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LETTER TO THE EDITOR

The number of convex polygons on the square and honeycomb lattices

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Abstract. A subset of the set of self-avoiding polygons (SAP) embeddable on the square lattice which display the property of convexity is defined. An algorithm for their enumeration is developed, and from the available series coefficients the exact generating function is found. The singularity structure appears similar to that of the unsolved SAP problem, but with different critical exponents and critical points.

The enumeration of convex polygons allows the extension of the existing series for the square lattice SAP by one term. For the honeycomb lattice similar results have been obtained, despite a less natural definition of convexity.

We are currently engaged in a project to substantially extend the series expansions of the square and honeycomb lattice self-avoiding polygon (SAP) generating functions, as well as determining the caliper diameter of square lattice polygons (Privman and Rudnick 1985). Our method consists of a refinement of the data structuring of the transfer matrix algorithm originally developed by Enting (1980) and generalised for other lattices by Enting and Guttmann (1985). In the latter paper we obtained the number of SAP on the square lattice to 46-step polygons. In an attempt to go further, we have reached 54 steps by direct enumeration, with the 56-step polygon given incompletely. In considering the missing component in the 56-step polygon enumeration, we came to realise that it was precisely the number of convex polygons of 56 steps. Convex polygons are defined as self-avoiding polygons whose number of steps equals the perimeter of their minimal bounding rectangle. Any vertical (horizontal) line drawn through the polygon between any two vertices of the graph will cut precisely two horizontal (vertical) bonds.

This led us to consider the enumeration of convex polygons, which was a far simpler computational process than the original SAP enumeration problem. Further, we realised that the convex polygons are a superset of the 'staircase polygons' considered by Lin *et al* (1987), and are hence of considerable interest in their own right.

Next, we show how the convex polygons may be enumerated, and later we determine the precise recurrence relation for the coefficients by systematic searching. We have solved this recurrence relation and obtained the exact solution in closed form. An analysis of the generating function shows a complex singularity structure which appears to be identical to that expected in the full SAP problem.

Earlier it was noted that the basic enumeration technique for self-avoiding polygons described by Enting (1980) could be augmented by a simple correction term, so that one extra term was obtainable with little extra effort. The basis for the algebraic technique of polygon enumeration is that any square lattice polygon of perimeter p must be embeddable in a rectangular grid of perimeter $p' \leqslant p$.

Thus, by counting all polygons that occur in any of the rectangles of perimeter $p' \leqslant 54$, we have counted all polygons with $p \leqslant 54$. However, if the series are retained to sufficient order, counting all polygons in rectangles $p' \leqslant 54$ also counts the majority of polygons with $p = 56$. In fact, the only polygons with $p = 56$ that are not counted by the above method will be 56-step polygons that fit into a rectangle of perimeter 56 but into no smaller rectangle, i.e. convex polygons.

If the honeycomb lattice is treated as a square lattice with certain bonds missing, then the above remarks apply equally well to enumerations of honeycomb lattice polygons. It should be noted that the definition of convexity (cutting any horizontal or vertical line twice at most) refers to the square lattice representation that is used in the algebraic enumeration techniques. This definition of convexity has no natural interpretation on the honeycomb lattice and so the class of convex polygons is of little interest except as correction terms. For this reason we postpone the discussion of the polygon generating function for convex polygons on the honeycomb lattice to a subsequent paper in which we utilise the convex polygon enumerations to extend the SAP series.

The enumeration of convex polygons appears to be related to some of the 'directed' lattice problems that have recently been of interest, such as crystal growth models or disorder point solutions (Enting 1977), spiral self-avoiding walks (Guttmann and Wormald 1984, Guttmann and Hirschhorn 1984, Szekeres and Guttmann 1985), directed percolation (Kinzel 1983, Baxter *et al* 1988) and cellular automata (Wolfram 1986). A subset of the set of convex polygons has recently been enumerated (in closed form) by Lin *et al* (1987). Lin *et al* considered the more restrictive problem of anisotropic spiral self-avoiding loops. In such loops a west (east) step cannot be followed by a north (south) step. Further, if the first step is north (south), the closing step cannot be west (east). These constraints restrict the shape of the polygon to be a rising staircase followed by a descending staircase. All such polygons satisfy our definition of convexity but, as we shall show, represent a fraction $n^{-2.5}$ of the total number of convex polygons.

While the convex polygon problem on the square lattice may repay further investigation in the context of directed problems, and is clearly of interest in its own right, the important point for the purpose of obtaining correction terms to the general polygon expansion is that convex polygons can readily be enumerated using transfer matrix techniques. The number of vector components in the transfer matrix formulation is very much smaller than in the general polygon enumeration problem. Furthermore, specific expressions describing the column-to-column evolution of the vectors can be written down.

The enumerations for bounding rectangles with N vertical steps and M horizontal steps are carried out separately for each N. Each iteration of relations (2.3)–(2.6) increases M by 1. There are four vectors involved for each 'column state'; we denote their components by R^j_{mm}, S^j_{mn}, T^j_{mn} and U^j_{mn}. They denote the number of ways loops can be built up column by column such that, in the jth of the M columns of horizontal bonds, the two horizontal bonds are in positions m and n out of the possible range 0–N. The indices are thus restricted to

$$0 < m < n < N. \qquad (1)$$

The four vectors refer to particular classes of a partly completed ring. The components of the vectors are simple integers rather than truncated series. It is not necessary to keep track of the number of steps; the convexity requirement determines this uniquely given the configuration of bonds and the history of contact with the bounding rectangle.

R refers to loops starting from the left that have not yet reached either the top (row 0) or the bottom (row N); S refers to loops starting from the left that have reached the top but not the bottom; T refers to loops starting from the left that have not yet reached the top but have reached the bottom; U refers to loops starting from the left that have reached both the top and the bottom; the number of convex polygons of $2(M+N)$ steps in the $M\times N$ rectangle is thus

$$C_{MN}=\sum_{n=1}^{N}\sum_{m=0}^{n-1}U^{M}_{mn}. \tag{2}$$

The initial conditions (always subject to constraint (1)) are

$$\begin{aligned}
&U^1_{0N}=1 && \\
&U^1_{ij}=0 && \text{otherwise} && (3)\\
&T^1_{iN=1} && 0<i<N && \\
&T^1_{ij}=0 && \text{otherwise} && (4)\\
&S^1_{0j}=1 && 0<j<N && \\
&S^1_{ij}=0 && \text{otherwise} && (5)\\
&R^1_{ij}=1 && 0<i<N && \\
&R^1_{0j}=0 && \text{for all } j && \\
&R^1_{0N}=0 && \text{for all } i. && (6)
\end{aligned}$$

The basis of the evolutionary equations for convex polygons, is that, if the upper (lower) branch of a loop has not yet reached the top (bottom) of the rectangle, then it cannot move away from the top (bottom). If the upper (lower)branch of a loop has reached the top (bottom) it cannot move towards the top (bottom). By considering all possible ways in which such elements can combine, as shown in figure 1, we obtain the equations:

$$R^{k+1}_{ij}=\sum_{m=i}^{j-1}\sum_{n=m+1}^{j}R^{k}_{mn} \qquad 0<i<j<N \tag{7}$$

$$S^{k+1}_{0j}=\sum_{n=1}^{j}S^{k}_{0n}+\sum_{m=1}^{j-1}\sum_{n=m+1}^{j}R^{k}_{mn} \qquad 0<j<N \tag{8a}$$

$$S^{k+1}_{ij}=\sum_{m=0}^{i}\sum_{n=i+1}^{j}S^{k}_{mn} \qquad 0<i<j<N \tag{8b}$$

$$T^{k+1}_{iN}=\sum_{m=i}^{N-1}T^{k}_{mN}+\sum_{m=i}^{N-2}\sum_{n=m+1}^{N-1}R^{k}_{mn} \qquad 0<i<N \tag{9a}$$

$$T^{k+1}_{ij}=\sum_{m=i}^{j-1}\sum_{n=j}^{N}T^{k}_{mn} \qquad 0<i<j<N \tag{9b}$$

$$U^{k+1}_{iN}=\sum_{m=0}^{i}U^{k}_{mN}+\sum_{m=0}^{i}\sum_{n=i+1}^{N-1}S^{k}_{mn} \qquad 0<i<N \tag{10a}$$

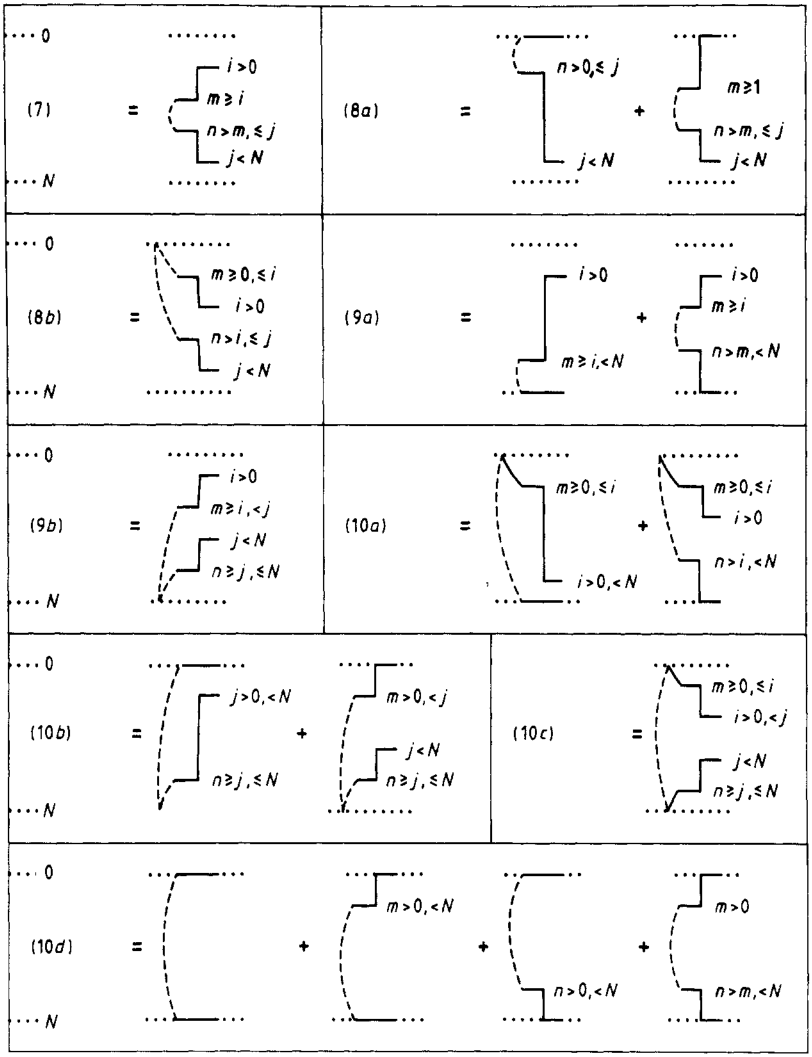

Figure 1. Graphical representation of the transfer matrix equations for generating convex polygons of width N. Each diagram represents one of the single or double summations in the specified equation (7)-(10), with the ordering of diagrams following the order of terms in the equation. The boundaries O and N are shown as dotted lines. The diagrams show the evolution from column k (left) to column $k+1$ (right). The broken curve shows (schematically) the connection to the left of column k and whether these connecting bonds pass through the O and/or N boundaries. The horizontal bonds are indexed i, j, m, n as in the equations and the limits on these indices (which define the limits on the summations) are shown. The index on the left of each inequality is the index of the bond opposite which the inequality is shown. Two-sided bounds ($a<j<b$) on a bond j are shown as $j<a$, $<b$.

$$U_{0j}^{k+1}=\sum_{n=j}^{N}U_{0n}^{k}+\sum_{m=1}^{j-1}\sum_{n=j}^{N}T_{mn}^{k}\qquad 0<j<N \tag{10b}$$

$$U_{ij}^{k+1}=\sum_{m=0}^{i}\sum_{n=j}^{N}U_{mn}^{k}\qquad 0<i<j<N \tag{10c}$$

$$U_{0N}^{k+1}=U_{0N}^{k}+\sum_{m=1}^{N-1}T_{mN}^{k}+\sum_{n=1}^{N-1}S_{0n}+\sum_{m=1}^{N-2}\sum_{n=m+1}^{N-1}R_{mn}^{k}. \tag{10d}$$

We can treat the honeycomb lattice as a square lattice with half the horizontal bonds missing. The columns of horizontal bonds alternate between having all even bonds missing and all odd bonds missing. We have to consider and sum over two classes of rectangle—those starting on an 'even' column and those starting on an 'odd' column. This corresponds to the algebraic polygon enumeration techniques which determine the number of polygons per pair of sites, so as to give series with integer coefficients. The two classes of rectangles must be considered separately. In each class, a restricted set of equations (2)-(10) apply. For class 1, the quantities R, S, T and U are zero unless both i and j are odd when k is odd and both even when k is even. For class 2 we require i, j to be both odd (even) when k is even (odd). These restrictions apply to all subscripts including the 0 and N that appear in special cases.

The above scheme for the square lattice was implemented as a FORTRAN program on a DEC Micro Vax II computer and, after development, transferred to the University of Melbourne Cyber 990. Utilising 64-bit integers, the program ran in a few seconds, producing polygons to 64 steps. Beyond this size, integer overflow occurred, and while we could have obtained longer series by using residue arithmetic, the series to 64 steps was more than adequate to enable the exact generating function to be obtained, and in any case gave us the required correction term. Because of the smaller numbers involved, the honeycomb case could, in principle, be extended further without causing integer overflow. However, initially 62-step polygons were enumerated on a PC compatible microcomputer as a test run and these proved more than adequate to determine the recurrence relation exactly. The coefficients obtained are shown in table 1.

We have analysed the series by searching for recurrence relations among the coefficients, as originally outlined by Guttmann and Joyce (1972) and Joyce and Guttmann (1973). This is equivalent to the method of differential or integral approximants subsequently discussed by Fisher and Au-Yang (1979) and Hunter and Baker (1979).

We define the generating function as

$$P(x)=x^{-2}\sum_{n=2}^{\infty}P_{2n}x^{n} \tag{11}$$

where the term $1/x^2$ takes into account the fact that the first non-zero coefficient is p_4. By a systematic search, we find that the coefficients p_{2n} satisy the recurrence relation

$$\begin{aligned}&[(n+1)^2-9.5(n+1)+15]p_{2n+6}-(8n^2-58n+57)p_{2n+4}\\&\qquad+[16(n-1)^2-80(n-1)+36]p_{2n+2}\\&\quad=7\delta_{n,2}+22\delta_{n,1}-44\delta_{n,0}+15\delta_{n,-1}.\end{aligned} \tag{12}$$

The class of recurrence relations within which the search was made is inspired by the exact results for the two-dimensional Ising model magnetisation and specific heat. We

Table 1. The number of convex polygons of N steps embeddable on the square and honeycomb lattices.

N	Square	Honeycomb
4	1	0
6	2	1
8	7	0
10	28	3
12	120	2
14	528	10
16	2 344	14
18	10 416	40
20	46 160	74
22	203 680	176
24	894 312	358
26	3 907 056	798
28	16 986 352	1 670
30	73 512 288	3 626
32	316 786 960	7 638
34	1 359 763 168	16 366
36	5 815 457 184	34 462
38	24 788 842 304	73 230
40	105 340 982 248	153 830
42	446 389 242 480	324 896
44	1 886 695 382 192	680 514
46	7 955 156 287 456	1 430 336
48	33 468 262 290 096	2 987 310
50	140 516 110 684 832	6 253 712
52	588 832 418 973 280	13 025 954
54	2 463 133 441 338 048	27 176 052
56	10 286 493 304 041 104	56 465 878
58	42 892 130 604 098 656	117 458 820
60	178 592 047 539 343 200	243 507 250
62	742 609 229 473 744 320	505 239 624
64	2 439 630 075 430 725 288	

seek recurrence relations whose coefficients are linear, quadratic, cubic, etc., polynomials in n, with an appropriate inhomogeneous term as shown. The 'depth' of the recurrence, i.e. the value of m where the coefficient P_n is expressed in terms of P_{n-1}, $P_{n-2}, \ldots, P_{n-m}$, is determined by the number of available series coefficients. Twelve terms of the series are needed to get the recurrence relation. The remaining 18 terms then provide a check on the recurrence relation. This recurrence relation among the coefficients is equivalent to the following differential equation for the generating function:

$$P''(x)(x^2-8x^3+16x^4)-P'(x)(8.5x-50x^2+64x^3)+P(x)(15-57x+36x^2)$$
$$=15-44x+22x^2-7x^3. \qquad (13)$$

To solve this equation, we first make the substitution $u=4x$, then write

$$f(u)=[(u-1)/u]^2P(u) \qquad (14)$$

which transforms the differential equation into

$$u(1-u)f''(u)+(4u-4.5)f'(u)-2.25f(u)=(1-u)p(u)/u^3 \qquad (15)$$

where $p(u) = 15 - 11u + 1.375u^2 + 0.109\,375u^3$. The corresponding homogeneous differential equation is readily seen to be the degenerate hypergeometric function:

$$F(-1/2, -9/2; -9/2; u) = (1-u)^{1/2} F(-4, 0; \ -9/2; u) = (1-u)^{1/2} \tag{16}$$

To solve the inhomogeneous equation by the method of reduction of order we write $f(u) = (1-u)^{1/2} v(u)$, which gives upon substitution

$$\mathrm{d}v/\mathrm{d}u = (1-u)^{3/2}(cu^{9/2} - 2u^{-3} + 4u^2 - 9/4u + \tfrac{9}{32} + u/32). \tag{17}$$

From the fact that the required solution is an expansion in powers of x, and hence u, it follows that $c = 0$ (or else powers of $u^{1/2}$ would be present). Integration of (3.7) and substitution of the early terms of the series to identify the constant of integration yields the solution

$$P(x) = (1 - 6x + 11x^2 - 4x^3)/(1-4x)^2 - 4x^2/(1-4x)^{3/2}. \tag{18}$$

That is, the generating function has a 'critical point' at $x = \frac{1}{4}$, with critical exponent 2 and confluent exponent 1.5. The generating function for the 'staircase model' studied by Lin *et al* is

$$P(x) = \sum_{n=0}^{\infty} p_{2n} x^n = \tfrac{1}{2} - x - \tfrac{1}{2}(1-4x)^{1/2} \tag{19}$$

which can be seen to have the same critical point as the convex polygon generating function, but with critical exponent $-\frac{1}{2}$. Thus there are $n^{2.5}$ more convex polygons than staircase polygons. The generating function for self-avoiding polygons on the square lattice in contrast has a critical point at $x \approx 0.143\,68\ldots$ with exponent $-\frac{3}{2}$ so that the convex polygons constitute an exponentially small subset of the SAP.

Note too that the recurrence relation (3.2) is not unique. Indeed, it is clear from the solution (3.8) that a homogeneous recurrence relation, and hence differential equation, will represent the solution (18).

The enumeration of convex polygons has allowed us to extend the enumeration of SAP on the square lattice to 56 terms and should allow us to extend the honeycomb SAP to 76 or 82 steps. The generation and analysis of this series is the subject of a subsequent paper (Guttmann and Enting 1988). The calculation of the generating function for convex polygons, while non-rigorous, is undoubtedly correct and constitutes an exact solution of an interesting combinatorial and statistical mechanical problem.

The singularity structure is also illuminating. A dominant exponent is followed by a confluent square root singularity. We believe a similar structure exists for the general SAP problem, with the additional subtlety that, as the exponent of the SAP generating function is -1.5, corresponding to a cusp-like singularity, the confluent square root singularity has an integral exponent, which 'folds into' the additive analytic background term. In contrast, the simpler staircase model of Lin *et al* (1987) displays no such confluence, prompting them to remark that their model does not support non-integral correction-to-scaling exponents in the self-avoiding walk problem. It is clear from our solution that such confluent exponents *are* to be expected.

An additional benefit of this solution is that it represents an exactly solvable model with a confluent exponent, and so should serve as a useful benchmark for methods of series analysis which lay claim to being able to unravel such singularity structures.

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