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Self-avoiding walks, neighbour-avoiding walks and trails on semiregular lattices

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Abstract. We study self-avoiding and neighbour-avoiding walks and lattice trails on two semiregular lattices, the (3.12^2) lattice and the (4.8^2) lattice. For the (3.12^2) lattice we find the exact connective constant for both self-avoiding walks, neighbour-avoiding walks and trails. For the (4.8^2) lattice we generate long series which permit the accurate estimation of the connective constant for self-avoiding walks and trails.

1. Introduction

There are only three regular tilings of the plane, the triangular, square and hexagonal tilings respectively. There are a further eight semiregular or Archimedean tilings (sometimes called homogeneous tilings) [9]. The defining feature of these tilings is that all vertices are of a single type. Note too that all edges are of equal length.

A self-avoiding walk (SAW) is an open connected path on edges of a lattice with the restriction that vertices on the path may not be revisited. They are normally considered distinct if they are distinct up to a translation.

A self-avoiding polygon (SAP) of n-steps is a SAW of $(n-1)$-steps whose starting point is adjacent to its ending vertex—and which can therefore be made into an n-step closed path by the addition of a single edge.

A neighbour-avoiding walk is a SAW with the additional restriction that adjacent vertices not connected by an edge cannot be occupied by the walk. The corresponding definition of neighbour-avoiding polygons (NAP) may also be given.

A lattice trail is defined like a SAW, except the restriction is not to vertices, but to edges. That is, trails are connected paths on the lattice subject to the restriction that edges may not be multiply occupied. Thus any SAW and any SAP is a trail on the same lattice. Trails too are usually defined up to a translation. Note that a trail can have either two or zero vertices of odd degree. Those with zero odd-degree vertices are sometimes called *trailgons*, in analogy with polygons.

Finally, it will turn out to be useful to define a new class of lattice path, which we call an *osculating polygon*. These are similar to trailgons, except the condition is imposed that edges may not cross at a vertex, but only touch. This is illustrated in figure 1(a) and (b) below. Thus the path shown in figure 1(c) corresponds to a single trail (or trailgon), but to two distinct osculating polygons, as shown in figure 1(d).

While SAW, NAW and lattice trails (T) on the regular lattices have been extensively studied, the other homogeneous lattices—with the exception of the kagomé lattice—have received less attention.

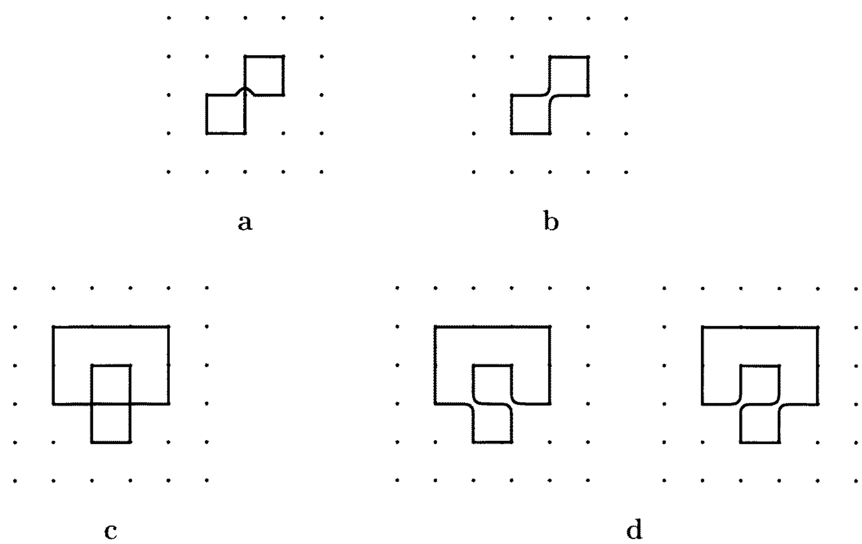

Figure 1. Illustration of lattice paths with (*a*) a crossing and (*b*) a vertex where two edges touch. (*c*) A single trailgon and (*d*) the two corresponding OP.

Table 1. The connective constants for various planar lattices.

Lattice	μ_{SAW}	η_T	μ_{NAW}
triangular	4.150 795(4)	4.524(4)	—
square	2.638 158 53(15)	2.720 62(6)	2.319 5272(5)
kagomé	2.560 6(2)	—	$\sqrt{2+\sqrt{2}}$
hexagonal	$\sqrt{2+\sqrt{2}}$	$\sqrt{2+\sqrt{2}}$	—
Manhattan	1.733 535(3)	1.733 535(3)	1.565 7(15)
L-lattice	1.565 7(15)	1.565 7(15)	—

Before reviewing the known results, it will be useful to state some general results that apply, in part, to these lattices. Recall that the covering lattice $\mathcal{L}^c$ of a lattice $\mathcal{L}$ is obtained by an edge-to-vertex transformation as follows. Each edge of the lattice $\mathcal{L}$ becomes a vertex of the covering lattice $\mathcal{L}^c$, and vertices of $\mathcal{L}^c$ are joined by an edge if the corresponding edges of $\mathcal{L}$ meet at a vertex of $\mathcal{L}$. Thus, for example, the covering lattice of the hexagonal lattice is the kagomé lattice.

It is known [14] that any n-step trail on a lattice $\mathcal{L}$ produces an $(n-1)$-step SAW on the covering lattice $\mathcal{L}^c$. However, in general there are SAW on the covering lattice that are not produced by trails on the original lattice, as this mapping is *injective*.

It is also known [18] that any n-step SAW on a lattice $\mathcal{L}$ produces an $(n-1)$-step NAW on the covering lattice $\mathcal{L}^c$. This mapping is 1 : 1, or *bijective*.

Finally, we mention a result [10] that Hughes [12] has generously called Guttmann's theorem to the effect that any regular lattice of coordination number 3 has the SAW and trail critical points equal. This theorem is immediately extendable *mutatis mutandis* to the homogeneous lattices, using either method of proof given in [10, 12].

The known connective constants (the reciprocals of the critical point) for SAW on a number of lattices are given in table 1. Apart from the hexagonal lattice [15] result, all these results are numerical estimates. The results quoted for the kagomé [13] and Manhattan lattices were derived from recently extended series [3]. The result for square lattice trails is also a numerical estimate derived from extended series [5], while that for the triangular lattice is an old, rather imprecise estimate [11]. As far as we are aware, no estimate has been made of the trail connective constant for the kagomé lattice, or the NAW connective constant for the triangular or hexagonal lattices. The corresponding table entries are accordingly left blank. For the hexagonal, Manhattan and L-lattices it follows from the theorem given above that the connective constant for trails is equal to the corresponding SAW value. The result for the connective constant for NAW on the square lattice is a recent numerical estimate [4], while those for the kagomé and Manhattan lattice follow from Watson's mapping [18].

Thus it can be seen that for SAW, NAW and trails, the connective constant is known exactly for only one lattice. It is clearly of considerable interest to find other lattices for which the connective constant can be exactly obtained. Another reason to look at the lattices we have considered is to determine whether the exponent universality that exists for regular tilings extends to non-regular tilings. With this is mind, and prompted by a query [1], we have investigated SAW and NAW on two such semiregular lattices, the so called (3.12^2) and (4.8^2) lattices, which are illustrated in figures 2 and 3, respectively. They both have vertices of coordination number three.

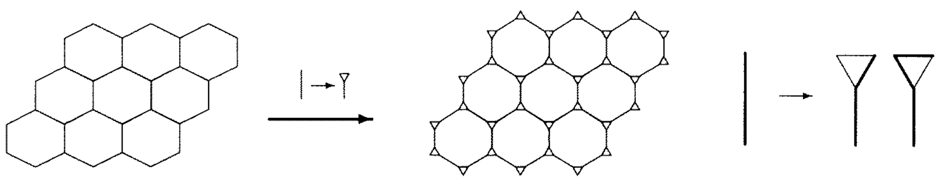

Figure 2. Transformation of the hexagonal lattice into the (3.12^2) lattice and how each step of a polygon on the hexagonal lattice maps to either two or three steps on the (3.12^2) lattice.

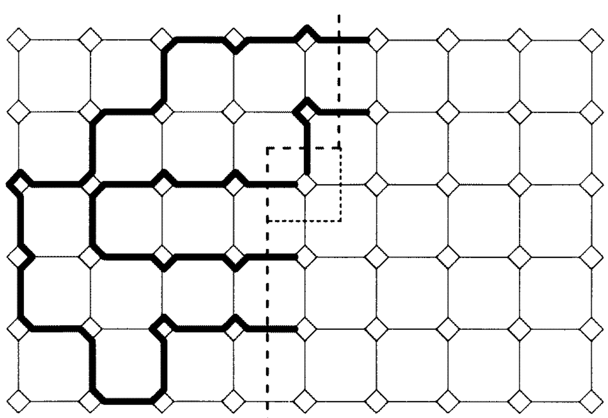

Figure 3. A snapshot of the intersection (broken line) during the transfer matrix calculation on the (4.8^2) lattice. Polygons are enumerated by successive moves of the kink in the intersection, as exemplified by the position given by the dotted line, so that one vertex at a time is added to the rectangle. To the left of the intersection we have drawn an example of a partially completed polygon.

2. The (3.12^2) lattice

We will first conside SAP on the (3.12^2) lattice. The smallest polygon is a triangle, and there is one triangle for every three vertices. Hence the lattice constant of the triangle is $\frac{1}{3}$. The next smallest polygon is the dodecagon, and each dodecagon shares an edge with six others. This connectivity is similar to that of hexagons on the hexagonal lattice. Indeed polygons on the two lattices map to one another if we observe that each step on the hexagonal lattice corresponds to either two or three steps on the (3.12^2) lattice. This is illustrated in figure 2 where we show how a step on the hexagonal lattice can be replaced by one step on a long edge of the dodecagon and either one step along an edge of a triangle or by a detour around the other two edges of the triangle.

Thus, apart from the initial term $\frac{1}{3}x^3$ corresponding to the triangle, the polygon generating function is obtained from that for the hexagonal lattice (given to 82 steps in [8]) by the mapping $x \to x^2 + x^3$. Hence the first few terms of the polygon generating function for the (3.12^2) lattice are

$$\frac{1}{3}x^3 + \frac{1}{2}(x^{12} + 6x^{13} + 15x^{14} + 20x^{15} + 15x^{16} + 6x^{17} + x^{18} + \cdots).$$

As the critical point for hexagonal lattice SAP is known [15], and is $x_c^2 = \frac{1}{2+\sqrt{2}}$, it follows that the critical point for (3.12^2) lattice SAP is given by the solution of a twelfth-degree polynomial, namely

$$1 - 4x^4 - 8x^5 - 4x^6 + 2x^8 + 8x^9 + 12x^{10} + 8x^{11} + 2x^{12} = 0.$$

Numerically, this gives $x_c = 0.584\,439\,4298\ldots$.

For SAW a similar mapping applies. Let $C_{\text{hex}}(x) = 1 + 3x + 6x^2 + \cdots$ be the generating function for hexagonal lattice SAW. Then the corresponding generating function for the (3.12^2) lattice is

$$C_{(3.12^2)}(t) = 1 + (C_{\text{hex}}(t^2 + t^3) - 1 - 3t^2)/t^2 = 1 + 3t + 6t^2 + 12t^3 + 18t^4 + \cdots.$$

For neighbour-avoiding SAW the mapping is even simpler. Nearest-neighbour contacts can only occur if the walker goes around two sides of a triangle. Forbidding this is equivalent to the mapping from the hexagonal lattice, $x \to x^2$. Hence the critical point for NAW on the (3.12^2) lattice is just $\frac{1}{\sqrt{\mu_{\text{hex}}}} = (2 + \sqrt{2})^{\frac{-1}{4}}$. From the theorem given above, it also follows that the connective constant for trails is equal to that for SAW.

A further consequence of these mappings is that the critical exponent for the SAW and SAP generating functions for both self- and neighbour-avoiding walks is the same as that for their hexagonal lattice counterpart.

Related ideas in the framework of percolation theory are contained in [16] and developed further in [17]. These ideas lead [19] to the critical occupation probability for site percolation on the (3.12^2) lattice, $p_c = \sqrt{1 - 2\sin\frac{\pi}{18}}$. Recently, Batchelor [2] studied the $\mathrm{O}(n)$ loop model on the (3.12^2) lattice, and the critical point was obtained.

3. The (4.8^2) lattice

For this lattice we have found a local mapping that connects SAW on the (4.8^2) lattice to those of osculating polygons on the square lattice. Unfortunately, we have limited enumerative results for the osculating polygon problem, so the mapping does not help us in determining the critical point. Further discussion of the mapping is given in the next section.

Table 2. The various 'input' states and the 'output' states (with corresponding weights) which arise as the boundary line is moved in order to include one more vertex of the lattice.

Input	Outputs		
'00'	'00'	(x^2+x^4)'12'	
'01'	(x^2+x^4)'01'	$2x^3$'10'	
'10'	$2x^3$'01'	(x^2+x^4)'10'	
'02'	(x^2+x^4)'02'	$2x^3$'20'	
'20'	$2x^3$'02'	(x^2+x^4)'20'	
'11'	$(x+x^3)$'$\overline{00}$'	x^4'11'	x^4'$\overline{12}$'
'22'	$(x+x^3)$'$\overline{00}$'	x^4'22'	x^4'$\overline{12}$'
'21'	$(x+x^3)$'00'	x^4'21'	x^4'12'
'12'	$x+x^3$'accumulate'	x^4'12'	

Accordingly, we have generated the polygon series to 150 terms. The method used to enumerate SAP on the (4.8^2) lattice is a generalization of the method devised by Enting [6] in his pioneering work on the enumeration of square lattice polygons. In our case we use transfer matrix techniques to count the number of polygons which span a rectangle $W+1$ edges wide and $L+1$ edges long. The transfer matrix technique involves drawing a line through the rectangle intersecting a set of $W+2$ edges. For each configuration of occupied or empty edges along the intersection we maintain a (perimeter) generating function for loops to the left of the line cutting the intersection in that particular pattern. Polygons in a given rectangle are enumerated by moving the intersection so as to add one vertex at a time as shown in figure 3. The allowed configurations along the intersection are described in [6]. Each configuration can be represented by an ordered set of edge states $\{n_i\}$, where

$$n_i = \begin{cases} 0 & \text{empty edge} \\ 1 & \text{lower part of loop closed to the left} \\ 2 & \text{upper part of loop closed to the left.} \end{cases} \tag{1}$$

Configurations are read from the bottom to the top. So the configuration along the intersection of the polygon in figure 3 is {0112122}.

In table 2 we have listed the possible local 'input' states and the 'output' states which arise as the kink in the intersection in propagated by one step. Some of these update rules are illustrated further in figure 4. The top row represents the 'input' states '10' or '20' and the possible output states are '01' and '10' or '02' and '20', respectively. The bottom row represents the 'input' state '11' as part of the configuration {01122}. In this case there are three possible output states. First, we can just connect the two loop ends (second and third picture), but in doing so we see that the upper part of the second loop before the move becomes the lower part of the one remaining loop after the move, that is the configuration {01122} becomes {00012}. This relabelling of the configuration is denoted by overlining in table 2. Secondly, we can connect the two loop ends and insert new loop ends (fourth picture), in which case we relabel the old configuration and insert a '12' so the configuration {01122} becomes {01212}. Thirdly, the two loop ends can simply be continued (fifth picture). The weights corresponding to these configuration transformations are simply calculated by counting the number of steps which have been added to the polygon. Similar considerations yield all of table 2. Note that the 'input' state '12' is special because connecting the two ends results in a closed loop, so this is only allowed if there are no other loops cut by the intersection and the result is a valid polygon which is accumulated in the total count for that particular length. We refer the interested reader to [6, 8] for further

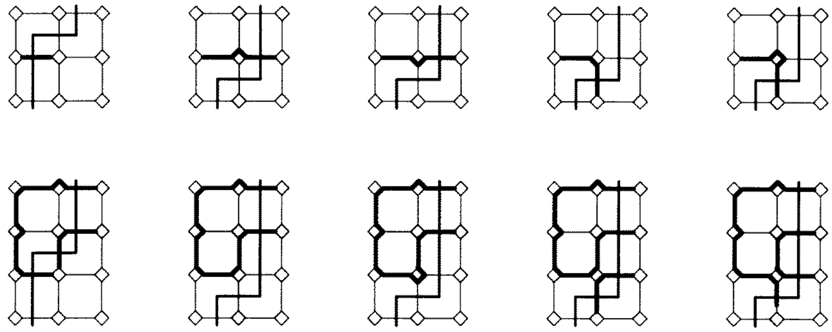

Figure 4. Some of the local configurations which occur as the kink in the intersection is moved one step. The leftmost pictures illustrate the 'input' state and the remaining pictures all the possible 'output' states.

details regarding the encoding and relabelling of configurations.

Due to the obvious symmetry of the lattice we need only consider rectangles with $L \geqslant W$. Any polygon spanning such a rectangle has a perimeter of length at least $8W + 6(L - W)$. By adding the contributions from all rectangles of width $W \leqslant W_{\max}$ and length $W \leqslant L \leqslant W + (8W_{\max} - 8W + 6)/6$, with contributions from rectangles with $L > W$ counted twice, the number of polygons per vertex of an infinite lattice is obtained correctly up to perimeter length $8W_{\max} + 6$.

The major difference between the method used to enumerate polygons in this work and the original method of Enting [6, 8] is that we require valid polygons to span the rectangle in *both* directions while the original method only required valid polygons to span the length-wise direction. The major drawback of this approach is that for most configurations we have to keep four distinct generating functions since the partially completed polygon to the left of the intersection could have reached neither, both, the lower, or the upper boundaries of the rectangle. The major advantage is that the memory requirement of the algorithm is exponentially smaller. Polygons spanning a rectangle with a width close to $W_{\max}$ have to be almost convex, so very convoluted polygons are not possible and thus configurations with many loop ends (non-zero entries) make no contribution at perimeter length $\leqslant 8W_{\max} + 6$. In fact in our calculation to 150 terms the maximum number of configurations appeared at $W = 15$ while $W_{\max} = 18$. Furthermore, for any W we know that contributions will start at $8W$ so for each configuration we need only retain $8(W_{\max} - W) + 6$ terms of the generating functions.

The series coefficients are listed in table 3. An analysis parallelling that of the square lattice polygon series [7] gives $x_c^2 = 0.305\,635\,99(2)$ and exponent $2 - \alpha = 1.500\,015(25)$ from which we conclude that, almost certainly, $\alpha = \frac{1}{2}$, as for other regular lattices. We also find an additional conjugate pair of singularities at $x_c^2 = -0.297\,38(1) \pm 0.300\,37(1)i$ with exponent 1.505(10), which is also almost certainly $\frac{3}{2}$ exactly.

From the theorem given above, it also follows that the connective constant for trails is equal to that for SAW.

4. A mapping between (4.8^2) polygons and square OP

There exists a somewhat contrived mapping between square lattice OP and SAP on the (4.8^2) lattice. Let us denote the perimeter of a square lattice OP by n, the number of right-

Table 3. The number, x_n, of embeddings of n-step polygons on the (4.8^2) lattice. Only non-zero terms are listed.

n	$2x_n$	n	$2x_n$
4	$\frac{1}{2}$	82	56 127 825 980 331 092
8	1	84	172 922 267 105 815 882
10	4	86	533 503 693 180 103 864
12	6	88	1 648 189 447 683 948 379
14	12	90	5 098 439 066 875 960 692
16	35	92	15 790 689 723 287 897 894
18	76	94	48 963 924 742 091 644 652
20	206	96	151 999 389 180 193 850 663
22	544	98	472 364 090 273 622 297 256
24	1349	100	1 469 477 588 844 668 049 380
26	3816	102	4 575 959 881 447 409 235 000
28	10 268	104	14 263 221 245 884 834 105 782
30	27 988	106	44 499 346 700 742 002 234 372
32	79 507	108	138 955 314 883 895 754 574 038
34	221 020	110	434 278 279 567 926 013 162 264
36	629 526	112	1 358 373 414 586 345 410 973 416
38	1 807 552	114	4 252 219 120 258 432 361 555 776
40	5 178 809	116	13 321 267 459 183 175 648 582 128
42	15 060 812	118	41 763 561 317 645 345 684 406 264
44	43 863 330	120	131 026 984 530 284 711 436 547 801
46	128 349 644	122	411 362 746 609 170 995 325 283 536
48	378 288 647	124	1 292 350 695 935 586 727 400 563 192
50	1 117 066 036	126	4 062 727 654 881 525 117 513 967 380
52	3 315 303 338	128	12 779 918 574 131 010 312 090 014 363
54	9 876 950 944	130	40 225 648 254 651 605 084 911 682 540
56	29 504 339 735	132	126 687 726 139 874 048 072 139 755 166
58	88 471 754 304	134	399 222 354 349 565 935 618 143 259 200
60	265 999 216 728	136	1 258 741 698 005 210 679 008 546 794 878
62	801 920 801 516	138	3 970 935 251 523 610 922 292 718 657 036
64	2 424 329 987 015	140	12 533 624 328 205 225 775 308 047 782 682
66	7 345 618 759 888	142	39 580 545 175 668 649 660 633 111 351 312
68	22 309 439 227 368	144	125 055 247 732 828 672 214 185 404 888 020
70	67 903 128 999 216	146	395 303 987 493 081 023 327 673 570 373 944
72	207 084 776 517 883	148	1 250 155 141 236 275 820 311 026 469 344 004
74	6 327 920 148 13052	150	3 955 438 296 377 927 612 702 201 033 518 280
76	1 937 110 494 938 538		
78	5 940 103 864 166 636		
80	18 245 304 336 182 817		

angle bends by b and the number of degree 4 vertices by c. Then there is a mapping between the square lattice OP generating function $O_{\text{sq}}(x, y, z)$ and the (4.8^2) lattice SAP generating function $P_{(4.8^2)}(x)$. In these generating functions, x, y, z are the variables conjugate to n, b, c respectively. The mapping in question consists of replacing each occurrence of x in $O_{\text{sq}}(x, y, z)$ by $(x^2 + x^4)^b x^{4c}(2x^3)^{n-b-2c}$. This results in a new generating function $\hat{O}(x, y, z)$ from which the perimeter generating function for SAP on the $(4.8)^2$ lattice can be obtained from

$$P_{(4.8)^2}(x) = \hat{O}(x, 1, 1).$$

By looking at the configurations in figure 4 the mapping becomes almost self-evident. If we ignore the small squares on the (4.8^2) lattice (let the length of the short edges vanish)

Table 4. The connective constants for the (3.12^2) and (4.8^2) lattices as obtained in this work.

Lattice	μ_{SAW}	η_T	μ_{NAW}
(3.12^2)	1.711 041...	1.711 041...	1.359 323...
(4.8^2)	1.808 830 01(6)	1.808 830 01(6)	—

we simply get a square lattice. Where a SAP on the (4.8^2) lattice has steps on both sides of a little square we get a degree 4 vertex in the OP on the square lattice. Otherwise, a step along one of the long edges on the (4.8^2) lattice is followed by another step in the same direction or a right-angle bend, which obviously corresponds to straight pieces and bends in the OP. The mapping simply says that each bend in the OP is either a long step followed by a short step or a long step followed by three short steps (detour round a little square) on the (4.8^2) lattice thus yielding the factor $(x^2 + x^4)^b$. A degree 4 vertex corresponds to a long step followed by a short step on either side of a little square thus yielding the factor x^{4c}. Since degree 4 vertices use two long steps we are left with $n - b - 2c$ straight pieces in the OP. Each of these are a long step followed by two short steps on the (4.8^2) lattice and since we can take a path along either side of any little square we get the factor $(2x^3)^{n-b-2c}$.

We have verified that this mapping gives results correct up to and including polygons of perimeter 34 on the (4.8^2) lattice. Up to order 30 we could have just as well use trailgons as OP, but at order 32 (and beyond) the different symmetries associated with the vertices of degree 4 manifest themselves.

5. Conclusion

We have obtained the exact critical point for SAW, trails and NAW on the (3.12^2) lattice, and have shown that the corresponding critical exponents for SAW, NAW and SAP are unchanged from their regular lattice counterparts.

Exact enumeration of SAP on the (4.8^2) lattice has resulted in an accurate estimate of the critical point and an estimate of the exponent in agreement with the regular lattice value. The same results hold for trails. The numerical values obtained are summarized in table 4.

A summary of corresponding connective constants for the regular lattices is given in table 1 in the introduction.

Acknowledgments

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