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High-precision determination of the critical exponent γ for self-avoiding walks

Sergio Caracciolo*
Scuola Normale Superiore and INFN, Sezione di Pisa, I-56100 Pisa, Italy

Maria Serena Causo†
Dipartimento di Fisica and INFN, Sezione di Lecce, Università degli Studi di Lecce, I-73100 Lecce, Italy

Andrea Pelissetto‡
Dipartimento di Fisica and INFN, Sezione di Pisa, Università degli Studi di Pisa, I-56100 Pisa, Italy

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We consider three-dimensional self-avoiding walks. We compute the exponent γ that controls the asymptotic behavior of the number of walks going from the origin to any lattice point in N steps. We get $\gamma = 1.1575 \pm 0.0006$ in agreement with renormalization-group predictions. Earlier Monte Carlo and exact-enumeration determinations are now seen to be biased by corrections to scaling. [S1063-651X(98)50202-4]

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The self-avoiding walk (SAW) is a well-known lattice model of a polymer molecule in a good solvent; moreover, because of its simplicity, it is an important test case in the theory of critical phenomena.

Much work has been done in computing critical exponents by a variety of theoretical approaches—Monte Carlo (MC), exact enumeration/extrapolation (EE), and renormalization group (RG)—with the aim of comparing these determinations with one another and with the experimental results. Small but persistent discrepancies have emerged among the predictions from different theoretical approaches. For example, extensive studies have been done on the exponent ν, which controls the critical behavior of the length scales. Early MC simulations and EE studies [1] in the seventies predicted $\nu = 3/5$ in agreement with the Flory theory. When the length of the walks that were simulated was increased [2–4] the value of ν decreased to $\nu = 0.592 \pm 0.002$. This value was also supported by extended EE studies, which provided an identical estimate [5]. On the other hand, field-theoretic RG computations [6–10] persistently gave $\nu = 0.588 \pm 0.001$ or even slightly lower. The discrepancy was clarified when the MC studies were extended to much longer walks: because of strong corrections with nonanalytic exponent $\Delta \approx 0.5$, the asymptotic regime is reached only for very long chains, and the results from shorter chains are systematically biased upward [11–14]. A simulation [14] with walks of length up to $N = 80\,000$, using a data analysis taking careful account of the corrections to scaling, gave $\nu = 0.5877 \pm 0.0006$ in good agreement with the renormalization-group estimates. Universality is also well satisfied: a simulation [13] in a slightly different geometry provided $\nu = 0.5867 \pm 0.0013$ (68% confidence limit) while a recent high-statistics simulation [15] for the off-lattice Kratky-Porod model with excluded volume gave $\nu = 0.5880 \pm 0.0018$.

One may ask if the same phenomenon occurs for the other critical exponents. We consider here the exponent γ, which, in spin systems, controls the critical behavior of the magnetic susceptibility. For SAW's γ is defined in terms of c_N, the number of walks going from the origin to any lattice point with N steps: for large N we have

$$c_N \approx a_0 \mu^N N^{\gamma - 1}, \tag{1}$$

where γ is universal, while μ, the connectivity constant, and a_0 are nonuniversal.

For the exponent γ, there are significant discrepancies in the existing theoretical predictions. MC and EE studies provide the estimates

$$\gamma = \begin{cases} 1.161 \pm 0.001 & \text{EE, Ref. [5]} \\ 1.1619 \pm 0.0001 & \text{EE, Ref. [17]} \\ 1.1608 \pm 0.0003 & \text{MC, Ref. [16].} \end{cases} \tag{2}$$

On the other hand the ϵ expansion predicts a lower value [7]: $1.157 \lesssim \gamma \lesssim 1.160$. Indeed a Borel-type resummation gives $\gamma = 1.160 \pm 0.004$ and $\gamma = 1.157 \pm 0.003$ if one forces the expansion to reproduce the exact value in two dimensions $\gamma = \frac{43}{32}$. One can also use the scaling relation $\gamma = (2 - \eta)\nu$ and the estimates for η and ν: the unconstrained ϵ expansion gives $\nu = 0.5885 \pm 0.0025$ and $\eta = 0.031 \pm 0.003$ so that $\gamma = 1.159 \pm 0.005$; using the exactly known values for $d = 2$, $\nu = \frac{3}{4}$ and $\eta = \frac{5}{24}$, one gets $\nu = 0.5880 \pm 0.0015$ and $\eta = 0.0320 \pm 0.0025$ so that $\gamma = 1.1572 \pm 0.0035$.

More controversial is the status of the expansions at fixed spatial dimension $d = 3$. In [7] γ is estimated as $\gamma = 1.1615 \pm 0.0020$ while in [9] the final estimate is $\gamma \approx 1.1613$. These estimates depend crucially on the critical value of the renormalized coupling constant $\overline{g}^*$: in [6,7] the estimate $\overline{g}^* = 1.421 \pm 0.008$ is used, while [9] uses $\overline{g}^* = 1.422 \pm 0.008$. However Nickel [18] has pointed out that the present estimates of $\overline{g}^*$ could be slightly higher than the correct value due to a possible nonanalyticity of the β function at $\overline{g}^*$, which is usually neglected in the standard

*Electronic address: caraccio@sns.it
†Electronic address: causo@le.infn.it
‡Electronic address: pelisset@ibmth.difi.unipi.it

analyses. A reanalysis of the series [10] indicates that $\overline{g^*}$ could be as low as 1.39 and predicts $\gamma=1.1569+0.10(\overline{g^*}-1.39)\pm 0.0004$.

In this paper we present a high-precision MC study for the exponent γ using walks up to length $N=40\,000$. Our results confirm the important role played by corrections to scaling; our final estimate $\gamma=1.1575\pm 0.0006$ is significantly lower than previous MC and EE results. It is also in agreement with the predictions of the ϵ expansion and with the RG results of Ref. [10]. It is in disagreement, however, with the estimates of [6,8,9] unless one uses a lower value of $\overline{g^*}$. Indeed we have reanalyzed the $O(g^7)$ series of [10] using the method presented in [6], but keeping $\overline{g^*}$ arbitrary. We get

$$\nu=0.5882+0.07(\overline{g^*}-1.421)\pm 0.0005, \tag{3}$$

$$\gamma=1.1616+0.11(\overline{g^*}-1.421)\pm 0.0004. \tag{4}$$

These estimates are in reasonable agreement with the Monte Carlo results for γ and ν if $\overline{g^*}\approx 1.395\pm 0.01$. Our data thus support a lower value for the renormalized coupling constant. The question that remains open is why standard analyses overestimate $\overline{g^*}$: it could be that the conjectured nonanalyticities are indeed present and play a larger role than expected, or, more simply, it could be a short-series effect. Of course one cannot hope to answer these questions numerically: only an analytic treatment could solve the controversy.

In the presence of strong corrections to scaling, in order to get a reliable estimate of the critical exponents one needs to perform the simulation in the large-N regime. This is only possible if the algorithm at hand does not exhibit too strong a critical slowing down. For the study of γ for SAW's on the lattice the best available algorithm is the *join-and-cut* algorithm [19]: in two dimensions the autocorrelation time, expressed in CPU units, behaves approximately as $N^{\approx 1.5}$ while in three dimensions the behavior is expected to be $N^{\approx 1.2}$. The algorithm is thus nearly optimal. Another advantage of this algorithm is that it does not require the determination of the connectivity constant, at variance with more standard algorithms.

The join-and-cut algorithm works in the unorthodox ensemble $T_{N_{\rm tot}}$ consisting of all pairs of SAW's (each walk starts at the origin and ends anywhere) such that the *total* number of steps in the two walks is some fixed number $N_{\rm tot}$. Each pair in the ensemble is given equal weight; therefore, the two walks are not interacting except for the constraint on the sum of their lengths.

One sweep of the algorithm consists of two steps: (1) Starting from a pair of walks (ω_1,ω_2), we update each of them independently using some ergodic fixed-length algorithm. We use the pivot algorithm [20,21,3], which is the best available one for the ensemble of fixed-length walks with free endpoints. (2) We perform a join-and-cut move: we concatenate the two walks ω_1 and ω_2 forming a new (not necessarily self-avoiding) walk $\omega_{\rm conc}$; then we cut $\omega_{\rm conc}$ at a random position creating two new walks ω'_1 and ω'_2. If ω'_1 and ω'_2 are self-avoiding we keep them; otherwise the move is rejected and we stay with ω_1 and ω_2. More details on the dynamical critical behavior and on the implementation of this algorithm can be found in [19].

Let us now discuss how the critical exponent γ can be estimated from the Monte Carlo data produced by the join-and-cut algorithm.

Let us start by noticing that the random variable N_1, the length of the first walk, has the distribution

$$\overline{\pi}(N_1)=\frac{c_{N_1}c_{N_{\rm tot}-N_1}}{Z(N_{\rm tot})} \tag{5}$$

for $1\leqslant N_1\leqslant N_{\rm tot}-1$, where $Z(N_{\rm tot})$ is the obvious normalization factor and c_N is the number of walks going from the origin to any lattice point with N steps, the asymptotic behavior of which, for large N, is given by Eq. (1). The idea is then to make inferences of γ from the observed statistics of N_1. Of course the problem is that Eq. (1) is an asymptotic formula valid only in the large-N regime. We will thus proceed in the following way: we will suppose that Eq. (1) is valid for all $N\geqslant N_{\rm min}$ for many increasing values of $N_{\rm min}$ and correspondingly we will get estimates $\hat{\gamma}(N_{\rm tot},N_{\rm min})$; these quantities are effective exponents that depend on $N_{\rm min}$ and that give correct estimates of γ as $N_{\rm min}$ and $N_{\rm tot}$ go to infinity.

The determination of γ from the data is obtained using the maximum-likelihood method. We will present here only the results: for a detailed discussion we refer the reader to [19].

Given $N_{\rm min}$ consider the function (from now on we suppress the dependence on $N_{\rm tot}$)

$$\theta_{N_{\rm min}}(N_1)=\begin{cases}1 & \text{if } N_{\rm min}\leqslant N_1\leqslant N_{\rm tot},\\ 0 & \text{otherwise}\end{cases} \tag{6}$$

and let X be the random variable

$$X=\ln[N_1(N_{\rm tot}-N_1)]. \tag{7}$$

Then define

$$X^{\rm cens}(N_{\rm min})=\frac{\langle X\theta_{N_{\rm min}}\rangle}{\langle\theta_{N_{\rm min}}\rangle}, \tag{8}$$

where the average $\langle\cdot\rangle$ is taken in the ensemble $T_{N_{\rm tot}}$ sampled by the join-and-cut algorithm. The quantity defined in Eq. (8) is estimated in the usual way from the Monte Carlo data obtaining is this way $X^{\rm cens}_{\rm MC}(N_{\rm min})$. Then $\hat{\gamma}(N_{\rm min})$ is computed by solving the equation

$$X^{\rm cens}_{\rm MC}(N_{\rm min})=[X]_{{\rm th},\hat{\gamma}}(N_{\rm min}), \tag{9}$$

where, for every function of N_1, we define

$$[f(N_1)]_{{\rm th},\gamma}(N_{\rm min})\equiv\frac{\sum_{N_1=N_{\rm min}}^{N_{\rm tot}-N_{\rm min}}f(N_1)N_1^{\gamma-1}(N_{\rm tot}-N_1)^{\gamma-1}}{\sum_{N_1=N_{\rm min}}^{N_{\rm tot}-N_{\rm min}}N_1^{\gamma-1}(N_{\rm tot}-N_1)^{\gamma-1}}. \tag{10}$$

The variance of $\hat{\gamma}(N_{\rm min})$ is then given by

$$\mathrm{var}[\hat{\gamma}(N_{\rm min})]=\frac{\mathrm{var}(X^{\rm cens}_{\rm MC}(N_{\rm min}))}{([X;X]_{{\rm th},\hat{\gamma}}(N_{\rm min}))^2} \tag{11}$$

TABLE I. Number of iterations and autocorrelation times for the various values of $N_{\rm tot}$.

$N_{\rm tot}$	$N_{\rm iter}$	$\tau_{{\rm int},Y(1)}$	$\tau_{{\rm int},Y(1000)}$
200	5×10^8	$1.479\,70\pm0.000\,55$	
2000	6.2×10^8	2.808 ± 0.022	
20 000	10^8	6.96 ± 0.18	9.35 ± 0.21
40 000	8.5×10^8	8.80 ± 0.23	10.78 ± 0.24

where $[X;X]=[X^2]-[X]^2$. We must finally compute $\text{var}(X_{\rm MC}^{\rm cens}(N_{\rm min}))$. As this quantity is defined as the ratio of two mean values [see formula (8)] one must take into account the correlation between denominator and numerator. Here we have used the standard formula for the variance of a ratio (valid in the large-sample limit)

$$\text{var}\left(\frac{A}{B}\right)=\frac{\langle A\rangle^2}{\langle B\rangle^2}\,\text{var}\left(\frac{A}{\langle A\rangle}-\frac{B}{\langle B\rangle}\right). \tag{12}$$

Finally, let us mention how to combine data from runs at different values of $N_{\rm tot}$. The approach we use consists in analyzing the data separately for each $N_{\rm tot}$ and then in constructing the usual weighted average of the resulting estimates $\hat{\gamma}(N_{\rm min})$ with weights inversely proportional to the estimated variances.

Let us now discuss our results. We have performed high-statistics runs at $N_{\rm tot}=200$, 2000, 20 000 and 40 000. The number of iterations is reported in Table I. The total simulation took 16 months on an AlphaStation 600 Mod 5/266. In the same table we report also, for two different values of $N_{\rm min}$, the autocorrelation times for the observable

$$Y(N_{\rm min})=\frac{X\theta_{N_{\rm min}}}{\langle X\theta_{N_{\rm min}}\rangle}-\frac{\theta_{N_{\rm min}}}{\langle\theta_{N_{\rm min}}\rangle} \tag{13}$$

which according to (12) controls the errors on γ. We use here a standard autocorrelation analysis ([3], Appendix C) with a self-consistent window of $15\tau_{{\rm int},Y}$, supplemented by an *ad hoc* prescription to take into account the fact that for $t>15\tau_{{\rm int},Y}$ the autocorrelation functions still have a long tail, which gives a sizeable contribution to $\tau_{{\rm int},Y}$ ([14], Appendix C). The contribution of the tail to $\tau_{{\rm int},Y}$ amounts to approximately 20% for the two larger values of $N_{\rm tot}$, 2% for $N_{\rm tot}=2000$, while for $N_{\rm tot}=200$ the autocorrelation function is already in the noise for $t>15\tau_{{\rm int},Y}$. The results are consistent with the expectation of $\tau_{{\rm int},Y}\sim N^{\approx0.3}$ so that, taking into account that the CPU time per iteration increases as $\sim N^{\approx0.9}$, we find that the CPU-time per independent walk increases roughly as $N^{\approx1.2}$.

In Table II and Table III we report, for various $N_{\rm min}$, the estimates of $X_{\rm MC}^{\rm cens}(N_{\rm min})$ that are needed for our analysis.

Let us now discuss the results. To determine γ we tried to be very conservative, in order to avoid underestimating the systematic errors. We have chosen the simplest possible strategy: we simply increase $N_{\rm tot}$ and $N_{\rm min}$ (this second parameter will play little role for larger values of $N_{\rm tot}$) until the estimates of γ become independent of these two parameters.

Let us consider first $N_{\rm tot}=200$. We see here that the estimates of γ increase with $N_{\rm min}$ and for $N_{\rm min}=50$ they give $\gamma\approx1.1605$. This value is in agreement with Monte Carlo studies [16] performed in the same range of values of N and exact-enumeration studies [5,17]. Consider now $N_{\rm tot}=2000$. One can see that the estimates of γ are lower and indicate $1.1580\lesssim\gamma\lesssim1.1585$; clearly the estimate at $N_{\rm tot}=200$ was biased upward by the corrections to scaling. Let us now consider the results of Table III, where we give the estimates of γ coming from the weighted average of the results with $N_{\rm tot}=20\,000$ and $N_{\rm tot}=40\,000$. The estimates are extremely flat and agree within error bars from $N_{\rm min}=1$ to $N_{\rm min}=8000$; they indicate $1.1574\lesssim\gamma\lesssim1.1578$. Again the new estimate is lower than the previous ones. At least at $N_{\rm tot}=2000$ there are still systematic deviations that are larger than the statistical error. Of course the same could be true for our results at the larger value of $N_{\rm tot}$. The most conservative way to solve the question would be to have data at a higher value of $N_{\rm tot}$, say $N_{\rm tot}=4\times10^5$, with comparable statistics. However, this is not possible with current computer resources. We have thus simply tried to estimate the systematic bias by comparing the results with different $N_{\rm tot}$ assuming that the systematic error vanishes as $N_{\rm tot}^{-\Delta}$ with $\Delta\gtrsim1/2$ [this is the behavior one expects if the corrections to c_N, formula (1), vanish as $N^{-\Delta}$]. Specifically we assume that the effective exponent $\hat{\gamma}(N_{\rm tot})$ behaves as

$$\hat{\gamma}(N_{\rm tot})=A+B/N_{\rm tot}^{\Delta}. \tag{14}$$

We neglect here the dependence on $N_{\rm min}$, which is small for $N_{\rm tot}=2000$ and irrelevant for larger values of $N_{\rm tot}$. In order to get an upper bound on B we assume $\Delta=1/2$, $\hat{\gamma}(2000)=1.1585$ and $\hat{\gamma}(40\,000)=1.1574$; that is we use for $N_{\rm tot}=2000$ the higher value of $\hat{\gamma}$ compatible with our data, and for $N_{\rm tot}=40\,000$ the lower value: this guarantees the

TABLE II. Raw data and estimates of γ for $N_{\rm tot}=200$ and $N_{\rm tot}=2000$.

	$N_{\rm tot}=200$			$N_{\rm tot}=2000$	
$N_{\rm min}$	$X_{\rm MC}^{\rm cens}$	γ	$N_{\rm min}$	$X_{\rm MC}^{\rm cens}$	γ
1	$8.701\,168\pm0.000\,052$	$1.152\,88\pm0.000\,11$	1	$13.298\,266\pm0.000\,068$	$1.15782\pm0.000\,13$
10	$8.842\,084\pm0.000\,036$	$1.158\,08\pm0.000\,21$	100	$13.452\,571\pm0.000\,046$	$1.15802\pm0.000\,28$
20	$8.943\,002\pm0.000\,026$	$1.158\,66\pm0.000\,34$	200	$13.551\,931\pm0.000\,033$	$1.15811\pm0.000\,45$
30	$9.017\,434\pm0.000\,019$	$1.158\,75\pm0.000\,53$	300	$13.625\,478\pm0.000\,025$	$1.15838\pm0.000\,71$
40	$9.074\,675\pm0.000\,014$	$1.159\,99\pm0.000\,84$	400	$13.682\,081\pm0.000\,018$	1.1598 ± 0.0011
50	$9.119\,083\pm0.000\,010$	1.1605 ± 0.0014	500	$13.725\,970\pm0.000\,013$	1.1584 ± 0.0019

TABLE III. Raw data for $N_{\rm tot}=20\,000$ and $N_{\rm tot}=40\,000$ and combined estimate of γ for various values of $N_{\rm min}$.

$N_{\rm min}$	$X_{\rm MC}^{\rm cens}(20\,000)$	$X_{\rm MC}^{\rm cens}(40\,000)$	γ
1	17.90 54 ± 0.000 26	19.288 50 ±0.000 10	1.157 63±0.000 18
200	17.943 30 ± 0.000 23	19.310 211±0.000 095	1.157 62±0.000 21
400	17.977 15 ± 0.000 21	19.329 406±0.000 090	1.157 58±0.000 24
600	18.006 87 ± 0.000 20	19.346 998±0.000 086	1.157 65±0.000 26
800	18.033 76 ± 0.000 19	19.363 292±0.000 083	1.157 60±0.000 28
1000	18.058 30 ± 0.000 17	19.378 624±0.000 080	1.157 64±0.000 30
1200	18.080 95 ± 0.000 16	19.393 077±0.000 077	1.157 54±0.000 32
1400	18.101 98 ± 0.000 15	19.406 824±0.000 074	1.157 49±0.000 34
1600	18.121 72 ± 0.000 14	19.419 918±0.000 071	1.157 44±0.000 36
1800	18.140 22 ± 0.000 13	19.432 477±0.000 069	1.157 55±0.000 38
2000	18.157 60 ± 0.000 12	19.444 488±0.000 067	1.157 49±0.000 40
2200	18.173 94 ± 0.000 12	19.456 041±0.000 065	1.157 46±0.000 42
2400	18.189 30 ± 0.000 11	19.467 169±0.000 063	1.157 39±0.000 45
2600	18.203 88 ± 0.000 11	19.477 901±0.000 061	1.157 41±0.000 47
2800	18.217 71 ± 0.000 10	19.488 255±0.000 059	1.157 39±0.000 50
3000	18.230 811 ± 0.000 093	19.498 275±0.000 058	1.157 48±0.000 52
3500	18.260 909 ± 0.000 081	19.521 898±0.000 053	1.157 53±0.000 58
4000	18.287 471 ± 0.000 069	19.543 763±0.000 049	1.157 72±0.000 66
5000	18.331 323 ± 0.000 049	19.582 986±0.000 043	1.157 49±0.000 83
6000	18.364 968 ± 0.000 034	19.617 183±0.000 037	1.1566 ±0.0010
7000	18.389 939 ± 0.000 021	19.647 298±0.000 032	1.1586 ±0.0013
8000	18.407 212 ± 0.000 011	19.673 754±0.000 027	1.1582 ±0.0017

most conservative estimate of the correction-to-scaling terms. Plugging the numbers in our ansatz we get $B\approx 0.06$, so that $B/\sqrt{40\,000}\approx 0.0003$. We have taken as our final estimate the value at $N_{\rm min}=2000$:

$$\gamma = 1.1575 \pm 0.0003 \pm 0.0003, \tag{15}$$

where the first error is the statistical one (68% confidence limits) while the second is a subjective estimate of the error due to the corrections to scaling.

To conclude, let us mention that we expect problems similar to those we find for γ also in the estimates of the connectivity constant μ defined in, Eq. (1). Indeed γ and μ are usually determined together and thus they are both affected by strong corrections to scaling. Therefore, also for μ we expect a large systematic bias; clearly large-N grand-canonical simulations would be welcome.

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