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Correction to scaling exponent for the two-dimensional self-avoiding walk

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A Monte Carlo series analysis for the scaling behavior of the two-dimensional self-avoiding walk is given. We have calculated the mean-square end-to-end distance on a square lattice with such a high accuracy that it is possible to analyze the data with ratio-type methods. From this we find for the correction-to-scaling exponent a value of $\Delta = 0.84$.

Recently there has been a large interest in the scaling behavior of self-avoiding walks (SAW). This is due to the availability of the exact result of Nienhuis,[1] who analyzed the two-dimensional $O(n)$ model. For the exponent ν, which describes the asymptotic behavior of the mean-square end-to-end distance he obtained the value $\frac{3}{4}$. In two dimensions, particular emphasis has been focused on the correction to scaling exponent Δ. Aside from the intrinsic interest of knowing the value of this exponent, one also needs it in order to make a reliable extrapolation for the value of the leading exponent ν. In this Rapid Communication we present a high-accuracy Monte Carlo study of the exponent Δ. We analyze the data with methods which previously have only been used in the context of exact-series enumeration. We find for Δ the value 0.84 ± 0.04, a result which differs markedly from all previously reported values. One expects the mean-square end-to-end distance to vary with N, the length of the chain, as[2]

$$\langle R^2(N)\rangle = AN^{2\nu}(1+BN^{-\Delta}+CN^{-1}+\cdots) \ . \quad (1)$$

This expression has been used by Majid, Djordjevic, and Stanley[3] to verify the value of ν and by Djordjevic, Majid, Stanley, and dos Santos[2] to estimate the value of Δ from exact enumeration data on the triangular lattice ($N \leq 18$). These authors observe that the assumption $\Delta > 1$ which had been made previously is incorrect and that as a consequence one cannot simply extrapolate the effective exponent $\nu(N)$ vs $1/N$ to obtain the critical exponent ν. This can be understood from the definition of $\nu(N)$:

$$\nu(N) = \ln\{[\langle R^2(N)\rangle / \langle R^2(N-1)\rangle]/2\ln[N/(N-1)]\} \ . \quad (2)$$

Inserting Eq. (1) into this definition results in the following expression:

$$\nu(N) = \nu - \frac{\Delta B}{2}N^{-\Delta} - \frac{C}{2}N^{-1} + \cdots \ . \quad (3)$$

From this it is clear that if $\Delta < 1$ a naive extrapolation versus $1/N$ gives wrong results. It is therefore very important to check if the correction to scaling exponent Δ is > 1 or not. If it is smaller, then one has to calculate it very accurately in order to do the extrapolation versus $N^{-\Delta}$. This has been done in Refs. 2 and 3 and leads to the conclusion that indeed $\nu = \frac{3}{4}$, in agreement with the Nienhuis[1] result. However, the estimate for $\Delta (0.66 \pm 0.07)$ strongly disagrees with Nienhuis's prediction of $\Delta = \frac{3}{2}$. The status of this exponent is not clear. It might be correct, but it is certainly not the smallest one. A more sophisticated analysis of somewhat shorter ($N \leq 16$) series results for the same lattice has been given by Privman.[4] His biased (with $\nu = \frac{3}{4}$) estimate ($\Delta = 0.65 \pm 0.08$) agrees completely with Djordjevic *et al.*[2]

A different method has been used by Adler[5] to study the generating function on the honeycomb lattice ($N \leq 34$). From this series she finds three different exponents: $\Delta_1 \sim 0.93$, $\Delta_2 \sim 1.2$, and $\Delta_3 \sim 1.5$. These results, however, are *not* confirmed by Guttmann[6] who studied the generating function for the triangular lattice ($N \leq 18$), the square lattice ($N \leq 24$), and the honeycomb lattice ($N \leq 34$). He does not find consistent evidence for the presence of a confluent singularity with $\Delta < 1$. It is interesting to note that his analysis of the 18-term triangular lattice series points to a correction to scaling exponent of $\Delta = 0.84$. He rejected this value because the other lattices did not show evidence for it.

We also have a prediction from field theory,[7] but in two dimensions one does not expect to find accurate results. Indeed, the value for the leading exponent ($\nu = 0.77$) differs so much from the accepted value 0.75 that the result for the confluent exponent ($\Delta = 1.15$) cannot be considered as a reliable estimate for the true value.

Havlin and Ben-Avraham[8] have performed a Monte Carlo simulation on the square lattice of only 10^4 SAW's of length 80, 160, and 320. To analyze their data they introduce the concept of a local fractal dimension. From the scaling behavior of this quantity they deduce $\nu = 0.753 \pm 0.004$ and $\Delta = 1.2 \pm 0.1$.

The wide range of estimates for the correction to scaling exponent necessitates a more careful study of this problem. To this end we have performed a high-accuracy Monte Carlo simulation of SAW chains up to a length of $N = 48$, using the simple sampling method.[9] This is a straightforward procedure in which one chooses the new direction from all directions with equal probability. The chain is stopped when a site is visited for the second time and one has to start a new chain. In this way no bias is introduced. The random numbers are generated using the well tested algorithm R250 of Kirkpatrick and Stoll.[10] The number of walks generated varies depending on N, the chain length, between 10^8 for

$N=10$ and 6×10^6 for $N=48$. The acceptance rate in this Monte Carlo procedure of course decreases rapidly with increasing N. For $N=48$ only $\sim 0.7\%$ of the attempts are accepted. This clearly makes it extraordinarily difficult to go to longer chain lengths using the simple sampling method. We claim, however, that the asymptotic behavior can already be studied with these lengths. This is numerically confirmed, because the lattice typical odd-even fluctuations, which are seen in a plot of $\nu(N)$ vs $1/N$ (Fig. 1), have almost vanished. Because in the asymptotic scaling regime there is no difference between the lattice and continuum approaches and one expects that lattice properties disappear, we conclude that for $N>30$ we can study the scaling behavior of the SAW. To estimate the accuracy of our data we have calculated the mean distance in the x direction. This quantity fluctuates around zero and from its absolute value we have estimated the error in $\langle R^2(N)\rangle^{1/2}$ to be 0.025% in the worst case ($N=29$) and usually is better than 0.01%.

The raw data for the mean-square displacement are analyzed using the following definition of $\nu(N)$:

$$\nu(N)=\frac{1}{2}\frac{\ln[\langle R^2(N+i)\rangle/\langle R^2(N-i)\rangle]}{\ln[(N+i)/(N-i)]} . \quad (4)$$

Together with the assumption for the scaling behavior of $\langle R^2(N)\rangle$ [Eq. (1)], this results again in the expression Eq. (3) for $\nu(N)$, independent of the choice of i. The symmetric definition of $\nu(N)$ has the advantage above the asymmetric definition [Eq. (2)] that in contrast with the latter, it does *not* introduce a bias for larger values of i. This is especially important when the ratio i/N is not very small. Also the difference between the two entries ($2i$) is always even, thereby eliminating the odd-even fluctuations to a great extent. In Fig. 1 we show a plot of $\nu(N)$ vs $1/N$ for $i=5$. One can clearly distinguish two different curves, which become parallel and almost identical for $N>30$. It is more convenient to study only one of these curves, namely, the one calculated from SAW's with an even number of monomers. This curve we show in Fig. 2, for $i=1$ and $i=5$. From the scatter of the points of the $i=1$ curve, we estimate the error of $\nu(N)$ to be roughly 0.001 or 1% for high-N values. For the $i=5$ curve this has been improved dramatically and it is not possible to give an error estimate for this curve. Note that the high i value does not introduce an observable bias. In this curve the low-N values extrapolate linearly to a ν value ~ 0.744, whereas the higher-N values give a value $\nu\sim 0.748$. The crossover point is $N\approx 27$, a value just above the maximum chain length which can be reached by exact enumeration. This explains why this technique gives the wrong prediction for Δ and shows at the same time that one cannot obtain ν from the series results using a simple extrapolation method.

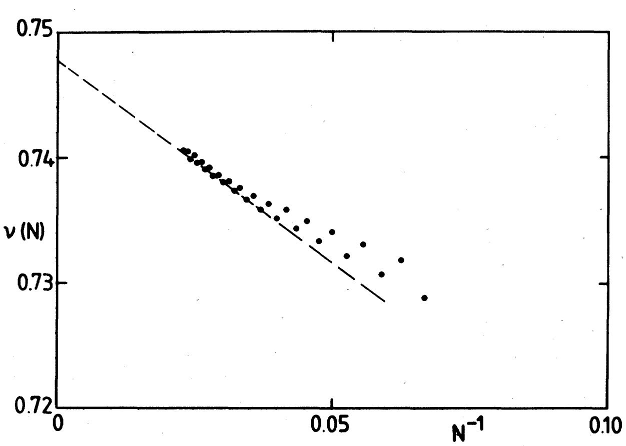

FIG. 1. Plot of $\nu(N)$ vs $1/N$ for all N values between 15 and 43. The parameter $i=5$. A linear extrapolation results in a ν value of 0.748.

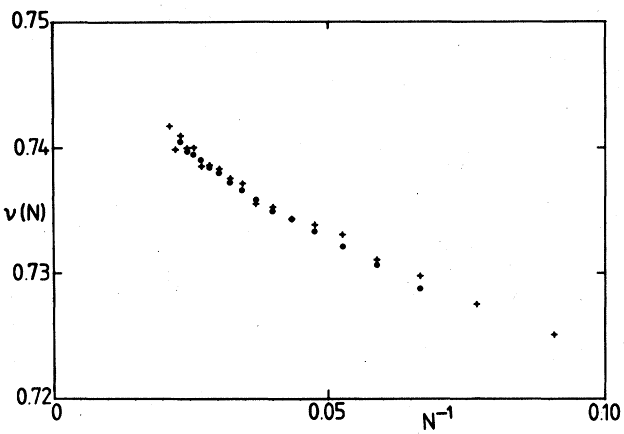

FIG. 2. Plot of $\nu(N)$ vs $1/N$ for the N values 11, 13, 15, . . . ,47. The parameter $i=1$ (●) and 5 (+).

To study the correction to scaling exponent Δ we assume $\nu=\frac{3}{4}$ and calculate the quantity

$$F(N)=\frac{N}{2i}\left[1-\frac{\langle R^2(N+i)\rangle/(N+i)^{2\nu}}{\langle R^2(N-i)\rangle/(N-i)^{2\nu}}\right]$$

$$=\Delta BN^{-\Delta}+CN^{-1}+\cdots . \quad (5)$$

The equality is obtained by inserting the assumed asymptotic behavior of $\langle R^2(N)\rangle$ [Eq. (1)] into the expression for $F(N)$. If $\Delta<1$, we can estimate it from the slope of the plot of $\ln S$ vs $\ln N$ for large enough N. This plot is shown in Fig. 3 for $i=5$. Again, this value does not introduce an observable bias with respect to $i=1$. There is a clear crossover at $N\simeq 27$. From the points below this value of N we estimate a slope of 0.64. This is in complete agreement with the results from series enumeration.[2,4] However, the slope for the larger-N values gives $\Delta=0.84$, distinctly different from the low-N value of the slope. From the slopes of all possible pairs of points in the asymptotic region we estimate an error of 0.04. Thus, assuming that for $N>30$ we are in a regime where the scaling behavior Eq. (1) holds, we find

$$\Delta=0.84\pm0.04 . \quad (6)$$

To complete this work we show in Fig. 4 a plot of $\nu(N)$ vs $N^{-\Delta}$. A linear extrapolation here points consistently to a value 0.750 for ν. Our confidence estimate for this value is 0.001.

From our discussion thus far it is clear that the analysis of the exact enumeration data[2-6] has been done on series which are too short and consequently cannot give correct results. Also the use of more sophisticated methods[4-6] to analyze the series has failed to give the correct result. A

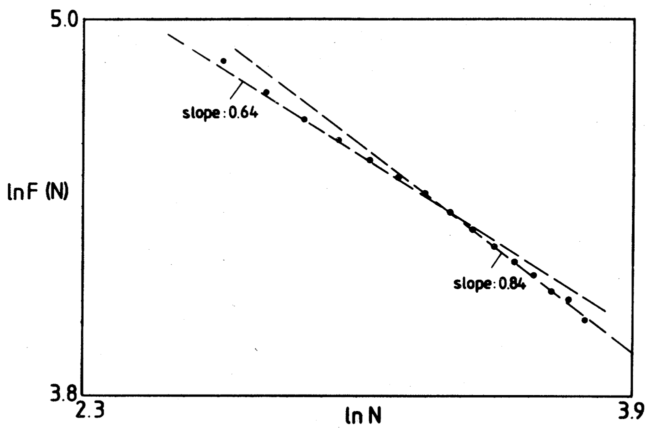

FIG. 3. Plot of $\ln F(N)$ with $i=5$. The slopes give the estimate for the correction exponent Δ for $N<30$ and $N>30$.

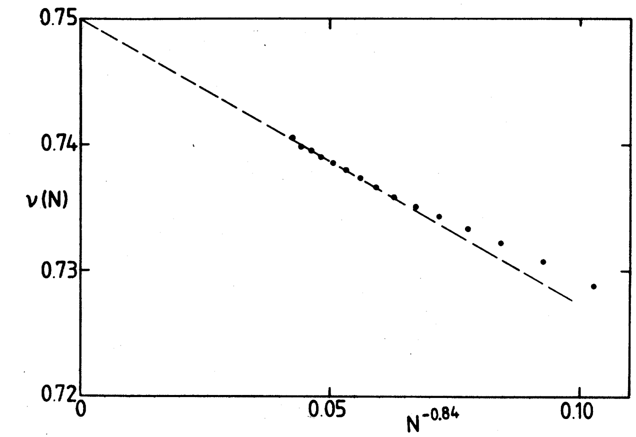

FIG. 4. Plot of $\nu(N)$ vs $N^{-0.84}$ with $i=5$. A linear extrapolation results in a ν value of 0.750.

possible exception is the Padé analysis of Guttmann[6] of the generating function series of the triangular lattice. It seems worthwhile to extend this series to obtain an independent check of our value for Δ.

The Monte Carlo estimates of Havlin and Ben-Avraham[8] are not reliable, due to the insufficient statistics of the Monte Carlo data. In addition, the method of data collapsing, though it shows the self-similarity very nicely, is not precise enough to calculate the correction to scaling exponent Δ.

In summary, we have shown that the asymptotic scaling regime for the SAW on a square lattice sets in only after a chain length of $N \simeq 30$. From a ratio-type analysis of high-accuracy Monte Carlo data we find for the correction-to-scaling exponent Δ the value 0.84 $(\sim \frac{5}{6})$, markedly different from *all* other predictions.

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