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Unidirectional-convex polygons on the honeycomb lattice

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Abstract. We obtain the exact generating function for a class of self-avoiding polygons on the honeycomb lattice which are convex in one of the three lattice directions. It is shown that the critical exponent α of these unidirectional-convex polygons is $\frac{3}{2}$.

The exact enumeration of self-avoiding polygons on a lattice has remained to this date an outstanding unsolved problem in lattice statistics. Let a_n be the number of topologically distinct self-avoiding polygons (SAP) having n sides that can be embedded on a d-dimensional lattice. The exact enumeration of a_n concerns with the closed-form evaluation of the generating function

$$G(x) = \sum_n a_n x^n \tag{1}$$

and the investigation of the singular behaviour

$$G(x) \approx A(x_c - x)^{2-\alpha} \tag{2}$$

from which one obtains the critical point x_c and the critical exponent α.

The evaluation of the generating function $G(x)$ for true self-avoiding polygons has remained elusive for any $d \geq 2$ lattices. However, it has been proven possible to evaluate the generating functions for restricted classes of polygons. For the square lattice, for example, it has been possible to evaluate $G(x)$ for the staircase (Temperley 1956, Polya 1969, Lin *et al* 1987), convex (Delest and Viennot 1984, Guttmann and Enting 1988b, Lin and Chang 1988, Kim 1988), and row-convex (Temperley 1956, Brak *et al* 1990) polygons. For the purpose of regarding restricted classes of polygons as approximations to the true SAP, the honeycomb lattice is of particular interest. The exact values of the honeycomb critical point and critical exponent are now known (Nienhuis 1982, 1984, Guttmann and Enting 1988a, Enting and Guttmann 1989) to be

$$x_c = 1 - \sqrt{2}/2 \qquad \alpha = 1/2. \tag{3}$$

On the other hand, however, the only restricted class that has previously been exactly solved for the honeycomb lattice is that of a certain class of polygons convex on the 'brick-wall' lattice (Guttman and Enting 1988b, Lin and Chang 1988) with $\alpha = 4$, which have no natural convexity interpretation on the honeycomb lattice (Enting and Guttmann 1989). To complete the description, we consider in this paper SAP on the

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honeycomb lattice which possess a genuine convexity meaning. Specifically, we obtain the exact solution of the generating function for SAP which are convex in one of the three lattice directions, presumably a class of polygons which are closer to the true SAP than those of the row-convex polygons for the square lattice.

Consider polygons drawn on the honeycomb lattice as shown in figure 1. The edges of a polygon are labelled by x, y, or z, such that all edges with the same label are parallel to the same direction. We define a polygon embedded on the lattice to be convex if all straight lines drawn on the dual lattice intersect the polygon at most twice. Thus, the polygon in figure 1(a) is convex, while the one in figure 1(b) is not. In the latter case, some lines on the dual lattice perpendicular to lattice edges labelled y and z cut the polygon at four points. By analogy with the definition of row-convex polygons of the square lattice (Brak *et al* 1990), we therefore define unidirectional-convex polygons as the ones for which the convexity property holds in one of the three lattice directions, namely, all lines on the dual lattice perpendicular to lattice edges in one direction cut the polygon at at most two points. Thus, the polygon in figure 1(b) is unidirectional-convex, since all dual lattice lines perpendicular to the edges labelled x possess this property. We now consider the generating function of these unidirectional-convex polygons.

It is convenient for our purposes to redraw the honeycomb lattice in the form of a 'brick-wall' lattice as shown in figure 2, with the edges labelling x pointing in the horizontal direction. We consider now more generally the generating function

$$G_{\mathrm{UC}}(x; y, z) = \sum_{l,m,n} a_{lmn} x^l y^m z^n \tag{4}$$

where a_{lmn} is the number of topologically distinct unidirectional-convex polygons with l, m, n edges labelled respectively by x, y, z. Clearly, (4) reduces to (1) by setting $x = y = z$. Following Temperley (1956) we write

$$G_{\mathrm{UC}}(x; y, z) = \sum_{r=1}^{\infty} g_r(x; y, z) \tag{5}$$

where $g_r(x; y, z)$ is the generating function for unidirectional-convex polygons whose left-most column contains an area of exactly $2r$ squares. By extending an argument used by Temperley (1956) for the square lattice to the present case, it is not difficult

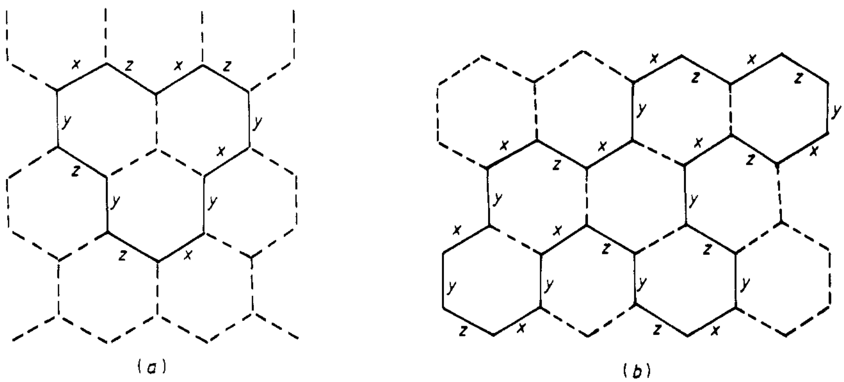

Figure 1. Polygons on the honeycomb lattice. (a) Convex polygon. (b) Unidirectional-convex polygon.

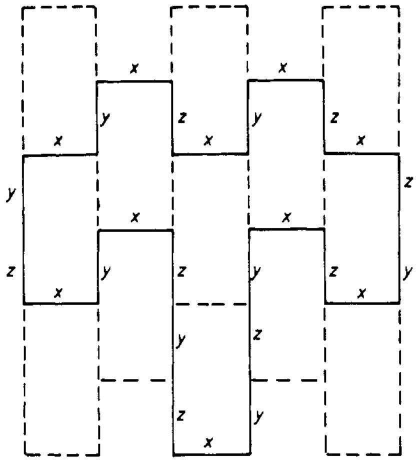

Figure 2. Polygon on the brick-wall lattice corresponding to the one shown in figure 1(*b*).

to see that the generating function g_r satisfies the relation

$$g_r = x^2(yz)^{2r}\left[1+\sum_{s=1}^{\infty} g_s\left(\sum_{n=1}^{\Delta(r,s)} \alpha\beta^{n-1}+|r-s|\beta^{\Delta(r,s)}\right)\right] \tag{6}$$

where

$$\Delta(r,s)=\min(r,s) \qquad \alpha=y^{-2}+z^{-2} \qquad \beta=(yz)^{-2}.$$

Here, the first term $x^2(yz)^{2r}$ on the RHS of (6) takes into account the polygon of the shape of precisely one column of $2r$ squares, and the term g_s takes into account those polygons whose left-most column contains $2r$ squares and the next column contains $2s$ squares. The coefficient of g_s in (6) is obtained by analysing corrections to perimeter weights when two columns of squares are in touch with each other, which can happen in $r+s$ different positions.

Writing

$$\Delta F_r \equiv F_r-(yz)^2F_{r-1} \tag{7}$$

for any function F_r and taking Δ^2 on both sides of (6), one obtains

$$\Delta^2 g_r = ag_{r-1}+b\sum_{s=r}^{\infty} g_s + c\sum_{s=1}^{\infty} sg_{r+s} \tag{8}$$

where

$$a=(xyz)^2(1-y^2)(1-z^2)$$
$$b=x^2(1-y^2z^2)(y^2+z^2-2y^2z^2)$$
$$c=x^2(1-y^2z^2)^2.$$

The infinite sums in (8) are eliminated by considering its double difference

$$\Delta^2(g_{r+4}-2g_{r+3}+g_{r+2})=(a-b+c)g_{r+3}-(2a-b)g_{r+2}+ag_{r+1} \tag{9}$$

which becomes, after using (7) in the LHS,

$$g_{r+4}-ug_{r+3}+vg_{r+2}-u(yz)^2g_{r+1}+(yz)^4g_r=0 \qquad r=1,2,3,\ldots \tag{10}$$

where

$$u = 2(1+y^2z^2)+x^2(1-y^2)(1-z^2)$$
$$v = 1+4y^2z^2+y^4z^4+x^2[4y^2z^2-(1+y^2z^2)(y^2+z^2)].$$

We further introduce the generating function

$$g(\lambda) = \sum_{r=1}^{\infty} g_r\lambda^{-r} \tag{11}$$

so that

$$G_{\mathrm{UC}}(x; y, z) = g(1). \tag{12}$$

Multiplying (10) by $\lambda^{-(r+4)}$ and summing over r from 1 to ∞, one obtains after some steps the following explicit expression for $g(\lambda)$:

$$g(\lambda) = N(\lambda)/D(\lambda) \tag{13}$$

where

$$N(\lambda) = (\lambda^3-u\lambda^2+v\lambda-uy^2z^2)g_1+(\lambda^2-u\lambda+v)g_2+(\lambda-u)g_3+g_4$$
$$D(\lambda) = \lambda^4-u\lambda^3+v\lambda^2-uy^2z^2\lambda+y^4z^4$$
$$= (\lambda-\lambda_1)(\lambda-\lambda_2)(\lambda-\lambda_3)(\lambda-\lambda_4).$$

Here, the four roots of $D(\lambda)$ are

$$\begin{aligned}\lambda_1 &= [B_+ + \sqrt{B_+^2-4y^2z^2}]/2\\ \lambda_2 &= [B_+ - \sqrt{B_+^2-4y^2z^2}]/2\\ \lambda_3 &= [B_- + \sqrt{B_-^2-4y^2z^2}]/2\\ \lambda_4 &= [B_- - \sqrt{B_-^2-4y^2z^2}]/2\end{aligned} \tag{14}$$

where

$$B_\pm = (u \pm \sqrt{F})$$
$$F = x^2[4(1-y^2z^2)^2+x^2(1-y^2)^2(1-z^2)^2].$$

The partial fraction expansion of (13) yields

$$g(\lambda) = \sum_{n=1}^{4} A_n/(\lambda-\lambda_n) \tag{15}$$

where A_n are constants to be determined from 'boundary' conditions, and the complete determination of $g(\lambda)$ requires an explicit knowledge of g_1, g_2, g_3 and g_4.

Writing $(\lambda-\lambda_n)^{-1} = \Sigma_{r=1}^{\infty} \lambda^{-r}\lambda_n^{r-1}$ and comparing (15) with (11), we obtain

$$g_r = \sum_{n=1}^{4} A_n\lambda_n^{r-1}. \tag{16}$$

It is easy to see that, for small x, y, z, we have $\lambda_1, \lambda_3 \approx \mathrm{O}(1)$ and $\lambda_2, \lambda_4 \approx \mathrm{O}(y^2z^2)$. Now by definition $g_r \approx x^2(y^2z^2)^{2r}$, it follows from (16) that we must have

$$A_1 = A_3 = 0 \tag{17}$$

giving rise to two boundary conditions, and

$$g(\lambda) = A_2/(\lambda-\lambda_2)+A_4/(\lambda-\lambda_4). \tag{18}$$

The remaining two boundary conditions are obtained by writing out (6) explicitly for $r=1,2$. This leads to, after using (11),

$$g_1 = x^2[y^2z^2 + (y^2+z^2-1)g(1) - g'(1)]$$
$$g_2 = x^2y^4z^4 + x^2(1-y^2)(1-z^2)g_1 + x^2[(1+y^2z^2)(y^2+z^2)-2]g(1) - x^2g'(1). \tag{19}$$

Substituting (18) and

$$g_1 = A_2 + A_4 \qquad g_2 = A_2\lambda_2 + A_4\lambda_4 \tag{20}$$

obtained from (16) into (19), we now have two equations containing the two unknowns A_2 and A_4. Using the computer algebra program REDUCE (Hearn 1968, Stauffer *et al* 1989) to solve these equations, we obtain

$$A_2 = [(1-y^2z^2)/8D](B_1 + B_2x^2/F^{1/2})$$
$$A_4 = [(1-y^2z^2)/8D](B_1 - B_2x^2/F^{1/2}) \tag{21}$$

where

$$D = (y^2+z^2)[1+2(y^2+z^2)+y^4+z^4-4y^2z^2(y^2+z^2)-y^2z^2(2y^4+3y^2z^2+2z^4)$$
$$+2y^4z^4(y^2+z^2)+y^4z^4(y^2+z^2)^2]+x^2y^2z^2[1-(y^2+z^2)^2(1-y^2z^2)] \tag{22}$$

$$B_j = a_j + b_jS^{1/2} + (c_j + d_jS^{1/2})T^{1/2}/[2(1+y^2z^2)+x^2(1-y^2)(1-z^2)] \qquad j=1,2$$

with

$$S = 1-2(x^2y^2+y^2z^2+x^2z^2) - 8x^2y^2z^2 + x^4y^4 + y^4z^4 + x^4z^4 - 2x^2y^2z^2(x^2+y^2+z^2)$$

$$T = 2(1-y^2z^2)^2 + 2x^2[2-(y^2+z^2)(1+y^2z^2)+2y^4z^4] + x^4(1-y^2)^2(1-z^2)^2$$
$$+2(1-y^2z^2)S^{1/2}$$

$$a_1 = x^2(1-y^2z^2)[-1-5(y^2+z^2)-3(y^2+z^2)^2+y^6+z^6+5(y^4z^2+y^2z^4)$$
$$+5y^2z^2(y^2+z^2)^2+y^2z^2(y^2+z^2)^3]$$
$$-x^4(y^2+z^2-y^4-z^4)[1-(y^2+z^2)^2(1-y^2z^2)]$$

$$b_1 = -x^2(1-y^2-z^2)[1-(y^2+z^2)^2(1-y^2z^2)]$$

$$c_1 = 2(y^2+z^2)(1+y^2+z^2)(1-y^2z^2)^2 + x^2[1+5(y^2+z^2)+y^4+5y^2z^2+z^4-3(y^6+z^6)$$
$$-12y^2z^2(y^2+z^2)-6y^2z^2(y^2+z^2)^2+2y^2z^2(y^2+z^2)(y^4+3y^2z^2+z^4)$$
$$+5y^4z^4(y^2+z^2)^2+y^4z^4(y^4+z^4)^3]$$
$$+(x^4y^2+z^2-y^4-z^4)[1-(y^2+z^2)^2(1-y^2z^2)]$$

$$d_1 = -2(y^2+z^2)(1+y^2+z^2)(1-y^2z^2) - b_1$$

$$a_2 = -2(1+y^2+z^2)(1+3y^2+3z^2)(1-y^2z^2)^3 + x^2(1-y^2z^2)[-1-6(y^2+z^2)$$
$$+2(y^4+z^4)+3y^2z^2+6(y^6+z^6)+17(y^4z^2+y^2z^4)-(y^2+z^2)^4$$
$$-5(y^8z^2+y^2z^8)-17(y^6z^4+y^4z^6)-y^{10}z^2-y^2z^{10}+y^8z^4$$
$$+y^4z^8+4y^6z^6+y^4z^4(y^2+z^2)^3]-x^4(1-y^2)(1-z^2)$$
$$\times(y^2+z^2-y^4-z^4)[1-(y^2+z^2)^2(1-y^2z^2)]$$

$$b_2 = -2[1-(y^2+z^2)^2](1-y^2z^2)^2 + (1-y^2)(1-z^2)b_1$$

$$\begin{aligned} c_2 = 2(1-y^2z^2)^2[&1+5(y^2+z^2)+3(y^4+z^4)+7y^2z^2-y^6-z^6+2(y^4z^2+y^2z^4) \\ &+2y^2z^2(y^2+z^2)^2]+x^2[1+6(y^2+z^2)-4(y^4+y^2z^2+z^4) \\ &-6(y^6+z^6)-19(y^4z^2+y^2z^4)+3(y^8+z^8)+10(y^6z^2+y^2z^6) \\ &+17y^4z^4+9(y^8z^2+y^2z^8)+20(y^6z^4+y^4z^6)-2(y^{10}z^2+y^2z^{10}) \\ &-11(y^8z^4+y^4z^8)-18y^6z^6-4(y^{10}z^4+y^4z^{10})-6(y^8z^6+y^6z^8)-y^{12}z^4 \\ &-y^4z^{12}+y^{10}z^6+y^6z^{10}+4y^8z^8+y^6z^6(y^2+z^2)^3] \\ &+x^4(1-y^2)(1-z^2)(y^2+z^2-y^4-z^4)[1-(y^2+z^2)^2(1-y^2z^2)] \end{aligned}$$

$$d_2 = 2(1-y^2z^2)(1-y^2-z^2)[1-(y^2+z^2)^2]-(1-y^2)(1-z^2)b_1.$$

Substituting (21) into (18) and specializing the result to $\lambda = 1$, we finally obtain the following explicit expression for the generating function:

$$\begin{aligned} G_{\mathrm{UC}}(x; y, z) &= g(1) \\ &= (1-y^2z^2)(a+bS^{1/2})/4D + (1-y^2z^2) \\ &\quad \times (c+dS^{1/2})T^{1/2}/4D[2(1+y^2z^2)+x^2(1-y^2)(1-z^2)] \end{aligned} \tag{23}$$

where

$$\begin{aligned} a = 1&+4(y^2+z^2)+3y^4+4y^2z^2+3z^4 \\ &-8y^2z^2(y^2+z^2)-6y^2z^2(y^4+z^4)-11y^4z^4+4y^4z^4(y^2+z^2) \\ &+3y^4z^4(y^2+z^2)^2+x^2[y^2+z^2-4y^2z^2(y^2+z^2)-y^6-z^6 \\ &+y^2z^2(y^6+z^6)+5y^4z^4(y^2+z^2)] \end{aligned}$$

$$b = (1-y^2z^2)[1-(y^2+z^2)^2]$$

$$\begin{aligned} c = -(1-y^2z^2)[&1+4(y^2+z^2)+3y^4+7y^2z^2+3z^4 \\ &+4y^2z^2(y^2+z^2)+y^2z^2(y^2+z^2)^2+x^2(y^2+z^2)(1-y^4-z^4)] \end{aligned}$$

$$d = -1+y^4+y^2z^2+z^4-y^2z^2(y^2+z^2)^2.$$

In the special case of $x = y = z$, (23) reduces to

$$\begin{aligned} G_{\mathrm{UC}}(x) &= (1-x^4)N/4x^2(2-x^2+x^4)D \\ &= x^6+3x^{10}+2x^{12}+12x^{14}+18x^{16}+63x^{18}+\dots \end{aligned} \tag{24}$$

where

$$N = a+bS^{1/2}+cT^{1/2}+d(ST)^{1/2}$$

$$D = 2+8x^2+5x^4-16x^6-18x^8+8x^{10}+12x^{12}$$

with

$$S = (1+x^2)(1-3x^2)$$

$$T = (1-x^4)[(1-x^2)(2+6x^2+x^4+x^6)+2(1+x^2)S^{1/2}]$$

$$a = 2+15x^2+17x^4-36x^6-38x^8+33x^{10}+7x^{12}-16x^{14}+24x^{16}$$

$$b = 2+x^2-10x^4-4x^6+8x^8-x^{10}+4x^{14}$$

$$c = -1-7x^2-7x^4+7x^6+8x^8$$

$$d = -1+3x^4-4x^8.$$

Comparison of (24) with the series expansions for unrestricted polygons (Enting and Guttmann 1989) shows that the first difference occurs at x^{18}.

The singular part of the generating function $G_{UC}(x)$ is that given by $S^{1/2}$ occurring at $x_c^2=\frac{1}{3}$. Hence we obtain the critical exponent $\alpha=\frac{3}{2}$. This exponent is the same as that of the row-convex polygons on the square lattice (Brak *et al* 1990), and is to be compared with the value $\alpha=4$ for the class of SAP convex on the 'brick wall' lattice (Guttmann and Enting 1988*b*, Lin and Chang 1988) and the value $\alpha=\frac{1}{2}$ for the true SAP (Nienhuis 1982, 1984). Thus, despite the fact that the class of polygons considered here is closer to the true SAP than those previously considered, it belongs to the same universality class as that of the square lattice row-convex polygons.

Expanding the generating function about the singularity, we obtain

$$G_{UC}(x)=c_0+c_1(1-3x^2)^{1/2}+c_2(1-3x^2)+c_3(1-3x^2)^{3/2}+O(1-3x^2)^2 \tag{25}$$

where

$$\begin{aligned}c_0&=8[13-4(7)^{1/2}]/171\\&=0.113\,076\ldots\\c_1&=32[-179\,(21)^{1/2}+140\,(3)^{1/2}]/68\,229\\&=-0.270\,99\ldots\\c_2&=2[2747\,479-707824\,(7)^{1/2}]/9074457\\&=0.192795\ldots\\c_3&=4[-80\,905\,507(21)^{1/2}+180\,290\,404(3)^{1/2}]/3620\,708\,343\\&=-0.064\,61\ldots.\end{aligned}$$

If we write as in (1)

$$G_{UC}(x)=\sum_n a_n x^{2n} \tag{26}$$

the asymptotic behaviour of a_n for large n is then given by

$$a_n=3^n n^{-3/2}\pi^{-1/2}[A+B/n+O(n^{-2})] \tag{27}$$

where

$$\begin{aligned}A&=-c_1/2=0.153\,495\ldots\\B&=-3c_1/16+3c_3/4=0.002\,353\ldots\end{aligned}$$

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