Critical exponents of self-avoiding walks in three dimensions

N. Eizenberg and J. Klafter
School of Chemistry, Tel Aviv University, Tel Aviv, 69978 Israel
(Received 6 July 1995)

We analyze Monte Carlo data of self-avoiding walks with up to about 8000 steps on a simple cubic lattice with emphasis on the question of the discrepancy between the scaling exponents obtained by renormalization group calculations and Monte Carlo simulations. This discrepancy has been recently investigated by Dayantis and Palierne [Phys. Rev. B **49**, 3217 (1994)] for self-avoiding walks of up to 3000 steps, and has been shown to originate from the finite size of chains generated in Monte Carlo simulations. Our analysis demonstrates this conjecture and shows that the exponents decrease for longer chains toward the renormalization group value.

Recently it has been indicated by several Monte Carlo (MC) simulations[1,2] that the critical exponent ν of the self-avoiding walk (SAW) in three dimensions exceeds the renormalization-group (RG) result[3] $\nu=0.588\pm0.001$ and does not reach an asymptotic value even for rather long chains. Table I presents MC simulation estimates of the critical exponents ν_R and ν_S, which correspond to the mean-square end-to-end distance and the mean-square radius of gyration, respectively.[1,4–7] The range of N, which is the number of steps of the SAW, is indicated for each result. As has been first noticed by Zifferer,[1] the critical exponent obtained through a log-log plot of the MC data in the range of short chains (99–999 steps in Ref. 1) is slightly larger than the critical exponent obtained in the range of longer chains (999–9999 steps in Ref. 1). This observation is also supported by the difference between the ν values obtained in previous MC simulations,[4–6] with chain lengths of up to 3000 steps at the most, and the results obtained for longer chains,[1,7] as shown in Table I. It should be noted, however, that the different ν values, obtained by dividing the data into two groups of short and long chains, are equal within the statistical uncertainty of the results.[1,7]

The observations discussed above have been conjectured recently by Zifferer[1] and by Dayantis and Palierne[2] to result from the finite size of the SAW's generated in the MC simulations. Namely, the chains generated in the MC simulations have not been sufficiently long to reach the asymptotic value of the critical exponent ν by fitting to a simple power law, and corrections to scaling have been necessary even for chain lengths of the order of 10^2-10^3 steps. According to the renormalization-group (RG) theory[3] one expects

$$\langle X_N\rangle = N^{2\nu}(C_0 + C_1 N^{-\Delta_1} + C_2 N^{-\Delta_2} + \cdots) \qquad (1)$$

where $\langle X_N\rangle$ is the averaged length property (for example, the mean-square end-to-end distance), $\nu=0.588\pm0.001$ and $\Delta_1=0.47\pm0.03$. Dayantis and Palierne[2] performed a detailed analysis of their data (for N up to 2999 steps) with respect to this scaling law in order to show that the MC result for ν tends towards the RG result as N is increased. Assuming that the asymptotic value of ν is the RG result, they obtained the set of scaling parameters for various length properties, taking $\Delta_1=0.5$ (the fitting result) or $\Delta_1=0.47$ (the RG result). Their results show that the scaling law in Eq. (1) describes correctly the data up to 50 steps, while the data above 50 steps are described successfully either by the scaling law or by a simple power law with $\nu=0.5919$. This suggests[2] that the difference between the MC and the RG results may originate from the slow decrease of ν towards the asymptotic value, which still allows a very good fit of the MC data to a simple power law.

TABLE I. Monte Carlo values of the critical exponent ν in three dimensions. The exponent ν_R corresponds to the mean-square end-to-end distance and the exponent ν_S to the mean-square radius of gyration.

	N range	ν_R	ν_S	A_R	A_S
Rapaport (Ref. 4)	200–2400	0.5919±0.0004	0.5933±0.0004	1.134±0.005	0.1772±0.0006
Madras and Sokal (Ref. 5)	200–3000	0.5907±0.0014	0.5939±0.0020	1.156±0.022	0.1768±0.0044
Zifferer (Ref. 1)	99–9999	0.5901	0.5916		
	99–999	0.5910	0.5925		
	999–9999	0.5895	0.5910		
Dayantis and Palierne (Ref. 6)	50–800		0.5919±0.0002		
Eizenberg and Klafter (Ref. 7)	200–7168	0.5904±0.0003	0.5914±0.0003	1.1594±0.0005	0.1820±0.0006
	200–3200	0.5908±0.0004	0.5921±0.0004	1.153±0.007	0.1803±0.0007

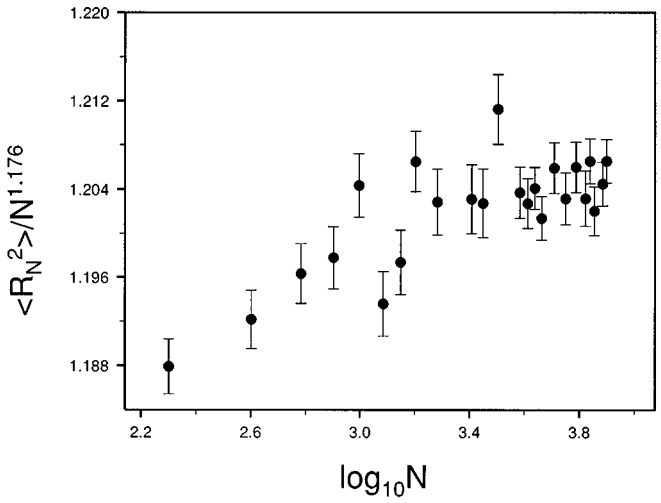

FIG. 1. $\langle R_N^2\rangle/N^{2\nu}$ vs $\log_{10}N$, using the renormalization-group (Ref. 3) prediction $2\nu=1.176$. $\langle R_N^2\rangle$ is the mean-square end-to-end distance of an N-step SAW. Error bars are the standard deviation.

In this comment we intend to further establish the assertion that ν decreases towards the RG result as the chain length is increased. Our first step has been to verify that ν, obtained from our MC data, indeed decreases as N increases. As mentioned already the decrease observed in previous MC simulations[1,7] was within the statistical uncertainty of the results. Here we improve the accuracy of the MC data in the range of relatively long chains ($N>3200$) in order to evidence this decrease. For this purpose we have continued our previous MC simulations[7] on a simple-cubic lattice to generate SAW's with N in the range from 3200 to 7936 steps. As before, we have used the pivot algorithm,[1,5,7,8] which has been proven to be extremely efficient for the study of global equilibrium properties of chains. Table II presents the obtained values of $\langle R_N^2\rangle$ and $\langle S_N^2\rangle$, which are the mean-square end-to-end distance and the mean-square radius of gyration, respectively. The results in Table II with N ranging from 200 to 3200 steps were taken from our previous work.[7] The standard deviations of $\langle R_N^2\rangle$ and $\langle S_N^2\rangle$ were determined as described in Ref. 7. The number of iterations for each run was 1.8×10^6 for $N\leqslant3200$ and 3.8×10^6 for $N>3200$. The computation time for generating 3.8×10^6 SAW's of 7936 steps, for example, was 76 h on the RS 6000. The initial chain required for the pivot algorithm was generated using the dimerization method,[9] and it took 1.5 h on the RS 6000 to generate an initial chain of 7936 steps.

Fitting our data with N ranging from 200 to 7936 steps to the power law $AN^{2\nu}$ through a log-log plot and using a weighted least-squares fit,[7] gave for $\langle R_N^2\rangle=A_RN^{2\nu_R}$,

$$\nu_R=0.5896\pm0.0002, \qquad A_R=1.171\pm0.004 \tag{2}$$

and for $\langle S_N^2\rangle=A_SN^{2\nu_S}$,

$$\nu_S=0.5908\pm0.0002, \qquad A_S=0.1834\pm0.0006. \tag{3}$$

These ν values are smaller than our previous results[7] for N between 200 and 7168, which were $\nu_R=0.5904\pm0.0003$ and $\nu_S=0.5914\pm0.0003$. The difference is due to the fact that, although the range of N has not been significantly changed, we have improved the statistics and accuracy of $\langle R_N^2\rangle$ and $\langle S_N^2\rangle$ in the range of relatively long chains ($N>3200$). Therefore, the proportional weight of the results in this range, when performing a weighted least-squares fit, is larger in comparison with our previous analysis. This indicates that the critical exponent ν tends to decrease as N increases. In order to show this trend more clearly we have

TABLE II. Estimates for the mean-square end-to-end distance $\langle R_N^2\rangle$ and the mean-square radius of gyration $\langle S_N^2\rangle$.

N	$\langle R_N^2\rangle$	$\langle S_N^2\rangle$
200	603.66±1.27	95.48±0.18
400	1 368.87±3.04	217.74±0.43
608	2 247.61±5.11	357.72±0.73
800	3 107.50±7.35	494.64±1.08
992	4 023.88±9.63	640.64±1.41
1 216	5 066.85±12.43	807.73±1.78
1 408	6 039.24±14.78	963.92±2.16
1 600	7 072.45±15.99	1 127.07±2.57
1 920	8 737.20±21.61	1 391.59±3.16
2 560	12 257.2±31.7	1 951.04±4.64
2 816	13 706.7±35.6	2 188.64±5.18
3 200	16 042.9±42.0	2 559.18±6.14
3 840	19 755.5±38.0	3 151.55±7.03
4 096	21 296.0±39.9	3 401.39±5.81
4 352	22 895.7±36.0	3 654.98±4.56
4 608	24 432.4±40.2	3 910.44±5.89
5 120	27 759.9±53.0	4 435.66±7.92
5 632	30 981.1±60.5	4 950.05±9.54
6 144	34 400.4±65.1	5 487.73±10.5
6 656	37 706.6±78.4	6 028.44±13.5
6 912	39 528.4±66.7	6 323.21±10.2
7 168	41 101.8±75.7	6 581.99±13.9
7 680	44 666.4±73.6	7 145.12±9.0
7 936	46 502.0±75.5	7 422.16±10.6

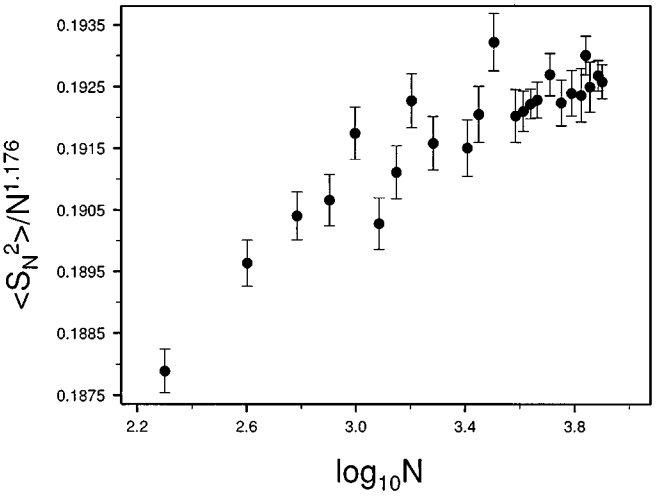

FIG. 2. $\langle S_N^2\rangle/N^{2\nu}$ vs $\log_{10}N$, using the renormalization-group (Ref. 3) prediction $2\nu=1.176$. $\langle S_N^2\rangle$ is the mean-square radius of gyration of an N-step SAW. Error bars are the standard deviation.

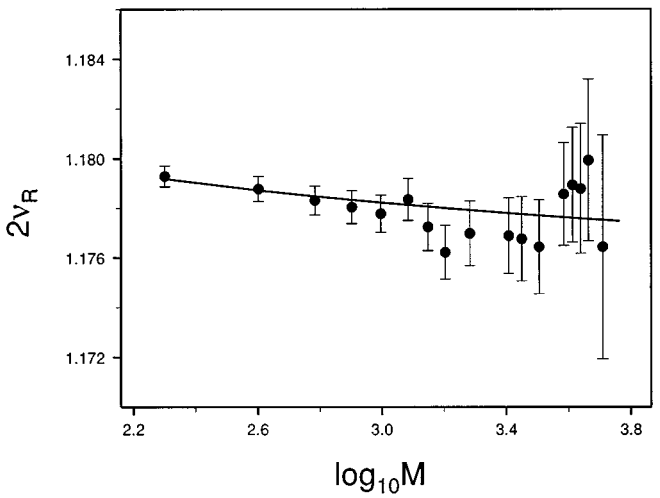

FIG. 3. Black circles, a plot of $2\nu_R$, obtained through a log-log fit of our MC data for $\langle R_N^2\rangle$ with N ranging from M to 7936 steps, vs $\log_{10}M$. Error bars are the standard deviation. Solid line, a plot of $2\nu_R$, obtained through a log-log fit of the reproduced $\langle R_N^2\rangle$ values with N ranging from M to 8000 steps, vs $\log_{10}M$.

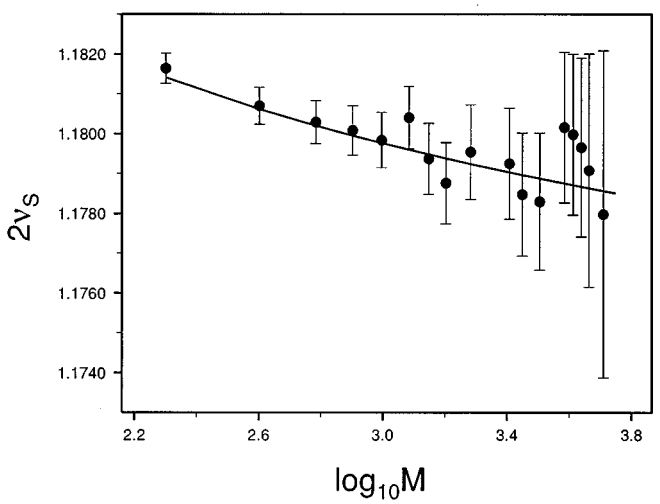

FIG. 4. Black circles, a plot of $2\nu_S$, obtained through a log-log fit of our MC data for $\langle S_N^2\rangle$ with N ranging from M to 7936 steps, vs $\log_{10}M$. Error bars are the standard deviation. Solid line, a plot of $2\nu_S$, obtained through a log-log fit of the reproduced $\langle S_N^2\rangle$ values with N ranging from M to 8000 steps, vs $\log_{10}M$.

divided our MC data into two groups: $N\leqslant 3200$ and $N\geqslant 3200$. The critical exponents obtained from our MC data with $N\leqslant 3200$ are[7]

$$\nu_R = 0.5908 \pm 0.0004, \qquad A_R = 1.153 \pm 0.007, \tag{4}$$

$$\nu_S = 0.5921 \pm 0.0004, \qquad A_S = 0.1803 \pm 0.0007,$$

and with $N\geqslant 3200$ are

$$\nu_R = 0.5882 \pm 0.0009, \qquad A_R = 1.200 \pm 0.020, \tag{5}$$

$$\nu_S = 0.5891 \pm 0.0009, \qquad A_S = 0.1887 \pm 0.0028.$$

It can be seen that the ν values which have been obtained for $N\geqslant 3200$ are significantly smaller than the ν values in the range of $N\leqslant 3200$. The difference between the exponents in Eq. (4) and Eq. (5) is not within the statistical uncertainty of the results, especially for ν_S. This provides evidence that ν really decreases as the chain length is increased. A further analysis of our results supports this observation.

As mentioned, the critical exponent ν is expected to decrease towards an asymptotic limit as $N\to\infty$, with the RG results as the asymptotic value. In Figs. 1 and 2 we present plots of $\langle R_N^2\rangle/N^{1.176}$ and $\langle S_N^2\rangle/N^{1.176}$ vs $\log_{10}N$. According to Eq. (1) these plots should approach a plateau for $N\gg 1$, as the scaling law in Eq. (1) approaches the asymptotic power-law behavior $C_0N^{2\nu}$ with $2\nu=1.176$. The curves in Figs. 1 and 2 clearly flatten as N increases although they are too scattered to prove the existence of a plateau. Figure 2, which is somewhat less scattered, indicates that the asymptotic limit for ν_S has not been recovered within the range of our MC simulation.

Our MC data for $\langle R_N^2\rangle$ and $\langle S_N^2\rangle$ have been fitted to the power law $AN^{2\nu}$ over the range of $N=M$ to $N=7936$ steps for different values of the lower bound M. The purpose of this analysis is to show the decrease of the critical exponent when the contribution of relatively short chains is gradually eliminated. A similar analysis has been performed in Ref. 8(b) for chains up to 800 steps. Our results are presented in Figs. 3 and 4 (black circles) which exhibit $2\nu_R$ and $2\nu_S$ vs $\log_{10}M$, respectively. The solid lines in Figs. 3 and 4 correspond to the following indirect analysis. First, we obtained the scaling parameters C_0 and C_1 in Eq. (1) using our MC data for $\langle R_N^2\rangle$ and $\langle S_N^2\rangle$. Then, substituting these parameters into Eq. (1), we obtained new values of $\langle R_N^2\rangle$ and $\langle S_N^2\rangle$ in the range 200–8000 steps. Finally, the fitting procedure which was described above was repeated using the new values of $\langle R_N^2\rangle$ and $\langle S_N^2\rangle$ to obtain "smoothed" curves of the plots in Figs. 3 and 4. The results of the indirect analysis (solid line) are consistent with the results of the direct analysis (black circles). It can be seen that the curves in Figs. 3 and 4 decrease as the lower bound M is increased, thus supporting our previous observations regarding the decrease of the critical exponent ν. The curves also show that ν_R obtained in the range 10^3-10^4 steps is within the RG results $2\nu=1.176\pm 0.002$, while ν_S in this range is still larger. The averages of ν_R and ν_S over the values obtained by direct analysis with M ranging from 1920 to 4352 (in this range the curves in Figs. 3 and 4 are relatively flat) are $\bar{\nu}_R=0.5886$ and $\bar{\nu}_S=0.5896$, and demonstrate the difference between ν_R and ν_S. Indeed, the results of previous MC simulations[1,4–7] of chains up to 10^4 steps, which were summarized in Table I, show that $\nu_S>\nu_R$. In addition, the results in Ref. 2 for the scaling parameters in Eq. (1) support the observation that ν_S approaches the asymptotic limit more slowly than ν_R.

In summary, we have extended previous MC simulation of SAW's on a simple-cubic lattice and improved the statistics and accuracy in the range of relatively long chains. We obtained the critical exponents ν_R and ν_S of the mean-squared end-to-end distance and the mean-square radius of gyration, respectively, at different ranges of the chain lengths between 200 and 7936 steps. Our results suggest that in the range 10^3-10^4 steps ν_R is within the RG result $\nu=0.588\pm 0.001$, while ν_S is still larger for the same number of steps.

[1] G. Zifferer, Macromolecules **23**, 3166 (1990).
[2] J. Dayantis and J. F. Palierne, Phys. Rev. B **49**, 3217 (1994).
[3] J. C. Le Guillou and J. Zinn-Justin, Phys. Rev. Lett. **39**, 95 (1977); Phys. Rev. B **21**, 3976 (1980).
[4] D. C. Rapaport, J. Phys. A **18**, 113 (1985).
[5] N. Madras and A. D. Sokal, J. Stat. Phys. **50**, 109 (1988).
[6] J. Dayantis and J. F. Palierne, J. Chem. Phys. **95**, 6088 (1991).
[7] N. Eizenberg and J. Klafter, J. Chem. Phys. **99**, 3976 (1993).
[8] (a) B. MacDonald, N. Jan, D. L. Hunter, and M. O. Steinitz, J. Phys. A **18**, 2627 (1985); (b) K. Kelly, D. L. Hunter, and N. Jan, *ibid.* **20**, 5029 (1987).
[9] Z. Alexandrowicz, J. Chem. Phys. **51**, 561 (1969); K. Suzuki and Y. Nakata, Bull. Chem. Soc. Jpn. **43**, 1006 (1970).