Scaling exponents of the self-avoiding-walk-problem in three dimensions

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(Received 5 April 1993; revised manuscript received 13 October 1993)

Monte Carlo simulations on self-avoiding walks traced on the simple cubic lattice and reported in a recent paper have been extended up to 2999 steps, using the same Alexandrowicz dimerization procedure. Through this extension, we are able to show that the discrepancy between ν_{RG}, the scaling exponent for the correlation length, as determined from renormalization-group calculations, and ν_{MC}, the same exponent determined through Monte Carlo simulations, is an artefact, originating in the fact that Monte Carlo simulations are restricted to relatively short chains, while to obtain the correct ν value using the latter method exceedingly large chains are required. This finding is in accord with a previous suggestion by Zifferer. We further show that $\langle r \rangle$, the modulus of the mean end-to-end distance, $\langle r^2 \rangle^{1/2}$, the root-mean-square end-to-end distance, $\langle r_g \rangle$, the mean radius of gyration, and $\langle r_g^2 \rangle^{1/2}$, the root-mean-square radius of gyration, cannot be correctly expressed for all N in the range $1<N<2999$ using a single correction to scaling exponent Δ_1. At least two such corrections to the scaling exponents are required, and the agreement with the Monte Carlo data is significantly improved if three corrections to the scaling exponents are introduced, so that one should write $\langle x \rangle = N^{0.588}[a_0^x + a_1^x N^{-\Delta_1} + a_2^x N^{-\Delta_2} + a_3^x N^{-\Delta_3}]$, where $\langle x \rangle$ stands for one of the above mean values. Consideration of a fourth correction to scaling exponent Δ_4 does not seem to be warranted for self-avoiding walks, where there is a lower cutoff for $N=1$. Further, such a fourth exponent seems devoid of physical significance because of the even-odd oscillations occurring for the lowest N values in the various mean values $\langle x \rangle$, where a fourth exponent has a non-negligible effect. A five-term expansion is however given here for completeness. The set of the corrections to the scaling exponents Δ_i, which, because of universality, is the same for the various mean values, as well as of the a_i^x's, which depend on the mean value considered, follows the somewhat arbitrary choice made, within a narrow range of values, for the first correction to the scaling exponent Δ_1. If the value $\Delta_1=0.50$ is adopted, as suggested by graphical analysis of our data, the set which minimizes the mean-square deviation of the Monte Carlo data is $\Delta_2=1.0$, $\Delta_3=2.0$, and $\Delta_4=4.0$. If the renormalization group value $\Delta_1=0.47$ is used instead, the corresponding set is $\Delta_2=1.05\pm0.02$, $\Delta_3=2.2\pm0.2$, and $\Delta_4=4.4\pm0.4$. These two sets are mathematically equivalent for the correct description of our Monte Carlo data. The precision of our data does not permit one to decide which set, on a physical basis, is the correct one. In any case, each successive correction to the scaling exponent is found to be, approximately if not exactly, the double of the preceding one.

I. INTRODUCTION

In a previous paper[1] it has been found using Monte Carlo (MC) simulations that for self-avoiding walk's (SAW's) in three dimensions, the correlation length exponent ν was equal to $\nu_{MC}=0.5919$. This value of ν, while in accord with that found by other investigators,[2-4,8] exceeds the value found by renormalization-group (RG) calculations, which was calculated to be $\nu_{RG}=0.588\pm0.001$.[5] One may object that the precision of the MC data and of the RG calculations, respectively, are not of such a quality as to be certain that the discrepancy is real and not simply an artefact. In this respect, Table I displays the values of ν_{MC} on the simple-cubic lattice found by various authors. The estimated error and the walk step range, from which these results have been deduced, is also indicated. Taking account of the error bars indicated, the least ν_{MC} value is $\nu_{MC}=0.5892$, while the greatest is $\nu_{MC}=0.5923$. This difference is considerably reduced if the results of Madras and Sokal[3] are not taken into account. In any case, taking account of error bars, the least MC value is larger and lies outside the range of the estimated RG calculations error. Of course, if the RG error bars are not correct, it cannot be excluded that the discrepancy between ν_{MC} and ν_{RG} is only apparent. However, since it is well known that ν_{MC} values are a function of the number of steps N in the walk,[6] and presumably tend to a limit as N becomes infinite, it is quite probable that the discrepancy is due, at least in part, to the fact that ν_{MC} has been estimated from finite N values. This argument is supported by the fact that if a series of MC data is divided in a group of smaller and a group of larger N step values, the second group always yields smaller ν_{MC} values. Such a statistical analysis has been performed in two instances in the past.[7,8] What had not been realized to date is that

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TABLE I. Monte Carlo values ν_{MC} for the correlation length critical exponent, for self-avoiding walks on the simple-cubic lattice.

Authors	ν_{MC}	Estimated error bars	Step range
Rapaport[a]	0.5919	±0.0004	120–2400
Madras and Sokal[b]	0.5907	±0.0014	200–3000
Dayantis and Palierne[c]	0.5919	±0.0002	50–800
Eizenberg and Klafter[d]	0.5908	±0.0004	200–3200

[a]Reference 4.
[b]Reference 3.
[c]Reference 1.
[d]Reference 8.

within the precision of MC simulation experiments, the limiting ν_{MC} value is not yet attained for several thousand steps.

Zifferer[7] has been the first to argue that the discrepancy between ν_{MC} and ν_{RG} is due to the fact that ν_{MC} has been deduced from finite values of N. The diagrams provided by Zifferer in support of his suggestion are not, however, convincing because of the excessive scattering of his MC simulation data. For this reason, we decided, in order to try to settle the question, to push our Alexandrowicz dimerization procedure,[1,9] as far as possible, account being taken of the computational means at our disposal. The major advantage of our version of the Alexandrowicz dimerization procedure is that each SAW configuration obtained is statistically independent of all others in the MC sample, since the successive dimerizations proceed from the beginning for each new tried configuration. The pivot algorithm,[3,7,8] on the other hand, though certainly significantly more efficient in order to obtain large samples of large N walks, introduces delicate problems of statistical independence of the configurations within the sample. We have thus calculated $\langle r \rangle$, the modulus of the mean end-to-end distance $\langle r^2 \rangle$, the mean square end-to-end distance $\langle r_g \rangle$, the mean radius of gyration, and $\langle r_g^2 \rangle$, the mean-square radius of gyration up to $N=2999$ steps. We have also proceeded to an exact determination of the above parameters up to the fourth moment, through exhaustive enumeration of all configurations, up to fifteen steps. Regarding the MC simulations, which range from 16 to 2999 steps, they may be divided into two classes: in the first class, from 16 to 250 steps, precise simulations, with sample sizes lying between 2.5 and 3.0×10^6 independent configurations, and from 399 to 2999 steps, limited precision simulations, with sample sizes lying between 1.6 and 2.4×10^4 independent configurations.

In Fig. 1 are shown the ratios $\langle r_g \rangle / N^{0.588}$ and $\langle r_g \rangle / N^{0.5919}$ as a function of $\ln N$. It is seen that the variation of the ratio $\langle r_g \rangle / N$ is not monotonous, whatever the value adopted for ν. Because of this, it is easy to show that $\langle r_g \rangle_N$, and generally all mean quantities $\langle x \rangle_N$ cannot be correctly expressed in all the N range using a single correction to scaling exponent Δ_1:

$$\langle x \rangle_N = N^{\nu}[a_0 + a_1/N^{\Delta_1}] . \quad (1)$$

At least two such correction to scaling exponents are needed, unless one is interested only in large values of N ($N > 1000$). More generally, one should write

$$\langle x \rangle_N = N^{\nu}\left[a_0^x + \sum_{i=1}^{k} a_i^x / N^{\Delta_i}\right] . \quad (2)$$

Here the superscript x refers to the mean quantity $\langle x \rangle$ considered, and k is an integer presently left unspecified but at least equal to two.

Now the sheer appearance of curves I and II in Fig. 1 makes one suspect that $\nu_{RG}=0.588$ is a more correct value than $\nu_{MC}=0.5919$. This, because curve I seems to tend to a finite limit as N increases, as physically required, while in such a case curve II would decrease to zero. This is a first indication that Zifferer's contention might be correct. A more stringent test for this is given

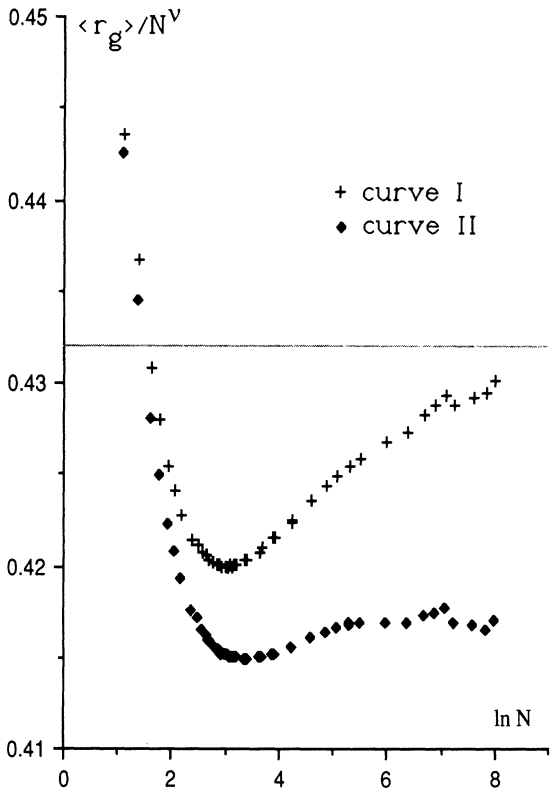

FIG. 1. Mean radius of gyration $\langle r_g \rangle$ over $N^{0.588}$ (curve I), and over $N^{0.5919}$ (curve II), where N is the number of steps in the self-avoiding walk. While curve I seems to tend to an upper limit of the order of 0.432 when N increases to infinity, curve II would apparently tend to zero. This excludes the Monte Carlo value $\nu_{MC}=0.5919$ for the correlation length critical exponent (scaling exponent for mean end-to-end distances in the present instance) from being correct. The discrepancy with the renormalization-group value $\nu_{RG}=0.588$ probably originates in the fact that ν_{MC} has been deduced from relatively short chains. (N less than a few thousand steps at most.) The shape of curve I indicates that $\langle r_g \rangle$ as a function of N, using for ν the renormalization-group value, cannot be adequately described using a single correction to scaling exponent Δ_1. At least two such correction to scaling exponents are required (see the text).

in the curve in Fig. 2. In this figure, the quantity ω, where $\omega/N=\langle r_g\rangle_{\rm MC}/0.417N^{0.5919}-1$, is plotted versus N. According to Eq. (1) [or Eq. (2), where the higher correction to the scaling terms is neglected], we have the approximate equality

$$\omega\simeq(a_1/a_0)N^{(1-\Delta_1)} . \tag{3}$$

Now theory and simulations (see Sec. III) both point to the fact that $\Delta_1\simeq 0.50$, that is $1-\Delta_1>0$. Further, graphical and numerical analysis of the MC data show that we always have $a_1<0$, whatever the set of Δ_i's considered (see below). Therefore, the curve in Fig. 2 should be continuously decreasing, contrary to what is actually found. This peculiar behavior can be explained only if it is assumed that the $\nu_{\rm MC}$ value used to draw the plot is too large. The argument goes as follows: from Fig. 1 it appears that the leading prefactor a_0 is approximately equal to 0.432 if ν is taken to be equal to 0.588, and 0.417 if ν is taken to be equal to 0.5919. For 2999 steps, our largest MC value, the ratio $R=0.417N^{0.5919}/0.432N^{0.588}$ equals 0.996. If now we consider the largest N value displayed in Fig. 2, i.e., $N=159$, the above ratio is equal to 0.984 only, which means that $0.417N^{0.5919}$ decreases more rapidly than $0.432N^{0.588}$ as N decreases. It follows that $\langle r_g\rangle/N^{0.5919}$ is larger than it should be in the expression for ω above, and ω increases (decreases in absolute value) as N increases, contrary to expectations. Of course, this demonstrates that $\nu=0.5919$ is too large but does not indicate the correct value of the exponent, as a plot of the kind displayed in Fig. 2 is unable to do so.

To obtain with precision the correct ν value directly through a plot as in Fig. 1, one should be able to obtain large samples ($E>10^6$) of exceedingly large chains ($N>10^6$ steps). Such data are quite beyond the possibilities of our Alexandrowicz dimerization procedure, and possibly also beyond the possibilities of the pivot algorithm. (Because in the pivot algorithm, among other circumstances, the relaxation time to obtain independent configurations increases with N). A more convenient procedure would be to plot, e.g., $\langle r_g\rangle$, versus $\ln N$, using precise MC data for chain lengths lying between 10^3 and 10^4 steps, as for such N values the correction to scaling becomes gradually negligible. In such a procedure, sample sizes of, say 5×10^6 independent walks would be required, and unfortunately, this also lies beyond the practical possibilities of our Alexandrowicz dimerization procedure.

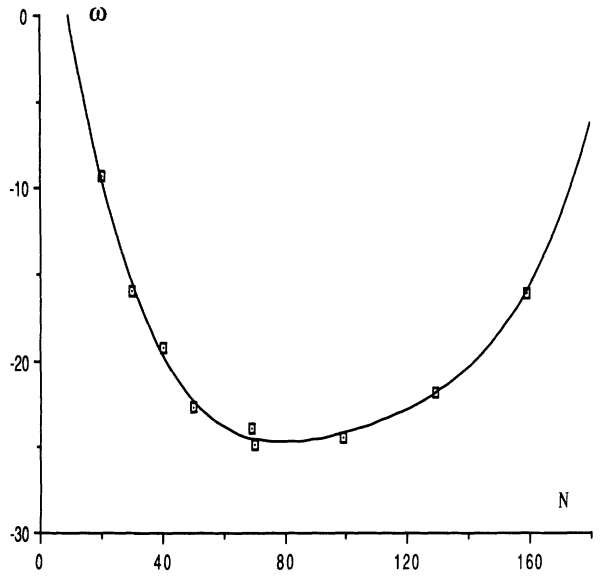

FIG. 2. ω versus N, where $\omega/N=[\langle r_g\rangle-0.417N^{0.5919}]/0.417N^{0.5919}$. If the value of the scaling exponent $\nu=0.5919$ deduced from MC simulations were correct, the plot in the figure should have been an ever decreasing curve with increasing N (see the text).

In what follows, we first give extensively our exact enumeration and Monte Carlo data, for the various mean values indicated above. Subsequently, assuming that the correct ν value is the RG value $\nu_{\rm RG}=0.588$, we shall try to specify the set of successive correction to scaling exponents Δ_i.

II. EXACT ENUMERATION AND MONTE CARLO RESULTS FOR $\langle r\rangle$, $\langle r^2\rangle$, $\langle r_g\rangle$, AND $\langle r_g^2\rangle$

In Table II we give the exact enumeration results for $\langle r\rangle$, $\langle r^2\rangle^{1/2}$, $\langle r_g\rangle$, and $\langle r_g^2\rangle^{1/2}$. Table III displays the precise Monte Carlo data for the same parameters, from 16 to 250 steps, and Table IV shows the limited precision data covering the range from 399 to 2999 steps. We present these data extensively, in order to avoid loss of information, as this would necessarily be the case if only small figures elaborated from these data were displayed. Further, in this way our calculations and conclusions can be checked, and different plots or calculations not considered here be performed, if so desired.

III. ANALYSIS OF THE MONTE CARLO DATA

Because the leading prefactor a_0 in Eq. (2) can only approximately be estimated from Fig. 1 and, because of the

TABLE II. Mean end-to-end distance $\langle r\rangle$, root-mean-square end-to-end distance $\langle r_2\rangle^{1/2}$, mean radius of gyration $\langle r_g\rangle$, and root-mean-square radius of gyration $\langle r_g^2\rangle^{1/2}$, for self-avoiding walks on the simple-cubic lattice, as a function of the number N of steps. Exact enumeration results from 1 to 15 steps.

N	$\langle r\rangle$	$\langle r^2\rangle^{1/2}$	$\langle r_g\rangle$	$\langle r_g^2\rangle^{1/2}$
1	1.000 00	1.000 00	0.500 00	0.500 00
2	1.531 37	1.549 19	0.696 63	0.699 21
3	1.907 57	1.969 77	0.848 74	0.854 40
4	2.275 77	2.356 63	0.986 87	0.994 86
5	2.577 42	2.689 67	1.109 70	1.120 31
6	2.884 47	3.011 73	1.227 22	1.239 98
7	3.149 17	3.301 10	1.335 64	1.350 68
8	3.417 77	3.584 00	1.440 47	1.457 55
9	3.657 14	3.844 55	1.538 98	1.558 21
10	3.899 91	4.100 88	1.634 93	1.656 11
11	4.120 87	4.340 67	1.726 15	1.749 34
12	4.344 73	4.577 43	1.815 41	1.840 46
13	4.551 47	4.801 26	1.900 93	1.927 88
14	4.760 67	5.022 80	1.984 89	2.013 61
15	4.955 93	5.233 84	2.065 79	2.096 31

TABLE III. The same mean values as in Table II, as determined through Monte Carlo sampling, from 16 to 250 steps. All Monte Carlo sample sizes ranging between 2.5 and 3.0×10^6 independent (noncorrelated) self-avoiding walks.

N	$\langle r\rangle$	$\langle r^2\rangle^{1/2}$	$\langle r_g\rangle$	$\langle r_g^2\rangle^{1/2}$
16	5.1542	5.4439	2.1455	2.1778
17	5.3396	5.6443	2.2226	2.2560
18	5.5254	5.8415	2.2983	2.3338
19	5.7025	6.0324	2.3717	
20	5.8841	6.2245	2.4451	2.4838
21	6.0550	6.4088	2.5161	
22	6.2280	6.5928	2.5862	
23	6.3885	6.7662	2.6540	2.6974
24	6.5584	6.9447	2.7220	
25	6.7176	7.1168	2.7884	2.8343
29	7.3326	7.7767	3.0439	3.0958
30	7.4853	7.9376	3.1054	
39	8.7475	9.2867	3.6280	3.6924
40	8.8840	9.4321	3.6839	
49	10.019	10.646	4.155	
50	10.140	10.776	4.205	4.283
69	12.276	13.057	5.094	5.190
99	15.204	16.191	6.314	6.437
129	17.778	18.941	7.390	7.537
159	20.140	21.458	8.370	8.537
199	22.987	24.500	9.562	9.756
200	23.062	24.581	9.591	9.786
249	26.237	27.972	10.919	11.142
250	26.303	28.045	10.947	11.171

statistical scattering of the MC data, the most satisfactory analysis of the data is obtained through a combination of graphical analysis and least-squares numerical analysis. The graphical method of analysis of the data is quite simple. Once a value for ν has been chosen (here $\nu=0.588$), a plot is made of $\ln\alpha_x$ versus $\ln N$, where

$$\alpha_x=a_0^x-\langle x\rangle/N^{0.588}=a_1^x/N^{\Delta_1}>0\ . \tag{4}$$

TABLE IV. The same mean values as in Tables I and II, as determined through Monte Carlo sampling, from 399 to 2999 steps. Monte Carlo sample sizes lying between 1.5 and 2.4×10^4 independent self-avoiding walks.

N	$\langle r\rangle$	$\langle r^2\rangle^{1/2}$	$\langle r_g\rangle$	$\langle r_g^2\rangle^{1/2}$
399	34.74	37.06	14.44	14.74
599	43.97	46.88	18.36	18.74
799	52.31	55.82	21.80	
999	59.65	63.68	24.89	
1199	66.52	70.97	27.74	
1399	72.85	77.65	30.34	
1999	89.87	95.95	37.46	
2000	89.57	95.60	37.43	38.26
2599	105.23	112.54	43.74	
2999	113.26	121.26	47.66	

The subscript or superscript x refers to the mean quantity considered. In the graphical analysis to follow $x=r_g$ exclusively. For large enough N values, such a plot should yield a straight line, whose slope gives Δ_1, and intercept the $\ln N$ axis, $\ln a_1$. A series of such plots should be drawn, taking in each instance a different value for a_0, which, fortunately enough, lie in a narrow range of values (see below). As soon as for a given a_0 value, Δ_1 and a_1 have been graphically determined, the quantity $\ln\beta$ is plotted versus $\ln N$, where

$$\beta=\langle r_g\rangle/N^{0.588}-a_0-a_1/N^{\Delta_1}>0\ . \tag{5}$$

Notice the change of sign of a_0 and $\langle r_g\rangle/N^{0.588}$ in the definitions of α and β, in order to keep these quantities positive. For N values not too small (though smaller than in the previous plot of $\ln\alpha$ versus $\ln N$), the plot of $\ln\beta$ versus $\ln N$ should again yield a straight line, from which Δ_2 and a_2 are determined. The procedure may be repeated, by introducing a third parameter

$$\gamma=\langle r_g\rangle/N^{0.588}-a_0-a_1/N^{\Delta_1}-a_2/N^{\Delta_2} \tag{6}$$

and plotting $\ln\gamma$ versus $\ln N$. However, in such a plot, the significant N values are quite small ($1\le N\le20$), and even-odd oscillations appear, which make the determination of a straight line uncertain. Remedy may be found to some extent to this situation, if one takes the mean of $\langle r_g\rangle$ for two successive N values, and makes the plot using half-integer N values. A fairly correct straight line can thus be obtained, and Δ_3 and a_3 are then unambiguously determined. However, as far as SAW's embedded on a lattice are concerned, the physical significance of Δ_3 becomes somewhat unclear, because in the series development of Eq. (2), Δ_3 is only a parameter that contributes to minimizing the least-squares error in the whole N range, and not actually yield the correct $\langle x\rangle_N$ value for small N values, where even-odd oscillations are predominant. This remark would, of course, become irrelevant if, e.g., in off-lattice SAW's, even-odd oscillations of the mean parameters disappear, and more generally in problems where the relevant parameter corresponding to N varies continuously and not discreetly. In such problems, the highest meaningful Δ_i would be determined by a lower cutoff, if any, introduced by the physics of the problem. To come back to the specific problem of SAW's on the simple-cubic lattice, a fourth correction to scaling exponent Δ_4 cannot really be determined by graphical means, and in any case is irrelevant as soon as N exceeds 3 or 4. Anticipating the results of the numerical analysis to follow, where introduction of a fourth correction to scaling exponent does not significantly improve the agreement between the result of the series expansion 2, and the actual values of the various mean values (except perhaps for the lowest N values), one may conclude that for SAW's on the cubic lattice the highest relevant correction to scaling exponent is the third one. In the numerical analysis to follow, we shall, however, consider a fourth correction to scaling exponent Δ_4 in the series expansion 2, to make a comparison possible with the fourth term up to Δ_3 expansion. In any case, as soon as N

exceeds 3 or 4, the two expansions are very nearly equivalent, in order to calculate the various mean values.

Graphical analysis of the results is time consuming and tedious, as the same procedure should be repeated for various a_0 values. Therefore, computer numerical analysis of the results may be used in support. To this end, a FIT algorithm has been devised. In this algorithm, arbitrary values of Δ_i are introduced ($2 \leq i \leq 7$) and the algorithm searches for the corresponding a_i prefactors, which minimize the squared error of the MC points. The FIT algorithm offers a possibility either to prescribe the value of a_0, the leading prefactor, or to let it vary freely. The first two corrections to scaling exponents are so chosen as to correspond approximately to the value found by graphical analysis, i.e., $\Delta_1 \simeq 0.50$ and $\Delta_2 \simeq 1.00$. A significant number of least-squares fits were thus performed, taking, in Eq. (2), $k=3$ or 4. It appears that the prefactor of the term in Δ_4 is always small and even in some instances zero, so that a four-term expansion

$$\langle x \rangle = N^{0.588}[a_0^x + a_1^x N^{-\Delta_1} + a_2^x N^{-\Delta_2} + a_3^x N^{-\Delta_3}] \quad (7)$$

is convenient, in accord with the findings of graphical analysis. A fortunate occurrence, disclosed by the FIT algorithm, is that when the leading prefactor a_0 is allowed to vary freely, the effect of varying Δ_3 and Δ_4 is negligible on the value taken by a_0, and that of varying Δ_2 is small. Thus, it appears that the leading prefactor varies within a quite narrow range of values when different sets of Δ_i values are introduced in the FIT algorithm. This fact could not have been guessed from a purely graphical analysis of the data, except perhaps after overwhelmingly time consuming and tedious work. Here the complementarity of graphical and numerical analysis appears clearly: the graphical analysis, taking a plausible but arbitrary value for a_0, suggests the approximate values of Δ_1 and Δ_2 to be introduced in the FIT algorithm; the FIT algorithm in turn, through successive trials, specifies which sets of Δ_i's lead to the smallest squared errors and displays the corresponding prefactors. The time required by the FIT algorithm to make a single calculation, depends, of course, on the number of terms considered in the series expansion, Eq. (2). For a five-term expansion, this time is of the order of 10 min, for 10 000 iterations, using a 50-MHz clock frequency PC. A summary of the results of the graphical and least squares analysis will now be given.

A. Graphical analysis

Graphical analysis of the MC data was performed using only the $\langle r_g \rangle$ data. Consideration of $\langle r_g \rangle$ instead of $\langle r \rangle$ (or of $\langle r_g^2 \rangle^{1/2}$ instead of $\langle r^2 \rangle^{1/2}$) reduces the relative importance of even-odd oscillations for small N values ($N < 20$). Also, as the distribution of r_g, the radius of gyration, is more narrow than that of $\langle r \rangle$, the end-to-end distance, the statistical scattering of the MC data is reduced when using the former parameter, for the same sample size, increasing correspondingly the precision of the determinations. Taking $\nu = 0.588$, the RG value, and $a_0 \simeq 0.432$, as suggested from Fig. 1, Fig. 3 displays a plot of $\ln\alpha$, defined through Eq. (4), versus $\ln N$. For the higher values of N, this plot should yield a straight line, from which the values of Δ_1 and a_1 are determined. Unfortunately, the high N points ($N > 250$), are also the less precise, and therefore unambiguous determination of the above parameters is not possible. However, a value for Δ_1 of 0.50 appears reasonable, and this leads to $a_1 = 0.106$. With these values for Δ_1 and a_1, β given by Eq. (5) has in turn been calculated, and a plot of $\ln\beta$ versus $\ln N$ made (Fig. 4). It is found that Δ_2 is slightly larger than one, the corresponding a_2 value being 0.247. Advantage may now be taken of the fact that $\Delta_1 \simeq 0.50$, $\Delta_2 \simeq 1.0$, to write $\alpha N \simeq a_1 N^{0.50} + a_2$. A plot of αN versus $N^{0.50}$ yields a good straight line (Fig. 5) from which it is found that $a_1 = 0.108$ and $a_2 = 0.238$, in good agreement with the previous determination. Finally a plot of $\ln\gamma$ versus $\ln N$ (not here reproduced), where half-integer values of N have been used to circumvent the effect of even-odd oscillations, leads to a value for Δ_3 somewhat larger than two.

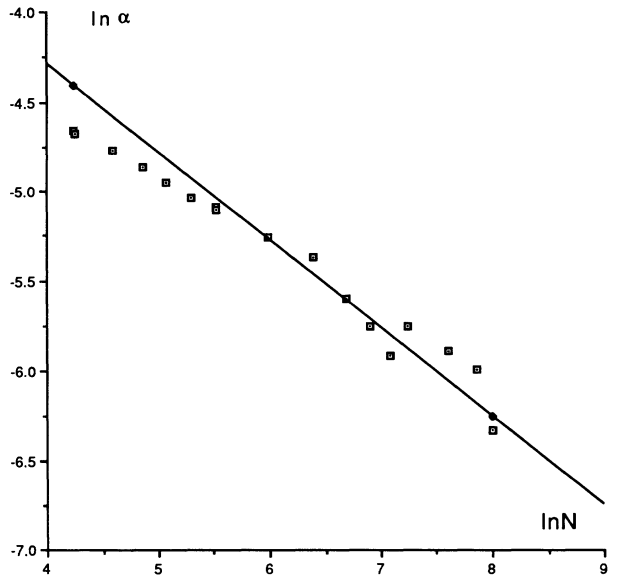

FIG. 3. Plot of $\ln\alpha$ versus $\ln N$. N is the number of steps in the self-avoiding walk and $\ln\alpha = \ln[0.432 - \langle r_g \rangle_{MC}/N^{0.588}] \simeq \ln a_1 - \Delta_1 \ln N$. $\langle r_g \rangle_{MC}$ is the mean radius of gyration as deduced from Monte Carlo simulations, Δ_1 the first correction to scaling exponent and a_1 the corresponding prefactor [see Eqs. (1) and (2)]. The high-N Monte Carlo points are scattered, so that the corresponding straight line cannot be precisely determined. However, a value $\Delta_1 = 0.49 \pm 0.02$ appears correct, with error bounds within the renormalization-group value $\Delta_1 = 0.47$. The corresponding a_1 value is 0.106.

B. Least-squares treatment

From the outset the assumption is made that $\langle r_g \rangle$, $\langle r_g^2 \rangle^{1/2}$, $\langle r \rangle$, and $\langle r^2 \rangle^{1/2}$ belong to the same universality class. Thus, the physically correct Δ_i's should be the same for all the above mean values. This assumption, which appears quite natural, is also born by the results of the FIT determinations, which show that whatever the mean value considered, it is always approximately the

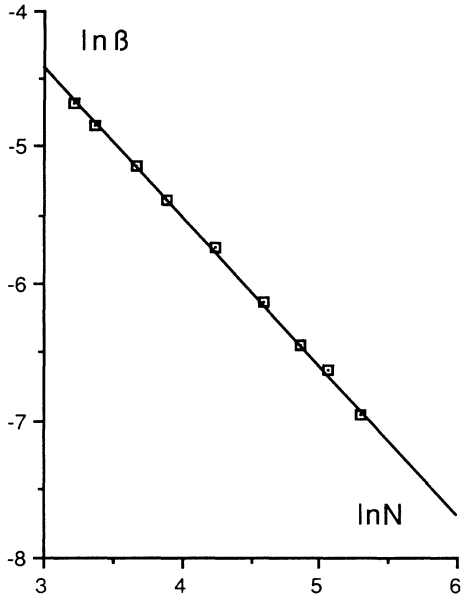

FIG. 4. Plot of $\ln\beta$ versus $\ln N$, with $\beta=\langle r_g\rangle_{MC}/N^{0.588}-0.432+0.106/N^{0.50}$. One has $\ln\beta=\ln a_2-\Delta_2\ln N$, so that the slope of the straight line yields the second correction to scaling exponent Δ_2 and the intercept with the $\ln N$ axis the prefactor a_2. The result is $\Delta_2\simeq 1.02$ and $a_2\simeq 0.247$.

same sets of Δ_i values that minimize the least-squares errors. The second assumption is that numerical analysis should lead to nearly the same prefactors a_i as the graphical analysis. With the numerical values $\nu=0.588$, $a_0=0.432$, $\Delta_1=0.50$, $\Delta_2=1.00$, and $\Delta_3=2.00$ the least-squares treatment yields the expansion

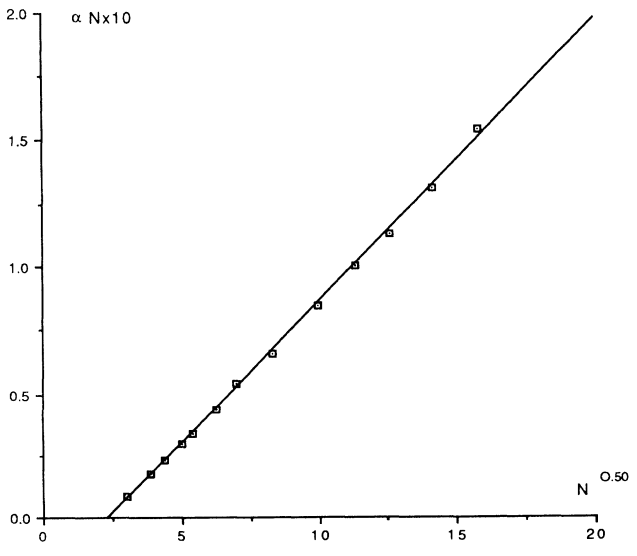

FIG. 5. Plot of αN, where $\alpha=0.432-\langle r_g\rangle_{MC}/N^{0.588}$ versus $N^{0.50}$. Because $\Delta_1\simeq 0.50$ and $\Delta_2\simeq 1$, one has $\alpha N\simeq a_1 N^{0.50}+a_2$, where a_1 and a_2 are, respectively, the prefactors to the first Δ_1 and second Δ_2, correction to scaling exponents. The straight line obtained yields $a_1=0.108$ and $a_2=0.238$, in good accord with the graphical analyses of Figs. 3 and 4.

$$\langle r_g\rangle=N^{0.588}[0.432-0.1107N^{-0.50}+0.2584N^{-1.00}-0.0797N^{0-2.00}]\,. \quad (8)$$

The agreement for a_1 and a_2 with the results of the graphical analysis is satisfactory. From here on, we shall therefore assume that there is not an important difference between the prefactors as determined by graphical or numerical analysis and shall determine the expansions for the mean values other than $\langle r_g\rangle$ only by the latter method. We remind the reader that our fit analysis was performed taking for ν the RG value $\nu_{RG}=0.588$. The Monte Carlo value $\nu_{MC}=0.592$ found by the present as well as numerous other investigators[1-4] is quite certainly not correct, for the reasons indicated in Sec. I. In any case, the correct ν value almost certainly lies within the error bounds set by the RG calculations,[10] that is $\nu=0.588\pm 0.001$. As for the value of Δ_1, this may be approximately determined from Fig. 3 to be $\Delta_1=0.49\pm 0.02$. Unfortunately, it is the high values of N, which are relevant for a precise determination of Δ_1, and in this range ($399<N<2999$), our MC samples of 1.6 to 2.4×10^4 SAW's are too small for an unambiguous two-digit determination of this parameter. Sample sizes of at least 10^6 SAW's are required for such a two-digit determination, and this lies outside the possibilities of our Alexandrowicz dimerization procedure. For this reason, two values have been chosen for the FIT algorithm calculations, $\Delta_1=0.50$ and $\Delta_1=0.47$. The former value is the one suggested by our graphical analysis and the later value is the one given by Le Guillou and Zinn-Justin.[5,10] Other values for Δ_1, complying with the error bounds set by Fig. 3, could have been used. However, in the present state of the matter, this would complicate things without adding anything fundamentally new. Further, from the raw data in Tables II–IV, one should be able, if so desired, to undertake such additional calculations.

Once the Δ_1 value is chosen, the corresponding complete sets of Δ_i's, which minimize the square error have been determined through a considerable amount of FIT trials. To dissipate any doubt, we have repeatedly checked by numerical analysis that a Taylor series expansion in powers of N^{-1} ($\Delta_1=1$, $\Delta_2=2$, $\Delta_3=3$, etc.) does not provide satisfactory results. This would have been contrary to what our graphical analysis did suggest and to the results of RG calculations. Now, for $\Delta_1=0.50$, the best set was found to be $\Delta_2=1.00\pm 0.01$, $\Delta_3=2.0\pm 0.1$, and Δ_4 essentially equal to 4.0. For the RG value $\Delta_1=0.47$, the best set was found to be $\Delta_2=1.05\pm 0.01$, $\Delta_3=2.2\pm 0.2$, and $\Delta_4=4.4\pm 0.4$. These sets concern all mean values, that is $\langle r\rangle$, $\langle r^2\rangle^{1/2}$, $\langle r_g\rangle$, and finally $\langle r_g^2\rangle^{1/2}$. Thus, the numerical analysis confirms the universality of the above parameters, as assumed from the outset.

Table V displays for $\langle r_g\rangle$, with the leading prefactor a_0 given prescribed values, the resulting prefactors a_i for the above two Δ_i sets. Four- and five-term series are successively shown. It is seen that adding a fifth term in the series changes very little the values of the preceding prefactors. In addition, a_4 is always small. Therefore, as already suggested, a four-term expansion appears satisfac-

TABLE V. Four- and five-term expansions of $\langle r_g \rangle$, the mean radius of gyration, with prescribed values for the correction to scaling exponents Δ_i ($i=1-3$ and $i=1-4$, respectively), and for the leading prefactor a_0, as indicated. The values of the prefactors are given in the first through fifth columns. The star in the superscript of a_0 emphasizes that this parameter is prescribed to the value indicated and not allowed to vary freely. The mean-square error is given in the sixth column. All data of Tables II to IV have been used to establish this table.

a_0^*	a_1	a_2	a_3	a_4	$E\times10^3$
		Set 0.50, 1.00, 2.00			
		Set 0.50, 1.00, 2.00, 4.00			
0.4320	−0.1107	0.2584	−0.0797		1.677
0.4320	−0.1105	0.2574	−0.0777	−0.0012	1.674
0.4319	−0.1101	0.2581	−0.0798		1.585
0.4319	−0.1097	0.2563	−0.0763	−0.0021	1.575
0.4318	−0.1090	0.2555	−0.0782		1.587
0.4318	−0.1082	0.2510	−0.0710	−0.0044	1.542
0.4317	−0.1082	0.2540	−0.0775		1.613
0.4317	−0.1071	0.2490	−0.0676	−0.0060	1.531
		Set 0.47, 1.05, 2.20			
		Set 0.47, 1.05, 2.20, 4.40			
0.4320	−0.0897	0.2338	−0.0762		1.659
0.4320	−0.0902	0.2370	−0.0849	0.0062	1.614
0.4319	−0.0890	0.2326	−0.0756		1.558
0.4319	−0.0897	0.2362	−0.0839	0.0054	1.449
0.4318	−0.0881	0.2305	−0.0741		1.598
0.4318	−0.0885	0.2324	−0.0789	0.0029	1.582
0.4317	−0.0874	0.2292	−0.0735		1.624
0.4317	−0.0876	0.2301	−0.0754	0.0013	1.621

tory, and three correction to scaling exponents will have, in general, to be considered. Also (not displayed in Table V), it was found that if the first few N values (say up to $N=3$) are truncated, addition of a fifth term in the expansion of Eq. (2) is completely irrelevant, as the term a_4/N^{Δ_4}, where Δ_4 equals at least 4, is completely negligible beyond $N=3$ or 4. As for the square error, it is found that the set 0.47, 1.05, 2.2, 4.4 is best for the highest allowed values of the leading prefactor a_0, while for the lowest allowed values of a_0 it is a regular set 0.50, 1.00, 2.0, 4.0, which is most satisfactory.

Table VI displays the set of a_i's for the two above five term expansions in Δ_i's for the various mean values. Here the leading prefactor a_0 is not prescribed but allowed to vary freely. The versatility of the FIT algorithm allows one to truncate the set of data at the two ends, so that one may choose, in order to specify the set of prefactors, either the full set of exact enumeration (EE) plus MC data, or only the MC data, or the EE plus the precise MC data, or only the precise MC data. To avoid, however, fastidious exposition of data of no particular interest, only two sets of data have been tabulated, the total data displayed in Tables II to IV and the MC data only displayed in Table III and IV. Elimination of the EE data may reduce the m.s. error, because of elimination of points that display important even-odd oscillations. On the other hand, the smallest m.s. errors are obtained if only the precise MC points are considered, eliminating thus errors originating in even-odd oscillations for small N values, and statistical errors due to limited precision of the data for large N values. However, from a physical standpoint, truncation of vast ranges of N values very probably has an effect on the correctness of the results obtained, and for this reason such results have not been tabulated.

Numerous trials with Δ_i values other than those here reported, always displayed a_0 values very close to those given in Table VI. In fact, it appears that only the value chosen for Δ_2 (since Δ_1 is specified either as 0.47 or 0.50) is of any significance for the corresponding value of a_0. This is a fortunate occurrence, as it considerably limits the range of values of a_0 to be considered when the value of this parameter is prescribed, as this is the case in Table V. Here lies the justification of the fact that in this table the leading prefactor a_0 is allowed to vary within the narrow range $a_0=0.4317$ to 0.4320 only. For $\langle r_g \rangle$, the

correct value of the leading prefactor quite certainly lies somewhere within the above narrow range. A similar remark can be made regarding the leading prefactors of all the other mean values here considered, and displayed in Table VI. We again emphasize the fact that if one fixes $\Delta_1=0.50$ or $\Delta_1=0.47$, the two corresponding sets of Δ_i's are, respectively, 0.50, 1.00, 2.0, 4.0 and 0.47, 1.05, 2.2, 4.4, and this usually happens for all mean values and all truncation of raw data considered. Therefore, these two sets are somewhat arbitrary only in the value chosen for the first correction to scaling exponent Δ_1. It thus becomes apparent that each successive correction to the scaling exponent is nearly the double of the preceding one. An exact relationship, $\Delta_i=2\Delta_{i-1}$, cannot be excluded.

IV. DISCUSSION AND CONCLUSION

The discussion will be based on Table VII, where set I and set II represent, respectively, the expansions

$$\langle r_g\rangle = N^{0.588}[0.4317-0.1072N^{-0.50}+0.2479N^{-1.00}-0.0562N^{-2.00}] \quad (9)$$

and

$$\langle r_g\rangle = N^{0.588}[0.4319-0.895N^{-0.47}+0.2349N^{-1.05}-0.0720N^{-2.20}] , \quad (10)$$

which have been deduced from Table VI. It is seen that the respective adequacies of these two expansions are mathematically indistinguishable, though from the physical viewpoint only one of these expansions should be correct, or, at least, more correct than the other, depending, in fact, on the physically correct value of Δ_1. Thus, no preference can be given here for either of these expansions. On the other hand, one should notice the excellent behavior of the simple law

$$\langle r_g\rangle = 0.417N^{0.5919} \quad (11)$$

TABLE VI. Prefactors a_i in five-term expansions for $\langle r_g\rangle$, the mean radius of gyration, $\langle r_g^2\rangle^{1/2}$, the root-mean-square radius of gyration $\langle r\rangle$, the mean (in modulus) end-to-end distance, and $\langle r^2\rangle^{1/2}$, the root-mean-square end-to-end distance. Two sets of corrections to scaling exponents Δ_i ($i=1$–4) have been considered: set I, 0.50, 1.00, 2.0, 4.0 and set II, 0.47, 1.05, 2.2, 4.4, respectively. The set of values used for each of the above mean values is, first, all the data in Tables II–IV (exact enumeration plus Monte Carlo data), and below, the Monte Carlo data only, from 16 to 2999 steps. Contrary to Table V, the leading prefactor a_0 is here left to vary freely, and the adequacy of the expansion estimated through the corresponding square error E (last column). Elimination of the exact enumeration data reduces E because the error originating in even-odd oscillations of the mean parameters for small N is suppressed. Both even-odd oscillations and Monte Carlo statistical errors are particularly important for $\langle r\rangle$ and $\langle r^2\rangle^{1/2}$.

	a_0	a_1	a_2	a_3	a_4	$E\times10^3$
			Set 0.50, 1.00, 2.0, 4.0			
All data $\langle r_g\rangle$	0.4317	−0.1071	0.2495	−0.0682	−0.0060	1.456
MC data only $\langle r_g^2\rangle^{1/2}$	0.4316	−0.1036	0.2293	0.0539	0.0004	1.143
All data	0.4411	−0.1191	0.2483	−0.0613	−0.0090	1.075
MC data only $\langle r\rangle$	0.4404	−0.1043	0.1747	0.3068	0.0026	0.448
All data	1.0359	−0.1098	0.0850	0.1136	−0.1194	13.323
MC data only $\langle r^2\rangle^{1/2}$	1.0311	−0.1261	0.1505	0.0461	0.0003	9.577
All data	1.1020	−0.1656	0.08368	0.0211	0.0410	10.448
MC data only	0.1021	−0.1743	0.1414	−0.1984	0.0007	9.696
			Set 0.47, 1.05, 2.2, 4.4			
$\langle r_g\rangle$						
All data	0.4318	−0.0888	0.2340	−0.0808	0.0038	1.479
MC data only $\langle r_g^2\rangle^{1/2}$	0.4318	−0.0873	0.2218	0.0307	0.0001	1.144
All data	0.4413	−0.0998	0.2314	−0.0728	0.0000	1.080
MC data only $\langle r\rangle$	0.4408	−0.0914	0.1842	0.1964	0.0009	0.514
All data	1.0310	−0.0973	0.0772	0.1134	−0.1242	13.114
MC data only $\langle r^2\rangle^{1/2}$	1.0313	−0.1073	0.1217	0.1474	0.0916	10.636
All data	1.1024	−0.1461	0.0565	0.0350	−0.0478	10.311
MC data only	1.1024	−0.1498	0.0801	−0.0105	0.0000	9.690

TABLE VII. Comparison of the values obtained for $\langle r_g \rangle$, the mean radius of gyration, by exact enumeration (*) or Monte Carlo samples (set II column), by the two single-term laws $\langle r_g \rangle = 0.432N^{0.588}$ and $\langle r_g \rangle = 0.417N^{0.5919}$ (third and fourth columns), and by two four-term expansions [see Eq. (2)], indicated by set I and set II, respectively: set I, $\Delta_1 = 0.50$, $\Delta_2 = 1.00$, $\Delta_3 = 2.00$, and $a_0 = 0.4317$, $a_1 = -0.1072$, $a_2 = 0.2479$, and $a_3 = -0.0562$. Set II, $\Delta_1 = 0.47$, $\Delta_2 = 1.05$, and $\Delta_3 = 2.2$, and $a_0 = 0.4319$, $a_1 = -0.0895$, $a_2 = 0.2349$, and $a_3 = -0.0720$. The excellent behavior of the simple law $\langle r_g \rangle = 0.417N^{0.5919}$, which, however, is not theoretically founded, is evident, as soon as N is not too small (see the text). Within the range of interest of N to polymer science, simple laws of the form $\langle x \rangle = a_x N^{0.592}$ are certainly more convenient than simple laws of the form $\langle x \rangle = a'_x N^{0.588}$.

N	EE* or MC	$0.432N^{0.588}$	$0.417N^{0.5919}$	Set I	Set II
5	1.109 70*	1.1130	1.0811	1.1109	1.1106
15	2.0658*	2.1234	2.0714	2.0656	2.0659
49	4.155	4.259	4.174	4.156	4.155
249	10.919	11.078	10.925	10.921	10.921
2999	47.66	47.86	47.66	47.60	47.60

from 50 to at least 3000 steps. This law had been adopted as correct in our previous paper.[1] Here, of course, lies the root of the confusion, namely, that RG calculations and MC simulations lead to different values for the correlation length critical exponent ν. In fact, the discrepancy is only apparent, and should be ascribed to the peculiar form of curve II in Fig. 1. If it were possible to obtain adequate samples of very large SAW's ($N > 10^6$), then the MC ν would undoubtedly be found to be equal to the RG ν, within the error bounds of the later calculations. Thus, Zifferer's conjecture quoted in the Introduction appears to be correct. Let us further notice that in Polymer Science, chains with repeat units lying between 50 and 10 000 cover most of the range of interest, so that for practical purposes, a simple law of the form $\langle x \rangle = a_x N^{0.5919}$, as assumed in Ref. 1, could be used to advantage, even if not theoretically correct.

The present investigation also shows that the successive correction to scaling exponents Δ_i, are approximately given by a simple law of the form

$$\Delta_i = 2^{i-2} \tag{12}$$

As previously noticed, an exact law of this form cannot be excluded, though our MC data are not precise enough to establish or discard that conjecture.

Finally, for the discreet problem involved in SAW's, Δ_i exponents beyond $i = 3$ [corresponding to a four term expansion in Eq. (2)] are of limited practical interest and possibly devoid of physical significance. However, there may exist problems in renormalization-group theory, where some continuously varying parameter is involved, instead of the discreet N of SAW's. In such instances, if any, higher i values might have to be considered, up to some highest value, corresponding to a cutoff originating in the physics of the problem.

ACKNOWLEDGMENTS

The authors wish to thank the following members of the Strasbourg Faculty for their assistance with this work: Professor Roger Hocquart (Institute Le Bel), Professor Jean Ladevèze (Ecole d'Application des Hauts Polymères), Dr. Jean Adloff (Institute de Physique), Dr. A. Fruchard (Institut de Recherches Mathematiques Avancées), Dr. François Lequeux (Institute de Physique), and Dr. Claude Picot (Institut Charles Sadron). They also thank Professor M. Allavena (Centre National de la Recherche Scientifique) for allowing the authors 125 hours of use of the IBM 3909 computer at the "Centre de Calcul de Strasbourg-Cronembourg." Finally, they are very grateful to Anne Helleboid and François Woehl, in charge of the computing facility of the Institut Charles Sadron, for their continuous assistance.

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