Enting[41] have obtained $\Delta_1 = 1$ and $\Delta_2 = 1.5$ from the analysis of 56-term series for the number of self-avoiding polygons on the sq lattice. Our method for this series yields $\Delta_1 = 0.9805$ by using the values $\mu = 2.638\,158\,5$ and $\alpha = 0.500\,06$ given by them, where α is the exponent for specific heat; the Δ_1 value is in excellent agreement with $\Delta_1 = 0.98$ for the SAW on the same lattice to support $\Delta_1 = 1$. We have also estimated $\Delta_1 = 0.70 \pm 0.06$ and 0.63 ± 0.06 from the 54-term series[41] for the span and square span of the polygon, respectively, where we used our estimate $\nu = 0.752 \pm 0.004$ in both cases. These Δ_1 values are reconciled with our corresponding result 0.66 ± 0.05 for the SAW; the value of ν is compared with 0.753 ± 0.007 of Guttmann and Enting.

TABLE XII. Exact series of C_N and S_N for the sq lattice.

N	$\frac{1}{4}C_N$	$\frac{1}{4}(N+1)^2C_NS_N^2$
1	1	1
2	3	14
3	9	116
4	25	722
5	71	3887
6	195	18 508
7	543	82 160
8	1479	340 180
9	4067	1 351 555
10	11 025	5 136 194
11	30 073	18 989 580
12	81 233	68 082 102
13	220 375	239 338 055
14	593 611	822 629 240
15	1 604 149	2 786 064 872
16	4 311 333	9 274 487 688
17	11 616 669	30 521 878 637
18	31 164 683	99 086 541 810
19	83 779 155	318 742 922 236
20	224 424 291	1 014 076 260 686
21	602 201 507	3 202 213 457 395

A universal relation[42] is generally predicted among the correction-to-scaling amplitudes as well as the leading critical amplitudes. Our estimates of B and B' in 3D suggest that they are universal excepting the values for R_N for the sc lattice and for C_N for the tet lattice; such a feature is not so clear for B in 2D. Note that B is negative for R_N in 3D whereas it is positive for S_N. Average estimates of the ratio A_S/A_R are 0.139 (3D) and 0.137 (2D) in contrast with the result by Lax, Barrett, and Domb:[43] $S_N^2/R_N^2 = 0.155$ (3D) and 0.140 (2D) as $N \to \infty$.

Critical quantities for SAW's are estimated from the exact series of R_N, S_N, and C_N for various lattices in 3D and 2D using a new method of series analysis; we have added new terms to the extant data of S_N for several lattices. The estimators of ν for R_N and γ for C_N in 3D are entirely consistent with the RG calculations $\nu = 0.588$ and $\gamma = 1.1615$ while those in 2D are in good agreement with Nienhuis's analytical values $\nu = \frac{3}{4}$ and $\gamma = \frac{43}{32}$; the estimates of μ are reconciled with other numerical results in 3D and 2D. Our values of ν for S_N are, however, somewhat larger than those for R_N contrary to expectation in both cases of 3D and 2D. The averages are $\nu = 0.598$ (3D) and 0.753 (2D); the former is very close to the Flory value $\frac{3}{5}$. The average estimates of the correction-to-scaling exponent are $\Delta_1=0.48$ (3D) and 0.65 (2D) for R_N, and $\Delta_1=1.19$ (3D) and 1.06 (2D) for S_N while $\Delta_1=0.99$ (3D) and 0.97 (2D) for C_N; the values for S_N and C_N are in favor of the analytic correction $\Delta_1=1$, whereas those for R_N are reconciled with the RG calculations.

ACKNOWLEDGMENTS

I am very grateful to Y. Arai for assistance with computational work.

[1]P. G. de Gennes, *Scaling Concepts in Polymer Physics* (Cornell University Press, Ithaca, NY, 1979).

[2]F. J. Wegner, Phys. Rev. B **5**, 4529 (1972); **6**, 1891 (1972).

[3]D. S. McKenzie, Phys. Rep. **27**, 35 (1976), and references therein.

[4]J. C. Le Guillou and J. Zinn-Justin, Phys. Rev. Lett. **39**, 95 (1977); Phys. Rev. B **21**, 3976 (1980).

[5]G. A. Baker, Jr., B. G. Nickel, M. S. Green, and D. I. Meiron, Phys. Rev. Lett. **36**, 1351 (1976); Phys. Rev. B **17**, 1365 (1978).

[6]B. Nienhuis, Phys. Rev. Lett. **49**, 1062 (1982); J. Stat. Phys. **34**, 731 (1984).

[7]I. Majid, Z. V. Djordjevic, and H. E. Stanley, Phys. Rev. Lett. **51**, 1282 (1983).

[8]S. Havlin and D. Ben-Avraham, Phys. Rev. A **27**, 2759 (1983).

[9]D. C. Rapaport, J. Phys. A **18**, 113 (1985).

[10]K. Kelly, D. L. Hunter, and N. Jan, J. Phys. A **20**, 5029 (1987).

[11]A. J. Guttmann, J. Phys. A **20**, 1839 (1987).

[12]Z. V. Djordjevic, I. Majid, H. E. Stanley, and R. J. dos Santos, J. Phys. A **16**, L519 (1983).

[13]V. Privman, Physica A **123**, 428 (1984).

[14]J. W. Lyklema and K. Kremer, Phys. Rev. B **31**, 3182 (1985).

[15]D. C. Rapaport, J. Phys. A **18**, L201 (1985).

[16]D. L. Hunter, N. Jan, and B. MacDonald, J. Phys. A **19**, L543 (1986).

[17]D. C. Rapaport, J. Phys. A **18**, L39 (1985).

[18]N. Madras and A. D. Sokal, J. Stat. Phys. **50**, 109 (1988).

[19]I. Majid, Z. V. Djordjevic, and H. E. Stanley, Phys. Rev. Lett. **51**, 143 (1983).

[20]J. Adler, J. Phys. A **16**, L515 (1983).

[21]A. J. Guttmann, J. Phys. A **17**, 455 (1984).

[22]S. McKenzie, J. Phys. A **12**, L267 (1979).

[23]T. Ishinabe, Phys. Rev. B **37**, 2376 (1988).

[24]F. T. Wall and J. J. Erpenbeck, J. Chem. Phys. **30**, 637 (1959).

[25]C. Domb and F. T. Hioe, J. Chem. Phys. **51**, 1915 (1969).

[26]H. Meirovitch, J. Chem. Phys. **79**, 502 (1983).

[27]T. A. Witten and L. Schäfer, J. Phys. A **11**, 1843 (1978).

[28]J. des Cloizeaux, J. Phys. (Paris) **42**, 635 (1981).

[29]M. K. Kosmas, J. Phys. A **14**, 2779 (1981).

[30]M. Benhamou and G. Mahoux, J. Phys. Lett. (Paris) **46**, 689 (1985).

[31]J. L. Martin, Proc. Cambridge Philos. Soc. **58**, 92 (1961).

[32]J. L. Martin and M. G. Watts, J. Phys. A **4**, 456 (1971).

[33]M. F. Sykes, A. J. Guttmann, M. G. Watts, and P. D. Roberts, J. Phys. A **5**, 653 (1972).

[34]T. Ishinabe, J. Phys. A **20**, 6435 (1987).

[35]The tables in Ref. 25 quote the values of S_N^2 but not $(N+1)^2 C_N S_N^2$.

[36]V. Privman and M. E. Fisher, J. Phys. A **16**, L295 (1983).

[37]S. Havlin and D. Ben-Avraham, J. Phys. A **15**, L311 (1982).

[38]Similar quantities are used in a somewhat different context in order to estimate Δ_1 for neighbor-avoiding walks; see G. Torrie and S. G. Whittington, J. Phys. A **10**, 1345 (1977).

[39]M. G. Watts, J. Phys. A **8**, 61 (1975).

[40]B. Derrida, J. Phys. A **14**, L5 (1981).

[41]A. J. Guttmann and I. G. Enting, J. Phys. A **21**, L165 (1988).

[42]A. Aharony and G. Ahlers, Phys. Rev. Lett. **44**, 782 (1980).

[43]M. Lax, A. J. Barrett, and C. Domb, J. Phys. A **11**, 361 (1978).