2-d Self-Avoiding Walks on a Cylinder

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We present simulations of self-avoiding random walks on 2-d 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 \( \mu \), 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 \( \gamma \) of SAW’s might be nonuniversal. Finally, we find that the amplitude for \( \langle W^2 \rangle \) does not agree with naive expectations from conformal invariance.

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Although self-avoiding random walks (SAW’s) are among the best studied critical phenomena, there have been recently speculations which, if true, would have very far reaching and surprising consequences [1]. One such consequence would be that the critical exponent \( \gamma \) of interacting SAW’s 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 \( \gamma \) for a-thermal SAW’s on the Manhattan lattice is different from \( \gamma \) on other 2-d lattices [2]. Numerical evidence for the former prediction is lacking [3,4], but it has been argued [5] that this is not conclusive since much longer SAW’s (10^9 steps) would be needed to refute the prediction unambiguously. As concerns the Manhattan lattice, the numerical evidence is unclear since non-universality was found in [6], but universality was found in [7].

The main question at stake here is the density of parallel contacts (i.e. the number of pairs of parallel steps on opposite sites of one plaquette) in a very long SAW. It is easily seen that parallel contacts are forbidden for 2-d 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 suggested by simulations in [6], but again it seems difficult to perform significant measurements on planar 2-d SAW’s.

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

\[
z = x + iy \rightarrow w = (L/2\pi) \ln z. \tag{1}
\]

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 (\( N^\nu \gg L \), 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 longitudinal size \( h \) (defined here as the average end-to-end distance, projected onto the direction parallel to the cylinder axis) scales as

\[h \sim N/L^{1/\nu-1}, \quad \nu = 3/4. \tag{2}\]

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

\[
\langle W^2 \rangle \approx A h/L \tag{3}
\]

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 one full turn. Finally, the connectivity constant (the critical monomer fugacity) should show the usual finite size behavior

\[
\mu(L) = \mu_\infty - b L^{-1/\nu}. \tag{4}
\]

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.(4) we obtain

\[
F(L, N) = F_\infty(N) - B h/L, \tag{5}
\]

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

\[n_\parallel \approx C h/L, \tag{6}\]

with \( C \) being yet another universal amplitude.

Finally, we can rewrite eq.(3) in terms of the Flory radius \( R \) of SAW’s 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

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

(7)

with $D$ being also universal. Using this, we can eliminate $h/L$ from eqs. (3), (5), and (6) to obtain $((W^2)), \ F_\infty(N) - F(L,N), \ n_0 = (A',B',C') \ (R/L)^{1/\nu}$, with universal amplitudes $A' = AD, \ B' = BD, \ and \ C' = CD$.

The main objective of the present paper was to test eqs. (4) by means of Monte Carlo simulations. Since we want to simulate lattices with large perimeters $L$, and with $N'' \gg L$ (we went up to $L = 128$ and $N = 60,000$), we need a fast algorithm. For SAW’s in planar geometry the fastest known algorithm is the pivot algorithm (at least if one is not interested in ergodic). We therefore used the pruned-enriched Rosenbluth method (PERM) (1) with markovian anticipation (2). In PERM one starts off by growing chains according to the well known Rosenbluth method (4), but when their weights become too large resp. too small one interferes by cloning resp. pruning. 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 $s = 0, \ldots, 2d - 1$. A sequence of $k + 1$ steps is then encoded as $S = (s_{-k}, \ldots, s_0) \equiv (s,s_0)$. By $P_{N,m}(S)$ we denote the statistical weight of all $N$-step chains in an unbiased sample which had followed the sequence $S$ during steps $N - m - k, \ldots, N - m$. This can be estimated either in a previous test run or during the present run. The ideal bias in $k$-step markovian anticipation is

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

(8)

with $N \gg m \gg 1$ (we used $m = 150$, and averaged $P_{N,m}(S)$ 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. Eq. (8) should not be used, of course, for the very first steps of the chain. There the probabilities $P_{N,m}(S)$ are not appropriate. Our remedy is ad hoc but efficient: When determining the bias for the $n$-th step in a chain, we replaced $P_{N,m}(S)$ by $P_{N,m}(S) + const/n$, with $const \approx 20$. The markovian anticipation bias is of course compensated by a weight factor $\propto 1/p(s_0|s)$, to guarantee correct sampling.

In our actual simulations we used semi-infinite cylinders. Knowing that the walks anyhow have to grow either parallel or antiparallel to the cylinder axis, 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. (3) 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 9 steps are encoded by integers from 0 to $4^9 - 1$, with the last step giving the most 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 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.

![fig.1](image-url)
In all simulations chain lengths were such that \( h/L > 80 \). Results for the connectivity constant are shown in fig.2 where we plotted \( \mu_\infty - \mu(L) \) with \( \mu_\infty = 2.638159 \) resp. \( \mu_\infty = 4.150795 \) for the square resp. triangular lattice. 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 plotting then 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 also 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: \( \lim_{N \to \infty} \langle R^2 \rangle / N^{2\nu} = 0.7710 \pm 0.0004 \) \[16\] for the square lattice, and 0.711 \[17\] for the triangular lattice. Both gave again consistent results, \( D = 0.9446 \pm 0.0006 \).

Finally, we consider the number of parallel contacts (measured only on the square lattice). A plot analogous to fig.4 shows a strong \( L \) dependence, but would not allow to estimate this dependence precisely. More instructive is a plot analogous to fig.3. For each \( L \), we first extracted

**FIG. 2.** Log-log plot of \( \mu_\infty - \mu(L) \) against \( L \). The straight lines have slope \(-4/3\), as predicted by eq.(1), and prefactors adjusted to fit the data. Error bars on the data points are comparable 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 \( h = h_0N + h_1 \) for fixed \( L \). Again, error bars on the data points are comparable or smaller than the symbol sizes. The straight lines have slope \(-1/3\) as predicted by eq.(2), with prefactors adjusted to fit the data.

**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 \( a_0 = a_0N + a_1 \) for fixed \( L \). According to the prediction of Ref. \[18\], one should have \( a_1 \sim 1/L^{1.333} \). The straight line is \( \text{const}/L^{2.25} \).
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

$$n_\parallel / \nu \sim L^{-1.92 \pm 0.03}.$$  

(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 1 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 $z^{1/2}$ [8], 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 [9]

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

(notice that we measure windings in units of $2\pi$). When the plane (punctuated at one of the end points of the chain) is mapped onto the cylinder by means of eq. (4), winding around this end point is mapped precisely onto wrapping around the cylinder. Taking into account that $\ln N = const + \nu^{-1} \ln |z| \to const + 2\pi h/\nu L$, we would predict $\langle W^2 \rangle = const + (1/\nu) h/L$, i.e. $A = 1/\nu = 0.4244$. This disagrees with our measured value by more than 10 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 $\langle W^2/\ln N \rangle \to (2\pi^2)^{-1}$ for $x \to x_c \equiv 1/\mu_\infty$, instead of eq. (11)). For any finite $L$, our results for the cylinder hold, in contrast, for $x_c(L) = 1/\mu(L) > x_c$, since only there $\langle N \rangle \to \infty$. Therefore, conformal invariance strictly spoken doesn’t give a prediction for $A$. In summary, we have shown by simulations of very long chains on cylinders that universality holds for 2-d SAW’s, 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 2-d SAW’s. 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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