EXACT SOLUTION OF TWO PLANAR POLYGON MODELS

ANTHONY J. GUTTMANN AND IWAN JENSEN

ARC Centre of Excellence for Mathematics and Statistics of Complex Systems
Department of Mathematics and Statistics
The University of Melbourne, Victoria 3010, Australia

Using a simple transfer matrix approach we have derived long series expansions for the perimeter generating functions of both *three-choice polygons* and *punctured staircase polygons*. In both cases we find that all the known terms in the generating function can be reproduced from a linear Fuchsian differential equation of order 8. We report on an analysis of the properties of the differential equations.

1. Introduction

A well-known long standing problem in combinatorics and statistical mechanics is the enumeration by perimeter of self-avoiding polygons (or walks) on a two- or three-dimensional lattice. Recently, we have gained a greater understanding of the difficulty of this problem, as Rechnitzer[14] has *proved* that the (anisotropic) generating function for square lattice self-avoiding polygons is not differentiably finite[15]. This property had been *conjectured*, on numerical grounds[5], but not proved. So the generating function cannot be expressed as a solution of an ordinary differential equation with polynomial coefficients. There are many simplifications of this problem that are solvable[1], but these simpler models impose an effective directedness or other constraint that reduce them, in essence, to one-dimensional problems.

One model, that of *three-choice polygons*, has remained unsolved despite the knowledge that its solution must be D-finite. Recent numerical work[7] resulted in an exact differential equation apparently satisfied by the perimeter generating function of three-choice polygons. Similarly for another model, that of *punctured staircase polygons*, that is a staircase polygon with an arbitrary staircase puncture. Again we found[8] that the perimeter generating function is apparently satisfied by an exact differential equation. While our results do not constitute rigorous mathematical proofs the numerical evidence is overwhelmingly compelling.

The next two sections consider these two models, in turn.

2

2. Three-choice polygons

Three-choice self-avoiding walks on the square lattice, $\mathbb{Z}^2$, were introduced by Manna[13] and can be defined as follows: Starting from the origin one can step in any direction; after a step upward or downward one can head in any direction (except backward); after a step to the left one can only step forward or head downward, and after a step to the right one can continue forward or turn upward. Alternatively put, one cannot make a right-hand turn after a horizontal step. Whittington[17] showed that the growth constant for three-choice walks is exactly 2, so that if w_n denotes the number of such walks of n steps on an infinite lattice, equivalent up to a translation, then $w_n \sim 2^{n+\mathrm{o}(n)}$. It is perhaps surprising that the best known result for the sub-dominant term is $2^{\mathrm{o}(n)}$, but attempts to improve on this have been unsuccessful. Even numerically, there is no firmly based conjecture for the sub-dominant term, unlike for ordinary self-avoiding walks, for which the sub-dominant term is widely believed to be $\mathrm{O}(\log n)$.

As usual one can define a polygon version of the walk model by requiring the walk to return to the origin. So a three-choice polygon[10] is simply a three-choice self-avoiding walk which returns to the origin, but has no other self-intersections. There are two distinct classes of three-choice polygons. The three-choice rule either leads to staircase polygons or *imperfect staircase polygons*[3] as illustrated in figure 1. In the case of staircase polygons any perimeter vertex can act as the origin of the three-choice walk (which then proceeds counter-clockwise), while for imperfect staircase polygons there is only one possible origin but the polygon could be rotated by 180 degrees. If we denote by t_n the number of three-choice polygons with perimeter $2n$ then, $t_n = 2nc_n + 2p_n$, where c_n is the number of staircase polygons and p_n is the number of imperfect staircase polygons with perimeter $2n$. Note that t_n, p_n and c_n all grow like 4^n and in particular we recall the well-known result that $c_{n+1} = C_n = \frac{1}{n+1}\binom{2n}{n}$ where C_n are the Catalan numbers.

In this paper we report on recent work[7] which has led to an exact Fuchsian[11] linear differential equation of order 8 apparently satisfied by the perimeter generating function, $\mathcal{T}(x) = \sum_{n\geq 0} t_n x^n$, for three-choice polygons (that is $\mathcal{T}(x)$ is conjectured to be one of the solutions of the ODE, expanded around the origin). The first few terms are

$$\mathcal{T}(x) = 4x^2 + 12x^3 + 42x^4 + 152x^5 + 562x^6 + \cdots .$$

(The generating function for the coefficients p_n is no simpler.)

If we distinguish between steps in the x and y direction, and let $t_{m,n}$ denote the number of three-choice polygons with $2m$ horizontal steps and
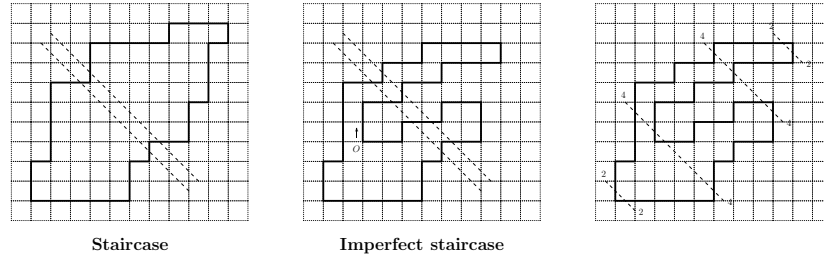
Figure 1.   Examples of the two types of three-choice polygons. In the middle panel we indicate the origin (O) and the direction of the first step (note that rotation by 180 degrees also leads to a valid three-choice polygon). The right panle shows the decomposition of an imperfect staircase polygon into a sequence of 2-4-2 non-intersecting walkers, each expressible as a Gessel-Viennot determinant.

$2n$ vertical steps, then the anisotropic generating function for $\mathcal{T}(x,y)$ is

$$\mathcal{T}(x,y) = \sum_{m,n} t_{m,n} x^m y^n = \sum_n H_n(x) y^n,$$

where $H_n(x) = \frac{R_n(x)}{S_n(x)}$ is the (rational[16]) generating function for three-choice polygons with $2n$ vertical steps. In earlier, unpublished, numerical work, we found that, for imperfect staircase polygons, the denominators are:

$$S_n(x) = (1-x)^{2n-1}(1+x)^{(2n-7)+} \qquad n \quad \text{even},$$

and

$$S_n(x) = (1-x)^{2n-1}(1+x)^{(2n-8)+} \qquad n \quad \text{odd}.$$

This was subsequently proved by Bousquet-Mélou[2]. Unfortunately, we still do not have enough information to identify the numerators.

It is also possible to express the generating function $\mathcal{T}(x)$ as a five-fold sum, with one constraint[2], of 4×4 Gessel-Viennot determinants[4]. This is clear from the right panel of figure 1, where the enumeration of the lattice paths between the dotted lines is just the classical problem of 4 non-intersecting walkers, and these must be joined to two non-intersecting walkers to the left, and to two non-intersecting walkers to the right. Then one must sum over different possible geometries. The fact that the generating function is so expressible implies that it is differentiably finite[12].

Next we discuss work leading to an ODE for the perimeter generating function of three-choice polygons. In[7] we generated the counts for three-choice polygons up to half-perimeter 260. Using numerical experimentation we found what we believe is the underlying ODE. This calculation required

4

the use of the first 206 coefficients with the resulting ODE then correctly predicting the next 54 coefficients. The possibility that this ODE is incorrect is extraordinarily small, but this does not of course constitute a proof. Unfortunately we cannot usefully bound the size of the underlying ODE, otherwise we could use the knowledge of D-finiteness to provide a proof. Bounds following from closure theorems[12] are too large to be useful.

The algorithm used to enumerate imperfect polygons is a slightly modified version of the algorithm of Conway *et al.*[3], and is described fully in[7].

2.1. *The Fuchsian differential equation*

Recently Zenine *et al.*[18,19,20] obtained linear differential equations whose solutions give the 3- and 4-particle contributions $\chi^{(3)}$ and $\chi^{(4)}$ to the Ising model susceptibility. In[7] we used their method to find an ODE which has as a solution the generating function $\mathcal{T}(x)$ for three-choice polygons. This involves a systematic search for a differential equation of the form:

$$\sum_{k=0}^{m} P_k(x) \frac{\mathrm{d}^k}{\mathrm{d}x^k} \mathcal{T}(x) = 0, \tag{1}$$

such that $\mathcal{T}(x)$ is a solution to this differential equation, where the $P_k(x)$ are polynomials. To make it as simple as possible we started by searching for a Fuchsian[11] equation. Such equations have only regular singular points.

We searched systematically for solutions by varying m and q_m, the degree of the polynomials $P_m(x)$. In this way a solution with $m = 10$ and $q_m = 12$ was first found, which required the determination of $L = 206$ unknown coefficients. With 260 terms in the half-perimeter series, there are more than 50 additional terms with which to check the correctness of this solution. Having found this conjectured solution the ODE was then turned into a recurrence relation and used to generate more series terms in order to search for a lower order Fuchsian equation. The lowest order equation found was eighth order and with $q_m = 30$, which requires the determination of $L = 321$ unknown coefficients. Thus from the original 260 term series this 8th order solution could not have been found. This raises the question as to whether perhaps there is an ODE of lower order than 8 that generates the coefficients? The short answer to this is no.

So the (half)-perimeter generating function $\mathcal{T}(x)$ for three-choice polygons is conjectured to be a solution of the linear ODE of order 8

$$\sum_{k=0}^{8} P_k(x) \frac{\mathrm{d}^k}{\mathrm{d}x^k} F(x) = 0 \tag{2}$$

with

$$P_8(x) = x^3(1 - 4x)^4(1 + 4x)(1 + 4x^2)(1 + x + 7x^2)Q_8(x), \qquad (3)$$

where $Q_8(x)$ is a polynomial of degree 25, which together with the remaining polynomials $P_k(x)$ are given in[7].

The singular points of the differential equation are given by the roots of $P_8(x)$. One can easily check that all the singularities (including $x = \infty$) are *regular singular points* so equation (2) is indeed of the Fuchsian type. Using the method of Frobenius one can obtain from the indicial equation the critical exponents at the singular points. These are listed in Table 2.1.

Singularity	Exponents
$x = 0$	$-1, 0, 0, 0, 1, 2, 3, 4$
$x = 1/4$	$-1/2, -1/2, 0, 1/2, 1, 3/2, 2, 3$
$x = -1/4$	$0, 1, 2, 3, 4, 5, 6, 13/2$
$x = \pm\,\mathrm{i}/2$	$0, 1, 2, 3, 4, 5, 6, 13/2$
$1 + x + 7x^2 = 0$	$0, 1, 2, 2, 3, 4, 5, 6$
$x = \infty$	$-2, -3/2, -1, -1, -1/2, 1/2, 3/2, 5/2$
$Q_8(x) = 0$	$0, 1, 2, 3, 4, 5, 6, 8$

A careful local analysis revealed that near the physical critical point $x = x_c = 1/4$ the singular behaviour is

$$\mathcal{T}(x) \sim A(x)(1 - 4x)^{-1/2} + B(x)(1 - 4x)^{-1/2}\log(1 - 4x), \qquad (4)$$

where $A(x)$ and $B(x)$ are analytic in the neighbourhood of x_c. Note that the terms associated with the exponents $1/2$ and $3/2$ become part of the analytic correction to the $(1 - 4x)^{-1/2}$ term. Near the singularity on the negative x-axis, $x = x_- = -1/4$ the singular behaviour is

$$\mathcal{T}(x) \sim C(x)(1 + 4x)^{13/2}, \qquad (5)$$

where again $C(x)$ is analytic near x_-. Similar behaviour is expected near the pair of singularities $x = \pm\,\mathrm{i}/2$, and finally at the roots of $1 + x + 7x^2$ one expects the behaviour $\mathcal{T}(x) \sim D(x)(1 + x + 7x^2)^2\log(1 + x + 7x^2)$.

We can simplify the 8th order differential operator found above. We first found three solutions of the ODE, each corresponding to an order one differential operator. Denoting these by $L_i^{(1)}$, with $i = 1,2,3$, we found that the differential operator could be written as $L^{(8)} = L^{(5)}L_1^{(1)}L_2^{(1)}L_3^{(1)}$, where $L^{(5)}$ is a fifth order differential operator, further decomposable as $L^{(5)} =$

6

$L^{(3)}L^{(2)}$. This then allows us to write down the form of the 8×8 matrix representing the differential Galois group of $L^{(8)}$, in an appropriate global solution basis. To determine the asymptotics one would need to calculate non-local connection matrices between solutions at different points. This is a huge task for such a large differential operator. Instead, we have developed a numerical technique that avoids all these difficulties, described below.

To analyse the asymptotic behaviour of the coefficients, we first transform the coefficients so that the critical point is at 1. The growth constant of staircase and imperfect staircase polygons is 4, so we consider a new series with coefficients $r_n = t_{n+2}/4^n$. Thus the generating function studied is $\mathcal{R}(y) = \sum_{n \geq 0} r_n y^n = 4 + 3y + 2.625y^2 + \cdots$. From equations (4) and (5) it follows that the asymptotic form of the coefficients is

$$[y^n]\mathcal{R}(y) = r_n = \frac{1}{\sqrt{n}} \sum_{i \geq 0} \left(\frac{a_i \log n + b_i}{n^i} + (-1)^n \left(\frac{c_i}{n^{7+i}} \right) \right) + \mathrm{O}(\lambda^{-n}). \quad (6)$$

The last term includes the effect of other singularities, further from the origin than the dominant singularities. These will decay exponentially since $\lambda > 1$ in the scaled variable $y = x/4$.

Using the recurrence relations for t_n (derived from the ODE) it is easy and fast to generate many more terms r_n. In[7] the first 100000 terms were generated and saved as floating point numbers with 500 digit accuracy (this calculation took less than 15 minutes). With such a long series it is possible to obtain accurate numerical estimates of the first 20 amplitudes a_i, b_i, c_i for $i \leq 19$ with a precision of more than 100 digits for the dominant amplitudes, shrinking to 10–20 digits for the the case when $i = 18$, or 19. In making these estimates the exponentially decaying terms were ignored. In this way an earlier conjecture[3] that $a_0 = \frac{3\sqrt{3}}{\pi^{3/2}}$, was confirmed. Other amplitude estimates include $b_0 = 3.173275384589898481765\ldots$ and $c_0 = \frac{-24}{\pi^{3/2}}$, though no one has been able to identify b_0. However, further sub-dominant amplitudes have been estimated[7], such as $a_1 = \frac{-89}{8\sqrt{3}\pi^{3/2}}$, $a_2 = \frac{1019}{384\sqrt{3}\pi^{3/2}}$, and $a_3 = \frac{-10484935}{248832\sqrt{3}\pi^{3/2}}$, and $c_1 = \frac{225}{\pi^{3/2}}$, $c_2 = \frac{-16575}{16\pi^{3/2}}$, and $c_3 = \frac{389295}{128\pi^{3/2}}$. It seems likely that the amplitudes $\pi^{3/2}\sqrt{3}a_i$ and $\pi^{3/2}c_i$ are rational.

We have also looked at the area generating function. For staircase polygons the area generating function is given by

$$A(q) = \sum_{n \geq 1} a_n q^n = \frac{J_1(1,1,q)}{J_0(1,1,q)},$$

where $J_i = \sum_{n \geq 0} \frac{(-1)^n q^{(n+i)(n+i+1)/2}}{(q)_n^2 (1-q^{n+1})^i}$, $i = 0, 1$. Based on a 500 term series, our analysis suggests that the area generating function is of the form

$\frac{F(q)+G(q)/\sqrt{1-q\eta}}{[J_0(1,1,q)]^2}$. That is to say, the leading singularity occurs at $q = 1/\eta$, where η is the first zero of $J_0(1, 1, q)$, and F and G are regular in the neighbourhood of $q = 1/\eta$. The coefficients thus behave asymptotically as

$$a_n = [q^n]A(q) \sim const.\eta^{-n}n^{3/2}.$$

The solution is not, however, of the simple product form as found for staircase polygons. We can see this by constructing Padé approximants of steadily increasing order, which don't stabilise.

3. Punctured staircase polygons

Punctured staircase polygons[6] are staircase polygons with internal holes which are also staircase polygons (the polygons are mutually- as well as self-avoiding). In[6] it was proved that the connective constant μ of k-punctured polygons (polygons with k holes) is the same as the connective constant of un-punctured polygons. Here we discuss only the case with a *single* hole (see figure 2). The perimeter length of a punctured staircase polygons is the outer perimeter plus the perimeter of the hole. We denote by p_n the number of punctured staircase polygons of total perimeter $2n$. The results of[6] indicate that the half-perimeter generating function has a simple pole at $x = x_c = 1/\mu = 1/4$, though the analysis[6] clearly indicated a more complicated critical behaviour.
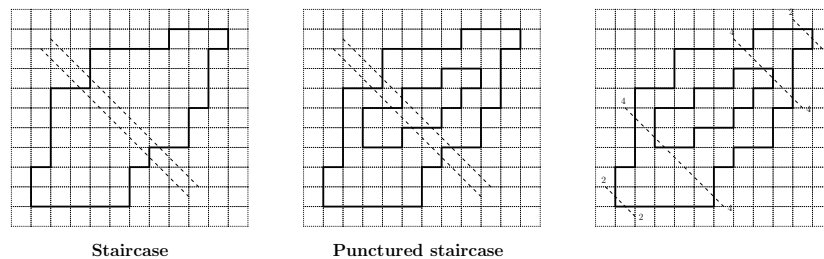

Staircase   Punctured staircase

Figure 2.   Examples of the types of staircase polygons studied in this paper. The right panle shows the decomposition of a punctured staircase polygon into a sequence of 2-4-2 vicious walkers, each expressible as a Gessel-Viennot determinant.

Here we report on recent work[8] which led to an exact Fuchsian linear differential equation of order 8 apparently satisfied by the perimeter generating function, $\mathcal{P}(x) = \sum_{n\geq 0} p_n x^n$, for punctured staircase polygons (that

8

is $\mathcal{P}(x)$ is one of the solutions of the ODE, expanded around the origin). The first few terms in the generating function are

$$\mathcal{P}(x) = x^8 + 12x^9 + 94x^{10} + 604x^{11} + 3463x^{12} + \cdots.$$

The situation is very similar to that of three-choice polygons. This is perhaps not surprising, as one can represent punctured staircase polygons as the fusion of two three-choice polygons, with some edges deleted. Again it is possible to express the generating function $\mathcal{P}(x)$ as a sum over 4×4 Gessel-Viennot determinants. This is clear from the right panel of figure 2. By arguments similar to those presented above, it follows that the generating function is D-finite. Again we cannot readily bound the size of the underlying ODE, otherwise we could use this observation to provide a proof of our results. However, from the counts of polygons up to half-perimeter 260, the underlying ODE was found experimentally from the first 206 coefficients[8]. The ODE then correctly predicted the next 54 coefficients. While the possibility that the underlying ODE is not the correct one is extraordinarily small, that still does not constitute a proof.

The enumeration algorithm[8] is again a modified version of the algorithm of Conway *et al.*[3] for the enumeration of imperfect staircase polygons.

We identified the ODE in a manner similar to that described above for three-choice polygons, and the (half-)perimeter generating function $\mathcal{P}(x)$ for punctured staircase polygons was found to satisfy an ODE of order 8

$$\sum_{k=0}^{8} P_n(x) \frac{\mathrm{d}^k}{\mathrm{d}x^k} F(x) = 0 \qquad (7)$$

with

$$P_8(x) = x^4(1-4x)^8(1+4x)(1+4x^2)(1+x+7x^2)Q_8(x), \qquad (8)$$

where $Q_8(x)$ is a polynomial of degree 22. All polynomials are given in[8]. The singular points as given by the roots of $P_8(x)$ and the associated critical exponents are listed in Table 3.

Detailed analysis of the local solutions of the ODE are given in[8]. Near the critical point $x = x_c = 1/4$ the following singular behaviour was found:

$$\mathcal{P}(x) \sim A(x)(1-4x)^{-1} + B(x)(1-4x)^{-1/2} + C(x)(1-4x)^{-1/2}\log(1-4x), \quad (9)$$

where $A(x)$, $B(x)$ and $C(x)$ are analytic in a neighbourhood of x_c. Note that the terms associated with the exponents $1/2$ and $3/2$ become part of the analytic correction to the $(1-4x)^{-1/2}$ term. Near the singularity on the negative x-axis, $x = x_- = -1/4$ the singular behaviour

$$\mathcal{P}(x) \sim D(x)(1+4x)^{13/2}, \qquad (10)$$

Singularity	Exponents
$x = 0$	$-1, 0, 0, 0, 1, 2, 3, 8$
$x = 1/4$	$-1, \ -1/2, -1/2, 1/2, 1, 3/2, 2, 3$
$x = -1/4$	$0, 1, 2, 3, 4, 5, 6, 13/2$
$x = \pm \mathrm{i}/2$	$0, 1, 2, 3, 4, 5, 6, 13/2$
$1 + x + 7x^2 = 0$	$0, 1, 2, 2, 3, 4, 5, 6$
$1/x = 0$	$-2, -3/2, -1, -1, -1/2, 1/2, 3/2, 5/2$
$Q_8(x) = 0$	$0, 1, 2, 3, 4, 5, 6, 8$

was found, where again $D(x)$ is analytic near x_-. Similar behaviour is expected near the pair of singularities $x = \pm \mathrm{i}/2$, and finally at the roots of $1 + x + 7x^2$ the behaviour $E(x)(1 + x + 7x^2)^2 \log(1 + x + 7x^2)$ is expected.

The asymptotic form of the coefficients was analysed as for three-choice polygons. The growth constant is 4 and we considered the new series with coefficients $r_n = p_{n+8}/4^n$. Using the recurrence relations for p_n (derived from the ODE) we generated many more terms r_n. From equations (9) and (10) it follows that the asymptotic form of the coefficients is

$$[x^n]\mathcal{R}(y) = r_n = \sum_{i \geq 0} \left(\frac{a_i}{n^i} + \frac{b_i \log n + c_i}{n^{i+1/2}} + (-1)^n \left(\frac{d_i}{n^{15/2+i}} \right) \right). \quad (11)$$

Any contributions from the other singularities are exponentially suppressed since their norm (in the scaled variable $y = x/4$) exceeds 1. From the first 100000 terms estimates for the amplitudes were obtained by fitting r_n to the form given above. This led to the refined asymptotic form

$$[x^n]\mathcal{R}(y) = r_n = 1024 \left(1 + \frac{1}{\sqrt{n}} \sum_{i \geq 0} \left(\frac{b_i \log n + c_i}{n^i} + (-1)^n \left(\frac{d_i}{n^{7+i}} \right) \right) \right). \quad (12)$$

We obtained accurate numerical estimates of many of the amplitudes and found that[8] $b_0 = -\frac{6\sqrt{3}}{\pi^{3/2}}$, $b_1 = \frac{305}{4\sqrt{3}\pi^{3/2}}$, $b_2 = \frac{86123}{192\sqrt{3}\pi^{3/2}}$, $c_0 = 1.55210340048879105374\ldots$ and $d_0 = \frac{48}{\pi^{3/2}}$, $d_1 = -\frac{2610}{\pi^{3/2}}$, $d_2 = \frac{640815}{8\pi^{3/2}}$, $d_3 = -\frac{116785575}{64\pi^{3/2}}$, $d_4 = \frac{70325480841}{2048\pi^{3/2}}$, though we have been unable to identify c_0. These amplitudes are known to at least 100 digits accuracy. The excellent convergence is solid evidence (though naturally not a proof) that the assumptions leading to equation (11) are correct.

We have also initiated an investigation of the *area* generating function. We find that the area generating function $A(q)$ is of the form

$$A(q) = (G(q) + H(q)\sqrt{1 - q/\eta})/[J_0(1, 1, q)^2],$$

10

where $J_0(x, y, q)$ is as described above. Here $q = \eta$ is the first zero of $J_0(1, 1, q)$, and G and H are regular in the neighbourhood of $q = \eta$. The coefficients thus behave asymptotically as

$$a_n = [q^n]A(q) \sim const.\eta^{-n}n.$$

Acknowledgments

References

1. Bousquet-Mélou M 1996 *Disc. Math.* **154** 1
2. Bousquet-Mélou M Private communication.
3. Conway A R, Guttmann A J and Delest M 1997 *Mathl. Comput. Modelling* **26** 51
4. Gessel I and Viennot X G 1989 Determinants, paths and plane partitions *preprint*
5. Guttmann A J and Conway A R 2001 *Ann. Comb.* **5** 319
6. Guttmann A J Jensen I Wong L H and Enting I G 2000 *J. Phys. A* **33** 1735
7. Guttmann A J and Jensen I 2006 Fuchsian differential equation for the perimeter generating function of three-choice polygons. *Séminaire Lotharingien de Combinatoire, in press Preprint:* math.CO/0506317
8. Guttmann A J and Jensen I 2006 Fuchsian differential equation for the perimeter generating function of punctured staircase polygons. *In preparation*
9. Guttmann A J and Jensen I 2006 Properties of Fuchsian differential equations for polygon enumeration problems *In preparation*
10. Guttmann A J, Prellberg T and Owczarek A L 1993 *J. Phys. A* **26** 6615
11. Ince E L 1927 *Ordinary differential equations* (London: Longmans, Green and Co. Ltd.)
12. Lipshitz L 1989 *J. Algebra* **122** 353
13. Manna S S 1984 *J. Phys. A: Math. Gen.* **17** L899
14. Rechnitzer A 2003 *Adv, Appl. Math.* **30** 228
15. Stanley R P 1980 *European J. Combin.* **1** 175
16. Stanley R P 1999 *Enumerative Combinatorics* vol. 2 (Cambridge: Cambridge University Press)
17. Whittington S G 1985 *J. Phys. A* **18** L67
18. Zenine N, Boukraa S, Hassani S and Maillard J M 2004 *J. Phys. A* **37** 9651
19. Zenine N, Boukraa S, Hassani S and Maillard J M 2005 *J. Phys. A* **38** 1875
20. Zenine N, Boukraa S, Hassani S and Maillard J M 2005 *J. Phys. A* **38** 4149