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The geometrical properties of planar lattice trails

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Abstract. We investigate the winding angle and mean square end-to-end distance of lattice trails on a square lattice, by both exact enumeration and Monte Carlo methods. We find similar behaviour to that of self-avoiding walks, to the extent that the complete distribution is found to agree with the recent exact calculation of the winding-angle distribution function for self-avoiding walks by Duplantier and Saleur, who found a Gaussian distribution. The exponent ν was found to be indistinguishable from $\frac{3}{4}$.

The last four years has seen a spate of interest in such geometrical properties as the winding angle of self-avoiding lattice walks (SAW). This property is of interest both as a measure of the geometry of the walk, and as a model of polymeric entanglement. For the related problem of Brownian motion in the plane Spitzer (1958) first obtained the winding-angle distribution. He found that the probability distribution at time t satisfies asymptotically as $t \to \infty$ a Cauchy law

$$P_t(\theta) = \ln(t)/[\theta^2 + (\ln(t)/2)^2]. \tag{1}$$

This distribution displays certain unusual features, notably infinite moments of all orders. This is because Brownian motion will return arbitrarily close to the origin, where the angle varies rapidly. Excluding the neighbourhood of the origin changes the distribution function dramatically; the new distribution function depends on the value of the exclusion (Rudnick and Hu 1987, 1988, Pitman and Yor 1986, Le Gall and Yor 1987).

For self-avoiding walks (SAW), however, the origin is automatically excluded by the self-avoiding constraint. Fisher *et al* (1984) first studied the winding-angle distribution for square lattice SAW by defining the winding angle θ, measured with respect to the direction of the first step. The origin of a polar coordinate system is taken as the origin of the walk, and the first step is directed along the x axis. As the walk progresses, it passes through points with coordinates (r_k, θ_k), and at each step the angular coordinate changes by an amount $\Delta\theta_k$ from the previous step. This increment may be positive or negative. The final value after N steps is denoted θ_N, and may be of either sign. By symmetry, it is clear that the odd moments of the distribution (if they are finite) vanish identically, $\langle\theta_N^{2k-1}\rangle = 0$, while the even moments are positive. Fisher *et al* calculated the second and fourth moments exactly for $N \leq 21$ for square lattice SAW, and obtained Monte Carlo estimates of the second moment for N up to 160.

Arguing by analogy with Spitzer's (1958) result for planar Brownian motion, in which the scale of θ grows as $\ln t$ (although the moments are infinite), they suggested that

$$\langle\theta_N^{2k}\rangle \approx a_k[\ln(N/b_k)]^{2k\psi_k}. \tag{2}$$

Their analysis is quite consistent with this assumption, and yielded the estimates $b_1 \approx 1.4$, $b_2 \approx 2.3$, $\psi_1 = 0.61 \pm 0.07$ and $\psi_2 = 0.52 \pm 0.04$. The ratio

$$R_N = \langle \theta_N^4 \rangle / \langle \theta_N^2 \rangle^2 \tag{3}$$

was found to lie between 2.9 and 3.2, which suggested a Gaussian distribution, for which this ratio is exactly 3, while the two 'exponents' ψ_1 and ψ_2 are then exactly $\frac{1}{2}$. Finally, they provided heuristic scaling arguments that supported these simple rational exponents.

Rudnick and Hu (1988) applied renormalisation group arguments to this problem, and obtained an ε expansion in which a $(4-\varepsilon)$-dimensional walker of N steps wraps around a $(2-\varepsilon)$-dimensional rod. To first order in ε they find a Gaussian distribution

$$P_N(\theta) = \exp[-\theta^2 \varepsilon / 8 \ln(N)] / (8\pi \ln(N)/\varepsilon)^{1/2} \tag{4}$$

so that θ scales as $(\ln N)^{1/2}$, compared with $\ln N$ for ordinary random walks (ORW). However, they also suggested that the crossover from ORW behaviour to SAW behaviour will only be seen for very large N, of order $\exp(16/\varepsilon)$. For $d = 2$ this gives a value of N around 3000 steps.

Very recently, Duplantier and Saleur (1988) have obtained the exact probability distribution for this problem in two dimensions using Coulomb-gas techniques and conformal invariance. They find the exact probability distribution to be

$$P_N(\theta) = \exp[-\theta^2 / 4 \ln(N)] / [4\pi \ln(N)]^{1/2} \tag{5}$$

in the large-N limit, which is in precise agreement with the renormalisation group result when $\varepsilon = 2$. The results of Fisher *et al* are also confirmed by this exact result.

In this paper we have studied lattice trails by both series analysis and Monte Carlo methods. Lattice trails are a superset of SAW. They are connected paths on an underlying lattice with the restriction that *bonds* cannot be multiply occupied (for SAW the restriction applies to *sites*). It is believed that they belong to the same universality class as SAW (Guttmann 1985a, b, Shapir and Oono 1984). We have enumerated lattice trails on the square lattice to 22 steps and on the triangular lattice to 15 steps, and calculated both the second and fourth moment of the winding angle, as well as the mean square end-to-end distance. In order to avoid difficulties with the definition of the distribution function, we have excluded the point at the origin. (While this exclusion is automatically applied for SAW by their constraint, for trails it has to be specifically invoked.) Our initial analysis of the exact data indicated that the series were too short for an accurate assessment of the winding angle. This is consistent both with the experience of the study in Fisher *et al* of the winding angle distribution of SAW and with our earlier study of critical exponents for trails (Guttmann 1985). In addition to these exact enumerations, we have performed high-precision Monte Carlo calculations on longer trails. We have used the fixed-N 'pivot' algorithm, originally invented by Lal (1969), but systematically analysed and applied to SAW by Madras and Sokal (1988). For various step lengths up to 512, we have generated between two and ten million independent realisations of N-step square lattice trails, and used these data to estimate the second and fourth moment of the winding angle and the mean square end-to-end distance. Our raw data are summarised in tables 1 and 2.

As observed in our earlier studies of lattice trails (Guttmann 1985a, b, Guttmann and Osborn 1988), and as noted above, the asymptotic regime for trails appears to correspond to larger N values than for SAW, and for that reason longer walks were considered necessary. This observation is borne out by the results shown in figure 1,

Table 1. Series data for the mean square end-to-end distance and the second and fourth moments of the winding angle distribution.

l	C_l	ΣR_l^2	Square lattice $\Sigma \theta_l^2$	$\Sigma \theta_l^4$
1	1	1		
2	3	8	1.233 700 550 136 169	$7.610\,085\,237\,031\,440\times10^{1}$
3	9	41	8.246 235 188 499 534	$1.536\,604\,804\,392\,356\times10^{1}$
4	25	176	$2.964\,908\,275\,147\,875\times10^{1}$	$9.397\,021\,962\,112\,685\times10^{1}$
5	75	683	$1.105\,575\,468\,731\,198\times10^{2}$	$4.887\,465\,204\,442\,500\times10^{2}$
6	211	2 492	$3.515\,609\,500\,020\,143\times10^{2}$	$1.848\,213\,695\,164\,414\times10^{3}$
7	609	8 705	$1.170\,218\,417\,408\,695\times10^{3}$	$7.312\,949\,097\,689\,575\times10^{3}$
8	1 703	29 480	$3.546\,605\,419\,613\,297\times10^{3}$	$2.460\,242\,390\,866\,012\times10^{4}$
9	4 853	97 389	$1.112\,521\,528\,615\,170\times10^{4}$	$8.686\,860\,160\,076\,602\times10^{4}$
10	13 531	315 668	$3.280\,633\,531\,874\,207\times10^{4}$	$2.710\,539\,893\,108\,322\times10^{5}$
11	38 229	1 007 069	$9.969\,845\,874\,482\,610\times10^{4}$	$8.977\,879\,585\,201\,158\times10^{5}$
12	106 227	3 171 288	$2.892\,884\,195\,446\,676\times10^{5}$	$2.712\,762\,509\,802\,989\times10^{6}$
13	298 257	9 876 033	$8.594\,631\,666\,516\,479\times10^{5}$	$8.578\,201\,955\,994\,304\times10^{6}$
14	827 235	30 468 380	$2.468\,920\,872\,755\,189\times10^{6}$	$2.545\,553\,853\,077\,603\times10^{7}$
15	2 312 077	93 222 341	$7.223\,355\,590\,262\,998\times10^{6}$	$7.814\,121\,183\,255\,652\times10^{7}$
16	6 400 035	283 200 848	$2.058\,750\,436\,722\,140\times10^{7}$	$2.286\,281\,912\,098\,709\times10^{8}$
17	17 828 445	854 865 749	$5.956\,664\,327\,344\,672\times10^{7}$	$6.874\,193\,351\,226\,631\times10^{8}$
18	49 275 803	2 566 034 164	$1.687\,956\,886\,786\,469\times10^{8}$	$1.991\,771\,987\,010\,146\times10^{9}$
19	136 899 957	7 663 397 997	$4.842\,728\,520\,787\,489\times10^{8}$	$5.897\,804\,479\,985\,227\times10^{9}$
20	377 884 807	22 783 089 464	$1.366\,057\,174\,980\,303\times10^{9}$	$1.695\,901\,548\,698\,672\times10^{10}$
21	1047 617 005	67 453 427 149	$3.893\,547\,479\,493\,469\times10^{9}$	$4.964\,030\,792\,533\,835\times10^{10}$
22	2888 550 643	198 963 085 748	$1.094\,297\,521\,672\,476\times10^{10}$	$1.418\,891\,752\,502\,458\times10^{11}$

l	C_l	ΣR_l^2	Triangular lattice $\Sigma \theta_l^2$	$\Sigma \theta_l^4$
1	1	1		
2	5	12	2.741 556 778 080 377	2.555 485 412 929 076
3	23	97	$2.284\,776\,527\,367\,392\times10^{1}$	$5.874\,332\,123\,949\,410\times10^{1}$
4	111	662	$1.402\,348\,288\,354\,481\times10^{2}$	$5.615\,130\,441\,555\,297\times10^{2}$
5	529	4 135	$7.971\,144\,420\,538\,182\times10^{2}$	$4.042\,186\,212\,783\,137\times10^{3}$
6	2 491	24 456	$4.320\,016\,269\,253\,037\times10^{3}$	$2.583\,797\,362\,537\,017\times10^{4}$
7	11 713	139 239	$2.260\,714\,897\,181\,434\times10^{4}$	$1.540\,960\,807\,475\,497\times10^{5}$
8	54 909	770 754	$1.156\,116\,637\,036\,761\times10^{5}$	$8.701\,782\,993\,030\,423\times10^{5}$
9	256 525	4 175 107	$5.820\,523\,136\,462\,224\times10^{5}$	$4.753\,612\,876\,624\,779\times10^{6}$
10	1 195 581	22 228 188	$2.893\,156\,381\,315\,119\times10^{6}$	$2.530\,565\,280\,365\,292\times10^{7}$
11	5 560 651	116 679 945	$1.423\,336\,462\,247\,378\times10^{7}$	$1.319\,500\,859\,890\,217\times10^{8}$
12	25 813 167	605 299 664	$6.945\,187\,562\,129\,392\times10^{7}$	$6.771\,353\,467\,107\,957\times10^{8}$
13	119 632 911	3 108 891 493	$3.365\,941\,917\,243\,509\times10^{8}$	$3.430\,648\,565\,608\,888\times10^{9}$
14	553 646 165	15 831 084 734	$1.621\,895\,837\,061\,260\times10^{9}$	$1.719\,565\,053\,231\,131\times10^{10}$
15	2558 871 815	80 015 551 627	$7.776\,847\,368\,166\,111\times10^{9}$	$8.541\,967\,880\,088\,253\times10^{10}$

in which we plot the dimensionless ratio R_N, defined by (3), against $1/N$. The Gaussian limit of 3 is quite consistent with these results, but this is only clear for reasonably large values of N. This Gaussian behaviour suggests that the distribution function for trails is likely to be similar to that for SAW, and the rest of our analysis is designed to test this suggestion. In figure 2 we plot $\langle\theta_N^2\rangle$ and $\langle\theta_N^4\rangle^{1/2}$ against $\log N$. These plots are seen to be totally linear to visual accuracy, and a least-squares straight line through

Table 2. Monte Carlo data for the mean square end-to-end distance and the second and fourth moments of the winding angle distribution. The data are uncertain in the last quoted digit.

l	Number of configurations	$\langle R_l^2 \rangle$	$\langle \theta_l^2 \rangle$	$\langle \theta_l^4 \rangle$
25	3 000 000	82.25	4.036	55.50
30	3 000 000	106.7	4.370	64.60
35	3 000 000	132.8	4.649	72.57
40	3 000 000	160.9	4.903	80.17
64	3 000 000	317.9	5.814	110.47
100	10 000 000	611.0	6.678	143.17
110	3 000 000	703.7	6.870	151.0
120	3 000 000	800.4	7.041	158.1
128	10 000 000	880.8	7.152	162.8
130	3 000 000	900.6	7.174	163.9
140	3 000 000	1005	7.346	171.2
150	3 000 000	1113	7.460	176.5
160	3 000 000	1225	7.583	182.2
192	3 000 000	1605	7.963	200.1
256	7 400 000	2464	8.508	226.9
320	3 000 000	3438	8.962	249.9
384	3 000 000	4512	9.316	270.0
512	2 100 000	6944	9.911	303.6

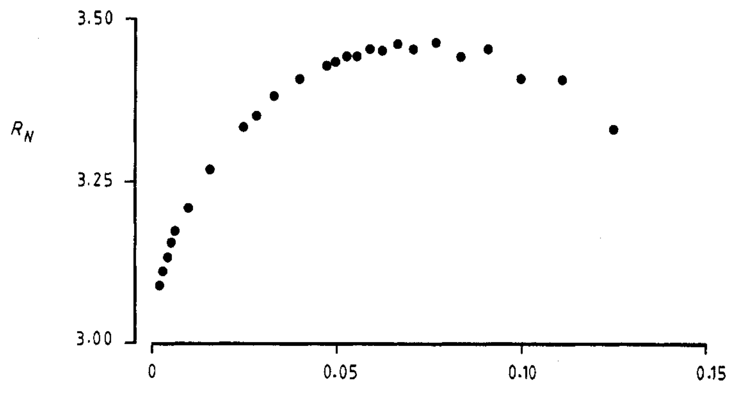

Figure 1. $R_N = \langle \theta_N^4 \rangle / \langle \theta_N^2 \rangle^2$ plotted against $1/N$. The approach to the Gaussian value of 3.0 can be seen.

these points has gradient 1.97 and intercept at $N = 1$ of -2.40 for the second moment, and gradient and intercept at $N = 1$ of 3.33 and -3.39 respectively for the square root of the fourth moment (using data for $N \geq 64$ only).

In terms of (2), this gives for the parameters a and b

$$\begin{aligned} a_1 &= 1.97 \qquad b_1 = 3.37 \\ a_2 &= 11.1 \qquad b_2 = 2.76. \end{aligned} \tag{6}$$

From (5) it follows that the constants a_1 and a_2 are precisely 2 and 12 respectively for SAW. Our numerical results for trails are quite close to these exact values, particularly

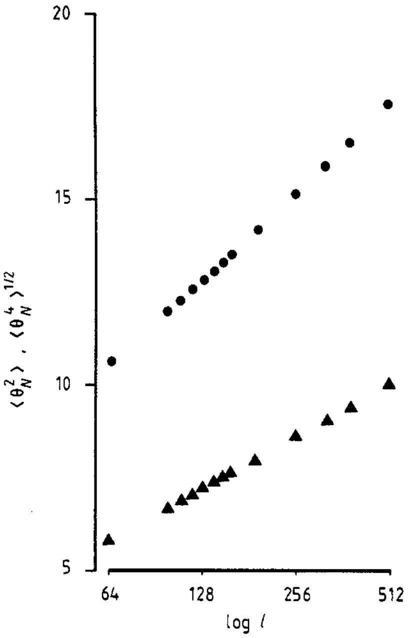

Figure 2. A plot of $\langle\theta_N^2\rangle$ (▲) and $\langle\theta_N^4\rangle^{1/2}$ (●) against log N.

the estimate of a_1, and sufficiently close that agreement seems quite likely, from which would follow the result that the distribution function of winding angles for lattice trails *is identical to* that for SAW.

Pursuing this possibility further, we show in figure 3 a histogram of winding angles obtained for 512 step trails, and a 'best-fit' Gaussian drawn through the points of the histogram. The Gaussian shape is extremely well reflected by the observed points. The 'best-fit' curve is found to be described by $\exp(-\theta^2/s \ln N)$, with $s = 3.07 \pm 0.06$. This is significantly different from the 'predicted' value from (5) of 4.0, but this difference reflects the fact that even 512 step trails are a long way from the infinite limit. In support of this interpretation, we fitted our data for 128 and 256 steps to a 'best-fit' Gaussian and found $s(N = 128) = 2.76$ and $s(N = 256) = 2.92$. A limit of 4.0 for this sequence as N approaches infinity appears entirely attainable.

In the light of Rudnick and Hu's comment that, for SAW one should only expect to see large-N behaviour for walks of several thousand steps, we also plotted $\langle\theta_N^2\rangle$ against $(\ln N)^2$, the expected ORW behaviour. The plot showed considerable curvature, suggesting that the crossover to SAW behaviour occurs at far smaller values of N than they predicted. This is consistent with the observations of Fisher *et al* for two-dimensional SAW and of Rudnick and Hu (1987) themselves for three-dimensional SAW.

As part of our simulations, we also kept track of the mean square end-to-end distance. This study complements the earlier Monte Carlo study of lattice trails by Guttmann and Osborn (1988), using the Berretti–Sokal (1985) algorithm. In that study we estimated the connective constant and the critical exponent corresponding to the growth in the number of n-step trails, γ. In this study our trails are restricted to those which do not revisit the origin. However, in analogy with random walks, we expect this to be a vanishingly small proportion of the total number of trails, and so the exponent will remain unchanged. A least-squares straight line through a log–log plot

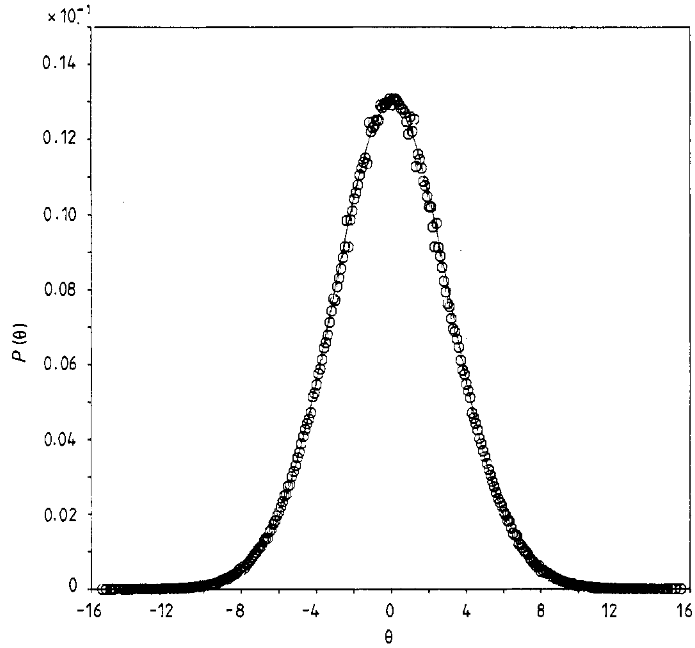

Figure 3. A histogram of winding angles for 512 step trails. $N(\theta)$ is the fraction of walks in the interval $\theta-\Delta\theta$ to $\theta+\Delta\theta$, where $\Delta\theta=0.05$. The Gaussian of best fit is shown as an unbroken curve.

of our data, given in table 2, from 64–512 steps gives $\nu=0.742$, data from 100–512 gives $\nu=0.744$, data from 160–512 gives $\nu=0.745$, and data from 256–512 gives $\nu=0.747$. These results are entirely consistent with the view that the model is in the same universality class as self-avoiding walks, for whch $\nu=0.75$ exactly. Indeed, this is perhaps the strongest numerical evidence to date in support of that view.

We conclude that the leading-order asymptotic behaviour of square lattice trails appears to be identical to that of square lattice SAW. It follows that the different constraint imposed on trails only affects the sub-dominant terms. That is to say, we might expect different correction-to-scaling exponents for trails, though our data are not sufficiently good to identify these sub-dominant terms.

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