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Lattice trails: II. Numerical Results

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Abstract. A numerical study of the properties of lattice trails on the honeycomb, square, triangular and simple cubic lattices is made. Critical points are estimated for all lattices, and upper and lower bounds established. Extensive series have been obtained, and series analysis of both trail generating functions and mean square end-to-end distance series are not inconsistent with the conclusion that the problem is in the same universality class as the self-avoiding walk problem. A pseudo star-triangle transformation is defined, and the analyticity properties of that function, coupled with previous exact results, clearly supports that conclusion for the triangular lattice, as well as providing excellent unbiased critical point estimates.

We also show that the connective constant for $d \geq 2$-dimensional hypercubic trails is strictly greater than the corresponding quantity for SAW's.

1. Introduction

In a previous paper (Guttmann 1985) hereafter referred to as I we developed a number of exact results about lattice trails. The fundamental question is whether this problem belongs to the same universality class as does the self-avoiding walk (SAW) problem, and we showed in I that this question can be answered in the affirmative for the honeycomb lattice, and for the L lattice (an oriented square lattice in which each step must be perpendicular to its predecessor). Recent series work by Zhou and Li (1984) raises the possibility that the two problems belong to different universality classes, and the purpose of this paper is to investigate our extended series expansions for the trail generating function and mean square end-to-end distances in order to establish critical point, critical exponent and amplitude estimates. We also obtain upper and lower bounds on the connective constants for some two- and three-dimensional lattices.

The layout of the paper is as follows. In § 2 we discuss and analyse our data on two-dimensional series, and in § 3 we do the same for the three-dimensional simple cubic lattice series. Section 4 is devoted to obtaining upper and lower bounds as well as proving that the connective constant for the $d \geq 2$-dimensional hypercubic lattice SAW series is less than that for trails. In § 5 we define a star-triangle substitution function, and argue on the basis of its singularity distribution that the triangular trails and SAW problem belong to the same universality class. Section 6 provides a summary of our results.

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2. Two-dimensional lattices

In table 1 we give the series coefficient t_n of the trail generating function (TGF)

$$T(x) = \sum_{n \geq 0} t_n x^n; \qquad t_0 = 1 \tag{2.1}$$

for the honeycomb (h), square (s) triangular (t) and simple cubic (sc) lattices. The expansions for the s and t lattices were obtained to 22 and 16 terms respectively. We used a simple back-tracking algorithm, similar to that used to generate SAWS, as described in Guttmann (1984). The program was written in FORTRAN and run on a Perkin-Elmer 3220 mini-computer using the Unix V7 operating system. The program was totally CPU bound, to the extent that re-writing it in C produced a time saving of

Table 1. Coefficients of the trail generating function for various lattices.

N	Honeycomb	Square	Triangular	Simple cubic
0	1	1	1	1
1	3	4	6	6
2	6	12	30	30
3	12	36	150	150
4	24	108	738	750
5	48	316	3 570	3 726
6	96	916	17 118	18 438
7	186	2 628	81 498	90 966
8	360	7 500	385 710	447 918
9	696	21 268	1 817 046	2 201 622
10	1 344	60 092	8 528 478	10 809 006
11	2 562	169 092	39 903 462	52 999 446
12	4 872	474 924	186 198 642	259 668 942
13	9 288	1 329 188	866 861 394	1 271 054 982
14	17 664	3 715 244	4 027 766 490	6 218 232 414
15	33 384	10 359 636	18 681 900 270	30 399 142 614
16	63 120	28 856 252	86 518 735 722	
17	119 280	80 220 244		
18	225 072	222 847 804		
19	423 630	618 083 972		
20	797 400	1 713 283 628		
21	1 499 256	4 742 946 484		
22	2 817 216	13 123 882 524		
23	5 286 480			
24	9 918 768			
25	18 592 080			
26	34 840 848			
27	65 228 874			
28	122 105 496			
29	228 402 168			
30	427 176 336			
31	798 373 662			
32	1 491 985 800			
33	2 786 515 176			
34	5 203 816 992			
35	9 712 725 234			
36	18 127 267 800			

less than 3%. Total run time was 50–150 hours on each lattice. Problems of integer overflow also occurred, but these were overcome by noting the (machine-dependent) property that if $2^{31} < i < 2^{32}$, then i is stored as $j = i - 2^{32}$.

For the honeycomb lattice we list 36 coefficients, obtained from the counting theorem given in I and the published data on honeycomb SAW's and polygons. It is also known that the connective constant $\lambda = (2+\sqrt{2})^{1/2}$ for this lattice (Nienhuis 1982, 1984) and that the critical exponent $\gamma = 43/32$ where $T(x) \sim A(1-\lambda x)^{-\gamma}$. Further, the amplitude A is exactly $4/(2+\sqrt{2})$ times that for SAWs, as proved in I.

In table 2 we present additional configurational information on the square lattice, including mean square end-to-end distances and other quantities used in establishing bounds.

Table 2. Square lattice configurational data. $\rho_n c_n = \Sigma_{c_n} r^2$, $\langle R_n^2 \rangle = \rho_n c_n / c_n$, bridging trails and irreducible bridging trails defined in text.

n	$c_n \rho_n$	$\langle R_n^2 \rangle$	Bridging trails	Irreducible bridging trails
1	4	1.000 000 000	1	1
2	32	2.666 666 667	3	2
3	164	4.555 555 556	7	2
4	704	6.518 518 518	17	2
5	2 748	8.696 202 528	41	2
6	10 096	11.021 834 06	101	4
7	35 524	13.517 503 81	259	18
8	121 056	16.140 800 00	669	48
9	402 420	18.921 384 24	1 731	96
10	1 311 504	21.824 935 10	4 499	194
11	4 205 476	24.870 934 17	11 705	398
12	13 304 864	28 014 722 36	30 623	992
13	41 612 324	31.306 575 14	80 443	2 614
14	128 878 736	34.689 171 42	211 851	6 496
15	395 767 092	38.202 799 02	558 999	15 512
16	1 206 315 296	41.804 295 86	1 477 983	37 536
17	3 652 739 252	45.533 883 59	3 914 393	92 366
18	10 995 977 424	49.342 992 08	10 384 023	231 544
19	32 927 997 988	53.274 311 40	27 585 099	583 442
20	98 139 646 880	57.281 611 32	73 366 563	1 464 452
21	291 246 749 300	61.406 290 44	195 341 557	3 680 362
22	860 965 104 720	65.602 926 84	520 640 553	9 310 622

We first analyse the mean square end-to-end distance data, which we expect to be more useful in that the 'critical point' is precisely known. As we are only interested in the answer to the question 'is the exponent the same as, or different from the corresponding exponent for the SAW model?', we focus on the exponent difference by computing $\langle R_n^2 \rangle_{\mathrm{SAW}} / \langle R_n^2 \rangle_{\mathrm{trails}}$. Denoting the corresponding exponents by $2\nu_{\mathrm{s}}$ and $2\nu_{\mathrm{t}}$ for SAW's and trails respectively, we expect that

$$r_n = \langle R_n^2 \rangle_{\mathrm{SAW}} / \langle R_n^2 \rangle_{\mathrm{trails}} \sim A n^{\phi}$$

where $\phi = 2(\nu_{\mathrm{s}} - \nu_{\mathrm{t}})$.

In order to estimate the exponent ϕ, we form the sequence $\{\phi_n\}$, where $\phi_n = \ln(r_n/r_{n-2})/\ln[n/(n-2)]$. Extrapolants of ϕ_n, formed from $\theta_n = [n\phi_n - (n-2)\phi_{n-2}]/2$ are also formed. (Alternate terms are used to minimise the oscillations characteristic of a loose-packed lattice.) In table 3 we show the data and the two sequences $\{\phi_n\}$ and $\{\theta_n\}$. It is clear that ϕ_n is decreasing, and the last eight extrapolants $\{\theta_n\}$ are all less than 0.008 in absolute value, implying that $|\nu_s - \nu_t| < 0.004$. The conclusion that they are equal seems inescapable.

Table 3. Analysis of square lattice mean square end-to-end distance series. $\{\phi_n\}$ and $\{\theta_n\}$ appear to be approaching zero.

n	$\langle R_n^2\rangle$ SAW's	$\langle R_n^2\rangle$ trails	r_n	ϕ_n	θ_n
5	9.563 380 28	8.696 202 53	1.099 719	0.186 081	0.465 202
6	12.574 358 97	11.021 834 06	1.140 859	0.135 204	0.183 549
7	15.556 169 43	13.517 503 81	1.150 817	0.134 980	0.007 229
8	19.012 846 52	16.140 800 00	1.177 937	0.111 175	0.039 089
9	22.411 359 72	18.921 384 24	1.184 446	0.114 611	0.043 318
10	26.242 539 68	21.824 935 10	1.202 411	0.092 156	0.016 078
11	30.017 657 03	24.870 934 17	1.206 937	0.093 739	−0.000 183
12	34.186 992 97	28.014 722 36	1.220 322	0.081 101	0.025 827
13	38.304 340 33	31.306 575 14	1.223 524	0.081 705	0.015 515
14	42.786 437 58	34.689 171 42	1.233 423	0.069 273	−0.001 693
15	47.2177 46 61	38.202 799 02	1.235 976	0.070 761	−0.000 374
16	51.992 500 70	41.804 295 86	1.243 712	0.062 208	0.012 755
17	56.716 411 65	45.533 883 59	1.245 587	0.061 886	−0.004 676
18	61.766 465 71	49.342 992 08	1.251 778	0.054 884	−0.003 708
19	66.765 782 72	53.274 311 40	1.253 245	0.055 110	−0.002 491
20	72.076 549 79	57.281 611 32	1.258 284	0.049 205	−0.001 911
21	77.336 744 50	61.406 290 44	1.259 427	0.049 163	−0.007 324
22	82.895 818 90	65.602 926 84	1.263 599	0.044 226	−0.005 559

Our analysis of the trail generating function is less successful because, in comparing it to the walk generating function we are seeking a second-order effect. That is, the dominant difference is in the critical points, and any exponent difference will be a secondary effect, whereas for the mean square distance series, the critical point is the same, being 1. We have tried several standard methods of analysis. Firstly, Dlog Padé approximants suggest a critical point and critical exponent of 0.2213 and 1.41 respectively for the triangular lattice, and 0.3679 and 1.39 respectively for the square lattice. The estimates of the critical parameters are slowly decreasing, and are clearly some way away from the SAW value of 1.343 75. A careful study of the distribution of singularities in the complex plane, as estimated by Dlog Padé approximants, gives some clue as to the reason for this slow convergence. Taking the triangular lattice first, the approximants to the SAW series suggest a branch cut along the positive real axis from $x_c \approx 0.241$ to ∞, plus two conjugate pairs of singularities at $x = (-0.40 \pm 0.32i)$ and $x = (-0.20 \pm 0.60i)$. For the trails series on the other hand, as well as a branch cut from $x_c \approx 0.221$ to ∞, there are two further branch cuts along the imaginary axis from $\pm 0.30i$. A conjugate pair of singularities at $x = (-0.50 \pm 0.30i)$ can also be discerned. Thus for the trails case, we have non-physical singularities much loser to the physical disc $|x| \leq x_c$ than for the SAW case, which we expect to slow the rate of convergence (Baker and Graves-Morris 1981). A similar situation exists for the square lattice series, where again there are branch cuts on the imaginary axis, with non-physical singularities quite close to the physical disc.

If we assume that $\gamma = 1.343\,75$, biased Padé approximants to $[f(x)]^{1/\gamma}$ give connective constant estimates of $\lambda = 4.525$ (triangular) and 2.7215 (square).

A ratio method analysis of the triangular lattice data is also quite instructive, and clearly shows the steady worsening of behaviour as one passes from the Ising problem to the SAW problem to the trails problem. Taking the values $\gamma = 1.75$ for the Ising model susceptibility and $\gamma = 1.343\,75$ for the SAW and trails generating function, we analyse the three series, given by $f(x) = \Sigma\, c_n x^n$ by forming the following sequences:

$$r_n = c_n / c_{n-1}$$

$$\beta_n = r_n / (1 + (\gamma - 1)/n)$$

$$\mu_n = [n^2 \beta_n - (n-1)^2 \beta_{n-1}] / (2n - 1)$$

$$\delta_n = [n^3 u_n - (n-1)^3 u_{n-1}] / (3n^2 - 3n + 1).$$

Each sequence should give successively more accurate estimates of the connective constant (or its Ising analogue). In table 4 we see that for the Ising model the last entries in the sequence $\{\delta_n\}$ are accurate to six figures, the exact value being $2 + \sqrt{3} = 3.732\,0508\ldots$. For the SAW problem, the last entries in the sequence $\{\delta_n\}$ are in excellent agreement with the current 'best' estimate (Guttmann 1984) of 4.150 75, being accurate to five figures. For the trails problem, the sequences $\{\beta_n\}$ and $\{\mu_n\}$ are still changing in the fourth decimal digit with increasing n, and from the sequence $\{\delta_n\}$ one cannot say any more than $\lambda = 4.525 \pm 0.006$, and even this may be considered excessively optimistic.

This behaviour is, we believe, due to two factors. The first we have already discussed, and that is the presence of non-physical singularities close to the physical disc. The second factor is the possible presence of confluent singularities. The rapid change in

Table 4. Analysis of triangular lattice data for the connective constant of the Ising, SAW and trails problem. As discussed in the text, it is clear that the series are increasingly difficult to analyse for this problem heirarchy.

			Ising model	
n	r_n	β_n	μ_n	δ_n
2	5.000 0000	3.636 3636	3.705 6277	4.235 0031
3	4.600 0000	3.680 0000	3.714 9091	3.718 8170
4	4.391 3043	3.697 9405	3.721 0069	3.725 4566
5	4.267 3267	3.710 7189	3.733 4360	3.746 4765
6	4.183 2947	3.718 4841	3.736 1324	3.739 8363
7	4.120 3550	3.721 6109	3.730 2697	3.720 2985
8	4.072 8227	3.723 7236	3.730 6251	3.731 3464
9	4.035 8595	3.725 4087	3.731 7527	3.734 4132
10	4.005 1500	3.726 6512	3.731 9480	3.732 4734
11	3.981 7152	3.727 5631	3.731 9056	3.731 7776
12	3.961 2741	3.728 2579	3.731 9132	3.731 9386
13	3.943 9265	3.728 8032	3.731 9443	3.732 0588
14	3.929 0201	3.729 2394	3.731 9695	3.732 0709
15	3.916 0731	3.729 5934	3.731 9862	3.732 0587
16	3.904 7229	3.729 8846	3.731 9975	3.732 0502

Table 4. (continued)

		SAW problem		
n	r_n	β_n	μ_n	δ_n
2	5.000 0000	4.266 6667	4.200 5168	4.800 5906
3	4.600 0000	4.127 1028	4.015 4517	3.937 5296
4	4.478 2609	4.123 8661	4.119 7047	4.195 7812
5	4.417 4757	4.133 3106	4.150 1008	4.181 9919
6	4.375 8242	4.138 7106	4.150 9831	4.152 1950
7	4.343 0437	4.139 7523	4.142 6371	4.128 4423
8	4.319 9954	4.142 0180	4.149 4195	4.163 1849
9	4.301 6731	4.143 4176	4.148 6866	4.146 9573
10	4.286 9207	4.144 4551	4.148 8779	4.149 3925
11	4.274 9161	4.145 3732	4.149 7454	4.152 3664
12	4.264 8407	4.146 0730	4.149 7544	4.149 7845
13	4.256 3043	4.146 6571	4.150 0216	4.151 0060
14	4.248 9675	4.147 1404	4.150 1653	4.150 7425
15	4.242 5908	4.147 5429	4.150 2635	4.150 6908
16	4.236 9982	4.147 8835	4.150 3556	4.150 7863
17	4.232 0517	4.148 1732	4.150 4203	4.150 7448
18	4.227 6451	4.148 4217	4.150 4742	4.150 7623

		Trails problem		
n	r_n	β_n	μ_n	δ_n
2	5.000 0000	4.266 6667	4.200 5168	4.800 5906
3	5.000 0000	4.485 9813	4.661 4330	4.855 5030
4	4.920 0000	4.530 6475	4.588 0754	4.534 5442
5	4.837 3984	4.526 2207	4.518 3509	4.445 1972
6	4.794 9580	4.535 1327	4.555 3872	4.606 2612
7	4.760 9534	4.538 1002	4.546 3181	4.530 8937
8	4.732 7542	4.537 7718	4.536 6989	4.517 1757
9	4.710 9123	4.537 6012	4.536 9589	4.537 5724
10	4.693 5950	4.537 6145	4.537 6712	4.539 5874
11	4.678 8491	4.537 0658	4.534 4532	4.524 7311
12	4.666 2278	4.536 2822	4.532 1594	4.524 4692
13	4.655 5731	4.535 6403	4.531 9433	4.531 1470
14	4.646 3789	4.535 0278	4.531 1936	4.528 1825
15	4.638 2779	4.534 3654	4.529 8883	4.524 2121
16	4.631 1529	4.533 7481	4.529 2681	4.526 3648

the sequencies $\{\beta_n\}$ and $\{\mu_n\}$ are indicative of the presence of a strong confluent term. A variety of methods were used to detect this term, but we found that none of the conventional methods were successful. This parallels our experience (Guttmann 1984) with the triangular lattice chain generating function. An alternative approach we adopted was to fit all the coefficients, suitably weighted, to an assumed functional form

$$T(x) = \sum_{n\geq 0} a_n x^n = A_1(1-\lambda x)^{-\gamma} + A_2(1-\lambda x)^{-\gamma+\Delta} + A_3(1-\lambda x)^{-\gamma+1}$$

with γ fixed at 43/32. The fitting was done by the nonlinear regression program P3R, available on the BMDP package. The coefficients were weighted by λ^n, (with $\lambda \approx 4.53$) so that higher-order coefficients were given much greater weight than earlier coefficients. This is in principle a powerful alternative method of series analysis, but much more work needs to be done before it can be widely used. At present it is extremely sensitive to starting estimates and is also sensitive to weighting functions. A large number of trials had to be carried out before we could be confident that we had found a global minimum rather than a local minimum. We are pursuing this approach in the hope that a new and powerful series analysis method will evolve, but for the present we simply state the results for this case, which are:

$$\lambda = 4.5256, \qquad \Delta = 0.51,$$
$$A_1 = 1.023, \qquad A_2 = -0.513, \qquad A_3 = 1.054.$$

No error estimates are quoted, though we expect λ to be accurate to about four significant figures, Δ to one figure, A_1 to two figures, and A_2, A_3 to one figure. The results as quoted fit the data extremely well, and it is for this reason we give more significant figures than the accuracy of the parameters warrants. The noteworthy feature is the presence of a strong confluent term, and when this is included the data is entirely consistent with our assumption that the trails problem belongs to the same universality class as the SAW problem.

For the square lattice, the characteristic odd–even oscillation added an extra complication to the above analysis. In the present primitive state of the new analysis method, we did not therefore pursue the square lattice analysis by that method. Apart from the Padé analysis mentioned previously, we also used the generalised ratio method of Sykes *et al* (1972), as applied by them to the SAW series. We again assumed that the exponent $\gamma = 43/32$, and that the antiferromagnetic exponent was similar to that for walks (though the results were insensitive to this assumption). Our analysis gives $\lambda = 2.7213 \pm 0.0007$, in excellent agreement with the Padé analysis. We believe this result rules out the possibility that $\lambda = e = 2.718\,28\ldots$ as suggested by Malakis (1975) and Zhou and Li (1984).

We have also obtained estimates for the critical amplitudes by forming Padé approximants to $(1/\lambda - x)[T(x)]^{1/\gamma}|_{x=1/\lambda}$. Using the estimates for λ quoted earlier, and $\gamma = 43/32$, the approximants were well converged, and we estimate $A_1 = 1.10$ (square) and $A_1 = 0.99$ (triangular), where $T(x) \sim A_1(1-\lambda x)^{-\gamma}$. The estimate of A_1 agrees to within 3% with that found by our nonlinear regression, which latter method also takes into account the confluent correction term.

3. Three-dimensional lattice

In table 1 we give the first 15 coefficients of the simple cubic lattice trail generating function—again representing about 50 hours CPU time on a PE 3220 mini-computer.

Padé analysis gave results consistent with the pattern observed for the two-dimensional series. Dlog Padé approximants were more scattered than their SAW counterparts, and many were defective. They appeared to converge to $\gamma \simeq 1.12$, $\lambda \simeq 4.8497$. This value of γ is significantly *lower* than the SAW exponent, believed to be around $\gamma \simeq 1.1615$ (Le Guillou and Zinn Justin 1980) from RG analysis. Again, we consider that this small discrepancy is due to closer non-physical singularities and confluent correction terms.

Padé approximants to $[T(x)]^{1/\gamma}$ with $\gamma = 1.1615$ give $\lambda = 4.8426 \pm 0.008$, while the confluent singularity analysis method of Adler *et al* (1982), while giving no convincing evidence of a confluent singularity, did indicate a critical point of $1/\lambda \simeq 0.2065 = 1/4.8426$ with an exponent of $\gamma \simeq 1.16$.

The extended ratio analysis (Sykes *et al* 1972) of the previous section was also used, and gave $\lambda = 4.843 \pm 0.002$, in agreement with the above analyses.

This was in fact the worst behaved trail generating function series of the three, and the only conclusions we can draw are that (a) there is no evidence for a different universality class for the trails problem in three dimensions compared to the walks problem and (b) if we accept that $\gamma = 1.1615$, the connective constant is then $\lambda = 4.8426 \pm 0.002$.

For the amplitude, Padé analysis as described in the previous section gave $A_1 \simeq 0.95$.

4. Bounds on connective constants

The various methods for determining upper and lower bounds on the value of the connective constant for self-avoiding walks are discussed in Guttmann (1983). These methods can all be applied *mutatis mutandis* to the trails problem.

To find upper bounds, we use the method of Ahlberg and Janson (1982), which, after making the necessary changes appropriate to the trails problem, gives

$$\lambda \leq \min(\lambda_a, \lambda_b) \tag{4.1}$$

where λ is the connective constant for trails,

$$\lambda_a = (t_n/t_1)^{1/(n-1)} \tag{4.2}$$

and λ_b is the positive root of

$$qx^{n-1} = [t_n - (q-2)t_{n-1}]x + (q-2)[(q-1)t_{n-1} - t_n] \tag{4.3}$$

where q is the coordination number of the lattice. From our configurational data in table 1 we readily obtain

$$\lambda < 4.929 \text{ (sc)}, \qquad \lambda < 4.745 \text{ (triangular)}, \qquad \lambda < 2.851 \text{ (square)}. \tag{4.4}$$

To find lower bounds for the hypercubic lattice, we apply the method of Kesten (1963). Consider a d-dimensional hypercubic lattice, with unit lattice spacing. A *terminally attached trail* (TAT) is a trail whose first step, rooted at the origin, is in the $+x$ direction, and which subsequently never crosses the $x = 1$ hyperplane. We denote the cardinality of n-step TAT's by r_n. Next we define *bridging trails*, with cardinality b_n, as those TAT's whose maximal x-coordinate is equal to the x-coordinate of the end-point vertex of the TAT. Finally, we define *irreducible bridging trails*, with cardinality s_n, as those trails which cannot be decomposed into two concatenated bridging trails. Clearly $t_n \geq r_n \geq b_n \geq s_n$.

Next, we outline a proof that $\lim_{n\to\infty} r_n^{1/n} = \lim_{n\to\infty} b_n^{1/n} = \lambda$. To prove this, we first define *loop trails* as trails whose first and last vertex are coincident. Let the cardinality of n-step loop trails be l_n. Following Hammersley (1961) we can transform these into bridging trails by first defining a right-most, top-most vertex and a left-most, bottom-most vertex and then cutting the loop trail at the first mentioned vertex and reflecting the 'top half' of the trail about the hyperplane through the other specified vertex (see figure 1(a)). Again following Hammersley (1961), it is possible to show that $\lim_{n\to\infty} l_n^{1/n} = \lambda$, while in I we proved that $\lim_{n\to\infty} t_n^{1/n} = \lambda$. The construction above shows that each loop trail can be transformed into a distinct bridging trail, so that

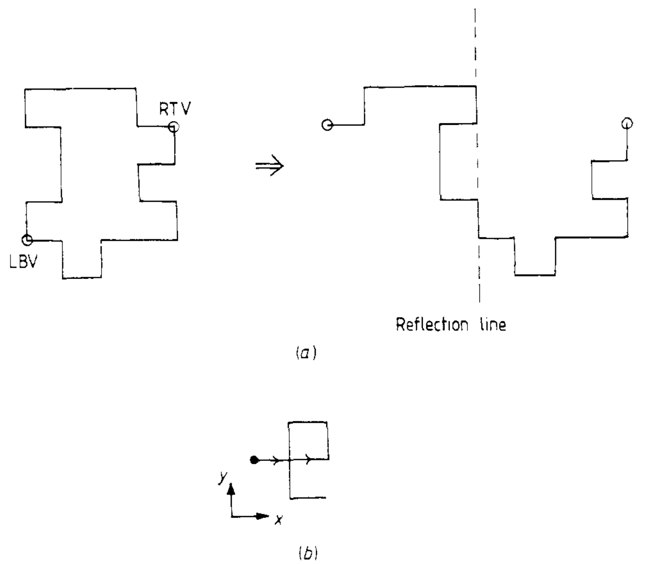

Figure 1. (*a*) shows the transformation of a polygon into a bridge. LBV = left, bottom vertex; RTV = right, top vertex. (*b*) shows a 7-step irreducible bridging trail that is *not an* irreducible bridging walk. Extending this trail in the $-y$ direction produces a similar realisation for any greater number of steps.

$t_n \geqslant r_n \geqslant b_n \geqslant l_n$. This observation is sufficient to complete the proof that $\lim_{n\to\infty} r_n^{1/n} = \lim_{n\to\infty} b_n^{1/n} = \lambda$.

The next step is to point out the lemma

$$b_n = \sum_{k=1}^{n} s_k b_{n-k} \qquad n \geqslant 1. \tag{4.5}$$

The proof is given by Kesten (1962) for SAW's, and follows from the observation that each bridging trail can be expressed as the concatenation of an irreducible bridging trail of length $m \in [1, n]$ and a bridging trail of length $p = (n-m) \in [0, n-1]$ since the first step of *every* bridging trail is an irreducible bridging trail.

If we now define the corresponding generating functions $B(x) = \Sigma_{n\geqslant 0} b_n x^n$ and $S(x) = \Sigma_{n\geqslant 1} s_n x^n$, it follows from the above lemma that $B(x) = 1/[1 - S(x)]$, and hence that λ^{-1} is the unique positive root of $S(x) = 1$. The proof of these last two remarks follows precisely Kesten's proof for the SAW analogue. Further, if λ_N is the (unique) positive root of the polynomial

$$\sum_{n=1}^{N} s_n \lambda_N^{-n} = 1 \tag{4.6}$$

then

$$\lambda_N \leqslant \lambda. \tag{4.7}$$

Thus the enumeration of irreducible bridges allows a monotonic, non-decreasing sequence of lower bounds on λ to be obtained, by solving the sequence of polynomials given by (4.6) with increasing N.

In table 2 we give the results for the first 22 terms of $B(x)$ and $S(x)$ for the square lattice. From these coefficients and the result (4.7) we finally obtain the bound $\lambda(\text{square}) > 2.6346$.

Following a suggestion of Whittington (private communication) we can also use a similar approach to prove that $\lambda > \mu$ for d-dimensional hypercubic lattices, where μ is the connective constant for self-avoiding walks, as follows. Let s_n be the cardinality of n-step irreducible bridging trails, as defined above, and let w_n be the corresponding quantity for self-avoiding walks. Then from Kesten's result for SAW's, and our analogous results for trails quoted above, we have that $W(x) = \sum_{n=1}^{\infty} w_n x^n$ is analytic in the disc $|x| < \mu^{-1}$ and continuous and strictly increasing in the interval $0 \leqslant x \leqslant \mu^{-1}$ and $W(\mu^{-1}) = 1$. An analogous result holds for the trails problem, where $S(x) = \sum_{n=1}^{\infty} s_n x^n$ is the analogue of $W(x)$ and $S(\lambda^{-1}) = 1$. By explicit construction (figure 1(*b*)) we show that $w_n < s_n$ for $n > 6$, while it is obvious by direct enumeration that $w_n = s_n$ for $n \leqslant 6$ (see table 2). Thus $W(x) < S(x)$ for all x such that $0 < x \leqslant \min(\mu^{-1}, \lambda^{-1})$. It thus immediately follows that $\lambda^{-1} < \mu^{-1}$, or $\lambda > \mu$.

For the simple cubic lattice we have not generated bridging trails, but a useful numerical 'bound' is the SAW connective constant, $\mu(\text{sc}) \simeq 4.6835$. This is of course only an estimate of μ, so doesn't constitute a bound in the proper sense, unlike the square lattice result. A very weak bound is provided by the SAW lower bound (Guttmann 1983), $\mu > 4.352$.

For the triangular lattice we have already proved in I that $\lambda > 4.222$. Summarising the results of this section, we find

$$\begin{aligned} 2.634 &< \lambda\ (\text{square}) &&< 2.851 \\ 4.222 &< \lambda\ (\text{triangular}) &&< 4.745 \\ (4.683) &< \lambda\ (\text{sc}) &&< 4.929 \end{aligned} \tag{4.8}$$

where the sc 'lower bound' is parenthesised to indicate its second-class status!

5. Substitution functions

As discussed in I, by relating trails on the triangular lattice to those on the honeycomb lattice we can obtain an analogue of the star-triangle transformation for trails. For the Ising problem, Fisher (1959) has given a transformation that relates the susceptibilities χ_{T} and χ_{H} of the triangular and honeycomb lattice respectively. That is

$$\chi_{\mathrm{T}}(v) = \tfrac{1}{2}\{\chi_{\mathrm{H}}(w) + \chi_{\mathrm{H}}(-w)\} \tag{5.1}$$

where

$$w^2 = h(v) = v(1+v)/(1+v^3) = v + v^2 - v^4 - v^5 + v^7 + v^8 - v^{10} - \dots \tag{5.2}$$

For the self-avoiding walk problem we denote by C_{T} and C_{H} the chain generating functions of the triangular and honeycomb lattice SAW model respectively. Then by analogy we write

$$C_{\mathrm{T}}(x) = \tfrac{1}{2}\{C_{\mathrm{H}}(y) + C_{\mathrm{H}}(-y)\} \tag{5.3}$$

which implicitly defines the function f through

$$y^2 = f(x). \tag{5.4}$$

Following the development of Guttmann and Sykes (1973) we can obtain the first 17 terms of the series expansion of f from the available expansions of C_T and C_H. In that way we find

$$f(x)=x+x^2-2x^4-x^5+3x^6+4x^7+12x^8+57x^9+127x^{10}+253x^{11}+907x^{12}$$
$$+4224x^{13}+14162x^{14}+43817x^{15}+150650x^{16}+538790x^{17}+\ldots \quad (5.5)$$

which corrects the last two coefficients of Guttmann and Sykes (1973).

For the trails problem we denote by T_T and T_H the trail generating functions for the triangular and honeycomb lattices respectively. Then we write

$$T_T(z)=\tfrac{1}{2}\{T_H(u)+T_H(-u)\} \quad (5.6)$$

which defines the function g through

$$u^2=g(z). \quad (57)$$

From the coefficients in table 1 and equations (5.6) and (5.7) we obtain the first 16 terms in the expansion of g as

$$g(z)=z+z^2+z^3+3z^4+3z^5+13z^6+47z^7+73z^8+273z^9+925z^{10}+2089z^{11}$$
$$+4935z^{12}+10403z^{13}+22319z^{14}-25515z^{15}-491241z^{16}\ldots. \quad (5.8)$$

For the Ising model, the critical temperatures are related through

$$\nu_H^{-2}=h(\nu_T^{-1}) \quad (5.9)$$

where $\nu_H=1/\tanh(J/kT_c^H)=\sqrt{3}$ and $\nu_T=1/\tanh(J/kT_c^T)=2+\sqrt{3}$. *Further, it follows from* (5.1) *that the susceptibilities on the two lattices have the same critical exponent unless the substitution function h is non-analytic at* $v=\nu_T^{-1}$. If h is non-analytic, further investigation is required to determine the change—if any—to the critical exponent. From (5.2) it is clear that h is non-analytic only at the cube roots of -1, thus confirming the well known universality of exponents for the two-dimensional Ising model.

For the SAW and trails problem we have the corresponding results

$$\mu_H^{-2}=f(\mu_T^{-1})=(2+\sqrt{2})^{-1} \quad (5.10)$$

and

$$\lambda_H^{-2}=g(\lambda_T^{-1})=(2+\sqrt{2})^{-1} \quad (5.11)$$

where μ and λ are the connective constants for the SAW and trails problem respectively, and we have used Nienhuis' (1982) result for μ_H and our earlier result (I) that $\lambda_H=\mu_H$.

Unlike the situation with the Ising problem f and g are not known except through their series expansions. If we accept the (unproven) assumption that a critical exponent exists for the previously defined generating functions, it again follows that this exponent must be the same for the triangular and honeycomb lattices provided that the substitution function is non-singular at $x=x_c=1/\mu_T$ for the SAW problem and at $z=z_c=1/\lambda_T$ for the trails problem.

Accordingly, we have investigated the singularity structure of the functions f and g by studying Padé approximants to the logarithmic derivative of f and g. It is well known (see e.g. Gaunt and Guttmann 1974) that the distribution of zeros of the denominator polynomials gives a good estimate of the singularity distribution.

Firstly, for the SAW substitution function f, a range of diagonal and off-diagonal Dlog Padé approximants clearly indicates a singularity at $x\simeq0.275$, and strongly suggests a conjugate pair of singularities very close to the imaginary x-axis at $x \approx \pm 0.45\mathrm{i}$. No other singularities are clearly discernible. As $x_c = \mu_T^{-1} \approx 0.2409$, the singularity at $x \simeq 0.275$ is well beyond the critical value of x, and so we conclude that exponent universality holds for the SAW generating function on the triangular and honeycomb lattices. This result is of course already widely accepted.

For the trail substitution function, a similar analysis gives a seemingly better converged sequence of estimates of singularity position. The singularities that are clearly indicated are at $z \approx 0.30$, $z \approx \pm 0.30\mathrm{i}$ and $z = -0.25 \pm 0.3\mathrm{i}$. In this case $z_c \approx 0.2210$, and again the substitution function $g(z)$ appears to be free of singularities in the physical disc $|z| \leq z_c$. This then implies the same exponent universality as for walks. As we have previously shown that the honeycomb lattice trail and SAW problem have the same exponent, this result implies that universality extends to the trails problem also.

Another useful aspect of the substitution functions is that they give unbiased estimates of the triangular lattice connective constants from (5.10) and (5.11). We have done this in two ways. Firstly, by truncating the substitution function at successively higher terms, and solving the resulting polynomials obtained from (5.10) and (5.11) we get a sequence of estimates of x_c and z_c. Secondly, by forming Padé approximants to $f(x) - \mu_H^{-2}$, the zeros of the *numerator* should give estimators of $x_c = 1/\mu_T$, and analogous results for the trails problem. The results of these calculations are shown in table 5. For the SAW problem, the first method gives a monotonic sequence

Table 5. Analysis of 'pseudo star-triangle substitution function' series as defined in text, in order to estimate connective constant for SAW and trails problems. (a) Polynomial truncation method, (b) Padé approximant method.

	Method (a)	
n	SAW	trails
7	0.241 43	0.221 43
8	0.241 33	0.221 21
9	0.241 22	0.221 02
10	0.241 16	0.220 88
11	0.241 13	0.220 81
12	0.241 10	0.220 78
13	0.241 07	0.220 76
14	0.241 05	0.220 76
15	0.241 04	0.220 76
16	0.241 02	0.220 77
17	0.241 01	

	Method (b)					
	$[N/N-1]$		$[N/N]$		$[N/N+1]$	
N	SAW	trails	SAW	trails	SAW	trails
4	0.241 48	0.222 43†	0.241 50	0.220 50	0.242 10†	0.220 76
5	0.241 40	0.220 74	0.241 17	0.220 71	0.241 04	0.220 67
6	0.240 95	0.220 58	0.241 04	0.220 70	0.241 04†	0.220 72
7	0.241 00	0.220 72	0.240 96	0.220 76	0.240 98	0.220 68
8	0.240 97	0.220 67	0.240 97	$\begin{cases}0.221\,56\\0.225\,40\end{cases}$	0.240 95	
9	0.240 99					

† Defective approximant. Pole-zero pair closer to the origin.

of estimates of μ_T^{-1}. *If* the coefficients of f continue to be non-negative (and we cannot prove this), then this sequence provides strict upper bounds to μ_T^{-1}, yielding $\mu_T > 4.1492$, which compares well with the best current estimate $\mu_T \approx 4.150\,75$. The Padé approximants are also decreasing, though less regularly, and suggest $\mu_T^{-1} < 0.240\,97$ or $\mu_T > 4.1499$.

For the trails problem, the sign change in the coefficients at the 15th term (which we at first thought signified an error in our series, but we now believe to be correct) means that the estimates cannot be monotonic, and we estimate from both methods $\lambda_T^{-1} = 0.2209 \pm 0.0005$, or $\lambda_T = 4.527 \pm 0.010$. While less precise than the estimates of § 2, this is an unbiased estimate, in that no critical exponent is assumed.

6. Summary and discussion

We find that the triangular lattice trail generating function is well fitted by

$$T(x) \simeq A_1(1-\lambda x)^{-\gamma} + A_2(1-\lambda x)^{-\gamma+\Delta} + A_3(1-\lambda x)^{-\gamma+1} + \mathrm{O}(1-\lambda x)^{1-\gamma},$$

where the critical parameters are shown in table 6 below. For the square and simple cubic lattices our analysis has provided estimates only of the leading critical parameters for reasons previously discussed, and these are also shown in table 6. For the square lattice our analysis shows that the exponent ν is the same as that for SAW's, and hence we conclude that the two problems belong to the same universality class.

Table 6. Summary of estimates of critical parameters for trail generating function and mean square end-to-end distance exponent ν, defined by $T(x) = A_1(1-\lambda x)^{-\gamma} + A_2(1-\lambda x)^{-\gamma+\Delta} + A_3(1-\lambda x)^{-\gamma+1}$ and $\langle R_n^2 \rangle \sim an^{2\nu}$.

	γ	Δ	ν	λ (Lower bound)	λ (Estimate)	λ (Upper bound)	A_1	A_2	A_3
Square	$1\frac{11}{32}$	—	$\frac{3}{4}$	2.634	2.7215 ± 0.002	2.851	1.10	—	—
Triangular	$1\frac{11}{32}$	0.51	—	4.222	4.524 ± 0.004	4.745	1.02	−0.51	1.1
Simple cubic	1.1615	—	—	(14.683)	4.843 ± 0.003	4.929	0.95	—	—

We define a pseudo star-triangle transformation function for the trail generating function, and use its analyticity properties to show that the generating function for trails is the same as that for SAW's.

Thus we find all the series data, when carefully interpreted, are not inconsistent with the conclusion that the trails problem and SAW problem are in the same universality class.

As well as our series estimates of the connective constant λ, we have obtained upper and lower bounds to λ. This derivation produced as a by-product, a proof that the connective constant for $d \geq 2$-dimensional hypercubic lattices for trails is strictly greater than the corresponding quantity for walks. This was already expected from the expansions obtained for the connective constant in I.

We remark in closing that the trail generating function series are less well behaved than their SAW counterparts. Accordingly, for comparable accuracy, much longer series than we have obtained would be necessary. This does not seem possible without a dramatically improved counting method. Alternatively, Monte Carlo methods should be readily applicable to trails and we are pursuing this approach.

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