Abstract

We present a high-statistics Monte Carlo determination of the exponent $\gamma$ for self-avoiding walks on a Manhattan lattice in two dimensions. A conservative estimate is $\gamma \gtrsim 1.3425 \pm 0.0003$, in agreement with the universal value 43/32 on regular lattices, but in conflict with predictions from conformal field theory and with a recent estimate from exact enumerations. We find strong corrections to scaling that seem to indicate the presence of a non-analytic exponent $\Delta < 1$. If we assume $\Delta = 11/16$ we find $\gamma = 1.3436 \pm 0.0003$, where the error is purely statistical.
1 Introduction

The self-avoiding walk (SAW) is a model which describes the universal properties of flexible chain polymers in a good solvent in the dilute regime. A simple but intriguing modification has been recently introduced to study polymers with an intrinsic orientation [1, 2]. This orientation could be due to the presence of dipole moments on the monomers of the chain or to an ordering in the sequence of monomer constituents. On the lattice one considers SAWs with a short-range interaction between different steps of the walk according to their relative orientation. The partition function is simply

\[ z_N = \sum_{\{\omega\}} e^{\beta_a m_a + \beta_p m_p}, \]  

where \( m_p \) and \( m_a \) are respectively the number of parallel and antiparallel interactions and the sum extends over all SAWs of length \( N \).

This model has a rich phase diagram [3–7] and can be analyzed theoretically [1, 2] by mapping it into a complex \( O(n) \) model in the limit \( n \to 0 \). In two dimensions, the theory with a repulsive interaction between parallel bonds, i.e. with \( \beta_a = 0, \beta_p < 0 \), was analyzed using conformal invariance techniques [2]. It was shown that the new interaction is truly marginal, giving rise to a line of fixed points. The main consequence is that the partition-function exponent \( \gamma \) should vary continuously with the strength of the orientation-dependent interaction. The exponent \( \gamma \) is defined from the asymptotic behaviour of the partition function \( z_N \), which should scale asymptotically as

\[ z_N = A \mu^N N^{\gamma-1}. \]  

Here \( A \) and \( \mu \) are non-universal constants, while \( \gamma \) is an exponent that, in the absence of the orientation-dependent interaction, is expected to be universal: it should not depend on the details of the interaction and it should assume the same value for any two-dimensional regular lattice. Using Coulomb-gas techniques, Nienhuis [8] predicted \( \gamma_{\text{reg}} = 43/32 \), a value that has been confirmed to high-precision by many numerical computations, see e.g. Ref. [4]. On the other hand, for interacting oriented SAWs with \( \beta = 0, \beta_p < 0 \), \( \gamma \) should be a function of \( \beta_p \). Unfortunately, conformal field theory does not provide definite numerical estimates, although it predicts that \( \gamma(\beta_p) \) should decrease monotonically as \( \beta_p \to -\infty \).

The square-lattice model was studied by exact enumerations in Ref. [3] and by transfer-matrix techniques in Ref. [10], finding a very tiny dependence of \( \gamma \) on \( \beta_p \), thereby supporting the field-theory analysis. When parallel interactions are forbidden, i.e. for \( \beta_p = -\infty \), Ref. [3] finds using unbiased approximants,

\[ 0.006 \lesssim \gamma_{\text{reg}} - \gamma \lesssim 0.013. \]  

The systematic uncertainty due to the extrapolations of two different series is taken into account in this range. The evidence for a non-universal behaviour is not overwhelming, keeping also into account that several problems affected the results of the analysis. As the authors report, they found small shifts of the critical fugacity \( \mu_c \) from the value it assumes for the ordinary SAW, in contrast with the theoretical result that
μc should not depend on βp. More worryingly, an analysis using biased differential approximants with fixed critical fugacity gave a smaller prediction for γreg − γ, although with much less confidence since most of the approximants were defective. The analysis of Koo [10], based on strips of width ≤ 8, was less precise. For the largest value of βp that was analyzed, βp = −3, he finds γreg − γ = 0.018 ± 0.012, a difference that is barely significant.

The evidence provided by Refs. [3,10] for a non-universal behaviour of γ was not conclusive and this spurred many workers to improve the result and/or to investigate the problem using different methods. The transfer-matrix analysis was improved in Ref. [3]: using larger strips they did not find any evidence of a non-universal behaviour and interpreted previous results as due to short-series effects and to the small size of the strips. Other field-theoretical predictions were also tested. Refs. [4,11] computed by Monte Carlo and exact-enumeration methods the mean value of mp for ordinary SAWs: they find that ⟨mp⟩ converges to a constant as N → ∞, in contrast with the field-theoretical prediction ⟨mp⟩ ∼ log N. Recently the behaviour of ⟨mp⟩ on a cylinder was determined by a Monte Carlo simulation [12], finding also in this case a result in disagreement with the field-theory predictions.

Recently it was shown [13] that Cardy’s original argument implies that the exponent γ for the Manhattan lattice should also be different from the exponent γreg. Indeed on this lattice a SAW is oriented by default and parallel interactions are automatically suppressed. From the analysis of long exact-enumeration series the authors of Ref. [13] report

\[ γ_{reg} − γ = 0.0053 ± 0.0030. \]  

(1.4)

The effect is extremely small. It differs from zero by less than two error bars. The evidence for γ ≠ γreg is therefore not overwhelmingly persuasive, and the theoretical importance of the problem asks for further investigations. Indeed one can suspect that the small deviation is simply a systematic effect due to the corrections to scaling that are not completely taken into account by the analysis.

We have therefore decided to investigate the problem by means of a Monte Carlo simulation, computing the exponent γ for SAWs on a Manhattan lattice. The advantage is that we are able to work with very long walks (N ≤ Nmax = 32000) and therefore to reduce the unknown systematic uncertainty due to the extrapolation N → ∞.

Our simulations were performed with two different algorithms. The first one, the join-and-cut algorithm [14], is a dynamic Monte Carlo algorithm that works in the ensemble of couples of walks with fixed total length. The algorithm is at present the best one to compute the exponent γ since the autocorrelation time in CPU units scales as N^{1.6}, while for other algorithms it behaves no better than N^{≈2}. The second algorithm is a variant of the pruned-enriched Rosenbluth method (PERM) [15]. This is a growth algorithm. Asymptotically, it is slower than the join-and-cut algorithm in generating independent configurations. The computer time to generate an independent configuration scales as N^2. But the constant in front of N^2 is very small, for instance the number of monomer additions needed to obtain one independent configuration was numerically found to increase as ≈ 0.008N^2 for N > 10000. Therefore
it is possible that the PERM is the most efficient one even for quite long walks. As we shall discuss, with a clever improvement, the Markovian anticipation, the PERM is more efficient in providing estimates of $\gamma$ than the join-and-cut algorithm as long as the length of the sampled walks is less than $10^4$. Only for longer walks the join-and-cut algorithm is faster. Another advantage in the present context is that it gives directly, together with the estimate of the partition sum for chains of length $N_{\text{max}}$ and without extra cost, also all partition sums for shorter chains. These estimates for different $N$ are not independent, but just because of this fact they are particularly useful for estimating $\gamma$.

The main sources of systematic errors in our analysis are the corrections to scaling, assumed to be of the form

$$\frac{z_N}{A_N N^{\gamma-1}} \approx 1 + \frac{a}{N^\Delta} + \frac{a_1}{N^{\Delta_1}} + \cdots$$

with $\Delta < \Delta_1 < \cdots$. All numerical evidence for SAWs on regular lattices (square, honeycomb and triangular) indicates that the leading correction is the analytic one \[16\] - \[18\]. On the other hand Saleur \[19\] predicted $\Delta = 11/16$, a result that was confirmed in numerical work on lattice trails \[20, 21\]. Why this exponent does not show up for SAWs on regular lattices is completely unclear.

For the Manhattan lattice, Ref. \[13\] showed that the enumeration data are very well fitted using an Ansatz with no non-analytic terms \[2\] with $\Delta < 1$. On the other hand a naive fit of our Monte Carlo data would indicate just the opposite: the results are well fitted assuming a correction-to-scaling exponent of order $\Delta \approx 0.5 - 0.7$. Of course one should not take this indication too seriously — our data are not precise enough for a serious attempt to determine $\Delta$ — but it is fair to say that $\Delta = 11/16$ is our preferred value. If we assume $\Delta = 11/16$ we obtain

$$\gamma = 1.3436 \pm 0.0003,$$

in very good agreement with $\gamma = \gamma_{\text{reg}} = 43/32 = 1.34375$. We have also tried to analyze our data assuming $\Delta = 1$. The quality of the fit is somewhat worse, although one could think that this is simply due to the additional neglected corrections to scaling \[2\] that are still relevant at the values of $N$ we are working (the determination of $\Delta$ depends mainly on the data with $N_{\text{tot}} = 2000$, i.e. on walks with $N \lesssim 1000$).

We do not know how reliable the estimate (1.6) is and a serious analysis of the systematic errors is practically impossible. In any case, without explicit assumptions

\[1\] An additional hint to $\Delta = 11/16$ is the numerical observation of Barkema and Flesia \[4\] that the average number of loops of length $l$ forming a parallel contact scales as $\langle m_p \rangle_l \sim l^{-1.65 \pm 0.05}$. From this they estimate that the total number of parallel contacts behaves as $\langle m_p \rangle \sim a - b/N^{0.65}$. On the other hand, $\langle m_p \rangle$ is proportional to $dz_N(T)/dT$ if one includes an orientation dependent interaction, whence there should be generically a term $\sim N^{-0.65} \approx N^{-11/16}$ in $z_N(T)$.

\[2\] Inclusion of a term with $\Delta = 11/16$ worsens the quality of the extrapolation \[22\].

\[3\] A similar phenomenon occurs for SAWs on the square lattice \[18\]. If one analyzes the end-to-end distance for short SAWs, with a single correction term, one finds $\Delta \approx 0.80$. Only the inclusion of longer walks and more correction terms with $\Delta_i > 1$ gives $\Delta \approx 1.0$. 


on \( \Delta \), we can still obtain the lower bound

\[
\gamma \gtrsim 1.3425 \pm 0.0003.
\]  

(1.7)

Although this result is lower than the estimate (1.6), it clearly supports the fact that \( \gamma = \gamma_{\text{reg}} \). The prediction of Ref. \([13]\), \( \gamma = 1.3385 \pm 0.003 \) is instead clearly excluded.

We should point out that if we analyze only data with small values of \( N \), we would obtain a lower estimate for \( \gamma \), in close agreement with the result (1.4). This shows the crucial role played in this problem by corrections to scaling and the importance of performing simulations for very large values of \( N \).

2 The join-and-cut algorithm on the Manhattan lattice

2.1 Description of the algorithm

In this Section we will define the pivot and the join-and-cut algorithm on a Manhattan lattice. The Manhattan lattice is a two-dimensional square lattice on which bonds are directed in such a way that adjacent rows (columns) have antiparallel directions, corresponding to the traffic pattern in Manhattan. Although bonds are directed, there is no overall directional bias. Explicitly we will assume the following orientations: a vertical bond connecting the points of coordinates \((x, y)\), \((x, y+1)\) is directed upward if \(x\) is even, downward if \(x\) is odd; a horizontal bond connecting the points of coordinates \((x, y)\) and \((x+1, y)\) is directed to the left if \(y\) is even, to the right if \(y\) is odd.

Let us now define the pivot algorithm \([23–25]\). It works in the ensemble of fixed-length walks with free endpoints: we will be interested in self-avoiding walks, but the algorithm can also be applied in a very efficient way to the Domb-Joyce model \([26,27]\), to power-law walks \([26]\), and to interacting polymers far from the \( \Theta \)-transition \([28,29]\).

The algorithm works as follows \([23]\). Given an \( N \)-step SAW \( \omega \) starting at the origin and ending anywhere, \( \omega \equiv \{\omega(0), \ldots, \omega(N)\} \), an iteration of the algorithm consists of the following steps:

1. Choose randomly, with uniform probability, an integer \( k \in \{0, 1, \ldots, N - 1\} \);
2. Choose with probability \( P(g) \) an element \( g \) of the lattice point symmetry group. The probability must satisfy \( P(g) = P(g^{-1}) \) to ensure detailed balance;
3. Propose a pivot move \( \omega \rightarrow \omega' \) defined by

\[
\omega'(i) = \begin{cases} 
\omega(i) & \text{for } 1 \leq i \leq k, \\
\omega(k) + g(\omega(i) - \omega(k)) & \text{for } k + 1 \leq i \leq N.
\end{cases} 
\]  

(2.1)

The proposed move is accepted if \( \omega' \) is self-avoiding; otherwise it is rejected and we stay with \( \omega \).
The probability \( P(g) \) must be such to ensure ergodicity: as discussed in Refs. [25,30], not all symmetry transformations are needed. In particular [30] the pivot algorithm is ergodic on a square lattice if \( P(g) \) is non-vanishing only for diagonal reflections, that is for reflections through lines of slope \( \pm 1 \).

For the Manhattan lattice the point symmetry group is much smaller than the symmetry group of the square lattice. Indeed the lattice is symmetric only with respect to lines of slope \( -1 \) going through lattice points \((x,y)\) with \( x + y \) even, and with respect to lines of slope \( +1 \) going through \((x,y)\) with \( x + y \) odd. Therefore we will modify step (ii) in the following way:

(ii) if \( \omega_x(k) + \omega_y(k) \) is even (resp. odd), let \( g \) be the reflection with respect to a line of slope \(-1\) (resp. \(+1\)), going through \( \omega(k) \).

Since \( g^2 = 1 \), detailed balance is automatically satisfied. The tricky point is ergodicity. It can be proved by slightly modifying the proof of Section 5 of Ref. [30]. Using the same definitions, the basic observation is the following: if \( \omega(k) \equiv (x_k, y_k) \) is a walk site belonging to a diagonal support line of slope \(-1\) (resp. \(+1\)), then \( x_k + y_k \) is even (resp. odd). Using this fact the proof works without any change.

We want now to define the join-and-cut algorithm [14]. The tricky point here is that in general, given two walks on the Manhattan lattice, their concatenation is a walk that does not respect the bond orientation of the lattice. More precisely, given two walks \( \omega_1, \omega_2 \) of lengths \( N_1 \) and \( N_2 \), the concatenated walk \( \omega = \omega_1 \circ \omega_2 \) respects the orientation of the lattice only if

\[
\text{mod}(\omega_{1x}(0) - \omega_{2x}(0), 2) = 0, \quad \text{mod}(\omega_{1y}(0) - \omega_{2y}(0), 2) = 0. \tag{2.2}
\]

This reflects the fact that only translations of two steps in each direction are symmetries of the lattice. A second consequence of the bond orientation of the Manhattan lattice is the following: consider a walk \( \omega \) and cut it into two parts \( \omega_1 \) and \( \omega_2 \) such that \( \omega = \omega_1 \circ \omega_2 \). In general there is no lattice translation \( T \) such the translated walk \( T\omega_2 \) respects the bond orientation of the lattice and satisfies \( (T\omega_2)(0) = \omega_1(0) = \omega(0) \). Indeed this happens only if

\[
\text{mod}(\omega_{1x}(0) - \omega_{2x}(0), 2) = 0, \quad \text{mod}(\omega_{1y}(0) - \omega_{2y}(0), 2) = 0. \tag{2.3}
\]

With these two observations in mind we define our ensemble in the following way: \( T_{N_{\text{tot}}} \) consists of all pairs \((\omega_1, \omega_2)\) of SAWs, each walk starting either in \((0,0)\) or in \((1,1)\) and ending anywhere, such that the total number of steps in the two walks is some fixed even number \( N_{\text{tot}} \). Moreover we require the lengths of \( \omega_1 \) and \( \omega_2 \) to be even. Explicitly

\[
T_{N_{\text{tot}}} = \bigcup_{k=1}^{N_{\text{tot}}/2-1} (S_{2k}(0,0) \cup S_{2k}(1,1)) \times (S_{N_{\text{tot}}-2k}(0,0) \cup S_{N_{\text{tot}}-2k}(1,1)) \quad \tag{2.4}
\]

where \( S_k(x,y) \) is the set of \( k \)-step walks starting from \((x,y)\) and ending anywhere. Each pair in the ensemble is given equal weight: therefore the two walks are not

\footnote{The only exception to this rule is when \( \omega_2 \) is a rod.}
interacting except for the constraint on the sum of their lengths. Notice that there is a one-to-one correspondence between $S_k(0,0)$ and $S_k(1,1)$ so that the ensemble defined in Eq. (2.4) is equivalent to

$$T_{N_{\text{tot}}} = \bigcup_{k=1}^{N_{\text{tot}}/2 - 1} S_{2k}(0,0) \times S_{N_{\text{tot}}-2k}(0,0) \quad (2.5)$$

One sweep of the algorithm consists of the following steps:

(i) Starting from a pair of walks $(\omega_1, \omega_2)$, we update each of them independently using some ergodic fixed-length algorithm. We use the pivot algorithm we described above.

(ii) With probability $1/2$ we interchange $\omega_1$ and $\omega_2$, i.e. $(\omega_1, \omega_2) \rightarrow (\omega_2, \omega_1)$.

(iii) We first check the parity of the endpoints: if $\text{mod}(\omega_1x(N_1) - \omega_2x(0), 2) = 1$, we stay with $(\omega_1, \omega_2)$. Otherwise we attempt a join-and-cut move. We choose with uniform probability $k \in \{1, \ldots, N_{\text{tot}}/2 - 1\}$. Then we concatenate the two walks $\omega_1$ and $\omega_2$ forming a new (not necessarily self-avoiding) walk $\omega_{\text{conc}} = \omega_1 \circ \omega_2$; then we cut $\omega_{\text{conc}}$ creating two new walks $\omega'_1$ and $\omega'_2$ of lengths $2k$ and $N_{\text{tot}}-2k$. If $\omega'_1$ and $\omega'_2$ are self-avoiding we keep them; otherwise the move is rejected and we stay with $\omega_1$ and $\omega_2$.

It is easy to see that the full algorithm is ergodic.

The algorithm defined on the Manhattan lattice works essentially in the same way as the standard one. The only important difference is that one must check the parities of $\omega_1(N_1)$ and $\omega_2(0)$ before attempting the join-and-cut move. This check is successfull in 50% of the cases and thus the algorithm we have defined above should be essentially equivalent to the standard algorithm in which one performs two pivot updates of each walk for every join-and-cut move (in the notation of Ref. [14] it corresponds to the algorithm with $n_{\text{piv}} = 2$). In principle it is easy to avoid this 50% rejection by modifying the third step of the algorithm in the following way:

(iii) [improved join-and-cut move]. If $\text{mod}(\omega_{1x}(N_1) - \omega_{2x}(0), 2) = 1$, let $\omega_{\text{conc}} = \omega_1 \circ R\omega_2$, where $R\omega_2$ is the walk reflected with respect to the line of slope +1 going through $\omega_2(0)$; if $\text{mod}(\omega_{1x}(N_1) - \omega_{2x}(0), 2) = 0$, let $\omega_{\text{conc}} = \omega_1 \circ \omega_2$. Then proceed as before.

This modification attempts twice the number of join-and-cut moves with respect to the previous one, and thus it should be more efficient. However the difference in performance is not expected to be large. Indeed from the analysis of the autocorrelation times of Ref. [14], we obtain\footnote{Notice that in Ref. [14] $\tau_{\text{int}}(n_{\text{piv}})$ is reported in units of two iterations, each iteration consisting of $n_{\text{piv}}$ pivot attempts and one join-and-cut attempt. In order to make a correct comparison we should multiply $\tau_{\text{int}}(n_{\text{piv}})$ by $n_{\text{piv}}$. Thus what we report as $\tau_{\text{int}}(n_{\text{piv}} = 2)$ corresponds to $2\tau_{\text{int}}(n_{\text{piv}} = 2)$ of Ref. [14].} that the ratio $\tau_{\text{int}}(n_{\text{piv}} = 2)/\tau_{\text{int}}(n_{\text{piv}} = 1)$ is equal to...
1.6, 1.5, 1.2 for \( N_{\text{tot}} = 500, 2000, 8000 \) respectively. For the algorithm on the Manhattan lattice we expect \( \tau_{\text{int}}(\text{non-impr})/\tau_{\text{int}}(\text{imp}) \) to be very similar to the previous ratio: therefore for \( N_{\text{tot}} = 8000 \) we expect that the autocorrelation time for the original algorithm to be only 20-30\% higher than the corresponding time for the improved one. One should also keep in mind that one iteration of the improved algorithm is slower than one iteration of the unimproved one, since one is doing twice the number of join-and-cut attempts. Therefore we expect that for \( N_{\text{tot}} = 8000 \) the improved algorithm is only 10-20\% better than the original one. Since the implementation of the improved algorithm required major changes of our codes, we decided to work with the unimproved version we described above.

### 2.2 Determination of \( \gamma \) from join-and-cut data

Let us now discuss how the critical exponent \( \gamma \) 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

\[
\pi(N_1) = \begin{cases} 
\frac{z_{N_1}z_{N_{\text{tot}}-N_1}}{Z(N_{\text{tot}})} & \text{if } N_1 \text{ is even,} \\
0 & \text{if } N_1 \text{ is odd}
\end{cases}
\]  

(2.6)

for \( 1 \leq N_1 \leq N_{\text{tot}} - 1 \); here \( Z(N_{\text{tot}}) \) is the obvious normalization factor and \( z_N \) is the number of \( N \)-step walks going from the origin to any lattice point whose asymptotic behaviour for large \( N \) is given by (1.2). The idea is then to make inferences of \( \gamma \) from the observed statistics of \( N_1 \). Of course the problem is that (1.2) is an asymptotic formula valid only in the large-\( N \) regime. We will thus proceed in the following way: we will suppose that (1.2) is valid for all \( N \geq N_{\text{min}} \) for many increasing values of \( N_{\text{min}} \) and correspondingly we will get estimates \( \hat{\gamma}(N_{\text{tot}}, N_{\text{min}}) \); these quantities are effective exponents that depend on \( N_{\text{min}} \) and that give correct estimates of \( \gamma \) as \( N_{\text{min}} \) and \( N_{\text{tot}} \) go to infinity.

The determination of \( \gamma \) from the data is obtained using the maximum-likelihood method (see e.g. [31]). We will present here only the results: for a detailed discussion we refer the reader to [14].

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

\[
\theta_{N_{\text{min}}}(N_1) = \begin{cases} 
1 & \text{if } N_{\text{min}} \leq N_1 \leq N_{\text{tot}} - N_{\text{min}}, \\
0 & \text{otherwise,}
\end{cases}
\]  

(2.7)

and let \( X \) be the random variable

\[
X = \log[N_1(N_{\text{tot}} - N_1)]
\]  

(2.8)

Then define

\[
X_{\text{cens}}(N_{\text{min}}) = \frac{\langle X \theta_{N_{\text{min}}} \rangle}{\langle \theta_{N_{\text{min}}} \rangle}
\]  

(2.9)
where the average $\langle \cdot \rangle$ is taken in the ensemble $T_{N_{\text{tot}}}$ sampled by the join-and-cut algorithm. The quantity defined in Eq. (2.9) is estimated in the usual way from the Monte Carlo data obtaining in this way $X_{MC}^{cens}(N_{\text{min}})$. Then $\hat{\gamma}(N_{\text{min}})$ is computed by solving the equation

$$X_{MC}^{cens}(N_{\text{min}}) = [X]_{th,\hat{\gamma}}(N_{\text{min}}), \quad (2.10)$$

where, for every function of $N_1$, we define

$$[f(N_1)]_{th,\hat{\gamma}}(N_{\text{min}}) \equiv \frac{\sum_{N_1=N_{\text{min}}}^{N_{\text{tot}}-N_{\text{min}}} f(N_1) N_1^{\gamma-1}(N_{\text{tot}} - N_1)^{\gamma-1}}{\sum_{N_1=N_{\text{min}}}^{N_{\text{tot}}-N_{\text{min}}} N_1^{\gamma-1}(N_{\text{tot}} - N_1)^{\gamma-1}}; \quad (2.11)$$

here the sum is extended over even values of $N_1$. The variance of $\hat{\gamma}(N_{\text{min}})$ is then given by

$$\text{Var} [\hat{\gamma}(N_{\text{min}})] = \frac{\text{Var} (X_{MC}^{cens}(N_{\text{min}}))}{(\langle X \rangle_{th,\hat{\gamma}}(N_{\text{min}}))^2}, \quad (2.12)$$

where $[X; X] = [X^2] - [X]^2$. We must finally compute $\text{Var} (X_{MC}^{cens}(N_{\text{min}}))$. As this quantity is defined as the ratio of two mean values (see Eq. (2.9)) 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)

$$\text{Var} \left( \frac{A}{B} \right) = \frac{\langle A \rangle^2}{\langle B \rangle^2} \text{Var} \left( \frac{A}{\langle A \rangle} - \frac{B}{\langle B \rangle} \right). \quad (2.13)$$

### 2.3 Dynamic behaviour

Let us first discuss the simulations using the join-and-cut algorithm. We have performed high-statistics runs at $N_{\text{tot}} = 500, 2000, 8000$ and $32000$. In Table 1 we report the number of iterations and the CPU time per iteration on an Alpha-Station 600 Mod 5/266. The total join-and-cut runs took 1 year of CPU on this machine.

In Table 2 we report the acceptance fraction of the pivot and of the join-and-cut moves, and, for two different values of $N_{\text{min}}$, the autocorrelation times for the observable

$$Y(N_{\text{min}}) = \frac{X_\theta N_{\text{min}}}{\langle X_\theta N_{\text{min}} \rangle} - \frac{\theta N_{\text{min}}}{\langle \theta N_{\text{min}} \rangle} \quad (2.14)$$

that, according to Eq. (2.13), controls the errors on $\gamma$. Notice that $Y(2) = X/\langle X \rangle - 1$, so that $\tau_{\text{int},Y}(2) = \tau_{\text{int},X}$.

To compute the autocorrelation times we used the recipe of Ref. [32, Appendix C]. Indeed the autocorrelation function has a very long tail with a very small amplitude, due to the fact that $\tau_{\exp} \gg \tau_{\text{int},Y}$. For this reason the self-consistent windowing method of Ref. [25, Appendix C] does not work correctly and underestimates the autocorrelation time. Following Ref. [32], we have computed $\tau_{\text{int},Y}$ as

$$\tau_{\text{int},Y} = \tau_{\text{int},Y} + \tau_{\text{tail},Y} \quad (2.15)$$

Here $\tau_{\text{int},Y}$ is the autocorrelation time computed using the self-consistent windowing method of Ref. [25, Appendix C] with window $W = 15\tau_{\text{int},Y}$ and

$$\tau_{\text{tail},Y} = \rho_Y(W) W \log \left( \frac{N}{Wf_{\text{piv}}} \right) \quad (2.16)$$
where \( \rho_Y(t) \) is the normalized autocorrelation function and \( f_{piv} \) is the acceptance fraction of the pivot algorithm. Of course Eq. (2.16) is a very rough ad hoc estimate of the contribution of the tail. For \( X \), it amounts to approximately 35% for \( N_{tot} = 32000 \), 24\% for \( N_{tot} = 8000 \), 15\% for \( N_{tot} = 2000 \), and 5\% for \( N_{tot} = 500 \). Based on our experience with the pivot algorithm we have assigned to \( \tau_{tail,Y} \) an error of 10\%. The error on \( \tau_{int,Y} \) was instead computed as in Ref. [25].

We have first analyzed the acceptance fractions. The general analysis of Ref. [14] predicts \( f_{piv} \sim N^{-p} \) and \( f_{jc} \sim N^{-q} \), with \( p \approx 0.19 \) and \( q \approx \gamma - 1 \approx 0.34 \). A least-square fit to the data of Table 2 gives

\[
p = 0.19605 \pm 0.00001 \quad \chi^2_1 = 603, \tag{2.17}
\]

\[
q = 0.32522 \pm 0.00004 \quad \chi^2_1 = 9197. \tag{2.18}
\]

The very large value of \( \chi^2 \) indicates that the quoted errors on \( p \) and \( q \), that are of purely statistical nature, are unreliable. Indeed a simple power law does not fit the data at this level of precision. A more realistic estimate of the errors would be

\[
p = 0.1960 \pm 0.0002, \quad q = 0.325 \pm 0.004. \tag{2.19}
\]

We have then performed an analogous analysis for the autocorrelation time \( \tau_{int,Y}(N_{min}) \). A least-square fit of the form

\[
\tau_{int,X} \sim N^z \tag{2.20}
\]

gives

\[
\chi^2_1 = 71 \quad \text{for } N_{min} = 1,
\]

\[
\chi^2_1 = 280 \quad \text{for } N_{min} = 100,
\]

\[
\chi^2_1 = 50 \quad \text{for } N_{min} = 200. \tag{2.21}
\]

Again, the very large value of \( \chi^2 \) indicates that the error bars are underestimated by at least a factor of ten. The results are somewhat higher than the estimate reported in Ref. [14], \( z = 0.70 \pm 0.03 \). This is evident if one directly compares our results of Table 2 with the values of \( \tau_{int} \) reported in Ref. [14] (see footnote [5]): \( \tau_{int} = 4.38(6), 9.47(21), 20.0(6) \) for \( N_{tot} = 500, 2000, 8000 \) respectively. For \( N_{tot} = 500 \) the autocorrelation times are similar, while for \( N_{tot} = 8000 \) there is a factor-of-two difference. It is very difficult to believe that the join-and-cut algorithm has a different dynamic behaviour on the square lattice and on the Manhattan lattice. We have thus tried to understand if the authors of Ref. [14] underestimated the autocorrelation times. Therefore we have determined \( \tau_{int} \) from our data using the self-consistent windowing procedure with a window of 5\( \tau_{int,X} \) as done in Ref. [14]. We obtain \( \tau_{int} = 4.166(2), 10.093(6), 29.13(2), 98.0(2) \) for \( N_{tot} = 500, 2000, 8000, 32000 \) respectively. A fit of these results gives \( z = 0.7271(2) \). This is now in good agreement with the results of Ref. [14].

In conclusion we believe a fair estimate would be

\[
z = 0.75 \pm 0.05. \tag{2.22}
\]

As noticed in Ref. [14], with a clever implementation of the algorithm, it is possible that the CPU-time per iteration increases as \( N^\sigma \) with \( \sigma < 1 \). In particular it was
predicted that $\sigma = 1 - p$ where $p$ is the exponent that controls the pivot acceptance fraction. In two dimensions we expect $p = 0.1953(21)$ \cite{25} and this is confirmed by our data on the acceptance fraction. From the data of Table 2 we obtain

$$\sigma = 0.865(1) \quad \chi^2 = 55$$

(2.23)

Keeping into account that the error bars are underestimated, we find reasonable agreement with the prediction $\sigma = 1 - p$. Of course what one is really interested in is the autocorrelation times expressed in CPU units.

We find

$$\tau_{\text{int}} \sim N^{z+\sigma} \sim N^{1.6}.$$  \hspace{1cm} (2.24)

The algorithm is not optimal, but still represents an improvement with respect to other algorithms that behave as $N^{z/2}$.

3 \hspace{1cm} PERM

3.1 \hspace{1cm} Description of the algorithm

The pruned-enriched Rosenbluth method (PERM) is a chain-growth algorithm based on the well-known Rosenbluth (inverse restricted sampling) \cite{33} algorithm. In the latter, chains are grown step by step. In unbiased sampling, steps are randomly generated, and, if a new step violates the self-avoidance constraint, the configuration is discarded and one restarts from scratch. This leads to exponential ‘attrition’, i.e. the number of attempts needed to generate a chain of length $n$ increases exponentially with $n$.

In Rosenbluth sampling, such steps are replaced (if possible) by ‘correct’ steps. This diminishes the attrition problem, but it leads to a bias that has to be compensated by a weight factor. If $m_n$ is the number of free sites where to place the $n$-th monomer (i.e., the number of allowed steps at time $n$), then the weight of a chain of length $N$ is $W_N \propto \prod_{n=1}^{N} m_n$. The proportionality factor depends on the ensemble one wants to simulate, e.g. it is constant for the canonical ensemble with fixed fugacity. The main problem with the Rosenbluth method is the fact that these weights show large fluctuations for large $N$. Thus even large samples can be completely dominated by just a few events, which leads to large statistical errors. Even worse, for very large $N$, the part of the distribution of weights which should dominate might not have been sampled at all, and this can lead to systematic errors. More precisely, while the method is guaranteed to give an unbiased estimate of the partition sum, due to these fluctuations and to the convexity of the logarithm, estimates of free energies are systematically too small.

The main idea in PERM \cite{15} is to watch the weight $W_N$ as $N$ is growing, and to compare it with the estimated average weight for this value of $N$. If $W_N$ is judged too big, a clone of the present configuration is made, both clones are attributed a weight $W_N/2$, and both are independently continued (‘enrichment’). On the other hand, if $W_N$ is too small, a (pseudo-) random number $r$ is drawn uniformly from
[0, 1]. If \( r < 1/2 \), the configuration is abandoned (‘pruning’), otherwise it is kept and its weight is doubled. This is most easily implemented by recursive function calls. A pseudocode is given in [17].

In this way the problem of large weight fluctuations is avoided, although not entirely. The set of generated configurations now is correlated due to cloning. Let us call a tour a set of configurations obtained by cloning from the same ‘ancestor’. Although the weights of individual configurations vary between narrow limits, the weights of tours can fluctuate very much. If so, we are back at basically the same problem. This can be avoided by making additional biases. For instance, before each step one might look ahead \( k \) steps, and choose the direction accordingly [34]. This is rather time consuming for large \( k \), nevertheless it can be efficient for dense (collapsed) systems.

For diluted systems, as it is the case here, the efficiency can be improved using Markovian anticipation [12,35]. Here one keeps the last \( k \) steps in memory, and biases the next step on the basis of the statistics of \((k+1)\)-step configurations accumulated during a previous run.

On the Manhattan lattice, an \( N \)-step walk with fixed starting point and fixed direction of the first step can be encoded as a binary sequence of length \( N - 1 \). A straight step is encoded as ‘0’, while a bend by \( \pm 90^\circ \) is encoded as ‘1’. Notice that one does not have to specify the direction of the bend, as only one bend is allowed at any time step. If the starting point has even \( x \) and \( y \) and the first step is upward, then the first bend is to the right (left) if it occurs at even (odd) times. After that, each bend is in the same (opposite) direction as the previous one if the number of in-between straight steps is even (odd). Let \( S = (s_{-k}, \ldots, s_0) \equiv (s, s_0) \) denote a binary string of length \( k + 1 \), and let \( C_{N,m}(S) \) be the cylinder set of all \( N \)-step walks starting upward from \((x, y) = (0,0)\), for which steps \( m-k, \ldots, m \) are given by \( S \). The total weight of this set in an unbiased ensemble is denoted by \( W_{N,m}(S) \). Finally, we consider

\[
    p_{N,m}(s_0|s) = \frac{W_{N,m}(S)}{\sum_{s_0'=0,1} W_{N,m}(s, s'_0)}. \tag{3.1}
\]

If SAW’s were a \( k \)-th order Markov process, we would obtain perfect importance sampling for \( N \)-step walks if we would select the \( m \)-th step according to \( p_{N,m}(s_0|s) \). Given the fact that SAW’s are not Markovian, Eq. (3.1) comes closest to importance sampling given a finite (\( k \)-step) memory.

In practice, Eq. (3.1) is not applicable as it stands, since it is practically impossible to acquire and store the needed statistics for all \( m \) and \( N \). First of all we use the fact that \( p_{N,m}(s_0|s) \) becomes independent of \( N \) and \( m \) in the limit \( m, N - m \gg k \). We therefore estimate it for large values of \( m \) and \( N \) by accumulating statistics for all \( N \) larger than some lower threshold (we used \( N > 400 \)), and \( N - m \) fixed (we used \( N - m = 200 \)). The fact that this \( p(s_0|s) \) does not give correct importance sampling for \( m \approx N \) is not serious and does not reduce much the efficiency. More serious is the fact that it would be inappropriate for small \( N \) and \( m \). In particular, for \( m < k \) we have no string \( s \) to condition upon. We dealt with this problem by tapering the symbol sequence with a string of \( k \) zeroes, and by taking step \( s_0 \) in the \( m \)-th step.
with probability
\[
p_m(s_0|s) = \frac{\text{const}/m + \lim_{m,N-m \to \infty} p_{N,m}(s_0|s)}{\sum_{s_0'=0,1} \text{const}/m + \lim_{m,N-m \to \infty} p_{N,m}(s_0|s)}.
\]

with \( \text{const} \approx 20 \).

Notice that all this fiddling is not crucial. The method per se is correct even if the probabilities for taking the \( m \)-th step were chosen badly, provided the probability is not set equal to zero for any allowed step. But efficiency can increase substantially with a good choice. Efficiency can be measured in several ways. The most straightforward method consists in measuring tour-to-tour fluctuations. Since subsequent tours are statistically strictly uncorrelated, this gives immediately estimates for the error bars of any measured observable. In practice, not to waste CPU time, we bunched tours in groups of typically \( 10^4 \) tours, and measured average values and fluctuations over these bunches.

A less direct but more instructive measure of efficiency is the number of tours in which a length \( N \) is reached in at least one configuration, normalized to the number of all tours. For other modified chain-growth algorithms such as incomplete enumeration [36] or the Berretti-Sokal (BS) algorithm [37], it seems that this number decreases as \( \text{const}/N \), provided the cloning and pruning parameters are adjusted so that the total number of generated walks is independent of \( N \). Improving the details of the algorithm cannot change this scaling law, but can change the constant considerably. For incomplete enumeration and the BS algorithm, the constant is \( O(1) \). For PERM without Markovian anticipation \( \text{const} \approx 10 \). For Markovian anticipation with \( k = 19 \) we found \( \text{const} \approx 130 \), see fig. [1].

A last check for efficiency is the following. As we said, the weights of tours can vary substantially, to the point that the distribution of these weights might not be properly sampled in the region which should dominate statistical averages. If this happens, the estimates of the free energies are too low, and all the errors are systematically underestimated. To show that this is not the case in the present simulation, we show in fig. [2] the measured distribution of tour weights for \( N = 32000 \), together with the weighted distribution. We see that the maximum of the weighted distribution occurs at a weight which is still well within our sampling distribution.

### 3.2 Determination of \( \gamma \) using PERM data

The raw data produced by PERM are estimates of the partition sum \( z_N \), for all \( N \leq N_{\text{max}} \). It is then straightforward to obtain estimates of \( \gamma \). Assuming Eq. (1.2), the exponent \( \gamma \) can be estimated from ratios of \( z_{N_i} \) for three different values of \( N_i \). Indeed, if one chooses two positive constants \( a < 1 < b \), and defines

\[
\gamma_{\text{eff}}(N) = \frac{x \log z_{aN} + y \log z_{bN} - \log z_N}{x \log a + y \log b},
\]

one checks easily that \( \gamma_{\text{eff}}(N) = \gamma \), provided that \[38\]
\[
x + y = 1, \quad ax + by = 1.
\]
Figure 1: Probabilities to reach length $N$ at least once in a tour, plotted against $N$. The curves are for PERM with $k$-step Markovian anticipation, with $k = 19, 10, 5,$ and $0$. The straight line is $130/N$.

Figure 2: Full line: histogram $P(\log W)$ of tours with fixed weight $W$, on a logarithmic horizontal scale. Normalization is arbitrary. Broken line: $W \times P(\log W)$, again with arbitrary normalization.
If Eq. (1.2) is not fulfilled exactly, Eqs. (3.3) and (3.4) define effective $N$-dependent exponents. These exponents still depend on $a$ and $b$. It is clear that statistical errors will be small if $a \ll 1 \ll b$, but then a wide range of chain lengths are needed. Since $N_{\text{max}}$ is fixed and cannot be exceeded, this means that $aN$ will be small, and systematic errors will become large if we want to reduce statistical errors. In addition to the ratio $b/a$, one has the product $a \times b$ at one’s disposal. For fixed $b/a$, its optimal value depends on the way how the statistical error on $z_N$ increases with $N$. In the present case, they increase roughly as $\sqrt{N}$. For practical reasons one also wants $a^{-1}$ and $b$ to be simple numbers. We found that good results were obtained with $a = 1/2, b = 4$ (and therefore $x = 6/7, y = 1/7$).

The computation of the error bars is not trivial. Indeed one should take into account the fact that different $z_N$ are correlated and therefore compute the full covariance matrix, which is practically impossible. Therefore we proceeded differently to obtain error estimates. For each bunch of tours we estimated $[\gamma_{\text{eff}}(N)]_{\text{bunch}}$ according to Eq. (3.3), and from these values we obtained the variance of the latter. Notice that we did not use this procedure to obtain $\gamma_{\text{eff}}(N)$ itself by taking the average over all bunches, as this would introduce a bias.

In addition, in order to improve the estimates of $X_{\text{cens}}(N_{\text{min}})$, cf. Eq. (2.9), obtained using the join-and-cut algorithm, we evaluated this quantity using the PERM estimates of $z_N$. The estimate of the mean value is trivial. For the error bars, we evaluated $[X_{\text{cens}}(N_{\text{min}})]_{\text{bunch}}$ over bunches of tours and then estimated their variance. We used the same trick as for $\gamma_{\text{eff}}$. Again, notice that we did not use this procedure to estimate the mean value itself, since this introduces a bias. We have checked however that this bias is extremely small.

### 3.3 Dynamic results

Let us now discuss the simulations using PERM. We have performed high-statistics runs using Markovian anticipation with $k = 19$. The dynamic data of the runs are reported in Table 3. The total PERM simulation would have taken approximately 7 months of CPU time on an Alpha-Station 600 Mod 5/266.

We have first of all performed an analysis of the CPU time per independent configuration, which we expect to scale as $aN^z$ with $z \approx 2$. Fitting the data of Table 3 and including in each fit only the data with $N \geq N_{\text{min}}$ in order to detect systematic effects, we have

$$ z \approx \begin{cases} 1.92 & N_{\text{min}} = 500, \\ 2.08 & N_{\text{min}} = 2000, \end{cases} \quad (3.5) $$

$$ a \approx \begin{cases} 0.00003 & N_{\text{min}} = 500, \\ 0.00001 & N_{\text{min}} = 2000. \end{cases} \quad (3.6) $$

The expected exponent $z \approx 2$ is clearly recovered. Let us now compare these results with the join-and-cut estimates. For the latter algorithm, the CPU time per independent configuration scales as (cf. tables 1 and 2) $\approx 0.0003 N^{1.6}$ and therefore the join-and-cut is faster in generating one independent configuration than the PERM as
long as $N \gtrsim 1000$. This is may not be however a fair comparison of the two algorithms. Indeed what we call an “independent configuration” for PERM is a bunch of walks which are correlated, but which still contain more information than a single walk. In order to make a fair comparison it is better to consider an observable and compare the CPU time needed to obtain the same error bars. We have therefore compared the results for our preferred observable $X_{\text{cens}}(N_{\text{min}})$, see table 4. We find that for $N_{\text{tot}} = 32000$ both algorithms require essentially the same CPU time to produce data with the same error bars. Only for longer walks the join-and-cut algorithm is more efficient. Notice that this result is true if we use the Markovian anticipation. In the absence of this improvement, PERM would be about ten times slower and therefore less efficient than the join-and-cut algorithm already for $N \approx 500$.

4 Estimate of $\gamma$

Let us now discuss the results for the critical exponent $\gamma$. We will first analyze the data using the method presented in section 2.2. This will allow us to use at the same time the data produced using the join-and-cut and the PERM. In table 4 we report, for various $N_{\text{min}}$, the estimates of $X_{\text{cens}}(N_{\text{min}})$ obtained using the two algorithms. We have checked that the raw data agree within error bars, therefore checking the correctness of our programs and error bars.

In table 5 we report the estimates of the effective exponents $\hat{\gamma}$ defined in Sec. 2.2. A graph of these estimates together with the results of the fits described below is reported in fig. 3. It is evident that the corrections to scaling are particularly strong and indeed $\hat{\gamma}$ clearly increases with $N_{\text{min}}$ and $N_{\text{tot}}$. Under the only assumption that in the interval $1000 \lesssim N \lesssim 32000$ the corrections to scaling have the asymptotic sign, i.e. if we exclude that $\hat{\gamma}$ will decrease for larger values of $N_{\text{min}}$ and $N_{\text{tot}}$, we obtain (using $N_{\text{tot}} = 32000, N_{\text{min}} = 2000$)

$$\gamma \gtrsim 1.3423 \pm 0.0018.$$ (4.1)

This clearly excludes the result of Ref. [13]. Under this very weak assumption, we can conclude that there is no evidence from our data of the non-universality predicted in Ref. [2]. More conservatively, our data indicate that, if the effect is really there, it is extremely small:

$$\gamma_{\text{reg}} - \gamma < 0.0014 \pm 0.0018.$$ (4.2)

We can improve this bound making additional assumptions on the corrections to scaling. For each value of $N_{\text{min}}$ we assume that $z_N$ is well approximated by

$$z_N = A \mu^N N^{\gamma - 1} \left(1 + a N^{-\Delta}\right)$$ (4.3)

for $N \geq N_{\text{min}}$. We are not able to determine $\Delta$ reliably and therefore we have performed fits for various fixed values of $\Delta$. Our analysis works as follows. For each triple $(N_{\text{min}}, N_{\text{tot}}, a)$ and for each value of $\Delta$, we can define an effective exponent $\hat{\gamma}(N_{\text{min}}, N_{\text{tot}}, a)$ (from now on we suppress the dependence on $\Delta$) using the natural generalization of Eqs. (2.10) and (2.11) with a corresponding error $\Delta \hat{\gamma}(N_{\text{min}}, N_{\text{tot}}, a)$. 


Then for each \( N_{\text{min}} \) and \( \Delta \) we determine the optimal value \( a_{\text{opt}} \) of \( a \) and an estimate of the exponent \( \gamma(N_{\text{min}}) \), by minimizing with respect to \( a \) and \( \gamma(N_{\text{min}}) \)

\[
\chi^2 = \sum_{N_{\text{tot}}} \left[ \frac{\hat{\gamma}(N_{\text{min}}, N_{\text{tot}}, a) - \gamma(N_{\text{min}})}{\Delta \hat{\gamma}(N_{\text{min}}, N_{\text{tot}}, a)} \right]^2,
\]

where the sum runs over \( N_{\text{tot}} = 2000, 8000, 32000 \). The statistical errors are obtained in a standard fashion.

In table 6 we report the results of the fits for various values of \( N_{\text{min}} \) and for two values of \( \Delta \), \( \Delta = 1 \) and \( \Delta = 11/16 \). First let us observe that the estimate of \( \gamma \) decreases with increasing \( \Delta \). Therefore a lower bound independent of any assumption on the value of \( \Delta \) is obtained using the results for \( \Delta = 1 \). From table 6 we can estimate

\[
\gamma \gtrsim 1.3425 \pm 0.0003.
\]

We can try to do more and see if we can obtain from the data a rough indication of the value of \( \Delta \). In principle we can consider the results for various \( N_{\text{min}} \) and see for which value of \( \Delta \) the estimates do not depend on \( N_{\text{min}} \). Notice however that the results with different \( N_{\text{min}} \) are strongly correlated — they are obtained essentially from the same data — and therefore an observed stability or upward trend should be interpreted with caution since it could simply be an effect of the correlations. If we consider the results of table 6 we see that the analysis with \( \Delta = 11/16 \) is extremely stable: \( a_{\text{opt}} \) and \( \gamma \) are essentially constant and we can estimate

\[
\gamma = 1.3436 \pm 0.0003.
\]

This result is in perfect agreement with the universal value \( \gamma_{\text{reg}} = 43/32 \). On the other hand the results for \( \Delta = 1 \) show an upward systematic trend. However the effect is barely statistically significant (the results for \( N_{\text{min}} = 100 \) and \( N_{\text{min}} = 500 \) differ approximately by 1.5 combined error bars) and one could just think that the systematic increase is simply an effect due to the neglected corrections to scaling and/or a result of the correlations. Without further hypotheses, we cannot confidently go beyond the lower bound (4.5). However if we assume \( \gamma = \gamma_{\text{reg}} \), then \( \Delta = 1 \) becomes less plausible and we can say that our data favour the presence of a non-analytic exponent. We cannot give a reliable estimate of \( \Delta \), but Saleur’s value 11/16 fits our data very well.

This conclusion is fully supported by the alternative analysis of the PERM data using Eq. (3.3). In fig. 4 we plot \( \gamma_{\text{eff}} \), obtained with \( a = 1/2, b = 4 \), against \( N^{-11/16} \). If \( \Delta \) has Saleur’s value, and if there are no other corrections to scaling, we should expect a straight line intersecting the \( y \)-axis at \( \gamma \). The most dramatic deviations from a straight line are strong period-four oscillations, observed also in [3]. Similar period-four oscillations are observed for SAWs on the square lattice [9]. They correspond to a singularity of the grand canonical partition sum at \( x = -1/\mu \) [3]. In fig. 4 one may also observe a slight curvature which might suggest that \( \Delta < 11/16 \). However, a more careful analysis, using also different pairs \( (a, b) \) and additional correction-to-scaling terms, suggests that this effect is not significant. In contrast, the fact that \( \Delta < 1 \) seems significant. Accepting for \( \Delta \) a value between 1/2 and 0.7, we find again perfect agreement with \( \gamma_{\text{reg}} = 43/32 \), while the estimate of [13] seems ruled out.
Figure 3: Estimates of the effective exponents $\hat{\gamma}$ for $N_{\text{tot}} = 2000$ (empty circle), 8000 (empty square), 32000 (empty triangle) and estimates obtained with the optimal amplitude method for $\Delta = 11/16$ (filled triangle) and $\Delta = 1$ (filled circle). The dotted lines represent $\gamma_{\text{reg}} = 43/32$ and the estimate of Ref. [13], $\gamma = 1.3385$.

Figure 4: Effective exponents $\gamma_{\text{eff}}$ defined by Eq. (3.3), plotted against $N^{-11/16}$. The extrapolation to the $y$-axis gives the estimate of $\gamma$. Only data with high statistics, i.e. $N < 1000$ are included.
Acknowledgments

We thank John Cardy, Tony Guttmann, Flavio Seno, and Antonio Trovato for very helpful discussions.
### Table 1: Number of iterations and CPU times per iteration for various values of $N_{\text{tot}}$. CPU-times are expressed in ms and refer to an Alpha-Station 600 Mod 5/266.

| $N_{\text{tot}}$ | $N_{\text{iter}}$ | CPU-time |
|------------------|--------------------|----------|
| 500              | $10^9$             | 0.248(1) |
| 2000             | $12 \cdot 10^8$    | 0.846(8) |
| 8000             | $33 \cdot 10^8$    | 2.41(3)  |
| 32000            | $23 \cdot 10^8$    | 9.08(2)  |

### Table 2: Acceptance fraction for the pivot move ($f_{\text{piv}}$), for the join-and-cut move ($f_{\text{jc}}$) and autocorrelation times for the various values of $N_{\text{tot}}$. Autocorrelation times are expressed in units of two iterations.

| $N_{\text{tot}}$ | $f_{\text{piv}}$ | $f_{\text{jc}}$ | $\tau_{\text{int,Y}(1)}$ | $\tau_{\text{int,Y}(100)}$ |
|------------------|------------------|-----------------|--------------------------|-----------------------------|
| 500              | 0.451943(11)     | 0.155468(11)    | 4.912 ± 0.031            | 8.171 ± 0.023               |
| 2000             | 0.3446316(86)    | 0.0998629(77)   | 14.30 ± 0.23             | 19.38 ± 0.12                |
| 8000             | 0.2624050(83)    | 0.0629925(65)   | 49.6 ± 1.2               | 55.8 ± 1.0                  |
| 32000            | 0.199693(46)     | 0.039330(31)    | 202.4 ± 7.4              | 206.7 ± 7.0                 |

### Table 3: Number of PERM tours (column 2) with $N \leq N_{\text{max}}$, total number of configurations with $N = N_{\text{max}}$ (column 3), number of independent configurations with $N = N_{\text{max}}$ (i.e., of tours which reached $N = N_{\text{max}}$; column 4), and CPU time per independent configuration (expressed in ms, on an Alpha-Station 600 Mod 5/266; column 5).

| $N_{\text{max}}$ | $N_{\text{tour}}$ | $N_{\text{config}}$ | $N_{\text{indep}}$ | CPU time |
|------------------|-------------------|---------------------|--------------------|----------|
| 500              | $1.0 \cdot 10^6$  | $1.140 \cdot 10^6$  | $2.637 \cdot 10^5$ | 4.985    |
| 2000             | $8.876 \cdot 10^8$ | $1.010 \cdot 10^9$  | $6.533 \cdot 10^7$ | 70.53    |
| 4000             | $1.756 \cdot 10^8$ | $2.016 \cdot 10^8$  | $6.359 \cdot 10^6$ | 298.6    |
| 8000             | $3.421 \cdot 10^8$ | $4.035 \cdot 10^8$  | $6.296 \cdot 10^6$ | 1272.6(4)|
| 32000            | $2.792 \cdot 10^7$ | $3.703 \cdot 10^8$  | $1.154 \cdot 10^6$ | 244(7) \cdot 10^4 |
Table 4: Raw data for $X_{\text{MC}}^{\text{cens}}$. We report separately the results obtained with the PERM and join-and-cut algorithms.
\[ \gamma(N_{\text{tot}}) \]

| \( N_{\text{min}} \) | \( \gamma(500) \) | \( N_{\text{min}} \) | \( \gamma(2000) \) | \( N_{\text{min}} \) | \( \gamma(8000) \) | \( N_{\text{min}} \) | \( \gamma(32000) \) |
|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| 2              | 1.32950 (3)    | 2              | 1.33263 (7)    | 2              | 1.33773 (21)   | 2              | 1.34059 (87)   |
| 20             | 1.32584 (5)    | 50             | 1.33423 (9)    | 100            | 1.33900 (25)   | 100            | 1.34097 (92)   |
| 40             | 1.32776 (7)    | 100            | 1.33516 (12)   | 200            | 1.33950 (29)   | 200            | 1.34105 (97)   |
| 60             | 1.32880 (9)    | 150            | 1.33569 (14)   | 300            | 1.33987 (33)   | 300            | 1.34105 (101)  |
| 80             | 1.32955 (12)   | 200            | 1.33609 (17)   | 400            | 1.34015 (36)   | 400            | 1.34106 (105)  |
| 100            | 1.33011 (15)   | 250            | 1.33638 (19)   | 500            | 1.34041 (40)   | 500            | 1.34112 (109)  |
| 120            | 1.33064 (20)   | 300            | 1.33661 (22)   | 600            | 1.34058 (44)   | 600            | 1.34122 (114)  |
| 140            | 1.33120 (28)   | 350            | 1.33681 (26)   | 700            | 1.34068 (48)   | 700            | 1.34136 (118)  |
| 160            | 1.33139 (40)   | 400            | 1.33692 (30)   | 800            | 1.34070 (53)   | 800            | 1.34143 (123)  |
| 180            | 1.33051 (63)   | 450            | 1.33705 (35)   | 900            | 1.34080 (58)   | 900            | 1.34139 (127)  |
| 200            | 1.33235 (132)  | 500            | 1.33711 (42)   | 1000           | 1.34077 (63)   | 1000           | 1.34143 (131)  |

Table 5: Estimates of \( \gamma(N_{\text{tot}}) \) for various values of \( N_{\text{min}} \) and \( N_{\text{tot}} \).

\[ \Delta = \frac{11}{16} \quad \Delta = 1 \]

| \( N_{\text{min}} \) | \( \Delta = 11/16 \) | \( \Delta = 1 \) |
|----------------|---------------------|----------------|
| \( \gamma \) | \( a_{\text{opt}} \) | \( \gamma \) | \( a_{\text{opt}} \) |
| 2              | 1.34306 (6) 0.43 (1) | 1.34159 (6) 0.85 (2) |
| 100            | 1.34300 (10) 0.51 (4)| 1.34200 (10) 1.75 (13)|
| 200            | 1.34318 (14) 0.54 (4)| 1.34198 (14) 1.93 (24)|
| 300            | 1.34344 (18) 0.57 (5)| 1.34192 (18) 1.98 (36)|
| 400            | 1.34357 (22) 0.59 (5)| 1.34230 (22) 2.23 (50)|
| 500            | 1.34356 (27) 0.59 (6)| 1.34251 (27) 2.40 (59)|

Table 6: Extrapolated estimates of \( \gamma \) for \( \Delta = 11/16 \) and \( \Delta = 1 \).
References

[1] J. Miller, J. Stat. Phys. 63, 89 (1991).

[2] J. L. Cardy, Nucl. Phys. B419, 411 (1994).

[3] D. Bennet-Wood, J. L. Cardy, S. Flesia, A. J. Guttmann, and A. L. Owczarek, J. Phys. A 28, 5143 (1995).

[4] G.T. Barkema and S. Flesia, J. Stat. Phys. 85, 363 (1996).

[5] A. Trovato and F. Seno, Phys. Rev. E 56, 131 (1997).

[6] T. Prellberg and B. Drossel, Phys. Rev. E 57, 2045 (1998).

[7] G. T. Barkema, U. Bastolla, and P. Grassberger, J. Stat. Phys. 90, 1311 (1998).

[8] B. Nienhuis, Phys. Rev. Lett. 49, 1062 (1982); J. Stat. Phys. 34, 731 (1984).

[9] A. Conway, I.G. Enting, and A.J. Guttmann, J. Phys. A 26, 1519 (1993).

[10] W.M. Koo, J. Stat. Phys. 81, 561 (1995).

[11] S. Flesia, Europhys. Lett. 32, 149 (1995).

[12] H. Frauenkron, M. S. Causo, and P. Grassberger, 2-d Self-Avoiding Walks on a Cylinder, cond-mat/9808075.

[13] D. Bennet-Wood, J. L. Cardy, I.G. Enting, A. J. Guttmann, and A. L. Owczarek, Nucl. Phys. B528, 533 (1998).

[14] S. Caracciolo, A. Pelissetto and A. D. Sokal, J. Stat. Phys. 67, 65 (1992).

[15] P. Grassberger, Phys. Rev. E 56, 3682 (1997).

[16] A. J. Guttmann and I. G. Enting, J. Phys. A 21, L165 (1988).

[17] A. R. Conway and A. J. Guttmann, Phys. Rev. Lett. 77, 5284 (1996).

[18] D. Bennett-Wood, S. Caracciolo, P. Grassberger, A. J. Guttmann, B. Li, A. Pelissetto, and A. D. Sokal, in preparation.

[19] H. Saleur, J. Phys. A 20, 455 (1987).

[20] A. R. Conway and A. J. Guttmann, J. Phys. A 26, 1535 (1993).

[21] I. Guim, H. W. J. Blöte, and T. W. Burkhardt, J. Phys. A 30, 413 (1997).

[22] A. J. Guttmann, private communication.

[23] M. Lal, Molec. Phys. 17, 57 (1969).
[24] B. MacDonald, N. Jan, D. L. Hunter and M. O. Steinitz, J. Phys. A 18, 2627 (1985).

[25] N. Madras and A. D. Sokal, J. Stat. Phys. 50, 109 (1988).

[26] S. Caracciolo, G. Parisi, and A. Pelissetto, J. Stat. Phys. 77, 519 (1994).

[27] P. Belohorec and B. G. Nickel, Accurate universal and two-parameter model results from a Monte-Carlo renormalization group study, Guelph university report (September 1997).

[28] G. Zifferer, Makromol. Chemie, Theory Simul. 2, 653 (1993).

[29] M. C. Tesi, E. J. Janse van Rensburg, E. Orlandini, S. G. Whittington, J. Stat. Phys. 82, 155 (1996).

[30] N. Madras, A. Orlitsky, and L. A. Shepp, J. Stat. Phys. 58, 159 (1990).

[31] see e.g. S. D. Silvey, Statistical Inference (Chapman and Hall, London, 1975).

[32] B. Li, N. Madras and A. D. Sokal, J. Stat. Phys. 80, 661 (1995).

[33] N. Madras and G. Slade, The Self-Avoiding Walk (Birkhäuser, Boston-Basel-Berlin, 1993)

[34] H. Meirovitch and H.A. Lim, J. Chem. Phys. 92, 5144 (1990).

[35] P. Grassberger, to be published.

[36] S. Redner and P.J. Reynolds, J. Phys. A 14, 2679 (1981).

[37] A. Berretti and A.D. Sokal, J. Stat. Phys. 40, 483 (1985).

[38] P. Grassberger, P. Sutter, and L. Schäfer, J. Phys. A 30, 7039 (1997).

[39] A. J. Guttmann and S. G. Whittington, J. Phys. A 11, 721 (1978).