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ADDENDUM

Addendum to 'On three-dimensional self-avoiding walk symmetry classes'

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Abstract

In two dimensions the universality classes of self-avoiding walks on the square lattice, restricted by allowing only certain two-step configurations to occur within each walk, has been argued to be determined primarily by the symmetry of the set of allowed two-step configurations. In a recent paper, primarily tackling the three-dimensional analogues of these models, a novel two-dimensional model was discovered that seemed either to break the classification of the models into universality classes according to microscopic symmetry or was itself a member of a novel universality class. This was supported by series analysis of exact enumeration data. Here we provide conclusive evidence that this model, known as 'anti-spiral walks', is in the directed walk universality class. We arrive at these conclusions from Monte Carlo simulations of these walks using a PERM algorithm modified for this problem. We point out that the behaviour of this model is unusual in that other models in the directed walk universality class remain directed when the self-avoidance condition is removed, whereas the behaviour of anti-spiral walks becomes that of a isotropic simple random walk. We also remark that the symmetry classification of walk models can be kept by adding a natural condition to the scheme that disallows models, all of whose configurations avoid some infinite region of the plane by virtue of their microscopic constraints.

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Two-step restricted walk (TSRW) models [1, 2] are oriented self-avoiding walks (SAW) where the allowed configurations have certain restrictions placed upon each pair of successive steps. The rules obeyed by the successive steps of TSRW models are most conveniently depicted by rule diagrams. Such a diagram describes all allowed pairs of steps by depicting the set of

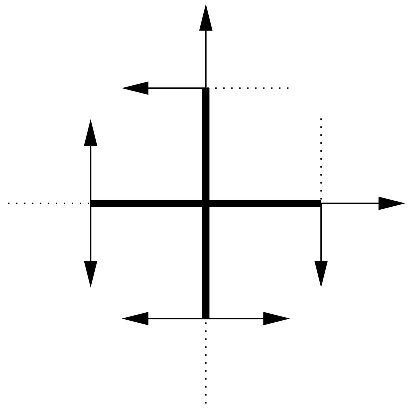

Figure 1. The rule diagram of the anti-spiral walk. The bold edge represents the current or last step of a walk of length $n - 1$ while the arrowed edges denote the allowed next steps to construct all possible walks of length n.

permissible continuing steps from each of the permissible lattice directions. In figure 1 the rule diagram for the so-called *anti-spiral walk* model is shown.

Guttmann *et al* [1] studied square lattice TSRW models in general and argued that certain properties of the rules could be used to determine into which universality class the model would fall. These properties included two types of conditions: firstly, conditions (*balanced*, *reverse-balanced* and *mixing*) that eliminate 'unbalanced' walks or rules, where certain directions are never taken, giving rise to trivial, one-dimensional or directed walks; secondly, a set of conditions regarding the symmetry of the rules further delineate the more interesting universality classes. While attempting to summarize this classification scheme of TSRW models in two dimensions Rechnitzer and Owczarek [2] recently found a TSRW model that is not excluded as trivial, one-dimensional or directed by the balanced, reverse-balanced and mixing conditions and was not in the original classification by Guttmann *et al* [1]. This model, given the name 'anti-spiral', appeared to be neither trivial nor directed when studied by exact enumeration [3]. Rechnitzer and Owczarek [2, 4] suggested a property of this model, which they called *region exclusion*, may be important in its classification, since it seemed directly related to the lack of spiral configurations.

Rechnitzer [3] enumerated the mean moment-of-inertia tensor series up to 50 terms using a parallelized backtracking algorithm and analysed the resulting series using the method of differential approximants [5]. Pathological results were obtained for the exponent ν extracted from the scaling of the mean moment-of-inertia tensor in its major and minor directions. Unbiased approximant analysis gave critical points far from the theoretical critical point of $x_c = 1$, and the exponent estimates from the same analysis gave anisotropic results which, however, did not approach the directed values of 1 and 1/2, as one may have expected. Rather, the analysis suggested that $2\nu_+ \approx 1.80(2)$, where ν_+ is associated with the line $x + y = 0$, and $2\nu_- \approx 1.15(2)$, where ν_- is associated with the line $x - y = 0$, with ν_+ decreasing and ν_- increasing. The symmetry of the walk rule for the anti-spiral TSRW model suggests a natural direction along the line $y = x$. However, the series analysis suggests growth of the walks occurs principally along the direction perpendicular to this. Since anti-spiral walks appear to be very anisotropic this seems to rule out the isotropic SAW universality class and the movement of the estimates of the exponents away from the directed-walk values as length increases seems to rule out the directed class the results tentatively suggest a novel universality class. On the other hand, the TSRW walk literature warns us about such badly behaved series analysis: aniso-spiral walks [6] (another TSRW square lattice model) display a turning point [7] in the estimates of their size exponents at a length of $O(10^2)$. In light of this, it is clearly prudent to examine much longer walks in the case of anti-spirals than is possible by exact enumeration methods.

With regard to the considerations above we have simulated anti-spiral walks up to lengths of $O(10^4)$ using an efficient Monte Carlo algorithm [8], PERM, that is easily modified for use with these TSRW models. These simulations allow us to conclude that anti-spiral walks fall into the directed universality class. Moreover, we can explain why the series analysis found spurious results: the true asymptotic behaviour is affected by huge corrections to scaling so that this is not seen for walks at least as large as $O(10^3)$. In fact, at short lengths analysis of the moment of inertia tensor would lead one to incorrectly identify the major and minor scaling directions: there is a crossover in the scaling of the two axes at around length 1000. This kind of unexpected pathology makes for a cautionary tale in accepting the results of brute force series analysis. However, we point out that careful analysis of corrections to scaling [9], as championed by Conway and Guttmann [10], would have indicated the presence of this pathology.

In our simulations we generated anti-spiral walks of lengths up to 16 384. We used the mean monomer-to-end distance as the measure of geometric size as it has proven better behaved than the end-to-end distance in previous analyses of similar models [7]. We implemented the algorithm on a LOBOS (lots of boxes on shelves) consisting of a cluster of 45 iMacs running LinuxPPC. We used about a week of LOBOS time to generate 45 million samples (1 million samples from each machine) of anti-spiral walks of length up to 16 384, which is equivalent to around one year of CPU time on an iMac. One of the disadvantages of using single-run data from a kinetic growth type algorithm is that data from different lengths are correlated, and so error analysis is subtle. We, however, used only data from lengths separated by factors of 2 which has proven sufficient in the past to render length correlations negligible [11]. We also ran some independent (smaller sample sizes) simulations at shorter lengths as a double check, and indeed our errors overlapped sufficiently to give us confidence in the utility of our data. Additionally, in PERM the enrichment process also adds some degree of correlation between data of the same length. Since we have performed 45 different simulations we simply calculated our errors empirically from the spread of the data in those 45 simulations. We also note that, even within a single run, the average number of samples we obtained from one tour of a walk that grows from length 0 and returns to length 0 was $O(10^2)$ compared to our individual sample sizes of $O(10^6)$.

Due to the anisotropy in evidence from the exact enumeration data we kept track of the components of the monomer-to-end distance in the directions given by the line $x - y = 0$, $\langle R_N^2 \rangle^-$, and by the line $x + y = 0$, $\langle R_N^2 \rangle^+$, in our simulations. One expects asymptotically

$$\langle R_N^2 \rangle^\pm \sim B_0 N^{2\nu_\pm} \qquad \text{as} \quad N \to \infty. \tag{1}$$

Estimates of $2\nu_\pm(N)$ were therefore found by eliminating B_0 using successive pairs of data points as

$$2\nu_\pm(N) \sim \frac{1}{\log 2} \left(\log \frac{\langle R_N^2 \rangle^\pm}{\langle R_{N/2}^2 \rangle^\pm} \right). \tag{2}$$

The estimates of $2\nu_\pm(N)$ are plotted in figure 2. The plot clearly shows a crossover of the estimates in two directions and allows us to identify the larger (parallel) exponent to be $\nu_\parallel = \nu_-$

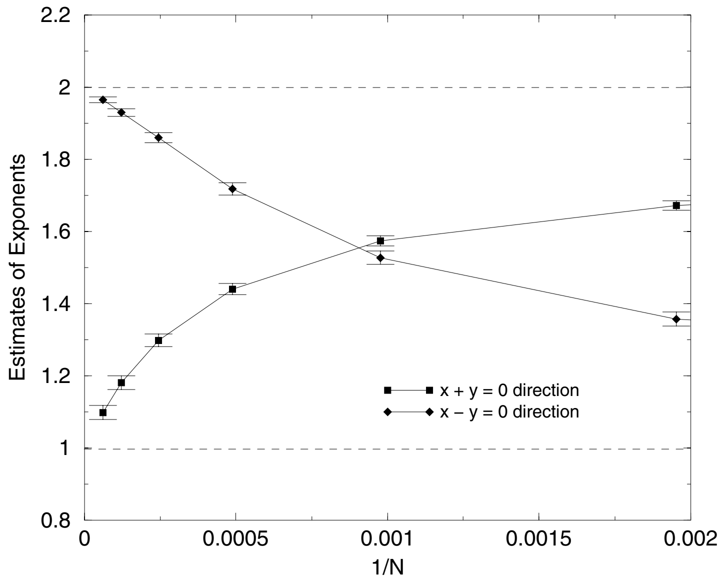

Figure 2. Plot of estimates of critical exponents, $2\nu_+(N)$ and $2\nu_-(N)$, in $x + y = 0$ and $x - y = 0$ directions, respectively, against $1/N$. This data clearly indicates that the model is affected by strong corrections to scaling and that there is a cross-over in the scaling axes at around $N = 1000$, and so we must conclude that $\nu_\parallel = \nu_-$ and $\nu_\perp = \nu_+$.

and the perpendicular exponent to be $\nu_\perp = \nu_+$. Moreover, it is also fairly clear that $2\nu_\parallel = 2$ and $2\nu_\perp = 1$, the directed universality class values, are the prime candidates for the asymptotic values of these exponents.

One might try to improve the analysis of the size exponents by including correction-to-scaling terms in the asymptotic forms like

$$\langle R_N^2 \rangle^{\pm} \sim N^{2\nu_\pm}\{B_0 + B_1 n^{-\Delta} + B_2 n^{-1} + \cdots\} \qquad \text{as} \quad N \to \infty. \tag{3}$$

First we plotted our data against $1/N$ and observed reasonably straight lines in the asymptotic region, $N > 2000$, of figure 2. This indicates little need to introduce further non-analytic corrections to scaling with $\Delta < 1$. Assuming analytic correction-to-scaling (Δ term absent), we performed a linear extrapolation of the last three data points of $2\nu_\parallel(N)$ and $2\nu_\perp(N)$ and found 2.000 ± 0.014 and 1.04 ± 0.03, respectively. If, however, we assume a square-root correction-to-scaling term exists ($\Delta = 1/2$), similar extrapolation finds 2.07 ± 0.06 and 0.90 ± 0.09, respectively, contradicting the theoretical bounds that $1 \leqslant 2\nu \leqslant 2$ in two dimensions (strictly speaking, $\nu_\parallel$ must always satisfy these bounds, but it is possible that $2\nu_\perp < 1$). This suggests that the assumption of stronger corrections to scaling will still lead to the conclusion that $\nu_\parallel = 2\nu_\perp = 1$. We note in passing that the corrections-to-scaling in this problem can still be viewed as strong, not because of the presence of a small exponent Δ but rather because of the relative size of the coefficients B_j.

Our data strongly indicates that the moment of inertia tensor for the TSRW model known as the *anti-spiral* scales anisotropically with a preferred direction exponent $\nu_\parallel = 2\nu_\perp$. Moreover, we can deduce that the size exponents take on the directed values $\nu_\parallel = 1$ and $\nu_\perp = 1/2$, and so that the anti-spiral TSRW is most likely in the directed universality class. It is interesting to note that, while other models in this universality class remain in the directed class when the self-avoidance condition is removed, the behaviour of anti-spiral walks becomes that of a random

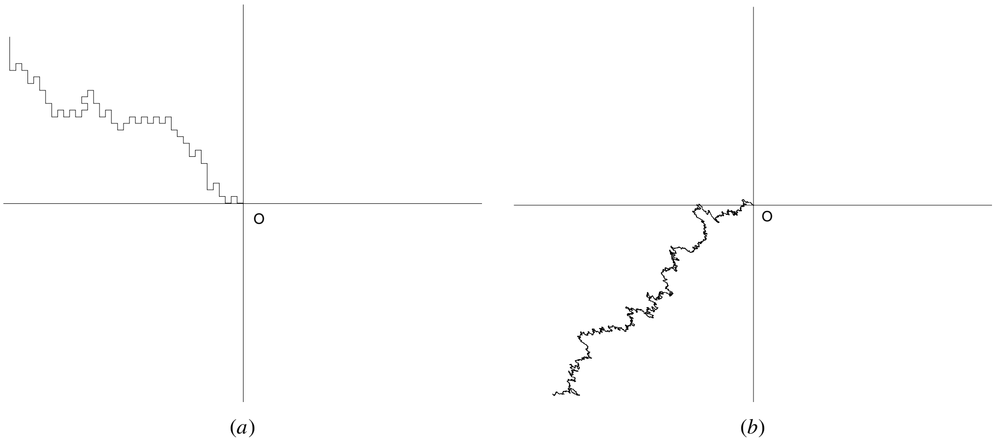

Figure 3. Typical instances of anti-spiral walks of length (*a*) 100 and (*b*) 10 000. They clearly illustrate the seemingly different preferred directions at these two length scales.

walk (with $\nu_\| = \nu_\perp = 1/2$). This completes the classification of all (balanced and reverse-balanced) TSRW models into six universality classes according to their size exponents [1]. The question of whether the rules making up the *aniso-spiral* (as opposed to the anti-spiral) class are also directed [12] is still of some debate—this question will require a new approach since Monte Carlo simulations of aniso-spiral walks up to length $O(10^5)$ produced inconclusive results [12]. If we use the original arguments in [1], anti-spiral walks might be predicted to be in class S (SAW) due to the symmetry of the walk rule. As suggested by Rechnitzer and Owczarek [2,4] the classification scheme should be altered to account for the *region exclusion* property of this rule. In [9] it is shown that the anti-spiral walk can never enter the first quadrant of the plane. We can therefore add the property that some walks must be able to access all parts of the plane (or at least no infinite regions are excluded) to the *mixing* condition so that the classification scheme still holds. However, the utility of the scheme would be called into question if further analysis of aniso-spiral models demonstrated that they too are part of the directed universality class.

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