

Two-dimensional self-avoiding walks on a cylinder

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We present simulations of self-avoiding random walks (SAWs) on two-dimensional lattices with the topology of an infinitely long cylinder, in the limit where the cylinder circumference L is much smaller than the Flory radius. We study in particular the L dependence of the size h parallel to the cylinder axis, the connectivity constant μ , the variance of the winding number around the cylinder, and the density of parallel contacts. While $\mu(L)$ and $\langle W^2(L,h) \rangle$ scale as expected [in particular, $\langle W^2(L,h) \rangle \sim h/L$], the number of parallel contacts decays as $h/L^{1.92}$, in striking contrast to recent predictions. These findings strongly speak against recent speculations that the critical exponent γ of SAWs might be nonuniversal. Finally, we find that the amplitude for $\langle W^2 \rangle$ does not agree with naive expectations from conformal invariance. [S1063-651X(99)51201-4]

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Although self-avoiding random walks (SAWs) are among the best studied critical phenomena, there have been recent speculations that, if true, would have very far reaching and surprising consequences [1]. One such consequence would be that the critical exponent γ of interacting SAWs on the square lattice would be temperature dependent if the interaction between neighboring bonds (i.e., steps of the walk on opposite edges of a plaquette) depends on the relative orientation of the steps. Another consequence would be that γ for a-thermal SAWs on the Manhattan lattice is different from γ on other two-dimensional (2D) lattices [2]. Numerical evidence in favor of the former prediction is lacking [3–9], but it has been argued [2] that this is not conclusive since much longer SAWs (10^9 steps) would be needed to refute the prediction unambiguously. With reference to the Manhattan lattice, the numerical evidence is unclear, since nonuniversality was found in [2], but universality was found in [10].

The main question at stake here is the density of parallel contacts (i.e., the number of pairs of parallel steps on opposite edges of one plaquette) in a very long SAW. It is easily seen that parallel contacts are forbidden for 2D self-avoiding closed loops. Therefore, it seems plausible that parallel contacts result only from spirals formed by the ends of the walks. This was indeed strongly suggested by simulations in [6], where it was shown that the probability for a contact to be parallel decreases as a power of the distance from the nearest chain end. But again the significance of this result was doubted in [2], where it was claimed that *much* larger systems were needed for measurements to be significant in planar topology.

As pointed out in [2], the natural geometry to study this problem is obtained by mapping the plane onto the surface of a cylinder by the conformal map

$$z = x + iy \rightarrow w = (L/2\pi) \ln z. \quad (1)$$

Except near the ends of the walk, parallel contacts can only occur when the walk wraps around the cylinder. In the limit of very long chains ($N \gg L$, where N is the number of steps) a typical SAW has to grow either parallel or antiparallel to the cylinder axis. Finite size scaling predicts that its longitu-

dinal size h (defined here as the average end-to-end distance, projected onto the direction parallel to the cylinder axis) scales as

$$h \sim N/L^{1/\nu-1}, \quad \nu = 3/4. \quad (2)$$

The scaling of the winding number variance follows from the facts that it must be linear in h , and that it is dimensionless,

$$\langle W^2 \rangle \approx Ah/L, \quad (3)$$

where A should be a universal amplitude. In the following, winding numbers will be measured in terms of wrappings around the cylinder, with $W=1$ corresponding to one full turn. Finally, the connectivity constant (the critical monomer fugacity) should show the usual finite size behavior

$$\mu(L) = \mu_\infty - bL^{-1/\nu}. \quad (4)$$

Here, the amplitude b is not universal. A universal amplitude can be obtained for the free energy $F = -\ln Z \approx N \ln \mu$, where Z is the partition sum. Using Eq. (2) we obtain

$$F(L,N) = F_\infty(N) - Bh/L, \quad (5)$$

up to terms logarithmic in N .

As discussed in [2], the predictions of [1] can be understood intuitively from the assumption that the density of parallel contacts follows essentially the winding number: If the walk wraps once around the cylinder, there should be $O(1)$ parallel contacts. Thus the prediction for the average number of parallel contacts is

$$n_{\parallel} \approx Ch/L, \quad (6)$$

with C as yet another universal amplitude.

Finally, we can rewrite Eq. (2) in terms of the Flory radius R of SAWs in planar geometry. More precisely, we define R as the rms end-to-end distance of a free SAW of N steps, $R \sim N^\nu$. Then we obtain

$$\frac{h}{L} = D \left(\frac{R}{L} \right)^{1/\nu}, \quad (7)$$

with D also universal. Using this, we can eliminate h/L from Eqs. (3), (5), and (6) to obtain $(\langle W^2 \rangle, F_\infty(N) - F(L, N), n_\parallel) = (A', B', C')(R/L)^{1/\nu}$, with universal amplitudes $A' = AD$, $B' = BD$, and $C' = CD$.

The main objective of the present paper was to test Eqs. (2)–(7) by means of Monte Carlo simulations. Since we want to simulate lattices with large perimeters L , and with $N^\nu \gg L$ (we went up to $L = 128$ and $N = 60\,000$), we need a fast algorithm. For SAWs in planar geometry, the fastest known algorithm is the pivot algorithm (at least if one is not interested in μ). But it is easy to see that the pivot algorithm doesn't work well on the cylinder (for sufficiently small L one can prove that it isn't even ergodic). We therefore used the pruned-enriched Rosenbluth method (PERM) [11] with Markovian anticipation [12,13]. In PERM one starts off by growing chains according to the well-known Rosenbluth method [14], but when their weights become too large and too small, respectively, one interferes by cloning and then pruning, respectively. Weights have to be used, since Rosenbluth sampling is biased, and the weights are needed to compensate the bias.

In k -step Markovian anticipation one uses an additional bias based on the statistics of sequences of $k+1$ successive steps. Let us number the $2d$ directions on a d -dimensional (hyper-)cubic lattice as $s=0, \dots, 2d-1$. A sequence of $k+1$ steps is then encoded as $\mathbf{S} = (s_{-k}, \dots, s_0) \equiv (\mathbf{s}, s_0)$. By $P_{N,m}(\mathbf{S})$ we denote the statistical weight of all N -step chains in an unbiased sample that had followed the sequence \mathbf{S} during steps $N-m-k, \dots, N-m$. This can be estimated either in a previous test run or during the present run. The ideal bias in k -step Markovian anticipation is

$$p(s_0|\mathbf{s}) = P_{N,m}(\mathbf{s}, s_0) \bigg/ \sum_{s'_0=0}^{2d-1} P_{N,m}(\mathbf{s}, s'_0), \quad (8)$$

with $N \gg m \gg 1$ [we used $m = 150$, and averaged $P_{N,m}(\mathbf{S})$ over all $N > 300$]. Thus a step s_0 is made more often if this step is anticipated to be more successful in the far (m steps ahead) future, based on previous experience. Equation (8) should not be used, of course, for the very first steps of the chain. There the probabilities $P_{N,m}(\mathbf{S})$ are not appropriate. Our remedy is *ad hoc* but efficient: When determining the bias for the n th step in a chain, we replaced $P_{N,m}(\mathbf{S})$ by $P_{N,m}(\mathbf{S}) + \text{const}/n$, with $\text{const} \approx 20$. The Markovian anticipation bias is of course compensated by a weight factor $\propto 1/p(s_0|\mathbf{s})$ to guarantee correct sampling.

In our actual simulations we used semi-infinite cylinders. Knowing that the walks have to grow either parallel or anti-parallel to the cylinder axis any way, we started them at height = 1 and put an absorbing barrier at height = 0, so that they had to grow into the positive h direction. The ratios on the right hand side of Eq. (8) depend then on the absolute orientation of the steps and on L . Obviously the longitudinal bias is larger for smaller L . Most of our simulations were done for the square lattice. Results for $L = 8$ are shown in Fig. 1. There, sequences of nine steps are encoded by integers from 0 to $4^9 - 1$, with the last step giving the most

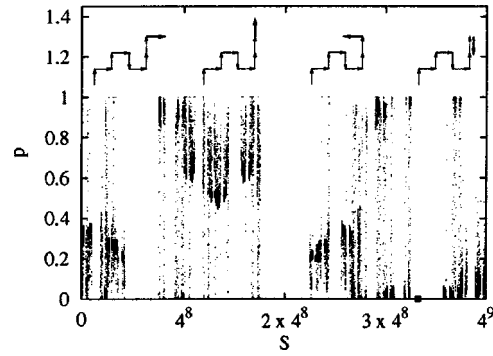


FIG. 1. Histogram ratio $p(s_0|\mathbf{s})$ used for biasing square lattice SAWs on cylinders with $L = 8$, based on sequences of length 9. Each sequence \mathbf{S} is encoded by a number between 0 and $4^9 - 1 = 262\,143$. The probability with which the next step is taken is $p(s_0|\mathbf{s})$, up to corrections for the very first steps. On all points, statistical errors are < 0.01 . The four heavy dots correspond to four sequences: $\mathbf{S} = \mathbf{s}, \mathbf{s} + 4^8, \mathbf{s} + 2 \times 4^8$, and $\mathbf{s} + 3 \times 4^8$. The chain segments corresponding to these sequences are also indicated. The probabilities to continue right (r), up (u), left (l), and down (d), after the segment $ururdruu$, are $p(r):p(u):p(l):p(d) = 0.28:0.52:0.20:0$.

significant digits. The upward direction is $s = 1$, downward is $s = 3$, and the directions perpendicular to the cylinder axis are 0 and 2. We see that there is both a strong anisotropy and a strong dependence on the shape of the last part of the chain. The former means that downward steps are likely to be less efficient, while the latter corresponds to the fact that a strongly curling walk will have problems to be continued. For large L we used isotropic Markovian anticipation with $k = 11$. It gave roughly a one order of magnitude improvement in speed over plain PERM. For small L , anisotropic anticipation with $k = 8$ gave up to one additional order of magnitude further improvement.

We also performed less extensive simulations on the triangular lattice in order to test for universality. There we have six local directions instead of four, so that we could not use memories with the same length. We used only isotropic anticipation there, with $k = 7$.

In all simulations chain lengths were such that $h/L > 80$. Results for the connectivity constant are shown in Fig. 2

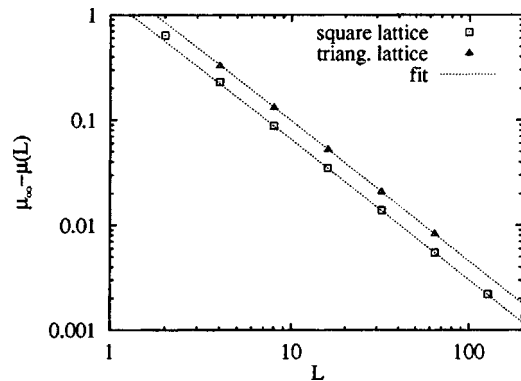


FIG. 2. Log-log plot of $\mu_\infty - \mu(L)$ against L . The straight lines have a slope of $-4/3$, as predicted by Eq. (4), and prefactors adjusted to fit the data. Error bars on the data points are comparable to or smaller than the symbol sizes.

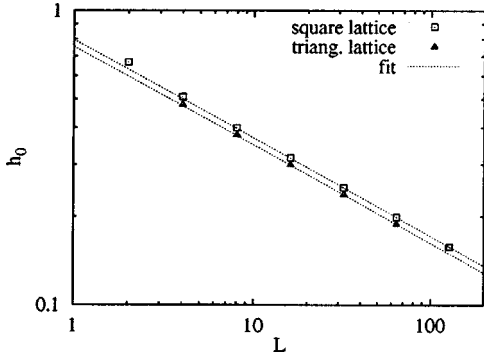


FIG. 3. Log-log plot of h_0 against L , with h_0 being the constant in a fit $h = h_0 N + h_1$ for fixed L . Again, error bars on the data points are comparable to or smaller than the symbol sizes. The straight lines have a slope of $-1/3$ as predicted by Eq. (2), with prefactors adjusted to fit the data.

where we plotted $\mu_\infty - \mu(L)$, with $\mu_\infty = 2.638159$ [15] and $\mu_\infty = 4.150795$, respectively [17] for the square and triangular lattice, respectively. We see perfect agreement with the theoretical prediction indicated by the slope of the straight lines. Equation (2) was tested by first making linear fits in plots of h versus N for fixed L (to avoid biases from the chain ends), and then plotting the slopes against L on a log-log plot. The result is shown in Fig. 3; again, we see perfect agreement with the theoretical prediction. Combining the results from Figs. 2 and 3, we find that the amplitude $B = 0.675 \pm 0.002$ is indeed universal (the error is just a rough but conservative estimate, as are the following error estimates).

Winding number variances, multiplied by L and divided by h , are shown in Fig. 4. For $L \leq 16$ we see finite size corrections. Apart from these, all curves coincide within the expected statistical fluctuations, as is expected from Eq. (3). Again we see that universality is satisfied, i.e., the constant A is the same for the square and triangular lattices, within the statistical errors. More precisely, we find $A = 0.475 \pm 0.004$.

In order to estimate the universal amplitude D , we use the following estimates for the end-to-end distances of free chains: $\lim_{N \rightarrow \infty} \langle R^2 \rangle / N^{2\nu} = 0.7710 \pm 0.0004$ [16] for the square lattice, and 0.711 [17] for the triangular lattice. Again, both gave consistent results: $D = 0.9446 \pm 0.0006$.

Finally, we consider the number of parallel contacts (mea-

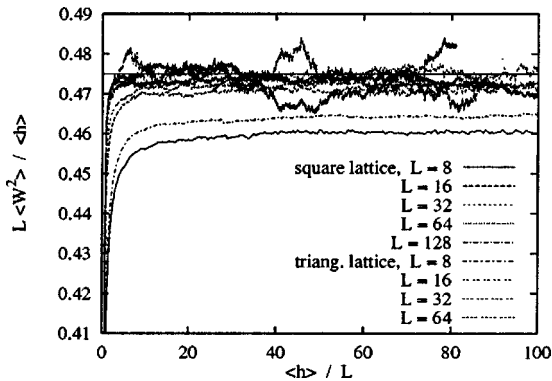


FIG. 4. Plot of $L\langle W^2 \rangle / h$ against h/L . The horizontal line is our best estimate for the constant A . Statistical errors are typically of the size of the visible fluctuations.

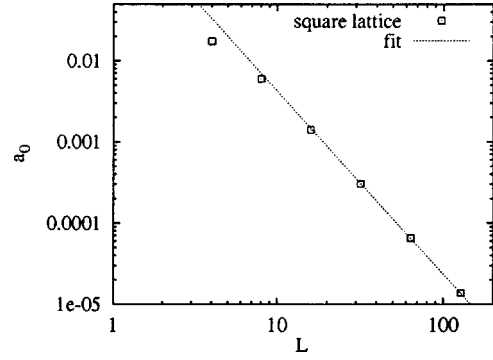


FIG. 5. Log-log plot of a_0 against L , where $n_{\parallel} = a_0 N + a_1$ for fixed L . According to the prediction of Refs. [1,2], one should have $a_1 \sim 1/L^{1.333}$. The straight line is $\text{const}/L^{2.25}$.

sured only on the square lattice). A plot analogous to Fig. 4 shows a strong L dependence, but would not allow us to estimate this dependence precisely. More instructive is a plot analogous to Fig. 3. For each L , we first extracted the coefficient a_0 in a fit $n_{\parallel} = a_0 N + a_1$. In Fig. 5 we then plot a_0 against L on double-logarithmic scale. From this figure we see that $n_{\parallel} \sim NL^{-2.25}$ or

$$n_{\parallel} / h \sim L^{-1.92 \pm 0.03}. \quad (9)$$

Again, the error estimate is just an educated guess. Indeed, our data show a slight downward curvature, suggesting that the true exponent might be closer to -2.0 . In any case, Eq. (6) is clearly ruled out.

Qualitatively this is indeed not surprising. It means that even if the walk winds once around the cylinder, the chance that it touches itself is much less than one and decreases with L . This agrees qualitatively with the behavior of a SAW confined to a strip of width L between two repelling walls. In that case the density of monomers at a distance z from a wall increases as $z^{1/\nu}$ [18], implying that the average distance between two contacts with the wall is $\sim L^2$. In the present case the previously placed part of the SAW acts like a wall, and during one wrapping around the cylinder the SAW fills a layer of typical width L in the longitudinal direction. We thus expect in the present case that the number of parallel contacts per wrapping is $\sim 1/L$. This argument is of course not rigorous, but it agrees within three standard deviations with our numerical result.

Finally, let us discuss the universal constant A . Naively, one could try to estimate it as follows. In planar geometry, it is known that the variance of the winding number around either end point is [19,8]

$$\langle W^2 \rangle = (2\pi^2)^{-1} \ln N, \quad N \rightarrow \infty \quad (\text{plane}) \quad (10)$$

(notice that we measure windings in units of 2π). When the plane (punctuated at one of the end points of the chain) is mapped onto the cylinder by means of Eq. (1), winding around this end point is mapped precisely onto wrapping around the cylinder. Taking into account that $\ln N = \text{const} + \nu^{-1} \ln |z| \rightarrow \text{const} + 2\pi h / \nu L$, we would predict $\langle W^2 \rangle = \text{const} + (1/\pi\nu)h/L$, i.e., $A = 1/\pi\nu = 0.4244$. This disagrees with our measured value by more than ten standard deviations, and seems definitely ruled out. To explain this discrepancy,

we notice that conformal invariance holds only for the canonical (fixed fugacity x) ensemble exactly at the critical point [in this ensemble N fluctuates of course, so that we should actually write $\langle W^2/\ln N \rangle \rightarrow (2\pi^2)^{-1}$ for $x \rightarrow x_c \equiv 1/\mu_\infty$, instead of Eq. (10)]. For any finite L , our results for the cylinder hold, in contrast, for $x_c(L) = 1/\mu(L) > x_c$, since only there, $\langle N \rangle \rightarrow \infty$. Therefore, conformal invariance strictly spoken does not give a prediction for A .

In summary, we have shown by simulations of very long chains on cylinders that universality holds for 2D SAWs, in contrast to recent claims. Our conclusion is based on the fact that parallel contacts are much more rare than predicted in

[1]. This suggests that the corresponding operator, which was predicted to be marginal, could play an irrelevant role, so that universality should hold for 2D SAWs. While counting parallel contacts with sufficient statistics would have been virtually impossible in planar geometry, it is feasible in cylinder geometry. At the same time our results on the constant A should serve as a warning that conformal invariance should not be applied too naively.

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