# Correction-to-scaling exponent for self-avoiding walks

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(Received 9 April 1990)

A Monte Carlo analysis for the scaling behavior of self-avoiding walks in two and three dimensions is given. We have calculated the mean-squared radius of gyration $S_N^2$, the mean-squared end-to-end distance $R_N^2$, and the total number of walks of $N$ steps $C_N^2$ to such a high accuracy that it is possible to analyze the data to obtain the correction-to-scaling exponent $\theta$. We find that both $S_N^2$ and $C_N^2$ give $\theta \simeq 1.1$, while $R_N^2$ gives $\theta \simeq 0.6$ in two dimensions. In three dimensions our data are consistent with $\theta \simeq 1.7$ and $\nu \simeq 0.597$ for both $R_N^2$ and $S_N^2$.

## I. INTRODUCTION

The self-avoiding-walk (SAW) model is one of the most successful models of long, flexible chain polymers in dilute solutions. It is directly related to the $n \to 0$ limit of the $n$-vector model.[1] In two dimensions, Nienhuis[2] had analyzed the $O(n)$ model and obtained the value $\nu = \frac{3}{4}$ for the exponent describing the asymptotic behavior of the mean-squared end-to-end distance $R_N^2$ or the mean-squared radius of gyration $S_N^2$. A number of efforts have been devoted to calculate the correction-to-scaling exponent $\theta$. Aside from the intrinsic interest of knowing its value, one also needs it in order to make a reliable extrapolation for the value of the leading exponent $\nu$. In two dimensions, Nienhuis[2] had made the prediction $\theta = \frac{3}{2}$. The status of this exponent is, however, not clear. Both invoking conformal invariance, Dotsenko[3] made the prediction $\theta = \frac{2}{3}$, while Saleur[4] had another prediction $\theta = \frac{11}{16} \simeq 0.687$. Most numerical calculations of this exponent can be essentially classified in two categories: (i) those using data for the total number of SAW's of $N$ steps $C_N$ and (ii) those using the data for the mean-squared end-to-end distance $R_N^2$. The first category includes the works of Adler[5] ($C_N$, $\theta \simeq 1.0$) and Guttmann[6] ($C_N$, $\theta \simeq 1.0$). The second category includes the works of Djordjevic *et al.*[7] ($R_N^2$, $\theta \simeq \frac{2}{3}$), Majid *et al.*[8] ($R_N^2$, $\theta \simeq \frac{2}{3}$), Privman[9] ($R_N^2$, $\theta \simeq 0.65$), Rapaport[10] ($R_N^2$, $\theta \simeq 1.0$), Havlin and Ben-Avraham[11] ($R_N^2$, $\theta \simeq 1.2$), and Lyklema and Kremer[12] ($R_N^2$, $\theta \simeq 0.84$). One observes that in the first category, the exponent $\theta$ is always greater than or equal to one while in the second category, with the exception of Rapaport and Havlin *et al.*, the exponent $\theta$ is always less than one. The case of Havlin and Ben-Avraham can be attributed to use of too few SAW configurations in their simulation (only $10^4$), as pointed out and corrected in Ref. 12. Recently, Ishinabe[13] reported results of an analysis using exact series of $C_N$, $R_N^2$, and $S_N^2$. He found $\theta \simeq 1.0$ for both $C_N$ and $S_N^2$ while for $R_N^2$, $\theta \simeq 0.63$. Therefore in two dimensions one has the conflicting situation that the correction to scaling exponent $\theta$ can be greater than or less than one depending on whether one analyzes $C_N$, $S_N^2$, or $R_N^2$, even though the leading exponent $\nu$ is exactly known. Ishinabe[13] even concluded that the leading exponent $\nu$ obtained using the $S_N^2$ data is different from that obtained using the $R_N^2$ data. The numerical evidence for such a conclusion ($\nu \simeq 0.755$ instead of 0.75) is, however, not strong. In addition there is also the prediction from field theory[14] based on the derivative of the marginal coupling constant at the fixed point that $\theta \simeq 1.7$. In this case there can be only one correction-to-scaling exponent. However, the same theory predicts $\nu \simeq 0.76$, quite far from the exact value of 0.75.

In three dimensions the situation is even worse since one does not have the good fortune of knowing the leading exponent $\nu$ exactly. Field theory predicts[14] $\nu \simeq 0.589$, $\theta \simeq 0.82$. Using Monte Carlo data for $R_N^2$, Kelley *et al.*[15] obtained $\theta \simeq 0.5$, $\nu \simeq 0.590$ while Majid *et al.*[8] obtained $\theta \simeq 0.47$, $\nu \simeq 0.5857$ by analyzing exact data for $R_N^2$. Rapaport,[16] using exact series data for $R_N^2$ concluded $\theta \simeq 1.0$, $\nu \simeq 0.592$. On the other hand, Guttmann[17] extended the series for the three-dimensional cubic lattice (20 terms) and reported a value $\nu$ of 0.592, in agreement with Rapaport. This value is close to Flory's prediction of 0.6 and thus Guttmann's result suggests the possibility that additional terms may push the series results towards 0.6. The aim of this paper is hopefully to clarify the situation both in two and three dimensions. In two dimensions we want to check if Ishinabe's results, which are obtained by the most extended series data and most sophisticated analysis so far, also hold true for larger-size $N$. In three dimensions we want to check if the conflicting situation of the exponent $\theta$ obtained using $C_N$, $S_N^2$, and $R_N^2$ also arises for large-size $N$. We do this by using a new Monte Carlo method to calculate the quantities $C_N$, $R_N^2$, and $S_N^2$, together with a new method of analyzing the data that avoids the use of ratio-type analysis which is not particularly accurate for Monte Carlo data.

## II. MONTE CARLO RESULT AND ANALYSIS

The Monte Carlo method used here, called the incomplete enumeration method had been described before and will only be briefly described here. It is a direct extension of the exact series expansion method[18,19] and had been applied to enumerate configurations of linear and branched polymers.[20–23] In the exact enumeration method, the SAW configurations are classified into a tree

 

structure according to their lineage and then enumerated using the backtracking method.[24] In the incomplete enumeration method for a $N$-step walk, one deletes with probability $(1-p_r)$ where $0<p_r<1$ and $r=2,3,\ldots,N$, all $r$-step configurations and their descendants from the genealogical tree. The remaining $N$-step configurations are then systematically enumerated using the backtracking method. Since the set $\{p_i\}$ is prechosen, the probability that a particular $r$-step SAW will be enumerated in a given trial is $p_2p_3\cdots p_r\equiv P_r$ and is the same for all configurations with the same $r$. The algorithm thus generates an unbiased sample of configurations. We have chosen here $p_1=1$, $p_i=\lambda^{-1}$ for $i\geq 2$, where $\lambda=2.5$, 4.0, and 4.5 for the square, triangular, and simple cubic lattices, respectively. The exact enumeration method is recovered by choosing $p_i=1$ for all $i$.

Let $X^2(n)$ denote either $R_n^2$ or $S_N^2$. Then asymptotically one has

$$X^2(n)=An^{2\nu}(1+B'n^{-\theta}) . \tag{1}$$

Furthermore, define $Q_n$ as

$$Q_n\equiv X^2(n)/n^{2\nu}=A+Bn^{-\theta} . \tag{2}$$

Integrating Eq. (2) from $M$ to $N$ one has

$$I_1(M,N)\equiv\int_M^N Q_n dn=(NQ_N-MQ_M)/(1-\theta) - A(N-M)\theta/(1-\theta) . \tag{3}$$

The second term on the right-hand of Eq. (3) can be eliminated by integrating Eq. (2) from another initial point $K<M$ and subtracting the resulting equation from Eq. (3). Then one has a $N$-dependent $\theta$ given by

$$\theta_N=1-\frac{N(M-K)Q_N-M(N-K)Q_M+K(N-M)Q_K}{(N-K)I_1(M,N)-(N-M)I_1(K,N)} . \tag{4}$$

The advantage of Eq. (4) is that we only have to integrate over our data and have thus avoided ratio-type analysis applied to neighboring data points such as that used by the authors in Ref. 12 on their Monte Carlo data. Such an analysis is fine for exact series data, but perhaps not accurate enough for Monte Carlo data.

We first discuss the results in two dimensions. We have calculated $R_N^2$, $S_N^2$, and $C_N^2$ for the square lattice up to $N=100$ using 120 000 trials. The results for $\theta_N$ as a function of $1/N$, calculated using Eq. (4) are shown in Fig. 1 for both $R_N^2$ and $S_N^2$. The $Q_N$ values in Eq. (2) are obtained using the exact exponent $\nu=\frac{3}{4}$. In calculating the integral $I_1(M,N)$ we have used Simpson's rule. Depending on the value of $N$, we have to choose the lower limits in the integral, $K$ and $M$, such that $(N-M)$ and $(N-K)$ are even integers. For any $K$ we can always find an integer $M>K$ so that the resulting $\theta_N$ values obtained using Eq. (4) become stable. Then plotting these $\theta_N$ values versus $1/N$ we find that asymptotically the $\theta_N$ values using different $K$ are independent of $K$. Therefore in all our analysis we have chosen $K=5$ or 6 and $M=15$ or 16. For large $N$, the values of $\theta_N$ obtained from the $S_N^2$ data become quite stable and they seem to approach the asymptotic value $\theta=1.1$. On the other hand, the values of $\theta_N$ obtained form the $R_N^2$ data show larger fluctuations but they seem to approach the asymptotic value $\theta\simeq 0.6$ for very large $N$. To check these results we have also calculated $R_N^2$ and $S_N^2$ for the triangular lattice up to $N=50$ using 12 000 trials. These results are also shown in Fig. 1 by crosses. They are consistent with the results for the square lattice.

The total number of walks of $n$ steps $C_n$ behaves asymptotically as

$$C_n=an^{\gamma-1}\mu^n(1+b'n^{-\theta}) , \tag{5}$$

where the universal exponent $\gamma=\frac{4}{3}$ (Ref. 2) is known ex-

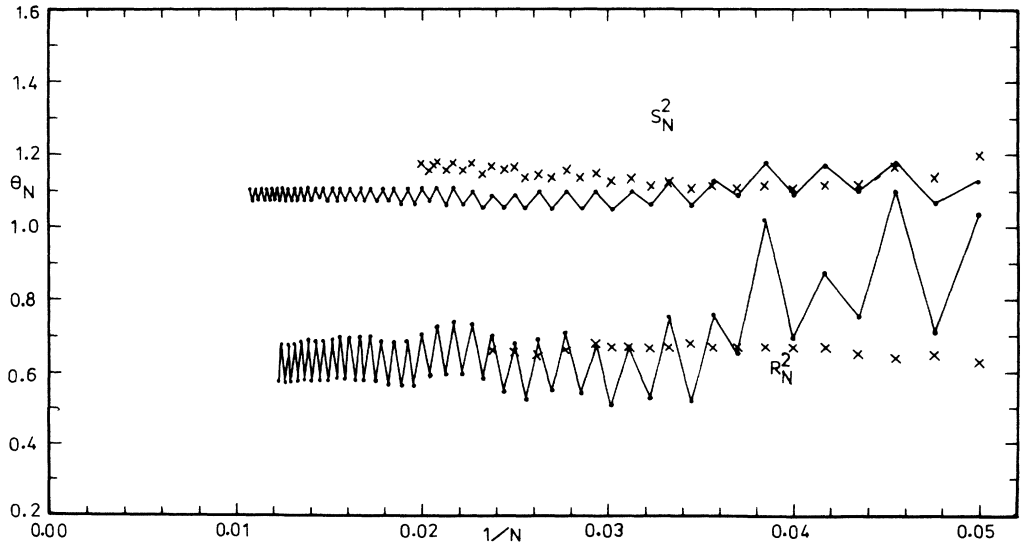


FIG. 1. The exponent $\theta_N$ as function of $1/N$, calculated using both $S_N^2$ and $R_N^2$ data. The dots and crosses represent results for the square and triangular lattices, respectively.

actly in two dimensions and $\mu$ is a lattice-dependent connectivity. For the square lattice Derrida obtained $\mu=2.6382\pm0.0002$ (Ref. 25) using a phenomenological renormalization scheme. Since this approach makes no assumption about the exponent $\gamma$, it is expected to be a reliable unbiased estimate. From Eq. (5) one can define

$$G_n \equiv C_n/(n^{\gamma-1}\mu^n)=a+bn^{-\theta} \tag{6}$$

The same analysis leading to Eq. (4) then gives an $N$-dependent expression for $\theta$

$$\theta_N=1-\frac{N(M-K)G_N-M(N-K)G_M+K(N-M)G_K}{(N-K)I_2(M,N)-(N-M)I_2(K,N)} \tag{7}$$

with

$$I_2(M,N)\equiv\int_M^N G_n dn \ . \tag{8}$$

The results for $\theta_N$ obtained using Eq. (7) and the $C_N$ data are shown in Fig. 2. These results are very sensitive to the value $\mu$ used in calculating $G_n$. One sees that the $\theta_N$ values approach the asymptotic value $\theta\simeq1.1$ or 1.2 for large $N$. Unfortunately lacking a corresponding accurate value of $\mu$ for the triangular lattice we cannot calculate the $\theta_N$ values for the triangular lattice using the $C_N$ data, because of their sensitivity to the connectivity constant $\mu$.

Thus our results in two dimensions are in good agreement with those of Ishinabe.[13] Even our numerical values for $\theta$ are similar to his: $\theta\simeq1.1$ obtained using $S_N^2$ and $C_N^2$ data and $\theta\simeq0.6$ obtained using $R_N^2$ data.

In three dimensions, since we do not have an exact value for the leading exponent $\nu$, we try to calculate $\theta$ using Eq. (4) for various values of $\nu$ in the range of known approximate values. The resulting values of $\theta_N$ obtained using $S_N^2$ data are shown in Fig. 3 and those using $R_N^2$ data are shown in Fig. 4. We have used $\nu$ values ranging from 0.592 to 0.600 in steps of 0.001. One sees that the resulting $\theta_N$ values are very sensitive to the $\nu$ values. From Fig. 3 we see that the $\theta_N$ values obtained from the $S_N^2$ data are becoming more and more sensitive to the $\nu$ values as the latter decrease from 0.595 to 0.592. At $\nu=0.592$, the resulting $\theta_N$ values are already quite erratic. On the other hand, from Fig. 4 we see that the $\theta_N$ values obtained from the $R_N^2$ data are getting more and more sensitive to the $\nu$ values as the latter *increase* from 0.598 to 0.600. At $\nu=0.600$ the $\theta_N$ values obtained from the $R_N^2$ data are already quite erratic. So we can say that the $\nu$ values giving good results for $\theta_N$ values for both $R_N^2$ and $S_N^2$ are in the range 0.595–0.598. In particular, for $\nu=0.597$, the extrapolated value of $\theta_N$ to $N\to\infty$ is 1.7 for both $R_N^2$ and $S_N^2$ data. In the lack of an exact value for $\nu$ we can only conclude that our data are consistent with $\theta\simeq1.7$ for both $R_N^2$ and $S_N^2$ with $\nu\simeq0.597$. Had we taken $\nu$ to be 0.592, we would have obtained $\theta\simeq0.5$ from our $R_N^2$ data, in agreement with that of Kelley *et al.*,[15] also using $R_N^2$ data. But then the same value for $\nu$ would have given $\theta>3.3$ for our $S_N^2$ data. Also the large fluctuations in the $\theta_N$ values at this value of $\nu$ for the $S_N^2$ data would suggest that we have made a bad choice for the exponent $\nu$. Lacking the knowledge of both the exponent $\gamma$ and the connectivity constant $\mu$, we did not attempt to calculate the correction-to-scaling exponent using our $C_N$ data.

To get an idea of the error estimates, let $X^2(n)$ from Eq. (1) be given by $\bar{X}^2(n)(1\pm\epsilon)$, where $\epsilon$ denotes the fractional error in $X^2(n)$. Then the quantity $Q_n$ in Eq. (2) will be given by $Q_n=\bar{Q}_n(1\pm\epsilon)$. If we assume that the errors in $Q_n$ do not affect the integrals $I_1(M,N)$ and $I_1(K,N)$, then the exponent $\theta_N$ is given by

$$\theta_N=\bar{\theta}_N\pm\epsilon(\bar{\theta}_N\mp1)\simeq\bar{\theta}_N\pm\epsilon(\bar{\theta}_N+1) \ .$$

We have for the square lattice $\epsilon\leq0.001$, 0.002 for $S_N^2$ and $R_N^2$, respectively. For the triangular lattice we have $\epsilon\leq0.001$, 0.0005 for $S_N^2$ and $R_N^2$, respectively, and for the simple cubic lattice we have $\epsilon\leq0.001$, 0.0005 for $S_N^2$ and $R_N^2$, respectively. For the $C_N$ data, if we have

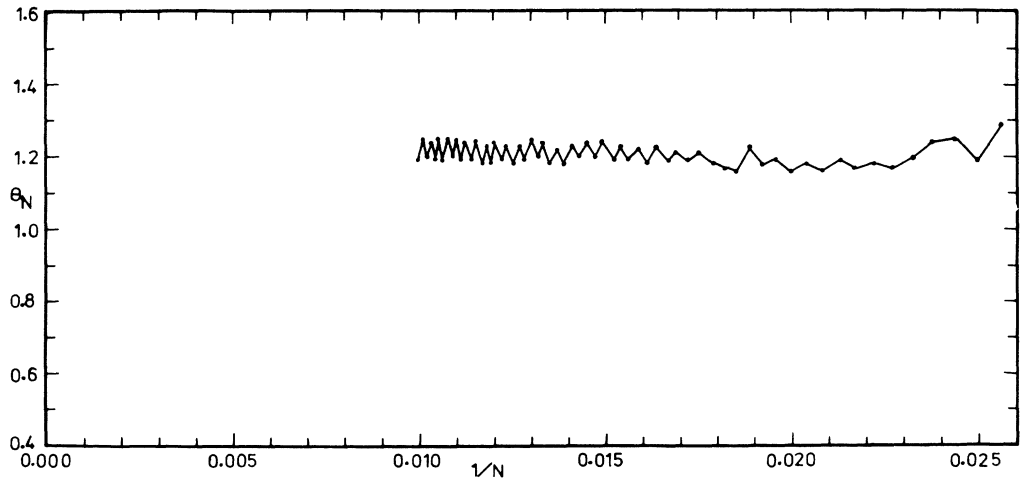


FIG. 2. The exponent $\theta_N$ as function of $1/N$, calculated using $C_N$ data for the square lattice.

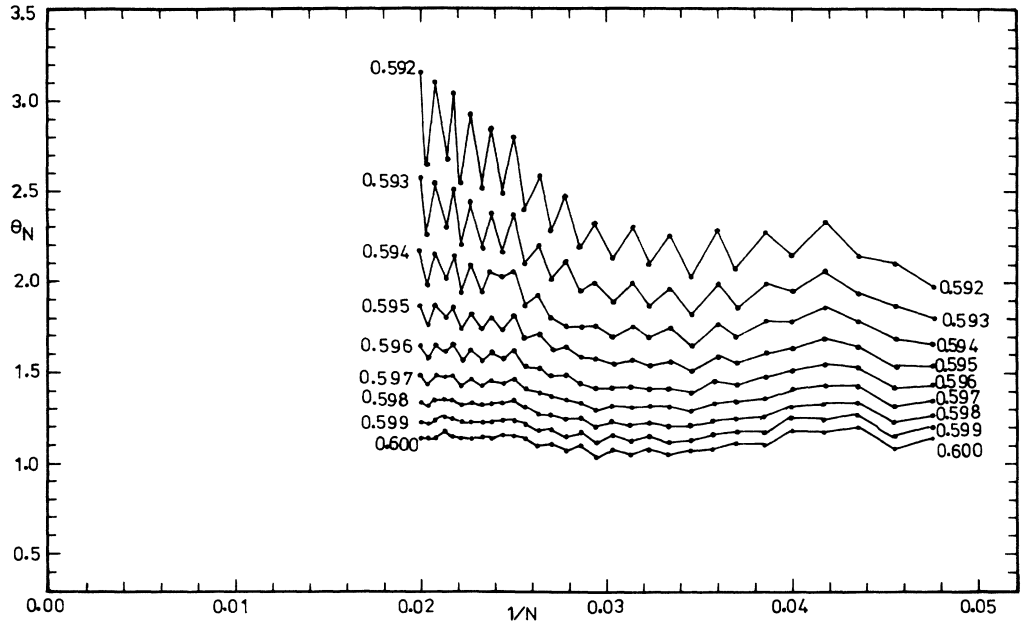


FIG. 3. The exponent $\theta_N$ as function of $1/N$, for the simple cubic lattice, calculated using the $S_N^2$ data and for various values of the leading exponent $\nu$ ranging from 0.592 to 0.600.

$C_N=\bar{C}_N(1\pm\epsilon)$, with $\epsilon$ a fractional error in the data $C_N$, then a similar analysis results also in an error for the exponent $\theta_N=\bar{\theta}\pm\epsilon(\bar{\theta}+1)$. We have for the square lattice $\epsilon\leq 0.007$ for the $C_N$ data.

In order to show that our data for $R_N^2$ and $S_N^2$ are consistent with the leading exponent $\nu=\frac{3}{4}$ in two dimensions and $\nu=0.597$ in three dimensions, we have plotted these exponents in Figs. 5 and 6 as a function of $1/N$. The $N$-dependent exponent $\nu_N$ are obtained in the following way. From Eq. (2) for large $N$, we have

$$X^2(n)=An^{2\nu}\ , \tag{9}$$

where $X_n^2$ denotes either $R_n^2$ or $S_n^2$. Taking the logarithm on both sides of Eq. (9) and integrating the resulting equation from $M$ to $N$ one obtains

$$\int_M^N \ln X^2(n)dn = NX^2(N)-MX^2(M)-2\nu(N-M)\ . \tag{10}$$

Defining the integral on the left-hand side of Eq. (10) as

$$I_3(M,N)\equiv\int_M^N \ln X^2(n)dn\ , \tag{11}$$

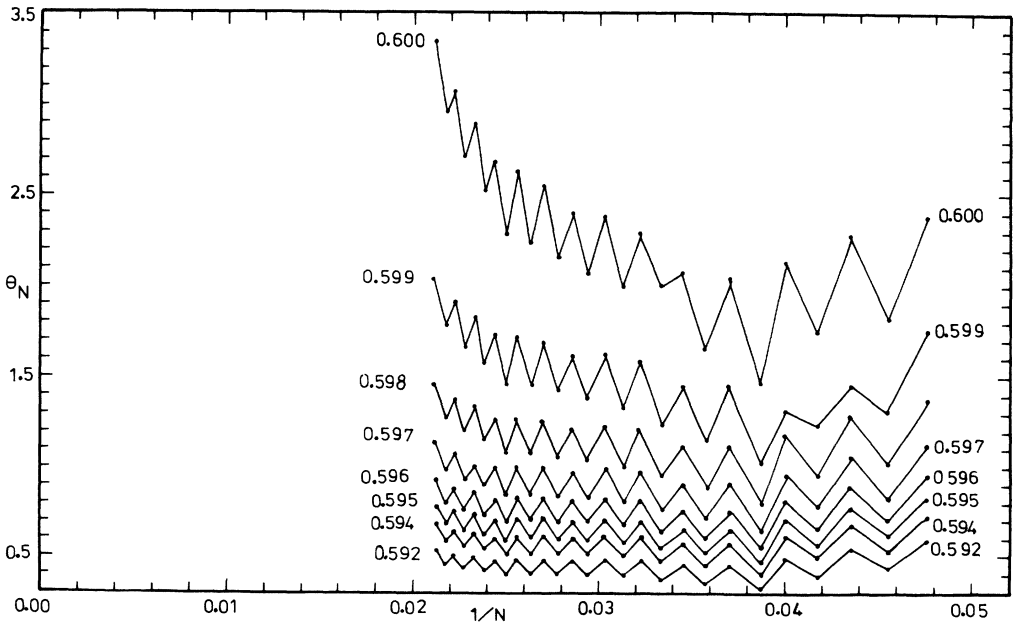


FIG. 4. Same as Fig. 3, but using the $R_N^2$ data.

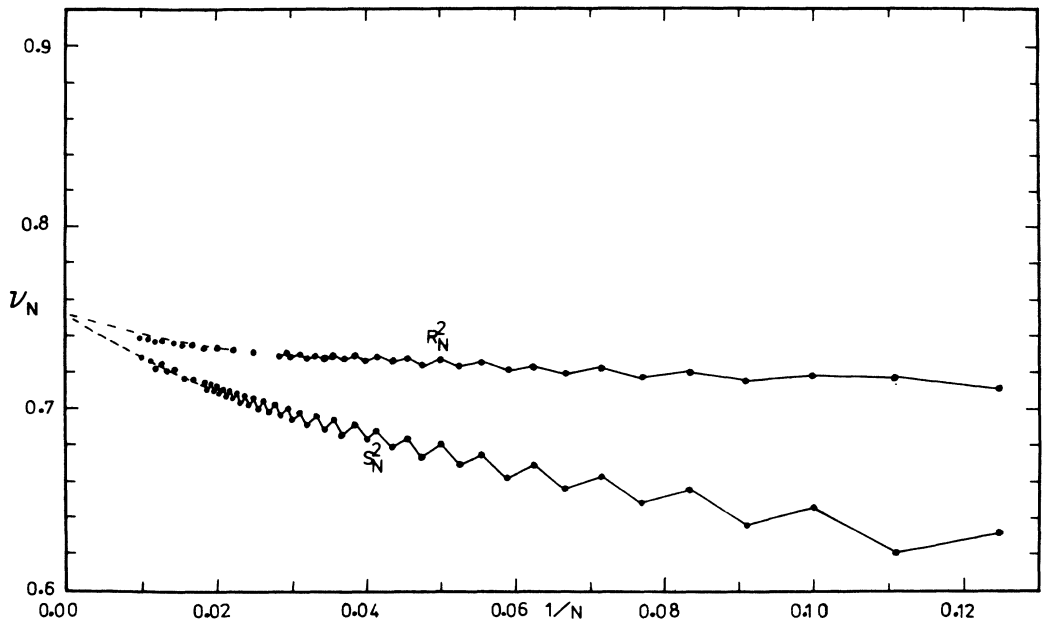


FIG. 5. The leading exponent $\nu$ as a function of $1/N$, calculated using both $S_N^2$ and $R_N^2$ data, for the square lattice.

one obtains a $N$-dependent exponent $\nu_N$ as

$$\nu_N=[N\ln X^2(N)-M\ln X^2(M)-I_3(M,N)]/[2(N-M)]\ . \tag{12}$$

The integral $I_3(M,N)$ is calculated using Simpson's rule. The lower limit $M$ is taken to be either 1 or 2 such that $(N-M)$ is an even integer. From the results of $\nu_N$ shown in Figs. 5 and 6 we see that in the asymptotic limit $\nu$ is consistent with the values $\frac{3}{4}$ and 0.597 in two and three dimensions, respectively, for $\nu_N$ calculated from both $S_N^2$ and $R_N^2$ data.

## III. DISCUSSIONS AND CONCLUSION

How are we going to understand the results presented above, especially for the different values of the exponent $\theta$ in two dimensions? In general, the critical quantities $R_N^2$ or $S_N^2$ obey the following asymptotic scaling law:[26]

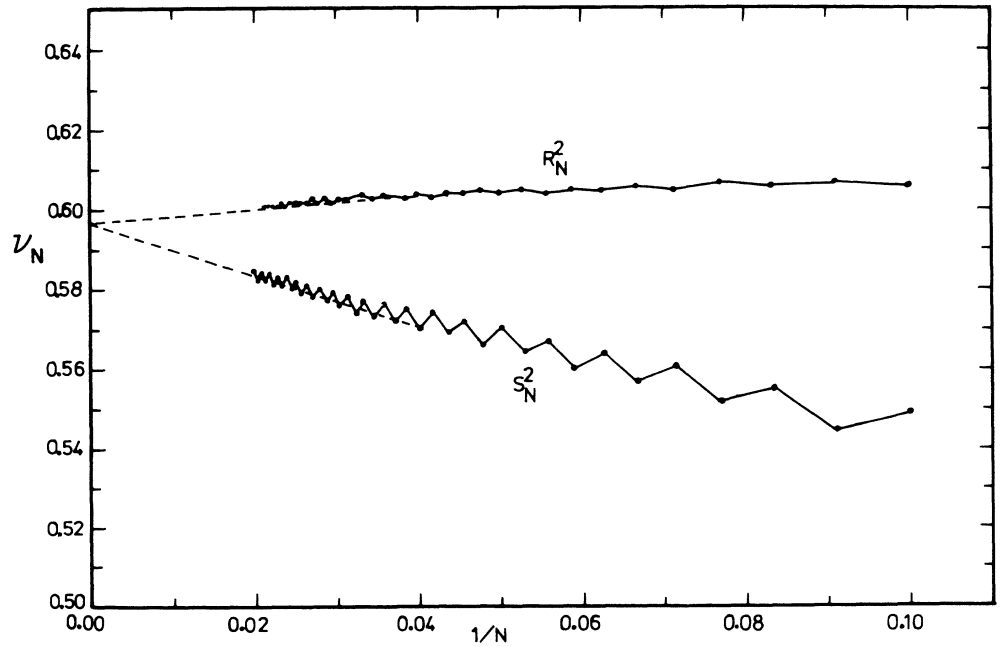


FIG. 6. Same as Fig. 5, but for the simple cubic lattice.

$$X_N^2 = A_i N^{2\nu}(1 + a_i N^{-1} + a_i' N^{-\Delta} + b_i N^{-2} + b_i' N^{-2\Delta} + c_i' N^{-(1+\Delta)} + \cdots), \quad (13)$$

where $X^2(N)$ and $i = R$ or $S$ represent either $R_N^2$ or $S_N^2$. The analytic correction terms with unprimed coefficients are due to nonlinear scaling fields, the nonanalytic terms with primed coefficients arise from the marginal scaling field, and $\Delta$ is a universal exponent. The coefficients in Eq. (13) are in general different from those introduced in Sec. II. In two dimensions, we found for the mean-squared end-to-end distance $R_N^2 = A_R N^{2\nu}(1 + BN^{-0.6})$. This means that the largest correction term is the nonanalytic term $a_i' N^{-\Delta}$, with $\Delta \simeq 0.6$. For the mean-squared radius of gyration $S_N^2$, we found $S_N^2 = A_S N^{2\nu}(1 + B' N^{-1.1})$. This implies that either $a_S' = 0$ and the largest correction term is the analytic correction term $a_S N^{-1}$ or that both coefficients $a_S$ and $a_S'$ are zero and the largest correction term is the nonanalytic correction term $b_S' N^{-2\Delta}$, with $2\Delta \simeq 1.1$, $\Delta \simeq 0.55$, in agreement with that found using $R_N^2$ data.

In three dimensions, our result

$$X^2(N) = A_i N^{2\nu}(1 + B_i N^{-1.7})$$

for both the mean-squared end-to-end distance and the mean-squared radius of gyration would imply that the coefficient $a_i = 0$ for both $i = R$ and $i = S$ and the largest correction term is the nonanalytic correction term $a_i' N^{-\Delta}$, with $\Delta \simeq 1.7$.

The critical quantity $C_N$ obeys the asymptotic scaling law

$$C_N^2 = A_C N^{\gamma-1} \mu^N (1 + a_C N^{-1} + a_C' N^{-\Delta} + b_C N^{-2} + b_C' N^{-2\Delta} + c_C' N^{-(1+\Delta)} + \cdots). \quad (14)$$

Our result that the exponent $\theta$ calculated from the $C_N$ data agrees with that calculated from the $S_N^2$ data implies that either $a_C' = 0$ or $a_C = a_C' = 0$.

## ACKNOWLEDGMENTS

This work was supported by the Sonderforschungsbereich 237 Unordnung und grosse Fluktuationen of the Deutsche Forschungsgemeinschaft.

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