

# ON 3-DIMENSIONAL LATTICE WALKS CONFINED TO THE POSITIVE OCTANT

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ABSTRACT. Many recent papers deal with the enumeration of 2-dimensional walks with prescribed steps confined to the positive quadrant. The classification is now complete for walks with steps in  $\{0, \pm 1\}^2$ : the generating function is D-finite if and only if a certain group associated with the step set is finite.

We explore in this paper the analogous problem for 3-dimensional walks confined to the positive octant. The first difficulty is their number: we have to examine no less than 11 074 225 step sets in  $\{0, \pm 1\}^3$  (instead of 79 in the quadrant case). We focus on the 35 548 that have at most six steps.

We apply to them a combined approach, first experimental and then rigorous. On the experimental side, we try to guess differential equations. We also try to determine if the associated group is finite. The largest finite groups that we find have order 48 – the larger ones have order at least 200 and we believe them to be infinite. No differential equation has been detected in those cases.

On the rigorous side, we apply three main techniques to prove D-finiteness. The algebraic kernel method, applied earlier to quadrant walks, works in many cases. Certain, more challenging, cases turn out to have a special *Hadamard structure* which allows us to solve them via a reduction to problems of smaller dimension. Finally, for two special cases, we had to resort to computer algebra proofs. We prove with these techniques all the guessed differential equations.

This leaves us with exactly 19 very intriguing step sets for which the group is finite, but the nature of the generating function still unclear.

## 1. INTRODUCTION

The enumeration of lattice walks is a venerable topic in combinatorics, which has numerous applications as well as connections with other mathematical fields such as probability theory. In recent years the enumeration of walks confined to cones has received a lot of attention, and the present article also explores this topic.

Let us recall a few results for walks on  $\mathbb{Z}^d$  that start at the origin and consist of steps taken in  $\mathcal{S}$ , a finite subset of  $\mathbb{Z}^d$ . Clearly, there are  $|\mathcal{S}|^n$  walks of length  $n$  (that is, using exactly  $n$  steps), and the associated (length) generating function,

$$\sum_w t^{|w|} = \sum_{n \geq 0} |\mathcal{S}|^n t^n = \frac{1}{1 - |\mathcal{S}|t},$$

is rational. Here, the sum runs over all walks  $w$ , and  $|w|$  denotes the length of  $w$ .

If we now confine walks to a (rational) half-space, typically by enforcing the first coordinate to be non-negative, then the resulting generating function becomes algebraic. This question was notably studied in one dimension (walks on the half-line  $\mathbb{N}$ ) [20, 16, 12, 2], but most methods can be extended to arbitrary dimension. These methods are effective and yield an explicit system of algebraic equations for the generating function.

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*Key words and phrases.* Lattice walks — Exact enumeration — D-finite series.

A.B. was supported by the Microsoft Research – Inria Joint Centre.

M.K. was supported by FWF Grants Y464-N18 and F50-04.

S.M. was supported by Inria, the Embassy of France in Canada, and an NSERC MSFSS.

In the past few years, the “next” natural case, namely walks confined to the intersection of two half-spaces, has been extensively studied in the form of walks on  $\mathbb{Z}^2$  confined to the positive quadrant  $\mathbb{N}^2$  [5, 8, 10, 11, 17, 18, 26, 31]. We call such walks *quadrant walks*. In the early days of this study, it was sometimes believed, from the inspection of examples, that the associated generating function was always *D-finite*, that is, satisfied a linear differential equation with polynomial coefficients. This is now known to be wrong, even for sets of *small* steps, that is, sets included in  $\{\bar{1}, 0, 1\}^2$ , with  $\bar{1} = -1$ . For example, the step set  $\mathcal{S} = \{(1, 1), (\bar{1}, 0), (0, \bar{1})\}$  is associated with a D-finite (and even algebraic) generating function [21, 9, 10], but D-finiteness is lost if the step  $(\bar{1}, \bar{1})$  is added [8].

In fact, Bousquet-Mélou and Mishna [11] observed that for quadrant walks with small steps, the nature of the generating function seemed to be correlated to the finiteness of a certain group of bi-rational transformations of the  $xy$ -plane associated with  $\mathcal{S}$ . Of the 79 non-equivalent step sets (or: *models*) under consideration, they proved that exactly 23 sets were associated with a finite group. Among them, they proved that 22 models admitted D-finite generating functions. The 23rd model with a finite group was proven D-finite (in fact, algebraic) by Bostan and Kauers [6]. These D-finiteness results extend to the trivariate generating functions that keep track of the length and the position of the endpoint. For 51 of the 56 models with an infinite group, Kurkova and Raschel [26] proved that this trivariate generating function is not D-finite, and Bostan *et al.* [8] proved that the (length) generating functions for walks returning to the origin is not D-finite. The nature of the length generating function for *all* quadrant walks is still unknown in those 51 cases. The remaining 5 models were proven to have non-D-finite length generating functions by Mishna and Reznitzer [31] and Melczer and Mishna [30].

It is now natural to move one dimension higher, and to study walks confined to the non-negative octant  $\mathbb{N}^3$ . A similar group of rational transformations can be defined: does the satisfactory dichotomy observed for quadrant walks (finite group  $\Leftrightarrow$  D-finite series) persist? Here, much less is known. Beyond a few explicit examples, all we have so far is an empirical classification by Bostan and Kauers [5] of the 83 682 (possibly trivial, possibly equivalent) models  $\mathcal{S} \subseteq \{\bar{1}, 0, 1\}^3 \setminus \{(0, 0, 0)\}$  with at most five steps. However, their paper does not discuss the associated group.

The aim of the present article is to initiate a systematic study of octant walks, their groups and their generating functions. We start from the 313 912 models with at most six steps, and apply various methods in order to identify provably and/or probably D-finite cases as well as probably non-D-finite cases. All our strategies for proving D-finiteness are illustrated by examples, and have been implemented. The software that accompanies this paper can be found on [Manuel Kauers’ website](#).

We now give an overview of the paper. First, we discard models that are in fact half-space models (and are thus algebraic), as well as models that are naturally in bijection to others (Section 2). This leaves us with (only) 35 548 models with at most six steps. Some of them are equivalent to a model of walks confined to the intersection of two half-spaces: we say they are *two-dimensional*. The remaining ones are said to be *three-dimensional*. The group of a model is defined at the end of Section 2.

In Section 3 we describe our experimental attempts to decide, for a given model, if the group is finite and if the generating function is D-finite. By the end of the paper we will have proven all our D-finiteness conjectures.

In Section 4 we present the so-called *algebraic kernel method*, a powerful tool that proves D-finiteness of many models with a finite group. This is a natural extension of the method applied in [11] to quadrant walks.

In Section 5 we show how the enumeration of walks of a *Hadamard model* reduces to the enumeration of certain quadrant walks. Together with the algebraic kernel method, this proves all our D-finiteness conjectures for three-dimensional models (Section 6). There remain 19 three-dimensional models with a finite group that may not be D-finite. Among them, a striking example is the 3D analogue of Kreweras' quadrant model [10].

In Section 7 we discuss 2-dimensional octant models. To simplify the discussion we only study their projection on the relevant quadrant. This includes the ordinary quadrant models studied earlier, but also models that have several copies of the same step. For all models with a finite group, we prove the D-finiteness of the generating function. In two cases, the only proofs we found are based on computer algebra. They are described in Section 8.

We conclude in Section 9 with some comments and questions.

## 2. PRELIMINARIES

Let  $\mathcal{S}$  be a subset of  $\{\bar{1}, 0, 1\}^3 \setminus \{(0, 0, 0)\}$ , which we think of as a set of *steps*, and often call *model*<sup>1</sup>. To shorten notation, we denote steps of  $\mathbb{Z}^3$  by three-letter words: for instance,  $\bar{1}10$  stands for the step  $(-1, 1, 0)$ . We say that a step is  $x$ -positive (abbreviated as  $x^+$ ) if its first coordinate is 1. We define similarly  $x^-$  steps,  $y^+$  steps and so on. Note that there are  $2^{26}$  different models.

We define an  $\mathcal{S}$ -walk to be any walk which starts from the origin  $(0, 0, 0)$  and takes its steps in  $\mathcal{S}$ . The present focus is on  $\mathcal{S}$ -walks that remain in the positive octant  $\mathbb{N}^3$ , with  $\mathbb{N} = \{0, 1, 2, \dots\}$ . We are interested in the generating function that counts them by the length (number of steps) and the coordinates of the endpoint:

$$O(x, y, z; t) = \sum_{i, j, k, n \geq 0} o(i, j, k; n) x^i y^j z^k t^n,$$

where  $o(i, j, k; n)$  is the number of  $n$ -step walks in the octant that end at position  $(i, j, k)$ . The dependence of our series on  $t$  is often omitted, writing for instance  $O(x, y, z)$  instead of  $O(x, y, z; t)$ , and this series is called the *complete* generating function of octant walks. We are particularly interested in the *nature* of this series: it is *rational* if it can be written as a ratio of polynomials, *algebraic* if there exists a non-zero polynomial  $P \in \mathbb{Q}[x, y, z, t, s]$  such that  $P(x, y, z, t, O(x, y, z; t)) = 0$ , and *D-finite* (with respect to the variable  $t$ ) if the vector space over  $\mathbb{Q}(x, y, z, t)$  spanned by the iterated derivatives  $D_t^m O(x, y, z; t)$  has finite dimension (here,  $D_t$  denotes differentiation with respect to  $t$ ). The latter definition can be adapted to D-finiteness in several variables, for instance  $x, y, z$  and  $t$ : in this case we require D-finiteness with respect to *each* variable separately [28]. Every rational series is algebraic, and every algebraic series is D-finite.

For a ring  $R$ , we denote by  $R[x]$  (resp.  $R[[x]]$ ) the ring of polynomials (resp. formal power series) in  $x$  with coefficients in  $R$ . If  $R$  is a field, then  $R(x)$  stands for the field of rational functions in  $x$ . This notation is generalised to several variables in the usual way. For instance,  $O(x, y, z; t)$  is a series of  $\mathbb{Q}[x, y, z][[t]]$ . Finally, if  $F(u; t)$  is a power series in  $t$  whose coefficients are Laurent series in  $u$ , say,

$$F(u; t) = \sum_{n \geq 0} t^n \left( \sum_{i \geq i(n)} u^i f(i; n) \right),$$

<sup>1</sup>Strictly speaking, a model would be a step set plus a region to which walks are confined, but the region will always be the non-negative octant in this paper, unless specified otherwise.

we denote by  $[u^{>0}]F(u; t)$  the *positive part of  $F$  in  $u$* :

$$[u^{>0}]F(u; t) = \sum_{n \geq 0} t^n \left( \sum_{i > 0} u^i f(i; n) \right).$$

This series can be obtained by taking a diagonal in a series involving one more variable:

$$[u^{>0}]F(u; t) = \Delta_{s,t} \left( \frac{s}{1-s} F(u/s, st) \right), \quad (1)$$

where the (linear) diagonal operator  $\Delta_{s,t}$  is defined by  $\Delta_{s,t}(s^i t^j) = \mathbb{1}_{i=j} t^j$ .

### 2.1. THE DIMENSION OF A MODEL

Let  $\mathcal{S}$  be a model. A walk of length  $n$  taking its steps in  $\mathcal{S}$  can be viewed as a word  $w = w_1 w_2 \dots w_n$  made up of letters of  $\mathcal{S}$ . For  $s \in \mathcal{S}$ , let  $a_s$  be the number of occurrences of  $s$  in  $w$  (also called multiplicity of  $s$  in  $w$ ). Then  $w$  ends in the positive octant if and only if the following three linear inequalities hold:

$$\sum_{s \in \mathcal{S}} a_s s_x \geq 0, \quad \sum_{s \in \mathcal{S}} a_s s_y \geq 0, \quad \sum_{s \in \mathcal{S}} a_s s_z \geq 0, \quad (2)$$

where  $s = (s_x, s_y, s_z)$ . Of course, the walk  $w$  remains in the octant if the multiplicities observed in each of its prefixes satisfy these inequalities.

**Example 1.** Take  $\mathcal{S} = \{0\bar{1}\bar{1}, \bar{1}10, \bar{1}11, 101\}$  (this is the third model of Figure 1). If we write  $a, b, c$  and  $d$  for the multiplicities of the four steps (taken in the above order), then the inequalities (2) read

$$d \geq b + c, \quad b + c \geq a, \quad c + d \geq a.$$

Note that if the first two inequalities hold, corresponding to a walk ending in the intersection of two half-spaces, then the third inequality is automatically satisfied.

**Definition 2.** Let  $d \in \{0, 1, 2, 3\}$ . A model  $\mathcal{S}$  is said to have dimension at most  $d$  if there exist  $d$  inequalities in (2) such that any  $|\mathcal{S}|$ -tuple  $(a_s)_{s \in \mathcal{S}}$  of non-negative integers satisfying these  $d$  inequalities satisfies in fact the three ones. We define accordingly models of dimension (exactly)  $d$ .

Examples are shown in Figure 1.



FIGURE 1. Four-step models of respective dimension 0, 1, 2 and 3. For each model, the first diagram shows steps of the form  $ij\bar{1}$ , the second shows steps  $ij0$ , and the third shows steps  $ij1$ .

It is clear that a model is 0-dimensional if and only if it is a subset of  $\{0, 1\}^3 \setminus \{000\}$ . Such models have a rational generating function:

$$O(x, y, z; t) = \frac{1}{1 - t \sum_{s \in \mathcal{S}} x^{s_x} y^{s_y} z^{s_z}}.$$

Let us also characterise models of dimension at most 1, or more precisely, those in which the first inequality in (2) (also called the *x-condition*) suffices to confine walks in the octant.

**Lemma 3.** Let  $\mathcal{S}$  be a model. The *y*- and *z*-conditions can be ignored when defining  $\mathcal{S}$ -walks in the octant if and only if the following two conditions hold:

- (a)  $\mathcal{S}$  contains no  $y^-$  step or every step  $ijk \in \mathcal{S}$  satisfies  $j \geq i$ ,

(b)  $\mathcal{S}$  contains no  $z^-$  step or every step  $ijk \in \mathcal{S}$  satisfies  $k \geq i$ .

*Proof.* Let us first recall the analogous result for quadrant walks [11, Section 2]: the  $y$ -condition can be ignored for a step set  $\mathcal{S} \subset \{\bar{1}, 0, 1\}^2$  if and only if  $\mathcal{S}$  contains no  $y^-$  step, or every step  $ij \in \mathcal{S}$  satisfies  $j \geq i$ .

Let us now consider a model in  $\mathbb{Z}^3$  such that the  $y$ - and  $z$ -conditions can be ignored. In particular, as soon as an  $\mathcal{S}$ -walk satisfies the  $x$ -condition, it satisfies the  $y$ -condition. By projecting walks on the  $xy$ -plane, and applying the above quadrant criterion, we see that either there are no  $y^-$  steps in  $\mathcal{S}$ , or any step  $ijk \in \mathcal{S}$  satisfies  $j \geq i$ . This is Condition (a). A symmetric argument proves (b). Conversely, it is easy to see that for any model satisfying (a) and (b), the  $y$ - and  $z$ -conditions can be ignored.  $\square$

For models of dimension at most 1, it suffices to enforce one of the three conditions for the other two to hold. This means that we are effectively counting walks confined to a half-space delimited, e.g., by the plane  $x = 0$ . As recalled in the introduction, such walks are known to have an algebraic generating function, and the proof of algebraicity is constructive. For these reasons, we do not discuss further 0- or 1-dimensional models.

For 2-dimensional models, we have not found an intrinsic characterisation that would be the counterpart of Lemma 3. In order to determine whether a given model is (at most) 2-dimensional, we used integer linear programming [35], as follows. For a model  $\mathcal{S}$  of cardinality  $m$  define the three linear forms  $I_1, I_2, I_3$  in the  $m$  variables  $(a_s)_{s \in \mathcal{S}}$  by (2). One condition, say the third, is redundant if the non-negativity of the corresponding linear form is implied by the non-negativity of the two others, e.g., if for all  $(a_s)_{s \in \mathcal{S}} \in \mathbb{N}^m$  we have  $(I_1 \geq 0) \wedge (I_2 \geq 0) \Rightarrow I_3 \geq 0$ . To check algorithmically whether this is the case we minimise the objective function  $I_3$  under the constraints  $I_1 \geq 0$  and  $I_2 \geq 0$  (and  $a_s \geq 0$  for all  $s$ ). The third condition is redundant if and only if the minimum is zero.

To check whether a given model has dimension at most two thus requires checking whether

$$(I_1 \geq 0) \wedge (I_2 \geq 0) \Rightarrow I_3 \geq 0 \quad \text{or} \quad (I_1 \geq 0) \wedge (I_3 \geq 0) \Rightarrow I_2 \geq 0 \\ \text{or} \quad (I_2 \geq 0) \wedge (I_3 \geq 0) \Rightarrow I_1 \geq 0.$$

This can be done by solving three small integer linear programming problems. It is worth mentioning that in each 2-dimensional case that we discovered, the 2-dimensionality can be explained (up to a permutation of coordinates) by the existence of two non-negative numbers  $\alpha$  and  $\beta$  such that for any  $ijk \in \mathcal{S}$ ,

$$k \geq \alpha i + \beta j.$$

The pairs  $(\alpha, \beta)$  that we find are  $(0, 0)$ ,  $(1, 0)$ ,  $(1, 1)$ ,  $(1/2, 1/2)$  and  $(1, 2)$ . In Example 1, this inequality holds for  $\alpha = \beta = 1$ .

## 2.2. EQUIVALENT MODELS

Two models are said to be *equivalent* if they only differ by a permutation of the step coordinates, or if they only differ by *unused steps*, that is, steps that are never used in a walk confined to the octant.

**Lemma 4.** *The model  $\mathcal{S}$  contains unused steps if and only if one of the following conditions holds:*

- (A<sub>x</sub>)  $\mathcal{S}$  contains an  $x^-$  step, but no  $x^+$  step,
- (B)  $\mathcal{S}$  is non-empty, and each step of  $\mathcal{S}$  has a negative coordinate,
- (C<sub>z</sub>)  $\mathcal{S}$  contains 001, any step  $ijk$  of  $\mathcal{S}$  satisfies  $i + j \leq 0$ , and  $\mathcal{S} \not\subset \{001, 00\bar{1}\}$ ,

(D) there exists a permutation of the coordinates which, applied to  $\mathcal{S}$ , gives a step set satisfying  $A_x$  or  $C_z$ .

In Case  $A_x$ , every  $x^-$  step is unused. In Case  $B$ , all steps are unused. In Case  $C_z$  all steps with a negative  $x$ - or  $y$ -coordinate are unused.

*Proof.* Let  $s$  be an unused step. Let us prove that  $s$  has at least one negative coordinate, say along the  $x$ -direction, such that all  $x^+$ -steps (if any) are also unused. We prove this by contradiction. Assume that for any negative coordinate of  $s$  there exists a used step which is positive in this direction. Let  $u_1, u_2, \dots$  be a collection of such used steps (at most three of them), one for each negative coordinate of  $s$ . Take an octant walk ending with  $u_1$ , concatenate it with an octant walk ending with  $u_2$ , and so on to obtain finally a walk  $w$ . Adding  $s$  at the end of  $w$  gives an octant walk containing  $s$ . We have thus reached a contradiction, and proved our statement.

So let us assume that  $\mathcal{S}$  contains an unused step with a negative  $x$ -coordinate, and that all  $x^+$  steps of  $\mathcal{S}$ , if any, are unused. Then all  $x^-$  steps are unused. If there is no  $x^+$  step, we are in Case  $A_x$ . Now assume that there are  $x^+$  steps, but that all of them are unused. Let us then prove that  $B$  or  $C_z$  (or its variant  $C_y$ ) holds.

- If each step of  $\mathcal{S}$  has a negative coordinate (Case  $B$ ), then all steps are indeed unused.
- We now assume that  $\mathcal{S}$  contains a non-negative step, that is, a step in  $\{0, 1\}^3$ . The steps 111, 110, 101 and 100 cannot belong to  $\mathcal{S}$ , since they are  $x^+$  and used. The step 011 cannot belong to  $\mathcal{S}$  either, otherwise any  $x^+$  step would be used.
- We are thus left with sets in which the non-negative steps are 001 and/or 010. In fact, they cannot be both in  $\mathcal{S}$ , otherwise any  $x^+$  step would be used. So assume that the only non-negative step of  $\mathcal{S}$  is 001. This forces every  $x^+$  step to be  $y^-$  (otherwise it would be used), and conversely every  $y^+$  step must be  $x^-$  (otherwise any  $x^+$  step would be used). In other words, we are in Case  $C_z$ .

The rest of the lemma is obvious.  $\square$

### 2.3. THE NUMBER OF NON-EQUIVALENT MODELS OF DIMENSION 2 OR 3

We now determine how many models are left when we discard models of dimension at most 1, models with unused steps, and when we moreover identify models that only differ by a permutation of the coordinates. We count these models by their cardinality.

**Proposition 5.** *The generating function of models having dimension 2 or 3, no unused step, and counted up to permutations of the coordinates, is*

$$\begin{aligned} I = & 73 u^3 + 979 u^4 + 6425 u^5 + 28071 u^6 + 91372 u^7 + 234716 u^8 + 492168 u^9 \\ & + 860382 u^{10} + 1271488 u^{11} + 1603184 u^{12} + 1734396 u^{13} + 1614372 u^{14} \\ & + 1293402 u^{15} + 890395 u^{16} + 524638 u^{17} + 263008 u^{18} + 111251 u^{19} \\ & + 39256 u^{20} + 11390 u^{21} + 2676 u^{22} + 500 u^{23} + 73 u^{24} + 9 u^{25} + u^{26}. \end{aligned}$$

This is big (11 074 225 models), but more encouraging than

$$(1 + u)^{26} = 1 + 26 u + 325 u^2 + 2600 u^3 + 14950 u^4 + 65780 u^5 + 230230 u^6 + O(u^7).$$

In particular, the number of non-equivalent interesting models of cardinality at most 6 is 35 548, which is about 9 times less than  $1 + 26 + \dots + 230230 = 313\,912$ .

The proof of this proposition involves inclusion-exclusion, Burnside's lemma, and the above characterisations of 0- and 1-dimensional models and of models with unused steps. We first determine the polynomial  $J$  that counts, up to permutations of the coordinates, sets having no unused step. We then subtract from  $J$  the polynomial  $K$  that counts models of dimension at most 1. The proof is rather tedious and given in Appendix A.

#### 2.4. THE GROUP OF THE MODEL

Given a model  $\mathcal{S}$ , we denote by  $S$  the Laurent polynomial

$$S(x, y, z) = \sum_{ijk \in \mathcal{S}} x^i y^j z^k, \quad (3)$$

and write

$$\begin{aligned} S(x, y, z) &= \bar{x}A_-(y, z) + A_0(y, z) + xA_+(y, z) \\ &= \bar{y}B_-(x, z) + B_0(x, z) + yB_+(x, z) \\ &= \bar{z}C_-(x, y) + C_0(x, y) + zC_+(x, y) \end{aligned} \quad (4)$$

where  $\bar{x} = 1/x$ ,  $\bar{y} = 1/y$  and  $\bar{z} = 1/z$ . We call  $S$  the *characteristic polynomial* of  $\mathcal{S}$ .

Let us first assume that  $\mathcal{S}$  is 3-dimensional. Then it has a positive step in each direction, and  $A_+$ ,  $B_+$  and  $C_+$  are non-zero. The *group of  $\mathcal{S}$*  is the group  $G$  of birational transformations of the variables  $[x, y, z]$  generated by the following three involutions:

$$\begin{aligned} \phi([x, y, z]) &= \left[ \bar{x} \frac{A_-(y, z)}{A_+(y, z)}, y, z \right], & \psi([x, y, z]) &= \left[ x, \bar{y} \frac{B_-(x, z)}{B_+(x, z)}, z \right], \\ \tau([x, y, z]) &= \left[ x, y, \bar{z} \frac{C_-(x, y)}{C_+(x, y)} \right]. \end{aligned}$$

By construction,  $G$  fixes the Laurent polynomial  $S(x, y, z)$ .

For a 2-dimensional model in which the  $z$ -condition can be ignored, the relevant group is the group generated by  $\phi$  and  $\psi$ .

### 3. COMPUTER PREDICTIONS AND SUMMARY OF THE RESULTS

We focus in this paper on models with at most 6 steps. Given such a model  $\mathcal{S}$ , we compute the first 1000 terms of the series  $O(x_0, y_0, z_0; t)$ , for all  $(x_0, y_0, z_0) \in \{0, 1\}^3$ , using the following step-by-step recurrence relation for the coefficients of  $O(x, y, z; t)$ :

$$o(i, j, k; n) = \begin{cases} 0 & \text{if } i < 0 \text{ or } j < 0 \text{ or } k < 0, \\ \mathbb{1}_{i=j=k=0} & \text{if } n = 0, \\ \sum_{abc \in \mathcal{S}} o(i-a, j-b, k-c; n-1) & \text{otherwise.} \end{cases} \quad (5)$$

From these numbers, we try to guess a differential equation (in  $t$ ) satisfied by  $O(x_0, y_0, z_0; t)$  using the techniques described in [5] and the references therein.

As described above in Section 2.4, we associate to  $\mathcal{S}$  a group  $G$  of rational transformations. Inspired by the quadrant case [11], where the finiteness of the group is directly correlated to the D-finiteness of the generating function, we also try to determine experimentally if  $G$  is finite. The procedure is easy: one simply writes out all words in  $\phi$ ,  $\psi$ , and  $\tau$  of some length  $N$ , removes words which correspond to the same transformation, and checks whether or not the remaining elements form a group (if not then this process is repeated with a larger  $N$ ).

Before we summarise our results for octant walks, let us recall those obtained for quadrant walks (Table 1). The most striking feature is of course the equivalence





Table 2 summarises our conjectures and results for 3D octant models. We find 170 groups of finite order (in fact, of order at most 48). The remaining ones have order at least 200. All models for which the length generating function  $O(1, 1, 1; t)$  was conjectured D-finite have a finite group, and we have in fact proved that their complete generating function  $O(x, y, z; t)$  is D-finite in its four variables. The table tells which of our main two methods (the kernel method and the Hadamard decomposition) proves D-finiteness. The main difference with the quadrant case is the following: *for 19 models with a finite group and zero orbit sum, we have not been able to guess differential equations, and it may be that these models are not D-finite*. Details are given in Section 6. In particular, we have computed much more than 1000 coefficients for these 19 intriguing models. Another difference between Tables 1 and 2 is the disappearance of algebraic models. For some models  $\mathcal{S}$ , we find certain algebraic specialisations  $O(x_0, y_0, z_0; t)$ . But then the walks counted by this series do not use all steps of  $\mathcal{S}$ , and deleting the unused steps leaves a model of lower dimension. We conjecture that, apart from these degenerate cases, there is no transcendental series in 3D models. In particular, we believe  $O(x, y, z; t)$  to be transcendental.

For 2D octant models, we have only studied the projection of the walks on the relevant quadrant. Since several 3D steps may project on the same 2D step, this means studying a quadrant model with steps *in a multiset*. It seems that the dichotomy established earlier for quadrant walks without multiple steps still holds: all models for which we found a finite group have been proved D-finite, and the others are conjectured to have an infinite group and to be non-D-finite. See Section 7 for details and a table classifying these models. Four D-finite models, shown in Figure 5, turn out to be especially interesting.

#### 4. THE ALGEBRAIC KERNEL METHOD

In this section, we adapt to octant walks the material developed for quadrant walks in Sections 3 and 4 of [11]. It will allow us to prove D-finiteness for a large number of models.

##### 4.1. A FUNCTIONAL EQUATION

Let  $\mathcal{S}$  be a model with associated generating function  $O(x, y, z; t) \equiv O(x, y, z)$ . Recall the definitions (3) and (4) of the characteristic polynomial of  $\mathcal{S}$  and of the polynomials  $A_+$ ,  $A_0$ ,  $A_-$ , etc. We also let

$$D_-(z) = [\bar{x}\bar{y}]S(x, y, z) := \sum_{k \text{ s.t. } \bar{1}\bar{1}k \in \mathcal{S}} z^k,$$

and define similarly

$$E_-(y) = [\bar{x}\bar{z}]S(x, y, z) \quad \text{and} \quad F_-(x) = [\bar{y}\bar{z}]S(x, y, z).$$

Finally, let  $\varepsilon$  be 1 if  $\bar{1}\bar{1}\bar{1}$  belongs to  $\mathcal{S}$  and 0 otherwise. The following functional equation translates the fact that a walk of length  $n$  must be a walk of length  $n - 1$  followed by a step in  $\mathcal{S}$ , provided that this step does not take the walk out of the octant:

$$\begin{aligned} O(x, y, z) &= 1 + tS(x, y, z)O(x, y, z) \\ &\quad - t\bar{x}A_-(y, z)O(0, y, z) - t\bar{y}B_-(x, z)O(x, 0, z) - t\bar{z}C_-(x, y)O(x, y, 0) \\ &\quad + t\bar{x}\bar{y}D_-(z)O(0, 0, z) + t\bar{x}\bar{z}E_-(y)O(0, y, 0) + t\bar{y}\bar{z}F_-(x)O(x, 0, 0) \\ &\quad - \varepsilon t\bar{x}\bar{y}\bar{z}O(0, 0, 0). \end{aligned} \tag{6}$$

The terms on the last three lines ensure that the restriction to the positive octant is enforced, and are given by the inclusion-exclusion principle. This is the series counterpart of the recurrence relation (5).

If the model is only 2-dimensional, so that, for instance, the positivity condition in the third variable can be ignored, the following simpler equation holds:

$$\begin{aligned} O(x, y, z) &= 1 + tS(x, y, z)O(x, y, z) \\ &\quad - t\bar{x}A_-(y, z)O(0, y, z) - t\bar{y}B_-(x, z)O(x, 0, z) \\ &\quad + t\bar{x}\bar{y}D_-(z)O(0, 0, z). \end{aligned} \quad (7)$$

It is then of the same nature as the equations studied for quadrant models, with the variable  $z$  playing no particular role [11].

#### 4.2. ORBIT SUMS FOR FINITE GROUPS

Let us multiply (6) by  $xyz$  and group the terms involving  $O(x, y, z)$ . This gives

$$\begin{aligned} xyzK(x, y, z)O(x, y, z) &= xyz - tyzA_-(y, z)O(0, y, z) \\ &\quad - txzB_-(x, z)O(x, 0, z) - txyC_-(x, y)O(x, y, 0) \\ &\quad + tzD_-(z)O(0, 0, z) + tyE_-(y)O(0, y, 0) + txF_-(x)O(x, 0, 0) \\ &\quad - t\varepsilon O(0, 0, 0). \end{aligned} \quad (8)$$

where  $K(x, y, z) := 1 - tS(x, y, z)$  is the *kernel* of the model. If the model is 2-dimensional (with the  $z$ -condition redundant), the terms in  $C_-$ ,  $E_-$ ,  $F_-$  and  $\varepsilon$  are not there, see (7). What is important in the above equation is that all unknown summands on the right-hand side involve at most two of the three variables  $x$ ,  $y$  and  $z$ . For instance, the second term,  $tyzA_-(y, z)O(0, y, z)$ , does not involve  $x$ .

Assume that the group  $G$  is finite. Let us write the  $|G|$  equations obtained from (8) by replacing the 3-tuple  $(x, y, z)$  by any element of its orbit. Then, we form the alternating sum of these  $|G|$  equations by weighting each of them by the sign of the corresponding group element (that is, minus one to the length of a minimal word in  $\phi, \psi$  and  $\tau$  that expresses it). Since each unknown term on the right-hand side involves at most two of the three variables  $x, y, z$ , and each of the involutions  $\phi, \psi$  and  $\tau$  fixes one coordinate, all unknown series cancel on the right-hand side, leaving:

$$\sum_{g \in G} \text{sign}(g) g(xyzO(x, y, z)) = \frac{1}{K(x, y, z)} \sum_{g \in G} \text{sign}(g)g(xyz), \quad (9)$$

where, for any series  $T(x, y, z)$  and any element  $g$  of  $G$ , the term  $g(T(x, y, z))$  must be understood as  $T(g(x, y, z))$ . The right-hand side is now an explicit rational function, called the *orbit sum*. In the left-hand side, we have a formal power series in  $t$  with coefficients in  $\mathbb{Q}(x, y, z)$ . We call (9) the *orbit equation*.

Assume that all the coordinates of all elements in the orbit of  $[x, y, z]$  are *Laurent polynomials* in  $x, y$  and  $z$ . This happens for instance in the example of Section 4.3 below (the orbit is shown in Figure 3). Assume moreover that for any element  $[x', y', z']$  in the orbit, other than  $[x, y, z]$ , there exists a variable, say  $x$ , such that  $x', y'$  and  $z'$  are in fact polynomials in  $\bar{x}$ . This is again true in Figure 3. Then the series  $x'y'z'O(x', y', z')$  occurring in the left-hand side of (9) consist of monomials  $x^i y^j z^k t^n$  where at least one of  $i, j$  and  $k$  is non-positive. In this case, extracting from (9) the monomials with positive exponents in  $x, y$  and  $z$  gives

$$xyzO(x, y, z; t) = [x^{>0}][y^{>0}][z^{>0}] \frac{1}{K(x, y, z; t)} \sum_{g \in G} \text{sign}(g)g(xyz). \quad (10)$$

By (1), the positive part of a series can be expressed as a diagonal. Thus  $O(x, y, z; t)$  is a diagonal of a rational series, and is D-finite in its four variables [27, 28].

More generally, the above identity holds if every orbit element  $[x', y', z']$  other than  $[x, y, z]$  satisfies:

$$\begin{aligned} \{x', y', z'\} \subset \mathbb{Q}(x, y)[\bar{z}] \quad \text{or} \quad \{x', y', z'\} \subset \mathbb{Q}(x)[\bar{y}, z] \\ \text{or} \quad \{x', y', z'\} \subset \mathbb{Q}[\bar{x}, y, z]. \end{aligned} \quad (11)$$

Indeed, in this case, the coefficient of  $t^n$  in  $x'y'z'O(x', y', z'; t)$ , once expanded as a (Laurent) series in  $z$ , then  $y$ , then  $x$ , consists of monomials with at least one non-positive exponent. Extracting the monomials where all exponents are positive gives (10). An example is detailed in Section 4.4.

Condition (11) does not cover all cases where the extraction of monomials with positive exponents in  $x$ ,  $y$  and  $z$  leads to (10). Two interesting two-dimensional examples are discussed in Section 7.2.

This procedure is what we call the *algebraic kernel method*.

#### 4.3. FIRST ILLUSTRATION OF THE KERNEL METHOD

Consider the step set  $\mathcal{S} = \{\bar{1}\bar{1}\bar{1}, \bar{1}\bar{1}1, \bar{1}10, 100\}$ . Denoting by  $a, b, c$  and  $d$  the number of steps of each type in an  $\mathcal{S}$ -walk, the positivity conditions read

$$d \geq a + b + c, \quad c \geq a + b, \quad b \geq a,$$

and it is clear that none is redundant. So the model is 3-dimensional. The functional equation (6) reads in this case

$$\begin{aligned} K(x, y, z)O(x, y, z) = 1 - t\bar{x}(y + \bar{y}z + \bar{y}\bar{z})O(0, y, z) - t\bar{x}\bar{y}(z + \bar{z})O(x, 0, z) - t\bar{x}\bar{y}\bar{z}O(x, y, 0) \\ + t\bar{x}\bar{y}(z + \bar{z})O(0, 0, z) + t\bar{x}\bar{y}\bar{z}O(0, y, 0) + t\bar{x}\bar{y}\bar{z}O(x, 0, 0) - t\bar{x}\bar{y}\bar{z}O(0, 0, 0), \end{aligned}$$

where the kernel is

$$K(x, y, z) = 1 - t(\bar{x}\bar{y}\bar{z} + \bar{x}\bar{y}z + \bar{x}y + x).$$

The images of  $[x, y, z]$  by the involutions  $\phi$ ,  $\psi$  and  $\tau$  are respectively

$$[\bar{x}(y + \bar{y}z + \bar{y}\bar{z}), y, z], \quad [x, \bar{y}(z + \bar{z}), z], \quad [x, y, \bar{z}].$$

By composing these involutions, one observes that they generate a group of order 8, shown in Figure 3. In fact,  $\phi$ ,  $\psi$  and  $\tau$  commute. Note that all coordinates in the orbit are Laurent polynomials in  $x$ ,  $y$  and  $z$ . The orbit equation (9) reads

$$\begin{aligned} xyzO(x, y, z) - \bar{x}yz(y + \bar{y}z + \bar{y}\bar{z})O(\bar{x}(y + \bar{y}z + \bar{y}\bar{z}), y, z) - x\bar{y}z(z + \bar{z})O(x, \bar{y}(z + \bar{z}), z) \\ - x\bar{y}\bar{z}O(x, y, \bar{z}) + \bar{x}\bar{y}z(y + \bar{y}z + \bar{y}\bar{z})(z + \bar{z})O(\bar{x}(y + \bar{y}z + \bar{y}\bar{z}), \bar{y}(z + \bar{z}), z) \\ + \bar{x}\bar{y}\bar{z}(y + \bar{y}z + \bar{y}\bar{z})O(\bar{x}(y + \bar{y}z + \bar{y}\bar{z}), y, \bar{z}) + x\bar{y}\bar{z}(z + \bar{z})O(x, \bar{y}(z + \bar{z}), \bar{z}) \\ - \bar{x}\bar{y}\bar{z}(y + \bar{y}z + \bar{y}\bar{z})(z + \bar{z})O(\bar{x}(y + \bar{y}z + \bar{y}\bar{z}), \bar{y}(z + \bar{z}), \bar{z}) \\ = \frac{(x - \bar{x}y - \bar{x}\bar{y}z - \bar{x}\bar{y}\bar{z})(y - \bar{y}z - \bar{y}\bar{z})(z - \bar{z})}{xyzK(x, y, z)}. \end{aligned}$$

Now let us examine the eight unknown series occurring in the left-hand side. The series  $xyzO(x, y, z)$  is *positive* in  $x$ ,  $y$  and  $z$ , meaning that all its monomials involve a positive power of each variable. In contrast, each of the other seven series is non-positive (and in fact, negative) in at least one variable, because Condition (11) holds. Hence, extracting the positive part in the above identity gives

$$xyzO(x, y, z) = [x^{>0}][y^{>0}][z^{>0}] \frac{(x - \bar{x}y - \bar{x}\bar{y}z - \bar{x}\bar{y}\bar{z})(y - \bar{y}z - \bar{y}\bar{z})(z - \bar{z})}{xyz(1 - t(\bar{x}\bar{y}\bar{z} + \bar{x}\bar{y}z + \bar{x}y + x))}.$$

We thus conclude that  $O(x, y, z; t)$  is D-finite in all variables. Moreover, the coefficient extraction can be performed explicitly, and gives rise to nice coefficients. Details of the extraction are left to the reader.

**Proposition 6.** *For the model  $\mathcal{S} = \{\bar{1}\bar{1}\bar{1}, \bar{1}\bar{1}1, \bar{1}10, 100\}$ , the number of walks of length  $n$  ending at  $(i, j, k)$  is non-zero if and only if  $n$  can be written  $8m + i + 2j + 4k$ , in which case*

$$o(i, j, k; n) = \frac{(i+1)(j+1)(k+1)n!}{(4m+i+j+2k+1)!(2m+j+k+1)!(m+k+1)!m!}.$$

**Note.** Throughout the paper,  $m!$  is defined to be infinite if  $m < 0$ .

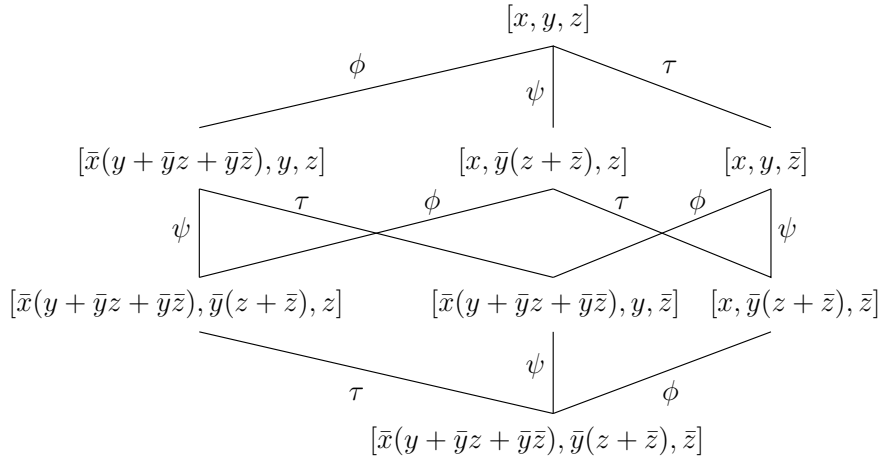


FIGURE 3. The orbit of  $[x, y, z]$  under the group generated by  $\phi$ ,  $\psi$  and  $\tau$ , when  $\mathcal{S} = \{\bar{1}\bar{1}\bar{1}, \bar{1}\bar{1}1, \bar{1}10, 100\}$ .

#### 4.4. SECOND ILLUSTRATION OF THE KERNEL METHOD

Let us now take  $\mathcal{S} = \{\bar{1}0\bar{1}, \bar{1}11, 0\bar{1}1, 10\bar{1}, 111\}$ . This model is also 3-dimensional. The functional equation (6) reads

$$K(x, y, z)O(x, y, z) = 1 - t\bar{x}(\bar{z} + yz)O(0, y, z) - t\bar{y}zO(x, 0, z) \\ - t\bar{z}(x + \bar{x})O(x, y, 0) + t\bar{x}\bar{z}O(0, y, 0),$$

where

$$K(x, y, z) = 1 - t(\bar{x}\bar{z} + \bar{x}yz + \bar{y}z + x\bar{z} + xyz).$$

The images of  $[x, y, z]$  by the involutions  $\phi$ ,  $\psi$  and  $\tau$  are respectively

$$[\bar{x}, y, z], \quad \left[ x, \frac{\bar{y}}{x + \bar{x}}, z \right], \quad \left[ x, y, \bar{z} \frac{x + \bar{x}}{\bar{y} + y(x + \bar{x})} \right].$$

As in the previous example, these three involutions commute, and thus generate a group of order 8. The coefficients of the series occurring in the orbit equation are

rational functions in  $x, y$  and  $z$ , but no longer Laurent polynomials:

$$\begin{aligned}
&xyzO(x, y, z) - \bar{x}y\bar{z}O(\bar{x}, y, z) - \frac{x\bar{y}z}{x + \bar{x}}O\left(x, \frac{\bar{y}}{x + \bar{x}}, z\right) \\
&\quad - \frac{xy\bar{z}(x + \bar{x})}{\bar{y} + y(x + \bar{x})}O\left(x, y, \frac{\bar{z}(x + \bar{x})}{\bar{y} + y(x + \bar{x})}\right) + \frac{\bar{x}\bar{y}z}{x + \bar{x}}O\left(\bar{x}, \frac{\bar{y}}{x + \bar{x}}, z\right) \\
&+ \frac{\bar{x}y\bar{z}(x + \bar{x})}{\bar{y} + y(x + \bar{x})}O\left(\bar{x}, y, \frac{\bar{z}(x + \bar{x})}{\bar{y} + y(x + \bar{x})}\right) + \frac{x\bar{y}\bar{z}}{\bar{y} + y(x + \bar{x})}O\left(x, \frac{\bar{y}}{x + \bar{x}}, \frac{\bar{z}(x + \bar{x})}{\bar{y} + y(x + \bar{x})}\right) \\
&\quad - \frac{\bar{x}\bar{y}\bar{z}}{\bar{y} + y(x + \bar{x})}O\left(\bar{x}, \frac{\bar{y}}{x + \bar{x}}, \frac{\bar{z}(x + \bar{x})}{\bar{y} + y(x + \bar{x})}\right) \\
&\quad = \frac{x - \bar{x}}{x + \bar{x}} \cdot \frac{\bar{y} - y(x + \bar{x})}{\bar{y} + y(x + \bar{x})} \cdot \frac{\bar{x}\bar{z} - \bar{x}yz - \bar{y}z + x\bar{z} - xyz}{K(x, y, z)}.
\end{aligned}$$

However, we observe that for any series  $O(x', y', z')$  occurring in this equation, other than  $O(x, y, z)$ , the variables  $x', y', z'$  satisfy Condition (11). By extracting the positive part first in  $z$ , then in  $y$ , and finally in  $x$ , we thus obtain:

$$xyzO(x, y, z) = [x^{>0}][y^{>0}][z^{>0}] \frac{x - \bar{x}}{x + \bar{x}} \cdot \frac{\bar{y} - y(x + \bar{x})}{\bar{y} + y(x + \bar{x})} \cdot \frac{\bar{x}\bar{z} - \bar{x}yz - \bar{y}z + x\bar{z} - xyz}{K(x, y, z)},$$

so that  $O(x, y, z; t)$  is again D-finite. Moreover, the coefficient extraction can be performed explicitly and gives rise to nice numbers. Details are left to the reader.

**Proposition 7.** *For the model  $\mathcal{S} = \{\bar{1}0\bar{1}, \bar{1}1\bar{1}, 0\bar{1}\bar{1}, 10\bar{1}, 11\bar{1}\}$ , the number of walks of length  $n$  ending at  $(i, j, k)$  is non-zero if and only if  $n$  can be written  $8m + 4i + 2j + 3k$ , in which case*

$$\begin{aligned}
o(i, j, k; n) &= \frac{(i + 1)(j + 1)(k + 1)}{(4m + 2i + j + 2k + 1)} \frac{(6m + 3i + 2j + 2k)!}{(3m + 2i + j + k + 1)!(3m + i + j + k)!} \\
&\quad \frac{n!}{(2m + i + k)!(2m + i + j + k + 1)!(4m + 2i + j + k)!}.
\end{aligned}$$

#### 4.5. WHEN THE ORBIT EQUATION DOES NOT SUFFICE

In the study of quadrant walks, there are four models with a finite group for which the complete generating function, denoted by  $Q(x, y)$ , cannot be extracted from the orbit equation

$$\sum_{g \in G} \text{sign}(g) g(xyQ(x, y)) = \frac{1}{K(x, y)} \sum_{g \in G} \text{sign}(g) g(xy).$$

They are shown in Figure 2. In each case, the orbit sum happens to be 0. This implies that  $Q(x, y) = 1$  solves the orbit equation, which does not determine  $Q(x, y; t)$  uniquely. Three of these four models can be solved using a half-orbit sum, followed by a more delicate extraction procedure [11]. The fourth one was first solved using intensive computer algebra [23, 6], and more recently using complex analysis [7].

For models in  $\mathbb{Z}^3$ , it also happens that we find a finite group but a non-conclusive orbit equation. This happens for 62 three-dimensional models, and then the orbit sum is zero<sup>2</sup>. This is the case for instance with  $S(x, y, z) = \bar{x} + xyz + x\bar{y} + x\bar{z}$ , or for the 3-dimensional analogue of Kreweras' walks,  $S'(x, y, z) = \bar{x} + \bar{y} + \bar{z} + xyz$ . For 43 of these 62 models, including  $S$ , we were able to guess differential equations, and we have then proved the D-finiteness of  $O(x, y, z; t)$  via a combinatorial construction described in Section 5 below. For the 19 others models, including  $S'$ , we have not

<sup>2</sup>For 2D octant models, we also find one non-conclusive orbit equation with a non-zero orbit sum, see Section 8.2 for details.

been able to guess any differential equation nor to prove D-finiteness. We refer to Section 6.2 for details on these 19 models.

## 5. HADAMARD WALKS

In this section, we describe how the study of some 3-dimensional models — called *Hadamard models* — can be reduced to the study of a pair of models, one in  $\mathbb{Z}$  and the other in  $\mathbb{Z}^2$ . Let us begin with an example.

### 5.1. EXAMPLE

Let  $\mathcal{S}$  be the step set with characteristic polynomial

$$S(x, y, z) = x + (1 + x + \bar{x})(yz + \bar{y} + \bar{z}).$$

The associated group is finite of order 12. The orbit of  $[x, y, z]$  contains  $[x, z, y]$ , and thus the orbit sum is zero. We will prove the D-finiteness of the series  $O(x, y, z; t)$  using a combinatorial argument.

Write  $U = x$ ,  $V = 1 + x + \bar{x}$ ,  $T = yz + \bar{y} + \bar{z}$ , so that  $S = U + VT$ . Let  $\mathcal{U}$ ,  $\mathcal{V}$  and  $\mathcal{T}$  denote the corresponding step sets, respectively in  $\{\bar{1}, 0, 1\}$  (for  $\mathcal{U}$  and  $\mathcal{V}$ ) and  $\{\bar{1}, 0, 1\}^2$  (for  $\mathcal{T}$ ). We thus have

$$\mathcal{S} = (\mathcal{U} \times \{0\}^2) \cup (\mathcal{V} \times \mathcal{T}),$$

and the union is disjoint.

Consider now an octant walk  $w$  with steps in  $\mathcal{S}$ , and project it on the  $x$ -axis. This gives a walk on  $\mathbb{N}$  with steps  $\bar{1}$ , 0 and 1. Colour white the steps that are projections of a step of  $\mathcal{U} \times \{0\}^2$  (that is, of a step 100), and colour black the projections of the steps of  $\mathcal{V} \times \mathcal{T}$ . This gives a coloured walk  $w_1$ . Now return to  $w$  and delete the steps of  $\mathcal{U} \times \{0\}^2$  (that is, the steps 100). The resulting walk lives in  $\mathbb{Z} \times \mathbb{N}^2$ . Project it on the  $yz$ -plane to obtain a second walk  $w_2$ , which has steps in  $\mathcal{T}$  and is a quarter plane walk.

The walk  $w$  can be recovered from  $w_1$  and  $w_2$  as follows. Start from  $w_1$ , and leave the white steps unchanged. Replace the  $j$ th black step of  $w_1$ , with value  $a \in \{\bar{1}, 0, 1\}$ , by  $abc$ , where  $bc \in \mathcal{T}$  is the  $j$ th step of  $w_2$ .

Conversely, let  $w_1$  be a walk in  $\mathbb{N}$  with steps in  $\mathcal{U} \cup \mathcal{V}$  having black and white steps, such that all steps of  $\mathcal{U} \setminus \mathcal{V}$  are white and all steps of  $\mathcal{V} \setminus \mathcal{U}$  are black. In other words, the only steps for which we can choose the colour are those of  $\mathcal{U} \cap \mathcal{V}$ . Let  $w_2$  be a walk in  $\mathbb{N}^2$  with steps in  $\mathcal{T}$ , whose length coincides with the number of black steps in  $w_1$ . Then the walk  $w$  constructed from  $w_1$  and  $w_2$  as described above is an octant walk with steps in  $\mathcal{S}$ .

Let  $C_1(x, v; t)$  be the generating function of coloured walks like  $w_1$ , counted by the length ( $t$ ), the number of black steps ( $v$ ) and the coordinate of the endpoint ( $x$ ). Let  $C_2(y, z; v)$  be the generating function of walks like  $w_2$ , counted by the length ( $v$ ) and the coordinates of the endpoint ( $y, z$ ). The above construction shows that

$$O(x, y, z; t) = C_1(x, v; t) \odot_v C_2(y, z; v)|_{v=1},$$

where  $\odot_v$  denotes the Hadamard product with respect to  $v$ :

$$\sum_i a_i v^i \odot_v \sum_j b_j v^j = \sum_i a_i b_i v^i,$$

and the resulting series is specialised to  $v = 1$ .

In our example,  $C_1(x, v; t)$  counts (coloured) walks on  $\mathbb{N}$  and is easily seen to be algebraic, while  $C_2(y, z; v)$  is the generating function of Kreweras walks, which is also algebraic [10]. Since the Hadamard product preserves D-finiteness [27], we conclude that  $O(x, y, z; t)$  is D-finite.

## 5.2. DEFINITION AND ENUMERATION OF HADAMARD WALKS

We can now generalise the above discussion to count octant walks for *Hadamard models*. Since this discussion works in all dimensions, we actually consider walks in  $\mathbb{N}^D$ , starting from the origin and taking their steps in a set  $\mathcal{S} \subset \{\bar{1}, 0, 1\}^D \setminus \{(0, \dots, 0)\}$ . We denote by  $S(x_1, \dots, x_D)$  the characteristic polynomial of  $\mathcal{S}$ :

$$S(x_1, \dots, x_D) = \sum_{(i_1, \dots, i_D) \in \mathcal{S}} x_1^{i_1} \cdots x_D^{i_D}.$$

We also denote by  $0^i$  the  $i$ -tuple  $(0, \dots, 0)$ . Assume there exist positive integers  $d$  and  $\delta$  with  $d + \delta = D$ , and three sets  $\mathcal{U} \subset \{\bar{1}, 0, 1\}^d \setminus \{0^d\}$ ,  $\mathcal{V} \subset \{\bar{1}, 0, 1\}^d$  and  $\mathcal{T} \subset \{\bar{1}, 0, 1\}^\delta \setminus \{0^\delta\}$ , such that

$$\mathcal{S} = (\mathcal{U} \times \{0^\delta\}) \cup (\mathcal{V} \times \mathcal{T}). \quad (12)$$

Note that the union is necessarily disjoint. The characteristic polynomial of  $\mathcal{S}$  reads

$$S(x_1, \dots, x_D) = U(x_1, \dots, x_d) + V(x_1, \dots, x_d)T(x_{d+1}, \dots, x_D).$$

We say that  $\mathcal{S}$  is  $(d, \delta)$ -Hadamard.

Let  $\mathcal{C}_1$  be the set of walks with steps in  $\mathcal{U} \cup \mathcal{V}$  confined to  $\mathbb{N}^d$ , in which the steps are coloured black and white, with the condition that all steps of  $\mathcal{U} \setminus \mathcal{V}$  are white and all steps of  $\mathcal{V} \setminus \mathcal{U}$  are black. We call these walks *coloured  $(\mathcal{U}, \mathcal{V})$ -walks*. Let  $C_1(x_1, \dots, x_d, v; t)$  be the associated generating function, where  $t$  keeps track of the length,  $x_1, \dots, x_d$  of the coordinates of the endpoint, and  $v$  of the number of black steps. Equivalently,

$$C_1(x_1, \dots, x_d, v; t) = \sum_w x_1^{i_1(w)} \cdots x_d^{i_d(w)} (1+v)^{|w|_{\mathcal{U} \cap \mathcal{V}}} v^{|w|_{\mathcal{V} \setminus \mathcal{U}}} t^{|w|}, \quad (13)$$

where the sum runs over all *uncoloured* walks  $w$  in  $\mathbb{N}^d$  with steps in  $\mathcal{U} \cup \mathcal{V}$ , the values  $i_1(w), \dots, i_d(w)$  are the coordinates of the endpoint and  $|w|_{\mathcal{W}}$  stands for the number of steps of  $w$  belonging to  $\mathcal{W}$ , for any step set  $\mathcal{W} \subset \mathcal{U} \cup \mathcal{V}$ . Let  $C_2(x_{d+1}, \dots, x_D; v)$  be the generating function of  $\mathcal{T}$ -walks confined to  $\mathbb{N}^\delta$ , counted by the length ( $v$ ) and the coordinates of the endpoint  $(x_{d+1}, \dots, x_D)$ .

**Proposition 8.** *Assume  $\mathcal{S}$  is  $(d, \delta)$ -Hadamard, given by (12). With the above notation, the series  $O(x_1, \dots, x_D; t)$  that counts  $\mathcal{S}$ -walks confined to  $\mathbb{N}^D$  is*

$$O(x_1, \dots, x_D; t) = C_1(x_1, \dots, x_d, v; t) \odot_v C_2(x_{d+1}, \dots, x_D; v)|_{v=1},$$

where  $\odot_v$  denotes the Hadamard product with respect to  $v$ .

*In particular,  $O$  is  $D$ -finite (in all its variables) if  $C_1$  and  $C_2$  are  $D$ -finite (in all their variables).*

The proof is a direct extension of the argument given in Section 5.1, and is left to the reader. We will also use the following simple observation.

**Observation 9.** *The generating function of  $\mathcal{S}$ -walks confined to  $\mathbb{N}^d \times \mathbb{Z}^\delta$ , counted by the length and the coordinates of the endpoint, is*

$$C_1(x_1, \dots, x_d, T(x_{d+1}, \dots, x_D); t).$$

We now specialise the Hadamard decomposition to octant walks.

### 5.3. THE CASE OF (1, 2)-HADAMARD WALKS

Assume that the model  $\mathcal{S}$  is  $(1, 2)$ -Hadamard:

$$S(x, y, z) = U(x) + V(x)T(y, z).$$

This was the case with the model of Section 5.1. Since the sets  $\mathcal{U}$  and  $\mathcal{V}$  are (at most) 1-dimensional, the generating function  $C_1(x, v; t)$  counting coloured  $(\mathcal{U}, \mathcal{V})$ -walks is always  $D$ -finite (in fact, algebraic). Proposition 8 specialises as follows.

**Proposition 10.** *If  $\mathcal{S}$  is (1,2)-Hadamard with  $\mathcal{S} = (\mathcal{U} \times \{0\}^2) \cup (\mathcal{V} \times \mathcal{T})$ , the generating function  $O(x, y, z; t)$  of  $\mathcal{S}$ -walks confined to the octant is D-finite as soon as the series  $C_2(y, z; t)$  that counts  $\mathcal{T}$ -walks in the quadrant is D-finite.*

#### 5.4. THE CASE OF (2, 1)-HADAMARD WALKS AND THE REFLECTION PRINCIPLE

Assume that the model  $\mathcal{S}$  is (2, 1)-Hadamard:

$$S(x, y, z) = U(x, y) + V(x, y)T(z).$$

Since the set  $\mathcal{T}$  is (at most) 1-dimensional, the generating function  $C_2(z; t)$  that counts  $\mathcal{T}$ -walks in  $\mathbb{N}$  is always D-finite (in fact, algebraic).

**Proposition 11.** *If  $\mathcal{S}$  is (2,1)-Hadamard with  $\mathcal{S} = (\mathcal{U} \times \{0\}) \cup (\mathcal{V} \times \mathcal{T})$ , then  $O(x, y, z; t)$  is D-finite as soon as the series  $C_1(x, y, v; t)$  that counts coloured  $(\mathcal{U}, \mathcal{V})$ -walks in the quadrant is D-finite.*

Moreover, if  $T(z) = z + \bar{z}$ , then

$$O(x, y, z; t) = [z^{\geq 0}](1 - \bar{z}^2)Q(x, y, z; t),$$

where  $Q(x, y, z; t)$  counts  $\mathcal{S}$ -walks confined to  $\mathbb{N}^2 \times \mathbb{Z}$ .

Note that  $T(z)$  must be equal to  $(z + \bar{z})$  for a 3D model.

*Proof.* The first statement just paraphrases the second part of Proposition 8. Now assume that  $T(z) = z + \bar{z}$ , and let us apply the first statement of Proposition 8. The reflection principle for walks on a line gives

$$C_2(z; v) = [z^{\geq 0}] \frac{1 - \bar{z}^2}{1 - v(z + \bar{z})} = \sum_{k \geq 0} v^k [z^{\geq 0}](1 - \bar{z}^2)(z + \bar{z})^k.$$

Let us now write  $C_1(x, y, v; t) = \sum_{k \geq 0} C_{1,k}(x, y; t)v^k$ . Then

$$\begin{aligned} O(x, y, z; t) &= \sum_{k \geq 0} C_{1,k}(x, y; t)[z^{\geq 0}](1 - \bar{z}^2)(z + \bar{z})^k \\ &= [z^{\geq 0}](1 - \bar{z}^2) \sum_{k \geq 0} C_{1,k}(x, y; t)(z + \bar{z})^k \\ &= [z^{\geq 0}](1 - \bar{z}^2)Q(x, y, z; t) \end{aligned}$$

by Observation 9. This identity can also be obtained by applying the reflection principle to  $\mathcal{S}$ -walks confined to  $\mathbb{N}^2 \times \mathbb{Z}$ , but this proof underlines the connection with Proposition 8.  $\square$

**Example 12. A (2, 1)-Hadamard model.** Take

$$S(x, y, z) = x + xy + (\bar{x} + \bar{x}\bar{y})(z + \bar{z}).$$

This is a (2, 1)-Hadamard model where  $\mathcal{U} \cap \mathcal{V} = \emptyset$ . The series  $C_1(x, y, v; t)$  counts the so-called Gessel walks by the length ( $t$ ), the coordinates of the endpoint  $(x, y)$ , and the number of  $x^-$  steps ( $v$ ). It can be expressed in terms of the complete generating function  $Q(x, y; t)$  of Gessel walks, which is known to be algebraic [6]. Indeed,

$$C_1(x, y, v; t) = Q(x\sqrt{\bar{v}}, y; t\sqrt{\bar{v}})$$

with  $\bar{v} = 1/v$ . The series  $C_2(y; v)$  is the (algebraic) generating function of  $\pm 1$ -walks in  $\mathbb{N}$ , and  $O(x, y, z; t)$  is thus D-finite. The associated group is finite of order 16, with a zero orbit sum.



## 6. THREE-DIMENSIONAL OCTANT MODELS

Starting from the 35 548 non-equivalent models with at most 6 steps that have dimension 2 or 3 (Proposition 5), we first apply the linear programming technique described at the end of Section 2.1 to determine their dimension. Doing this using the built-in solver of Sage [39] requires no more than a few minutes of computation time (in total). We thus obtain 20 804 truly three-dimensional models.

We analyse them with the tools of Sections 3 to 5. Our results are summarised by Table 2 displayed in Section 3. On the experimental side, we go through all models and determine which of them appear to have a finite group. We find only 170 models with a finite group, of order 8, 12, 16, 24 or 48. The 20 634 remaining models have a group of order at least 200, which we conjecture to be infinite. This includes for instance the highly symmetric model  $S = xy\bar{z} + \bar{x}y\bar{z} + \bar{x}\bar{y}z + xyz$  mentioned in [6, Sec. 4.1].

Among the 170 models with a finite group, 108 have a non-zero orbit sum. The algebraic kernel method of Section 4 proves that their complete generating function is D-finite: up to a permutation of coordinates, the series  $xyzO(x, y, z; t)$  is obtained by extracting the positive part in  $z$ ,  $y$  and  $x$  in a rational function, as in (10). The correctness of the extraction argument is guaranteed by Condition (11), which holds in each of these 108 cases.

There are 62 models left where the orbit sum is zero. Among these, 43 can be recognised as Hadamard and have a D-finite generating function. The remaining 19 are not Hadamard.

### 6.1. THE HADAMARD MODELS WITH ZERO ORBIT SUM

Let us give a few details on these 43 Hadamard models. Among them, 31 are (1, 2)-Hadamard and 17 are (2, 1)-Hadamard (up to a permutation of coordinates). This means that 5 are both (1, 2)- and (2, 1)-Hadamard; this happens when  $\mathcal{U} = \emptyset$  or  $\mathcal{V} = \emptyset$ . For the (1, 2)-Hadamard models, we apply Proposition 10. The set  $\mathcal{T}$  is found to be either Kreweras' model  $\{\bar{1}0, 0\bar{1}, 11\}$ , or its reverse  $\{10, 01, \bar{1}\bar{1}\}$  or Gessel's model  $\{10, \bar{1}0, 11, \bar{1}\bar{1}\}$ . In all three cases, the generating function  $C_2(y, z; v)$  is known to be algebraic [21, 10, 6], so that  $O(x, y, z; t)$  is D-finite by Proposition 10.

For the (2, 1)-Hadamard models, we apply Proposition 11, and thus need to check if  $C_1(x, y, v; t)$  is D-finite. The set  $\mathcal{U} \cup \mathcal{V}$  is found to be either Kreweras' model, or its reverse, or Gessel's model (in each case, possibly with an additional null step 00). Since there are only three steps in Kreweras' model, the associated complete generating function  $Q(x, y; t)$  records in fact the number of steps of each type (after some algebraic changes of variables). Moreover, adding a null step and recording its number of occurrences preserves algebraicity. This implies that in the Kreweras case, the series  $C_1(x, y, v; t)$  defined by (13) is obtained by algebraic substitutions in  $Q(x, y; t)$  and is thus algebraic. The same holds in the reverse Kreweras case. This leaves us with five models for which  $\mathcal{U} \cup \mathcal{V}$  is Gessel's model (possibly with a null step). It is known that the associated complete generating function  $Q(x, y; t)$  is algebraic, but does it imply that  $C_1(x, y, v; t)$  is also algebraic? The answer is yes. In all five cases,  $\mathcal{U} \cap \mathcal{V} = \emptyset$ , so that we just have to check that we can keep track of the number of  $\mathcal{V}$ -steps (see (13)). The five sets  $\mathcal{V}$  are  $\{\bar{1}0, \bar{1}\bar{1}\}$  (this is Example 12),  $\{10, 11\}$ ,  $\{01, \bar{1}\bar{1}\}$ ,  $\{0\bar{1}, 11\}$  and finally  $\{00\}$  (in the latter case, the model is also (1, 2)-Hadamard). In each case, it is readily checked that  $C_1(x, y, v; t)$  is obtained by algebraic substitutions in  $Q(x, y; t)$  and is thus algebraic.

### 6.2. THE NON-HADAMARD MODELS WITH ZERO ORBIT SUM

These 19 models, shown in Figure 4, remain mysterious. We are tempted to believe that they are not D-finite, which would mean that the nice correspondence

between a finite group and D-finiteness observed for quadrant walks does not extend to octant walks. We note that models associated with isomorphic groups may behave very differently: for instance, if we change the sign in the  $x$ -coordinate of each step of the second model of Figure 4, we obtain a model with an isomorphic group (see [11, Lemma 2]), but a non-zero orbit sum. This new model can be solved using the kernel method and has a D-finite series.

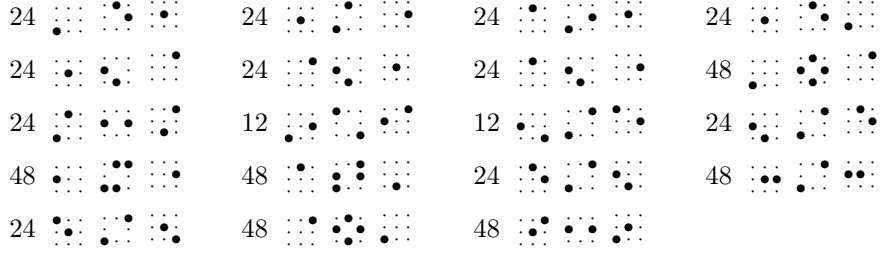


FIGURE 4. The 19 non-Hadamard 3D models with a zero orbit sum, with the order of the associated group. The first one on the second line is the natural 3D analogue of Kreweras' model.

We have tried hard to guess differential equations for the 19 mysterious models. In each case, we have calculated the first 5000 terms of the generating functions  $O(x_0, y_0, z_0; t)$  for any choice of  $x_0, y_0, z_0$  in  $\{0, 1\}$ , but we did not find any equation. It could still be that some or all of the models are D-finite but the equations are so large that 5000 terms are not enough to detect them. Unfortunately, it is quite hard to compute more terms, even if the calculations are restricted to a finite field for better efficiency. The default algorithm based on the recurrence relation (5) then still takes  $O(n^4)$  time and  $O(n^3)$  space, which already for  $n = 5000$  required us to employ a supercomputer (the one we used has 2048 processors and 16000 gigabyte of main memory).

For getting an idea about the expected sizes of equations, we have also guessed equations for all the 43 Hadamard models with finite group and zero orbit sum. The formulas given in Section 5 for their generating functions give rise to more efficient algorithms for computing their series expansion. It turns out that the biggest equation appears for the model  $\begin{smallmatrix} \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \end{smallmatrix}$ , for  $x = y = z = 1$ . It has order 55 and degree 3815, and we needed 20000 terms to construct it. This suggests that we may not have enough terms in our 19 models to guess differential equations.

However, we observed that even for the models where  $O(1, 1, 1; t)$  satisfies only extremely large equations, at least one of the other specialisations  $O(x_0, y_0, z_0; t)$  with  $(x_0, y_0, z_0) \in \{0, 1\}^3$  satisfies a small equation that can be recovered from a few hundred terms already. This is in contrast to the 19 non-Hadamard step sets, where none of these series satisfies an equation that could be found with 5000 terms. For this reason, we have some doubts that these models are D-finite.

## 7. TWO-DIMENSIONAL OCTANT MODELS

We are now left with the 14 744 two-dimensional models found among the 35 548 octant models with at most 6 steps (Proposition 5). At the moment, we have only studied their projection on the relevant quadrant:

*For a 2D octant model where the  $z$ -condition is redundant, we focus on the series  $Q(x, y; t) := O(x, y, 1; t)$ . This series counts quadrant walks with steps in  $\mathcal{S}' = \{ij : ijk \in \mathcal{S}\}$ , which should be thought of as a multiset of steps.*

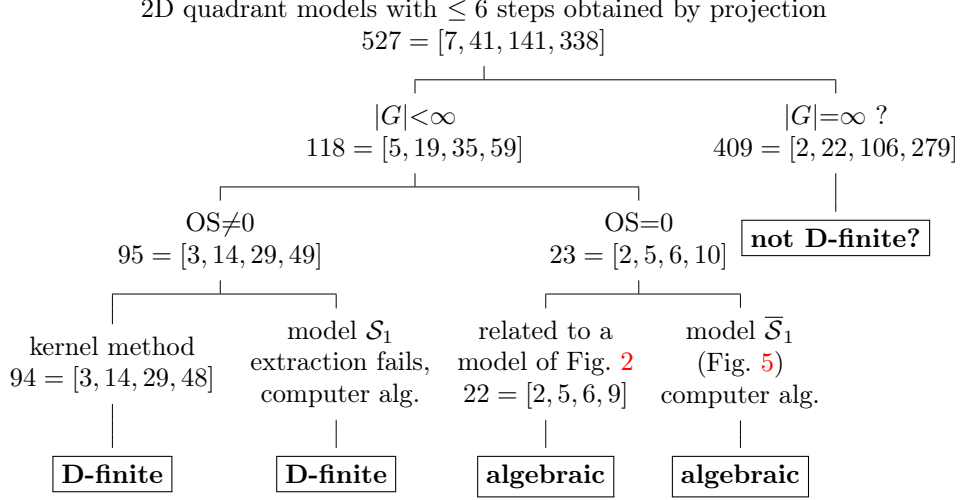


TABLE 3. Summary of our results and conjectures for the 527 quadrant models with at most 6 steps obtained by projection of a 2D octant model. The numbers in brackets give for each class the number of models of cardinality 3, 4, 5 and 6.

For instance, if  $\mathcal{S}$  is the 2D model of Example 1, then  $\mathcal{S}' = \{0\bar{1}, \bar{1}1, \bar{1}\bar{1}, 10\}$  contains two copies of the step  $\bar{1}1$ .

Note that the nature of  $Q(x, y; t)$  is not affected by adding a step 00 to  $\mathcal{S}'$ : it corresponds to substituting  $t \mapsto t/(1-t)$  in the generating function. This is why we do not consider models with a null step.

### 7.1. QUADRANT MODELS OBTAINED BY PROJECTION

We obtain by projection 527 models of cardinality at most 6 (after deleting the 00 step, and identifying models that only differ by an  $xy$  symmetry). Those with no repeated step were previously classified by Bousquet-Mélou and Mishna [11], but we also have models with repeated steps.

As in the 3D case, we first try to determine, experimentally, when the group  $G$  is finite and when the specialisations of  $Q(x, y; t)$  obtained when  $\{x, y\} \subset \{0, 1\}$  are D-finite. Our results are summarised in Table 3.

We find 118 models with a finite group, of order at most 8 (more precisely, of order 4, 6 or 8). The remaining ones have a group of order at least 200, which we conjecture to be infinite. (This is known for models with no repeated step [11], and it is likely that the methods of [11] can prove the other cases as well.) We observe that for each model for which  $Q(1, 1; t)$  is guessed D-finite, the group is finite.

Among the 118 models with a finite group, 95 have a non-zero orbit sum. For 94 of them, the algebraic kernel method establishes the D-finiteness of  $Q(x, y; t)$ . For 92 of these 94 models, the extraction of the positive part in  $x$  and  $y$  is justified by the fact that every element  $[x', y']$  of the orbit, other than  $[x, y]$ , satisfies the 2D counterpart of (11), namely

$$\{x', y'\} \subset \mathbb{Q}(x)[\bar{y}] \quad \text{or} \quad \{x', y'\} \subset \mathbb{Q}[\bar{x}, y] \quad (14)$$

(up to a permutation of coordinates). This property *does not hold* for the remaining two models  $\mathcal{S}_0$  and  $\bar{\mathcal{S}}_0$ , shown in Figure 5, but the extraction is still valid, as detailed in Section 7.2. The 95th model with a finite group and a non-zero orbit sum is the model  $\mathcal{S}_1$  also shown in Figure 5. As will be detailed in Section 8.2, it shares

with models with a zero orbit sum the property that the orbit equation does *not* characterise the series  $Q(x, y; t)$ . We will prove by computer algebra that this series is still D-finite, but transcendental (see Section 8.2).

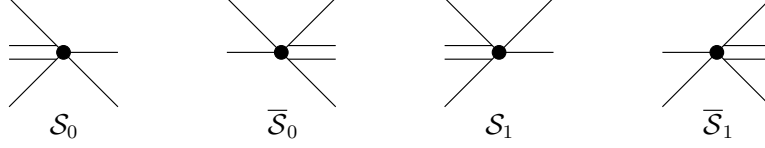


FIGURE 5. Four interesting quadrant models with repeated steps, only differing by a symmetry of the square. All are D-finite, and  $\bar{S}_1$  is even algebraic. See Section 7.2 for  $S_0$  and  $\bar{S}_0$ , Section 8.1 for  $\bar{S}_1$  and Section 8.2 for  $S_1$ . Note that with only one copy of the repeated step, none of these models would be D-finite [8].

We are now left with the 23 models having a zero orbit sum. Exactly 22 of them are obtained from the four algebraic quadrant models of Figure 2 by possibly repeating some steps. In each of these 22 cases, the generating function of the models with multiple steps can be written as an algebraic substitution in the complete generating function of the model with no repeated steps. This is obvious in the Kreweras or reverse Kreweras case, since their complete generating function actually keeps track of the number of occurrences of each step. This is also obvious in the double Kreweras case: it has already 6 steps, so that it only occurs in our list with non-repeated steps. In the Gessel case, the steps are at most duplicated, and the set  $\mathcal{V}$  of duplicated steps is  $\{\bar{1}0, \bar{1}\bar{1}\}$ ,  $\{10, 11\}$ ,  $\{01, \bar{1}\bar{1}\}$ , or  $\{0\bar{1}, 11\}$ . This is the same list as that of Section 6.1, and in each case, the complete generating function of the model with repetitions is obtained by an algebraic substitution in the (algebraic) generating function of Gessel's walks.

The 23rd model with a finite group and zero orbit sum is the model  $\bar{S}_1$  of Figure 5. Using the technique applied to Gessel's model in [6], we will prove that its generating function  $Q(x, y; t)$  is algebraic (Section 8.1). Moreover, the series  $Q(0, y; t)$  has nice hypergeometric coefficients.

## 7.2. TWO INTERESTING APPLICATIONS OF THE KERNEL METHOD

We discuss here the two models for which the orbit sum is non-zero, and where the kernel method works even though Condition (14) does not hold. These models are  $S_0 = \{\bar{1}\bar{1}, \bar{1}0, \bar{1}0, \bar{1}1, 10, 1\bar{1}\}$  (with a repeated west step) and its reverse  $\bar{S}_0 = \{11, 10, 10, 1\bar{1}, \bar{1}0, \bar{1}1\}$  (Figure 5). In both cases, the group  $G$  has order 6.

For  $S_0$ , the non-trivial elements in the orbit of  $[x, y]$  are

$$[\bar{x}(1+y), y], \quad [\bar{x}(1+y), \bar{y} + \bar{x}^2\bar{y}(1+y)^2], \quad [\bar{x} + (x + \bar{x})\bar{y}, \bar{y} + \bar{x}^2\bar{y}(1+y)^2], \\ [\bar{x} + (x + \bar{x})\bar{y}, \bar{y}(1+x^2)], \quad [x, \bar{y}(1+x^2)].$$

All coordinates are Laurent polynomials in  $x$  and  $y$ . Moreover, all elements  $[x', y']$  satisfy (14), with the exception of the third. Still, all monomials  $x^i y^j$  occurring in this element satisfy  $i + j \leq 0$ . Hence this is also true for the monomials occurring in  $x' y' Q(x', y')$ , so that this series does not contribute when one extracts the positive part (in  $x$  and  $y$ ) of the orbit sum. One thus obtains

$$xyQ(x, y) = [x^{>0}][y^{>0}] \frac{(x - \bar{x} - x\bar{y} - \bar{x}\bar{y})(x - \bar{x} - \bar{x}y)(\bar{x}y - x\bar{y} - \bar{x}\bar{y})}{1 - t(1 + \bar{y})(x + \bar{x}(1 + y))}.$$

The coefficient extraction can be performed explicitly and gives rise to nice numbers. Details of the extraction are left to the reader.

**Proposition 13.** For the model  $\mathcal{S}_0 = \{\bar{1}\bar{1}, \bar{1}\bar{0}, \bar{0}\bar{1}, \bar{1}\bar{1}, 10, \bar{1}\bar{1}\}$ , the number of walks of length  $n$  ending at  $(i, j)$  is zero unless  $n$  can be written as  $2m + i$ , in which case

$$q(i, j; n) = \frac{(i+1)(j+1) [(2i+3j+6)m + i^2 + 5i + 2ij + 3j + 6] n!(3m+i+2)!}{m!(m+i)!(m-j)!(2m+i+j+3)!(m+i+1)(m+i+2)(m+1)}.$$

**Remark.** The asymptotic behaviour of  $q(0, 0; 2m)$ , which is of the form  $c27^m n^{-4}$ , prevents the series  $Q(0, 0; t)$  from being algebraic [19].

Let us now address the model with reversed steps,  $\bar{\mathcal{S}}_0 = \{11, 10, 10, \bar{1}\bar{1}, \bar{1}\bar{0}, \bar{1}\bar{1}\}$ . Now the orbit of  $[x, y]$  involves rational functions which are not Laurent polynomials. Besides  $[x, y]$  itself, the orbit contains the following five pairs:

$$\begin{aligned} & \left[ \frac{\bar{x}y}{1+y}, y \right], \quad \left[ \frac{\bar{x}y}{1+y}, \frac{\bar{x}^2 y}{(1+y)^2 + \bar{x}^2 y^2} \right], \quad \left[ \frac{\bar{x}}{1+y(1+\bar{x}^2)}, \frac{\bar{x}^2 y}{(1+y)^2 + \bar{x}^2 y^2} \right], \\ & \left[ \frac{\bar{x}}{1+y(1+\bar{x}^2)}, \frac{x^2 \bar{y}}{1+x^2} \right], \quad \left[ x, \frac{x^2 \bar{y}}{1+x^2} \right]. \end{aligned}$$

Let  $[x', y']$  be one of these pairs,  $i, j$  two non-negative integers, and let us expand the series  $x'^i y'^j$  first in  $y$ , and then in  $x$ . We claim that the resulting series (a Laurent series in  $y$  whose coefficients are Laurent series in  $x$ ) does not contain any monomial  $x^a y^b$  with  $a$  and  $b$  positive. This is obvious for all pairs, except the fourth one, for which we have to perform the following calculation: for  $i > 0$ ,

$$x'^i y'^j = \sum_{n \geq 0} (-1)^n \binom{n+i-1}{i-1} y^{n-j} \bar{x}^i (1+\bar{x}^2)^{n-j}.$$

This expansion shows that if the exponent of  $y$  is positive ( $n > j$ ), then the exponent of  $x$  is negative. Hence the only series that contributes when expanding the orbit equation in  $y$  and  $x$  is  $xyQ(x, y)$  and finally

$$xyQ(x, y) = [x^{>0}][y^{>0}] \frac{y(x - \bar{x} + xy + \bar{x}y)(x - \bar{x} + x\bar{y})(xy + \bar{x}y - x\bar{y})}{(1+x^2)((1+y)^2 + \bar{x}^2 y^2)(1-t(1+y)(\bar{x} + x(1+\bar{y})))}.$$

As opposed to the previous example, the numbers  $q(i, j; n)$  do not appear to be hypergeometric in  $i, j$  and  $n$ , but only in  $i$  and  $n$ , for  $j$  fixed. For instance,

$$q(i, 0; 2m+i) = \frac{(i+1)(i+2)(2m+i)!(3m+2i+3)!}{m!(m+i)!(m+i+2)!(2m+i+2)!(m+i+1)(2m+2i+3)}.$$

Of course, the series  $Q(0, 0; t)$ , being the same as for the model  $\mathcal{S}_0$  studied previously, is transcendental.

### 7.3. ALGEBRAICITY

We have also tried to guess – and then prove – algebraic equations for the specialisations  $Q(x_0, y_0; t)$  with  $\{x_0, y_0\} \subset \{0, 1\}$ . Here is a summary of our results.

First, we have of course the 23 models with finite group and zero orbit sum, for which the complete generating function  $Q(x, y; t)$  is algebraic over  $\mathbb{Q}(x, y, t)$  (see Table 3). This explains for instance why the octant models with characteristic polynomials  $\bar{z} + \bar{x}(\bar{y} + 1 + y) + xyz$  or  $\bar{x}\bar{z}(\bar{y} + 1 + y) + xy + z$  were conjectured to have an algebraic length generating function  $O(1, 1, 1; t)$  in [5, Table 2]: both are 2-dimensional, with the  $y$ -condition redundant, and their projections on the  $xz$ -plane are  $\{0\bar{1}, \bar{1}\bar{0}, \bar{1}\bar{0}, \bar{1}\bar{0}, 11\}$  and  $\{\bar{1}\bar{1}, \bar{1}\bar{1}, \bar{1}\bar{1}, 10, 01\}$ . These are respectively versions of Kreweras' model and of its reverse, with multiple steps, and they are algebraic.

For models with a finite group and a *non-zero* orbit sum, we conjecture that the complete generating function  $Q(x, y; t)$  is transcendental. However, we have also found experimentally, and then proved, a few algebraic specialisations of these series. This is for instance the case for the specialisation  $Q(0, 0; t)$  of the model  $\mathcal{S}_1$

of Figure 5: this series is the same as for the model  $\overline{\mathcal{S}}_1$ , which is algebraic. The other models with algebraic specialisations are  $\{0\bar{1}, 10, \bar{1}\bar{1}\}$  (possibly with repeated steps) and  $\{0\bar{1}, 10, \bar{1}\bar{1}, \bar{1}0, 01, \bar{1}\bar{1}\}$ . Both models are known to have certain algebraic specialisations [11, Section 5.2]. Our algebraic guesses are all consequences of the following two results.

- For  $\mathcal{S} = \{0\bar{1}, 10, \bar{1}\bar{1}\}$ , the generating function  $Q(1, 1; t)$  is algebraic [11, Prop. 9]. With the same proof, one shows that this remains true with a weight  $\delta$  for diagonal steps  $\bar{1}\bar{1}$ .
- For  $\mathcal{S} = \{0\bar{1}, 10, \bar{1}\bar{1}, \bar{1}0, 01, \bar{1}\bar{1}\}$ , the generating function  $Q(1, 1; t)$  is algebraic [11, Prop. 10]. One step of the proof is to prove that  $xQ(x, 0) + \bar{x}(1 + \bar{x})Q(0, \bar{x})$  is algebraic. Setting  $x = 1$ , and using the  $xy$ -symmetry, shows that  $Q(0, 1; t)$  is also algebraic.

**Example 14.** Consider the octant model  $\mathcal{S} = \{0\bar{1}0, 101, \bar{1}\bar{1}\bar{1}, \bar{1}\bar{1}0, \bar{1}\bar{1}1\}$ , which was conjectured to have an algebraic length generating function  $O(1, 1, 1; t)$  in [5, Table 2] (up to a permutation of  $x$  and  $y$ , it is the first model in that table). The  $z$ -condition is easily seen to be redundant, and  $\mathcal{S}$  is two-dimensional. Let  $\mathcal{U}$  be the set obtained by projecting  $\mathcal{S}$  on the  $xy$ -plane and deleting repeated steps:  $\mathcal{U} = \{0\bar{1}, 10, \bar{1}\bar{1}\}$ . Let  $Q(x, y; t)$  be the quadrant series associated with  $\mathcal{U}$ . Denoting by  $a(w)$ ,  $b(w)$  and  $c(w)$  the number of occurrences of  $0\bar{1}$ ,  $10$  and  $\bar{1}\bar{1}$  in a  $\mathcal{U}$ -walk  $w$ , we have

$$Q(X, Y; T) = \sum_w (\bar{Y}T)^{a(w)} (XT)^{b(w)} (\bar{X}YT)^{c(w)}.$$

Moreover, by lifting every  $\mathcal{U}$ -walk  $w$  into all  $\mathcal{S}$ -walks that project on it, we obtain

$$O(x, y, z; t) = \sum_w (\bar{y}t)^{a(w)} (xzt)^{b(w)} (\bar{x}y(1 + z + \bar{z})t)^{c(w)}.$$

Comparing these two identities shows that

$$O(x, y, z; t) = Q\left(\frac{xz}{Z^{1/3}}, yZ^{1/3}; tZ^{1/3}\right) \quad \text{where } Z = 1 + z + z^2.$$

Since  $Q(x, y; t)$  is D-finite we have that  $O(x, y, z; t)$  is D-finite. Furthermore,  $Q(x, \frac{1}{x}; t)$  is algebraic [11, Prop. 9], so  $O(x, y, \frac{1}{xy}; t)$ , and specifically  $O(1, 1, 1; t)$ , is also algebraic.

## 8. COMPUTER ALGEBRA SOLUTIONS

As discussed in the previous section, there are two D-finite quadrant models (with repeated steps) for which we have only found proofs based on computer algebra. We now give details on these proofs. The two models in question are  $\mathcal{S}_1 = \{11, 10, \bar{1}\bar{1}, \bar{1}0, \bar{1}0, \bar{1}\bar{1}\}$  and its reverse  $\overline{\mathcal{S}}_1 = \{\bar{1}\bar{1}, \bar{1}0, \bar{1}\bar{1}, 10, 10, 11\}$  (Figure 5). We will show that  $\mathcal{S}_1$  is D-finite (but transcendental) and  $\overline{\mathcal{S}}_1$  algebraic. We begin with the latter model.

### 8.1. THE MODEL $\overline{\mathcal{S}}_1 = \{\bar{1}\bar{1}, \bar{1}0, \bar{1}\bar{1}, 10, 10, 11\}$ IS ALGEBRAIC

The group of this model is finite of order 6. The orbit sum is zero, which implies that the orbit equation does not characterise  $Q(x, y)$  (in fact,  $Q(x, y) = 1$  is another solution). We first establish the algebraicity of the series  $Q(0, 0; t)$ , which counts quadrant walks ending at the origin, often called *excursions*.

**Lemma 15.** *For the quadrant model  $\overline{\mathcal{S}}_1 = \{\bar{1}\bar{1}, \bar{1}0, \bar{1}\bar{1}, 10, 10, 11\}$ , the generating function  $Q(0, 0; t)$  is*

$$Q(0, 0; t) = \sum_{n \geq 0} \frac{6(6n+1)!(2n+1)!}{(3n)!(4n+3)!(n+1)!} t^{2n}. \quad (15)$$

It is algebraic of degree 6. Denoting  $Q_{00} \equiv Q(0, 0; t)$ , we have

$$16t^{10}Q_{00}^6 + 48t^8Q_{00}^5 + 8(6t^2 + 7)t^6Q_{00}^4 + 32(3t^2 + 1)t^4Q_{00}^3 \\ + (48t^4 - 8t^2 + 9)t^2Q_{00}^2 + (48t^4 - 56t^2 + 1)Q_{00} + (16t^4 + 44t^2 - 1) = 0. \quad (16)$$

A parametric expression of  $Q(0, 0; t)$  is

$$t^2Q(0, 0; t) = Z(1 - 6Z + 4Z^2),$$

where  $Z \equiv Z(t)$  is the unique power series in  $t$  with constant term 0 satisfying

$$Z(1 - Z)(1 - 2Z)^4 = t^2.$$

*Proof.* We prove the first claim (15) by computer algebra, using the method applied in [23] for proving that the number of Gessel excursions is hypergeometric — the so-called *quasi-holonomic ansatz* (see also [24]). As the details of this approach are already explained in this earlier article, we give here only a rough sketch of our computations.

First compute the coefficients  $q(i, j; n)$  of  $Q(x, y; t)$  for  $0 \leq i, j, n \leq 50$ , using the quadrant counterpart of the recurrence relation (5). Then, use this data to guess [22] a system of multivariate linear recurrence equations with polynomial coefficients (in  $i, j$  and  $n$ ) satisfied by the numbers  $q(i, j; n)$ . Then use the algorithm from [24] to prove that these guessed recurrences indeed hold. Then use linear algebra (or a variant of Takayama's algorithm [40], as was done in [23]) to combine these recurrences into a linear recurrence of the following form: for all  $i, j$  and  $n$ ,

$$\sum_{a, b, c, i', j', n' \geq 0} \kappa(a, b, c, i', j', n') i^a j^b n^c q(i + i', j + j'; n + n') = 0,$$

where  $\kappa(a, b, c, i', j', n') \in \mathbb{Q}$  is non-zero for only finitely many terms, and  $\max(a, b) > 0$  whenever  $\max(i', j') > 0$ . Upon setting  $i = j = 0$ , this recurrence gives a recurrence in  $n$  for the coefficients  $q(0, 0; n)$  of  $Q(0, 0; t)$ . We found in this way a recurrence of order 8 and degree 14. It is then routine to check that the coefficients of (15) satisfy this recurrence and that the right number of initial values match.

Now, the polynomial equation (16) has clearly a unique power series solution (think of extracting by induction the coefficient of  $t^n$ ). Using algorithms for holonomic functions [34, 29], one can construct a linear differential equation satisfied by this solution, and then a recurrence relation satisfied by its coefficients. It suffices then to check that the coefficients of (15) satisfy this recurrence and the right number of initial conditions.

The parametric form of the solution can be found with the `algcures` package of Maple. Using this parametrisation, one can also recover the expansion (15) of  $Q(0, 0; t)$  using the Lagrange inversion formula.  $\square$

We now extend Lemma 15 to the algebraicity of the complete series  $Q(x, y; t)$ .

**Proposition 16.** *For the quadrant model  $\bar{\mathcal{S}}_1 = \{\bar{1}\bar{1}, \bar{1}0, 1\bar{1}, 10, 10, 11\}$  (with an east repeated step), the generating function  $Q(x, y; t) \equiv Q(x, y)$  is algebraic of degree 12. It satisfies*

$$Q(x, y) = \frac{xy - t(1 + x^2)Q(x, 0) - t(1 + y)Q(0, y) + tQ(0, 0)}{xy(1 - t(1 + \bar{y})(\bar{x} + x(1 + y)))}. \quad (17)$$

The specialisations  $Q(x, 0; t)$  and  $Q(0, y; t)$  can be written in parametric form as follows. Let  $T \equiv T(t)$  be the unique power series in  $t$  with constant term 0 such that

$$T(1 - 4T^2) = t.$$

Let  $S \equiv S(t)$  be the unique power series in  $t$  with constant term 0 such that

$$S = T(1 + S^2).$$

Equivalently,  $S(1-S^2)^2 = t(1+S^2)^3$ . Then  $Q(x, 0; t)$  has degree 12 and is quadratic over  $\mathbb{Q}(x, S)$ :

$$Q(x, 0; t) = \left( \frac{1+S^2}{1-S^2} \right)^3 \times \frac{x(1+6S^2+S^4) - 2S(1-S^2)(1+x^2) - (x-2S+xS^2)\sqrt{(1-S^2)^2 - 4xS(1+S^2)}}{2x(1+x^2)S^2}. \quad (18)$$

Let also  $W \equiv W(y; t)$  be the unique power series in  $t$  with constant term 0 such that

$$W(1 - (1+y)W) = T^2.$$

Then  $Q(0, y; t)$  has degree 6 and is rational in  $T$  and  $W$ :

$$Q(0, y; t) = t^{-2}W(1 - 4T^2 - 2W). \quad (19)$$

Moreover, its coefficients are doubly hypergeometric:

$$Q(0, y; t) = \sum_{n \geq j \geq 0} \frac{6(2j+1)!(6n+1)!(2n+j+1)!}{j!^2(3n)!(4n+2j+3)!(n-j)!(n+1)} y^j t^{2n}.$$

*Proof.* We prove the claims again by computer algebra, this time using the technique applied in [6] for proving that Gessel's model is algebraic. Again, as there is nothing new about the logical structure of the argument, we give here only a summary of our computations (and complete a missing argument in [6]).

The functional equation defining  $Q(x, y)$  reads

$$xy(1 - t(1+\bar{y})(\bar{x} + x(1+y)))Q(x, y) = xy - t(1+x^2)Q(x, 0) - t(1+y)Q(0, y) + tQ(0, 0).$$

This is of course equivalent to (17). Recall that  $Q(0, 0)$  is known from Lemma 15. The (standard) kernel method [13, 10] consists in cancelling the kernel by an appropriate choice of  $x$  or  $y$  to obtain equations relating the series  $Q(x, 0)$  and  $Q(0, y)$ . Applied to the above equation, it gives:

$$\begin{cases} (1+x^2)Q(x, 0) + (1+Y)Q(0, Y) &= xY/t + Q(0, 0), \\ (1+X^2)Q(X, 0) + (1+y)Q(0, y) &= XY/t + Q(0, 0), \end{cases} \quad (20)$$

where  $X$  and  $Y$  are power series in  $t$  with Laurent coefficients in  $y$  and  $x$ , respectively, defined by

$$\begin{aligned} X \equiv X(y; t) &= \frac{1 - \sqrt{1 - 4t^2\bar{y}^2(1+y)^3}}{2t\bar{y}(1+y)^2} \\ &= t(1+\bar{y}) + \bar{y}^3(1+y)^4t^3 + O(t^5) \quad \in \mathbb{Q}[y, \bar{y}][[t]], \\ Y \equiv Y(x; t) &= \frac{1 - t\bar{x} - 2tx - \sqrt{1 - 2t\bar{x} - 4tx + t^2\bar{x}^2}}{2tx} \\ &= (\bar{x} + x)t + (\bar{x} + x)(\bar{x} + 2x)t^2 + O(t^3) \quad \in \mathbb{Q}[x, \bar{x}][[t]]. \end{aligned}$$

It follows from (20) and [6, Lemma 7] that  $(Q(x, 0), Q(0, y))$  is in fact the unique pair of formal power series  $(F, G) \in \mathbb{Q}[[x, t]] \times \mathbb{Q}[[y, t]]$  satisfying the functional equations

$$\begin{cases} (1+x^2)F(x) + (1+Y)G(Y) &= xY/t + Q(0, 0), \\ (1+X^2)F(X) + (1+y)G(y) &= XY/t + Q(0, 0). \end{cases} \quad (21)$$



Let us now define  $F$  and  $G$  by the right-hand sides of (18) and (19) respectively (these expressions have been guessed from the first coefficients of  $Q(x, y)$ ). We claim that  $F$  and  $G$  belong to  $\mathbb{Q}[x][[t]]$  and  $\mathbb{Q}[y][[t]]$  respectively. This is obvious for  $G$ , since  $T$  is a series in  $\mathbb{Q}[[t]]$  and  $W$  belongs to  $t^2\mathbb{Q}[y][[t]]$ . Let us now consider the series  $F$ , that is, the right-hand side of (18), and ignore the initial factor, which is clearly in  $\mathbb{Q}[[t]]$ . Then the numerator is a power series in  $S$  with polynomial coefficients in  $x$ . It is readily checked that it vanishes at  $x = 0$  and  $x = \pm i$ , so that these coefficients are always multiples of  $x(1 + x^2)$ . Moreover, the numerator is  $O(S^2)$ , so that we can conclude that  $F$  belongs to  $\mathbb{Q}[x][[S]]$ , and hence to  $\mathbb{Q}[x][[t]]$ .

We want to prove that  $F$  and  $G$  satisfy the system (21). Since  $X, Y, F, G$  and  $Q(0, 0)$  are algebraic, this can be done by taking resultants, and then checking an appropriate number of initial values.

This concludes the proof of (18) and (19). The fact that  $Q(x, y)$  has degree 12 is obtained by elimination (it has degree 4 over  $\mathbb{Q}(x, y, T)$ ). The (computational) proof of the hypergeometric series expansion of  $Q(0, y)$  is similar to the proof of the expansion of  $Q(0, 0)$  in Lemma 15: the key step is to derive from the algebraic equation satisfied by  $Q(0, y)$  a differential equation (in  $t$ ) for this series, and then a recurrence relation for the coefficient of  $t^n$ .  $\square$

## 8.2. THE MODEL $\mathcal{S}_1 = \{\bar{1}\bar{1}, \bar{1}1, \bar{1}0, \bar{1}0, 10, 11\}$ IS D-FINITE

The kernel of this model is

$$K(x, y) = 1 - t(1 + y)(\bar{x}(1 + \bar{y}) + x).$$

The functional equation defining  $Q(x, y)$  reads:

$$xyK(x, y)Q(x, y) = xy - tQ(x, 0) - t(1 + y)^2Q(0, y) + tQ(0, 0).$$

Again, the group has order 6. The orbit equation reads:

$$\begin{aligned} & xyQ(x, y) - \bar{x}(1 + \bar{y})Q(\bar{x}(1 + \bar{y}), y) + \frac{x(1 + y)}{(1 + y)^2 + x^2y^2} Q\left(\bar{x}(1 + \bar{y}), \frac{x^2y}{(1 + y)^2 + x^2y^2}\right) \\ & - \frac{xy(1 + y + x^2y)}{(1 + y)^2 + x^2y^2} Q\left(\bar{x}(1 + y) + xy, \frac{x^2y}{(1 + y)^2 + x^2y^2}\right) \\ & + \frac{\bar{x}\bar{y}(1 + y + x^2y)}{1 + x^2} Q\left(\bar{x}(1 + y) + xy, \frac{\bar{y}}{1 + x^2}\right) - \frac{x\bar{y}}{1 + x^2} Q\left(x, \frac{\bar{y}}{1 + x^2}\right) \\ & = \frac{(1 + y(1 - x^2))(1 - y^2(1 + x^2))(1 - x^2 + y(1 + x^2))}{xy(1 + x^2)K(x, y)((1 + y)^2 + x^2y^2)}. \end{aligned}$$

The right-hand side is non-zero, but this equation does not define  $Q(x, y; t)$  uniquely in the ring  $\mathbb{Q}[x, y][[t]]$ . In fact, the associated *homogeneous* equation (in  $Q(x, y)$ ) seems to have an infinite dimensional space of solutions. It includes at least the following polynomials in  $x$  and  $y$ :

$$x, \quad 2xy + x^3y, \quad x^2y + x^2 + y + 2, \quad x^3y^2 - x^3y + x^3 + 2xy^2.$$

We show in this subsection that  $Q(x, y; t)$  is D-finite in  $x, y$  and  $t$ , but transcendental. To our knowledge, it is the first time that the D-finiteness of a (non-algebraic) quadrant model is proved via computer algebra.

**Proposition 17.** *The complete generating function  $Q(x, y; t)$  for the model  $\mathcal{S}_1$  is D-finite in its three variables.*

*Proof.* Saying that  $Q(x, y; t)$  is D-finite means that the  $\mathbb{Q}(x, y, t)$ -vector space generated by  $Q(x, y; t)$  and all its derivatives  $D_x^i D_y^j D_t^k Q(x, y; t)$  (for  $i, j, k \in \mathbb{N}$ ) has finite dimension. This vector space is isomorphic to the algebra  $\mathbb{Q}(x, y, t)[D_x, D_y, D_t]/\mathcal{I}$ ,

where  $\mathbb{Q}(x, y, t)[D_x, D_y, D_t]$  is the Ore algebra of linear partial differential operators with rational function coefficients, and  $\mathfrak{J}$  is the left ideal consisting of all the operators in this algebra which map  $Q(x, y, t)$  to zero. The condition that  $Q(x, y, t)$  be D-finite is thus equivalent to  $\mathfrak{J}$  having Hilbert dimension 0.

The structure of the argument is similar to the proof of Proposition 16, but now with differential equations instead of polynomial equations. Again, it suffices to prove that the specialisations  $Q(x, 0)$  and  $Q(0, y)$  are D-finite.

First, we calculate the coefficients  $q(i, j, n)$  of  $Q(x, y, t)$  for  $0 \leq i, j, n \leq 100$  using the combinatorial recurrence relation. From these, two systems of differential operators annihilating  $Q(x, 0; t)$  and  $Q(0, y; t)$ , respectively, can be guessed. The ideals  $\mathfrak{J}_x$  and  $\mathfrak{J}_y$  generated by the guessed operators have Hilbert dimension 0, as can be checked by a Gröbner basis computation. We used Koutschan's package [25] for this and all the following Gröbner basis computations. The generators of  $\mathfrak{J}_x$  and  $\mathfrak{J}_y$  are somewhat too lengthy to be reproduced here. They are available on [Manuel Kauers' website](#). We simply report that  $\dim_{\mathbb{Q}(x, t)} \mathbb{Q}(x, t)[D_x, D_t]/\mathfrak{J}_x = \dim_{\mathbb{Q}(y, t)} \mathbb{Q}(y, t)[D_y, D_t]/\mathfrak{J}_y = 11$ , and that the Gröbner bases for  $\mathfrak{J}_x$  and  $\mathfrak{J}_y$  with respect to a degree order are roughly 1Mb long.

The proof consists in showing that these guesses are correct. As in the previous proof, we will first exhibit a pair of series ( $F \equiv F(x; t), G \equiv G(y; t)$ ) in  $\mathbb{Q}[[x, t]] \times \mathbb{Q}[[y, t]]$  that satisfy the guessed differential equations and certain initial conditions. Then, we will prove that they satisfy the system

$$\begin{cases} F(x) + (1 + Y)^2 G(Y) = xY/t + Q(0, 0), \\ F(X) + (1 + y)^2 G(y) = Xy/t + Q(0, 0), \end{cases} \quad (22)$$

which, by the standard kernel method, characterises the pair  $(Q(x, 0), Q(0, y))$  in  $\mathbb{Q}[[x, t]] \times \mathbb{Q}[[y, t]]$ . Here, the algebraic series  $X$  and  $Y$  that cancel the kernel are given by

$$\begin{aligned} X \equiv X(y; t) &= \frac{1 - \sqrt{1 - 4t^2 \bar{y}(1 + y)^3}}{2t(1 + y)} \\ &= t\bar{y}(1 + y)^2 + \bar{y}^2(1 + y)^5 t^3 + O(t^5) \quad \in \mathbb{Q}[[y, \bar{y}]][[t]], \\ Y \equiv Y(x; t) &= \frac{1 - tx - 2t\bar{x} - \sqrt{1 - 2tx - 4t\bar{x} + t^2 x^2}}{2t(x + \bar{x})} \\ &= \bar{x}t + (2\bar{x}^2 + 1)t^2 + O(t^3) \quad \in \mathbb{Q}[[x, \bar{x}]][[t]]. \end{aligned}$$

To exhibit a power series of  $\mathbb{Q}[[x, t]]$  annihilated by  $\mathfrak{J}_x$ , we construct a nonzero element of  $\mathfrak{J}_x \cap \mathbb{Q}(x, t)[D_t]$ , free of  $D_x$ . For such an operator it is easy to check that it admits a solution in  $\mathbb{Q}(x)[[t]]$ . To determine this series uniquely, we prescribe the first coefficients of its expansion in  $t$  to coincide with those of  $Q(x, 0)$ . It remains to prove that this series, henceforth denoted  $F \equiv F(x; t)$ , actually belongs to  $\mathbb{Q}[x][[t]]$ . In order to do so, we look at the recurrence relation satisfied by its coefficients (this recurrence can be derived from the differential equation in  $t$ ). Alas, it reads

$$P(n, x)f_n(x) = \sum_i P_i(n, x)f_{n-i}(x),$$

where  $P$  and the  $P_i$ 's are polynomials, and  $P$  actually involves  $x$  (we denote by  $f_n(x)$  the coefficient of  $t^n$  in the series  $F(x; t)$ ). However, once we apply a desingularisation algorithm to this recurrence [1], the leading coefficient becomes free of  $x$ . Since the first values of  $f_n(x)$  are polynomials in  $x$ , this implies that our series  $F(x; t)$  lies in  $\mathbb{Q}[x][[t]] \subseteq \mathbb{Q}[[x, t]]$ . In the same way we construct a series  $G(y; t)$

in  $\mathbb{Q}[[y, t]]$  that is cancelled by  $\mathfrak{J}_y$  and coincides with  $Q(0, y; t)$  far enough to be uniquely determined by these two conditions.

It remains to prove that the pair  $(F, G)$  satisfies (22). Using algorithms for D-finite closure properties, together with the defining algebraic equations for  $X, Y$  and  $Q(0, 0)$  (Lemma 15), we can compute differential equations in  $t$  for the left-hand side and the right-hand side of these identities (which are both power series in  $t$ , with coefficients in  $\mathbb{Q}[y, \bar{y}]$  or  $\mathbb{Q}[x, \bar{x}]$ , respectively). After checking an appropriate number of initial terms, it follows that  $F$  and  $G$  form a solution of (22), and this concludes our proof.  $\square$

The next result proves that the D-finite generating function  $Q(x, y; t)$  for the model  $\mathcal{S}_1$  is transcendental. We have not been able to find a direct proof of this; arguments based on asymptotics for coefficients of several specialisations are not enough, since for instance, the coefficients of  $Q(1, 0; t)$  appear to grow like  $c(2 + \sqrt{3})^n/n^{3/2}$ , for some constant  $c$ , and those of  $Q(0, 1; t)$  appear to grow like  $c(4\sqrt{2})^n/n^{3/2}$ , for some constant  $c$ , but these asymptotic behaviours are not incompatible with algebraicity [19]. We present a more sophisticated argument, reducing the transcendence question to linear algebra. Our reasoning is inspired by Section 9 in [42]. The main idea can be traced back at least to [32]; similar arguments are used in [14, 3] and [15, §2]. The argument may be viewed as a general technique for proving transcendence of D-finite power series;<sup>3</sup> even though based on ideas in [42], we write down the proof in detail, since we have not spotted out such a proof elsewhere in the literature. The needed background on linear differential equations can be found in [41, §4.4.1] or [33, §20].

**Proposition 18.** *The complete generating function  $Q(x, y; t)$  for the model  $\mathcal{S}_1$  is not algebraic.*

*Proof.* It is sufficient to prove that the series

$$Q(1, 0; t) = 1 + t + 4t^2 + 8t^3 + 39t^4 + 98t^5 + O(t^6)$$

is not algebraic.

Assume by contradiction that  $Q(1, 0; t)$  is algebraic. Recall that it is D-finite, and denote by  $\mathcal{M}(t, D_t)$  the monic linear differential operator in  $\mathbb{Q}(t)[D_t]$  of minimal order such that  $\mathcal{M}(Q(1, 0; t)) = 0$ . Denote by  $\mathcal{L}$  the 11th order linear differential operator in  $\mathbb{Q}(t)[D_t]$  computed in the proof of Proposition 17 such that  $\mathcal{L}(Q(1, 0; t)) = 0$ . By minimality,  $\mathcal{M}$  right-divides  $\mathcal{L}$  in  $\mathbb{Q}(t)[D_t]$ . Moreover,  $\mathcal{M}$  strictly right-divides  $\mathcal{L}$ , since otherwise  $\mathcal{L}$  would have a basis of algebraic solutions [15, §2], which is ruled out by a local analysis showing that logarithms occur in a basis of solutions of  $\mathcal{L}$  at  $t = 0$ . Therefore, the order  $n$  of  $\mathcal{M}$  is at most 10. On the other hand, it follows from [15, §2.2] that  $\mathcal{M}$  is Fuchsian and has the form

$$\mathcal{M} = D_t^n + \frac{a_{n-1}(t)}{A(t)} D_t^{n-1} + \dots + \frac{a_0(t)}{A(t)^n}, \quad (23)$$

where  $A(t)$  is a squarefree polynomial and  $a_{n-i}(t)$  is a polynomial of degree at most  $\deg(A^i) - i$ .

To get a contradiction (thus proving that  $Q(1, 0; t)$  is transcendental), we use the following strategy: (i) get a bound on the degree of  $A$ —and thus on the degrees of the coefficients of  $\mathcal{M}$ —in terms of  $n$  and of local information of  $\mathcal{L}$ ; (ii) use this bound and linear algebra to show that such an operator  $\mathcal{M}$  cannot annihilate  $Q(1, 0; t)$ .

<sup>3</sup>There exists an alternative algorithmic procedure based on [37], that allows in principle to answer this question [36]. It involves, among other things, factoring linear differential operators, and deciding whether a linear differential operator admits a basis of algebraic solutions. However, this procedure would have a very high computational cost when applied to our situation.

For (i), it is sufficient to bound the number of singularities of  $\mathcal{M}$  (i.e., the roots of  $A(t)$ , and possibly  $t = \infty$ ). Let us write  $A(t) = A_1(t)A_2(t)$ , where the roots of  $A_1(t)$  are the finite *true* singular points of  $\mathcal{M}$ , and the roots of  $A_2(t)$  are the finite *apparent* singular points of  $\mathcal{M}$  (these are the roots  $p \in \mathbb{C}$  of  $A(t)$  such that the equation  $\mathcal{M}(y(t))=0$  possesses a basis of analytic solutions at  $t = p$ ).

Since  $\mathcal{M}$  right-divides  $\mathcal{L}$ , the true singularities of  $\mathcal{M}$  form a subset of the true singularities of  $\mathcal{L}$ . Now,  $\mathcal{L}$  is explicitly known, and its local analysis shows that it is Fuchsian and that it admits the following local data, presented below as pairs (point  $p$ , (sorted) list of exponents of  $\mathcal{L}$  at  $p$ ):

$$\begin{aligned} 0, & \quad [-2, -2, -3/2, -1, -1/2, 0, 1, 2, 3, 4, 5], \\ 1, & \quad [-1, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9], \\ \infty, & \quad [1, 5/3, 2, 7/3, 8/3, 3, 10/3, 11/3, 4, 13/3, 5], \\ \pm \frac{\sqrt{3}}{9}, & \quad [0, 1, 3/2, 2, 5/2, 3, 3, 4, 5, 6, 7], \\ 3 \pm 2\sqrt{2}, & \quad [0, 1/2, 1, 3/2, 2, 5/2, 3, 4, 5, 6, 7], \\ 55 \text{ apparent singularities,} & \quad [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 11]. \end{aligned}$$

Therefore,  $\mathcal{L}$  has 6 finite true singularities, and this implies that  $\deg A_1$  is at most 6. It remains to upper bound  $\deg A_2$ ; this will result from an analysis of the apparent singularities of  $\mathcal{M}$ . To do this, for any point  $p$  in  $\mathbb{C} \cup \{\infty\}$  we denote by  $S_p(\mathcal{M})$  the following quantity:

$$S_p(\mathcal{M}) = (\text{sum of local exponents of } \mathcal{M} \text{ at } p) - (0 + 1 + \dots + (n - 1)).$$

If  $p$  is an ordinary point of  $\mathcal{M}$ , then  $S_p(\mathcal{M}) = 0$ ; therefore  $S_p(\mathcal{M})$  is an interesting quantity only for singularities  $p$  of  $\mathcal{M}$ . Moreover, the quantities  $S_p(\mathcal{M})$  are globally related by the so-called Fuchs' relation [41, §4.4.1]:

$$\sum_{p \in \mathbb{C} \cup \{\infty\}} S_p(\mathcal{M}) = \sum_{p \text{ singularity of } \mathcal{M}} S_p(\mathcal{M}) = -n(n - 1). \quad (24)$$

If  $p$  is an apparent singularity of  $\mathcal{M}$ , then  $S_p(\mathcal{M}) \geq 1$ , since the local exponents of  $\mathcal{M}$  at  $p$  are  $n$  distinct non-negative integers, the largest one being at least equal to  $n$  [15, Lemma 2.2]. We use this observation in conjunction with Fuchs' relation (24) in order to bound the number of apparent singularities of  $\mathcal{M}$ :

$$\#\{\text{apparent singularities of } \mathcal{M}\} \leq -n(n-1) - \sum_{p \text{ true singularity of } \mathcal{M}} S_p(\mathcal{M}). \quad (25)$$

For any true singularity  $p$  of  $\mathcal{M}$ , the list of local exponents of  $\mathcal{M}$  at  $p$  is a sublist of the list of exponents of  $\mathcal{L}$  at  $p$ . Therefore  $S_p(\mathcal{M}) \geq S_p^{(n)}(\mathcal{L})$ , where  $S_p^{(n)}(\mathcal{L})$  denotes the sum of the smallest  $n$  elements from the list of exponents of  $\mathcal{L}$  at  $p$ , minus  $(0 + 1 + \dots + (n - 1))$ . Thus, the sum  $\sum_{p \text{ true singularity of } \mathcal{M}} S_p(\mathcal{M})$  is minimal

if the true singularities of  $\mathcal{M}$  are precisely those true singularities  $p$  of  $\mathcal{L}$  for which  $S_p^{(n)}(\mathcal{L})$  is non-positive. It then follows from (25) that

$$\deg(A_2) \leq -n(n - 1) - \sum_{p \text{ true singularity of } \mathcal{L}} \min(0, S_p^{(n)}(\mathcal{L})). \quad (26)$$

For instance, for  $n = 10$ , the quantities  $S_p^{(n)}(\mathcal{L})$  where  $p$  runs through the set  $\{0, 1, \infty, \frac{\sqrt{3}}{9}, -\frac{\sqrt{3}}{9}, 3 + 2\sqrt{2}, 3 - 2\sqrt{2}\}$  of true singularities of  $\mathcal{L}$  are equal respectively to  $-42, -10, -17, -17, -17, -39/2, -39/2$ . Therefore, the inequality (26) reads  $\deg(A_2) \leq -10 \times 9 - (42 + 10 + 17 + 17 + 17 + 39/2 + 39/2) = 52$ , and thus  $\deg(A) = \deg(A_1) + \deg(A_2) \leq 6 + 52 = 58$ .

A similar computation for  $n = 1, 2, \dots, 9$  implies the respective upper bounds 9, 12, 15, 19, 24, 31, 40, 47, 53 for the degree of  $A$ . We conclude that the minimal-order annihilating operator  $\mathcal{M}$  has the form (23) with  $n \leq 10$  and coefficients of degree  $\deg(A) \leq 58$  and  $\deg(a_{n-i}) \leq 57i$  for  $0 \leq i \leq n - 1$ .

To summarise, under the assumption that  $Q(1, 0; t)$  is algebraic, we proved that there exists a non-zero linear differential operator that annihilates it (namely  $A(t)^n \cdot \mathcal{M}$ ), of order at most 10 and polynomial coefficients of degrees at most 580. Moreover, this operator writes  $\hat{\mathcal{M}} = \sum_{i=0}^{10} \sum_{j=0}^{570+i} m_{i,j} t^j D_t^i$ . The equality  $\hat{\mathcal{M}}(Q(1, 0; t)) = 0 \pmod{t^{6400}}$  then yields a linear system of 6400 equations in the 6336 unknowns  $m_{i,j}$ , and a linear algebra computation shows that its unique solution is the trivial one  $m_{i,j} = 0$  for all  $i$  and  $j$ , contradicting the fact that  $\mathcal{M} \neq 0$ .

In conclusion,  $Q(1, 0; t)$  is transcendental.  $\square$

## 9. FINAL COMMENTS AND QUESTIONS

We have determined strategies for classifying the generating functions of walks with small steps in the positive octant, based on the algebraic kernel method, reductions to lower dimensions, and computer algebra.

In this way, we have been able to prove D-finiteness for all models for which we had guessed a differential equation. All these models have a finite group. However, we have not ruled out the possibility of non-D-finite models having a finite group. Indeed, for the 19 models discussed in Section 6.2 and listed in Figure 4, the group is finite but we have not discovered any differential equations. If one of these models was proved to be non-D-finite, it would be the end of the correspondence between finite groups and D-finiteness that holds for quadrant walks. One approach to prove non-D-finiteness might be a 3D extension of [8].

Here are other natural questions that we leave open.

- **Groups.** Can one prove that the groups that we conjecture infinite are infinite indeed? Some techniques that apply to quadrant models are presented in [11, Section 3].
- **Transcendence.** For the complete generating function of many models with a finite group, we have proved D-finiteness but not algebraicity. Can one prove that these models are in fact transcendental, either using an asymptotic argument or by adapting the proof of Proposition 18?
- **Non-D-finiteness.** Can one prove the non-D-finiteness of certain quadrant models with repeated steps with the technique of [8]? Can it be extended to octant models?
- **Human proofs.** Can one give “human proofs” for the computer algebra results of Section 8?
- **Repeated steps.** If we investigate systematically quadrant models with repeated steps (and arbitrary cardinality), do we find more attractive models, like those of Figure 5?
- **Closed form expressions.** Can one express all the D-finite length generating functions that we obtained in terms of hypergeometric series, as was done for quadrant walks in [4]?

**Acknowledgements.** S.M. would like to thank Simon Fraser University and the Inria-MSR joint lab, where he was working while the majority of this research was completed.

## REFERENCES

- [1] S. A. Abramov and M. van Hoeij. Desingularization of linear difference operators with polynomial coefficients. In *Proceedings of ISSAC'99*, pages 269–275, 1999.

- [2] C. Banderier and P. Flajolet. Basic analytic combinatorics of directed lattice paths. *Theoret. Comput. Sci.*, 281(1-2):37–80, 2002.
- [3] D. Bertrand and F. Beukers. Équations différentielles linéaires et majorations de multiplicités. *Ann. Sci. École Norm. Sup. (4)*, 18(1):181–192, 1985.
- [4] A. Bostan, F. Chyzak, M. van Hoeij, M. Kauers, and L. Pech. Explicit differentially finite generating functions of walks with small steps in the quarter plane. In preparation, 2014.
- [5] A. Bostan and M. Kauers. Automatic classification of restricted lattice walks. In *21st International Conference on Formal Power Series and Algebraic Combinatorics (FPSAC 2009)*, Discrete Math. Theor. Comput. Sci. Proc., AK, pages 201–215. Assoc. Discrete Math. Theor. Comput. Sci., Nancy, 2009.
- [6] A. Bostan and M. Kauers. The complete generating function for Gessel walks is algebraic. *Proc. Amer. Math. Soc.*, 138(9):3063–3078, 2010. With an appendix by Mark van Hoeij.
- [7] A. Bostan, I. Kurkova, and K. Raschel. A human proof of Gessel’s lattice path conjecture. [ArXiv:1309.1023](https://arxiv.org/abs/1309.1023), 2013.
- [8] A. Bostan, K. Raschel, and B. Salvy. Non-D-finite excursions in the quarter plane. *J. Combin. Theory Ser. A*, 121:45–63, 2014.
- [9] M. Bousquet-Mélou. Counting walks in the quarter plane. In *Mathematics and computer science 2, (Versailles, 2002)*, Trends Math., pages 49–67. Birkhäuser, Basel, 2002.
- [10] M. Bousquet-Mélou. Walks in the quarter plane: Kreweras’ algebraic model. *Ann. Appl. Probab.*, 15(2):1451–1491, 2005.
- [11] M. Bousquet-Mélou and M. Mishna. Walks with small steps in the quarter plane. In *Algorithmic probability and combinatorics*, volume 520 of *Contemp. Math.*, pages 1–39. Amer. Math. Soc., Providence, RI, 2010.
- [12] M. Bousquet-Mélou and M. Petkovšek. Linear recurrences with constant coefficients: the multivariate case. *Discrete Math.*, 225(1-3):51–75, 2000.
- [13] M. Bousquet-Mélou and M. Petkovšek. Walks confined in a quadrant are not always D-finite. *Theoret. Comput. Sci.*, 307(2):257–276, 2003.
- [14] G. V. Chudnovsky. Rational and Padé approximations to solutions of linear differential equations and the monodromy theory. In *Complex analysis, microlocal calculus and relativistic quantum theory (Proc. Internat. Colloq., Centre Phys., Les Houches, 1979)*, volume 126 of *Lecture Notes in Phys.*, pages 136–169. Springer, Berlin-New York, 1980.
- [15] O. Cormier, M. F. Singer, B. M. Trager, and F. Ulmer. Linear differential operators for polynomial equations. *J. Symbolic Comput.*, 34(5):355–398, 2002.
- [16] P. Duchon. On the enumeration and generation of generalized Dyck words. *Discrete Math.*, 225(1-3):121–135, 2000.
- [17] G. Fayolle, R. Iasnogorodski, and V. Malyshev. *Random walks in the quarter-plane*, volume 40 of *Applications of Mathematics (New York)*. Springer-Verlag, Berlin, 1999.
- [18] G. Fayolle and K. Raschel. On the holonomy or algebraicity of generating functions counting lattice walks in the quarter plane. *Markov Process. Related Fields*, 16(3):485–496, 2010. [Arxiv:1004.1733](https://arxiv.org/abs/1004.1733).
- [19] P. Flajolet. Analytic models and ambiguity of context-free languages. *Theoret. Comput. Sci.*, 49(2-3):283–309, 1987.
- [20] I. M. Gessel. A factorization for formal Laurent series and lattice path enumeration. *J. Combin. Theory Ser. A*, 28(3):321–337, 1980.
- [21] I. M. Gessel. A probabilistic method for lattice path enumeration. *J. Statist. Plann. Inference*, 14(1):49–58, 1986.
- [22] M. Kauers. Guessing handbook. Technical Report 09-07, RISC-Linz, 2009. Available at [http://www.risc.jku.at/publications/download/risc\\_3814/demo.nb.pdf](http://www.risc.jku.at/publications/download/risc_3814/demo.nb.pdf).
- [23] M. Kauers, C. Koutschan, and D. Zeilberger. Proof of Ira Gessel’s lattice path conjecture. *Proc. Nat. Acad. Sci. USA*, 106(28):11502–11505, 2009. [ArXiv:0806.4300](https://arxiv.org/abs/0806.4300).
- [24] M. Kauers and D. Zeilberger. The quasi-holonomic Ansatz and restricted lattice walks. *J. Difference Equ. Appl.*, 14:1119–1126, 2008. [ArXiv:0806.4318](https://arxiv.org/abs/0806.4318).
- [25] C. Koutschan. HolonomicFunctions (User’s Guide). Technical Report 10-01, RISC Report Series, University of Linz, Austria, January 2010. Available at [http://www.risc.jku.at/publications/download/risc\\_3934/hf.pdf](http://www.risc.jku.at/publications/download/risc_3934/hf.pdf).
- [26] I. Kurkova and K. Raschel. Explicit expression for the generating function counting Gessel’s walks. *Adv. in Appl. Math.*, 47(3):414–433, 2011.
- [27] L. Lipshitz. The diagonal of a D-finite power series is D-finite. *J. Algebra*, 113(2):373–378, 1988.
- [28] L. Lipshitz. D-finite power series. *J. Algebra*, 122:353–373, 1989.
- [29] C. Mallinger. Algorithmic manipulations and transformations of univariate holonomic functions and sequences. Master’s thesis, J. Kepler University, Linz, August 1996.

- [30] S. Melczer and M. Mishna. Singularity analysis via the iterated kernel method. *Combin. Probab. Comput.*, 23(5):861–888, 2014.
- [31] M. Mishna and A. Rechnitzer. Two non-holonomic lattice walks in the quarter plane. *Theoret. Comput. Sci.*, 410(38-40):3616–3630, 2009. [ArXiv:math/0701800](https://arxiv.org/abs/math/0701800).
- [32] M. Ohtsuki. On the number of apparent singularities of a linear differential equation. *Tokyo J. Math.*, 5(1):23–29, 1982.
- [33] E. G. C. Poole. *Introduction to the theory of linear differential equations*. Oxford Univ. Press, London, 1936.
- [34] B. Salvy and P. Zimmermann. Gfun: a Maple package for the manipulation of generating and holonomic functions in one variable. *ACM Transactions on Mathematical Software*, 20(2):163–177, 1994. Reprint doi:10.1145/178365.178368.
- [35] A. Schrijver. *Theory of linear and integer programming*. Wiley-Interscience Series in Discrete Mathematics. John Wiley & Sons Ltd., Chichester, 1986.
- [36] M. F. Singer. Private communication, 2014.
- [37] M. F. Singer. Algebraic solutions of  $n$ th order linear differential equations. In *Proceedings of the Queen's Number Theory Conference, 1979 (Kingston, Ont., 1979)*, volume 54 of *Queen's Papers in Pure and Appl. Math.*, pages 379–420. Queen's Univ., Kingston, Ont., 1980.
- [38] R. P. Stanley. *Enumerative combinatorics 2*, volume 62 of *Cambridge Studies in Advanced Mathematics*. Cambridge University Press, Cambridge, 1999.
- [39] W. A. Stein et al. Sage mathematics software. <http://www.sagemath.org>, 2013.
- [40] N. Takayama. An algorithm of constructing the integral of a module. In *Proceedings of IS-SAC'90*, pages 206–211, 1990.
- [41] M. van der Put and M. F. Singer. *Galois theory of linear differential equations*, volume 328 of *Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]*. Springer-Verlag, Berlin, 2003.
- [42] M. van Hoeij. Factorization of differential operators with rational functions coefficients. *J. Symbolic Comput.*, 24(5):537–561, 1997.



## APPENDIX A. THE NUMBER OF NON-EQUIVALENT 2D OR 3D MODELS

We now want to prove Proposition 5. To begin with, we determine the polynomial counting models with no unused step.

### A.1. MODELS WITH NO UNUSED STEP

**Proposition 19.** *The generating function of step sets that contain no unused step, counted up to permutations of the coordinates, is*

$$\begin{aligned}
 J = & 1 + 3u + 21u^2 + 179u^3 + 1294u^4 + 7041u^5 + 28917u^6 + 92216u^7 + 235338u^8 \\
 & + 492509u^9 + 860520u^{10} + 1271528u^{11} + 1603192u^{12} + 1734397u^{13} \\
 & + 1614372u^{14} + 1293402u^{15} + 890395u^{16} + 524638u^{17} + 263008u^{18} \\
 & + 111251u^{19} + 39256u^{20} + 11390u^{21} + 2676u^{22} + 500u^{23} + 73u^{24} + 9u^{25} + u^{26}.
 \end{aligned}$$

We prove this using Burnside's lemma [38, Lem. 7.24.5]:

$$J = \frac{1}{6} \sum_{\sigma \in \mathfrak{S}_3} J^\sigma, \tag{27}$$

where  $J^\sigma$  counts sets that contain no unused step and are left invariant under the permutation  $\sigma$ . By symmetry, it suffices to determine  $J^\sigma$  when  $\sigma = \text{id}$ , when  $\sigma$  is the 2-cycle  $(1, 2)$  and when  $\sigma$  is the 3-cycle  $(1, 2, 3)$ . This is done in Sections A.1.1, A.1.2, and A.1.3, respectively.

**A.1.1. No prescribed symmetry: the series  $J^{\text{id}}$ .** There are  $26 = 3^3 - 1$  non-trivial steps, and thus the generating function of all models is  $(1 + u)^{26}$ .

Now we want to remove sets that contain unused steps, using the characterisation of Lemma 4. We use the notation  $A_x$  for the generating function of models that satisfy Condition  $(A_x)$ , and so on. We extrapolate this so that  $A_{xy}$  counts models

satisfying  $(A_x)$  and the condition  $(A_y)$  obtained from  $(A_x)$  by replacing  $x$  by  $y$ . Similarly,  $A_x C_z$  counts models satisfying both  $(A_x)$  and  $(C_z)$ , and is *not* the product of the series  $A_x$  and  $C_z$ . We hope this will not raise any confusion. Let us note that

$$A_z C_z = B C_z = C_y C_z = 0 \quad \text{and} \quad A_{xyz} = A_{xy z} B.$$

Using inclusion-exclusion, obvious symmetries ( $A_x = A_y$  for instance) and the above relations, we obtain

$$J^{\text{id}} = (1+u)^{26} - 3A_x - B - 3C_z + 3A_{xy} + 3A_x B + 6A_x C_z - 3A_{xy} B - 3A_{xy} C_z. \quad (28)$$

Let us now determine the series  $A_x$ ,  $B$  and  $C_z$ . We will then give without details the values of the other five series.

For  $A_x$ , we count models containing no  $x^+$ -step, but at least one  $x^-$ -step. Among the 26 steps,  $26 - 9 = 17$  are not  $x^+$ . Among these 17 steps, 8 are not  $x^-$  either. Hence

$$A_x = (1+u)^{17} - (1+u)^8 = [17] - [8],$$

where we denote  $[i] = (1+u)^i$ .

For  $B$ , we count non-empty models in which each step has a negative coordinate. There are  $26 - 7 = 19$  such steps, and thus

$$B = [19] - 1.$$

Finally, a model satisfying  $(C_z)$  must contain 001 and consists otherwise of steps  $ijk$  with  $i + j \leq 0$ . There are  $26 - 9 = 17$  steps satisfying this inequality, among which 001, which is necessarily in  $\mathcal{S}$ . Thus

$$C_z = u([16] - [1])$$

as the model must not be a subset of  $\{001, 00\bar{1}\}$ .

Let us now list the values of the other series occurring in (28):

$$\begin{aligned} A_{xy} &= [11] - 2[5] + [2] \\ A_x B &= [14] - [5] \\ A_x C_z &= u([13] - [4]) \\ A_{xy} B &= [10] - 2[4] + [1] \\ A_{xy} C_z &= u([10] - 2[4] + [1]). \end{aligned}$$

Returning to (28), this now gives the generating function of models with no unused step:

$$\begin{aligned} J^{\text{id}} &= [26] - [19] - 3[17] + 3[14] + 3[11] - 3[10] + 3[8] - 9[5] + 6[4] + 3[2] - 3[1] + 1 \\ &\quad + 3u(-[16] + 2[13] - [10]). \quad (29) \end{aligned}$$

**A.1.2. With an  $xy$ -symmetry: the series  $J^{(1,2)}$ .** We now count models  $\mathcal{S}$  with no unused step that have an  $xy$ -symmetry:  $ijk \in \mathcal{S} \Leftrightarrow jik \in \mathcal{S}$ . We revisit the above argument with this additional constraint. The set of all 26 steps has 17 orbits under the action of the 2-cycle  $(1, 2)$ : 8 of them are singletons, and 9 are pairs. Hence the generating function of  $xy$ -symmetric sets is  $[8][[9]]$  where  $[[j]]$  stands for  $(1+u^2)^j$ . We recycle the notation  $A_x$ ,  $B$ , and so on, but we add bars to indicate that we only count models with an  $xy$ -symmetry:  $\overline{A_x}$ ,  $\overline{B}$ , etc. We apply again inclusion-exclusion to count symmetric models with no unused step, noting that

$$\overline{A_x} = \overline{A_y} = \overline{A_{xy}}, \quad \overline{C_x} = \overline{A_z C_z} = \overline{B C_z} = 0 \quad \text{and} \quad \overline{A_{xz} B} = \overline{A_{xz}}.$$

We thus obtain:

$$J^{(12)} = [8][[9]] - \overline{A_x} - \overline{A_z} - \overline{B} - \overline{C_z} + \overline{A_x B} + \overline{A_z B} + \overline{A_x C_z}.$$



Let us determine  $\overline{A_x}$ . We observe that 5 singleton orbits are not  $x^+$  (among which 2 are not  $x^-$  either), and that 3 orbits of size 2 are not  $x^+$  (all of them are  $x^-$ ). This gives

$$\overline{A_x} = [5][[3]] - [2].$$

For  $\overline{A_z}$ , we find that 5 singleton orbits are not  $z^+$  (among which 2 are not  $z^-$  either), and that 6 orbits of size 2 are not  $z^+$  (among which 3 are not  $z^-$  either). This gives

$$\overline{A_z} = [5][[6]] - [2][[3]].$$

We further obtain

$$\begin{aligned} \overline{B} &= [5][[7]] - 1 \\ \overline{C_z} &= u([4][[6]] - [1]) \\ \overline{A_x B} &= [4][[3]] - [1] \\ \overline{A_z B} &= [4][[5]] - [1][[2]] \\ \overline{A_x C_z} &= u([4][[3]] - [1]), \end{aligned}$$

so that finally

$$\begin{aligned} J^{(1,2)} &= [8][[9]] - [5]([7] + [6] + [3]) + [4]([5] + [3]) + [2]([3] + 1) \\ &\quad - [1]([2] + 1) + 1 - u[4]([6] - [3]). \end{aligned} \quad (30)$$

**A.1.3. With an  $(x, y, z)$ -symmetry: the series  $J^{(1,2,3)}$ .** We finally count how many models with no unused step are left invariant under the action of the cycle  $(1, 2, 3)$ . That is, if  $ijk \in \mathcal{S}$ , then  $jki$  (and  $kij$ ) also belong to  $\mathcal{S}$ . The set of our 26 steps has 10 orbits under the action of the 3-cycle: 2 of them are singletons, and 8 contain 3 elements. Hence the generating function of symmetric models is  $[2]\langle 8 \rangle$ , where  $\langle j \rangle = (1 + u^3)^j$ . We now use tildes above our generating functions to indicate the invariance under  $(1, 2, 3)$ . Noting that

$$\widetilde{A_x} = \widetilde{A_y} = \widetilde{A_z} = \widetilde{A_x B} \quad \text{and} \quad \widetilde{C_z} = 0,$$

the inclusion-exclusion reduces to

$$J^{(1,2,3)} = [2]\langle 8 \rangle - \widetilde{B} = [2]\langle 8 \rangle - [1]\langle 6 \rangle + 1, \quad (31)$$

since there are 1 non-positive singleton orbit and 6 non-positive orbits of size 3.

*Proof of Proposition 19.* We apply Burnside's formula (27) with  $J^{\text{id}}$ ,  $J^{(1,2)}$  and  $J^{(1,2,3)}$  given by (29), (30) and (31) respectively.  $\square$

## A.2. MODELS WITH NO UNUSED STEP AND DIMENSION AT MOST 1

We now establish the counterpart of Proposition 19 for models of dimension at most 1.

**Proposition 20.** *The generating function of models of dimension at most 1, having no unused step, counted up to permutations of the coordinates, is*

$$\begin{aligned} K &= 1 + 3u + 21u^2 + 106u^3 + 315u^4 + 616u^5 + 846u^6 + 844u^7 \\ &\quad + 622u^8 + 341u^9 + 138u^{10} + 40u^{11} + 8u^{12} + u^{13}. \end{aligned}$$

As before, we prove this using Burnside's lemma:

$$K = \frac{1}{6} \sum_{\sigma \in \mathfrak{S}_3} K^\sigma, \quad (32)$$

where  $K^\sigma$  is the generating function of 0- or 1-dimensional models with no unused step, left invariant by the permutation  $\sigma$ . Again, we only need to determine  $K^{\text{id}}$ ,  $K^{(1,2)}$  and  $K^{(1,2,3)}$ .

**A.2.1. Small dimension, no prescribed symmetry: the series  $K^{\text{id}}$ .** By definition, a model is at most one-dimensional if it suffices to enforce one non-negativity condition to confine walks in the octant. We denote by  $K_x^{\text{id}}$  the generating function of models (with no unused step) for which it suffices to enforce the  $x$ -condition. We denote similarly by  $K_{xy}^{\text{id}}$  the generating function of models for which it suffices to enforce the  $x$ -condition or the  $y$ -condition, and adopt a similar notation  $K_{xyz}^{\text{id}}$  for models for which it suffices to enforce any of the three conditions. This is the case, for instance, if  $\mathcal{S} = \{\bar{1}\bar{1}\bar{1}, 111\}$ . By inclusion-exclusion,

$$K^{\text{id}} = 3K_x^{\text{id}} - 3K_{xy}^{\text{id}} + K_{xyz}^{\text{id}}. \quad (33)$$

**The generating function  $K_x^{\text{id}}$ .** This polynomial count models with no unused step satisfying Lemma 3. To begin with, let us count *all* models satisfying this lemma, or equivalently, one (and exactly one) of the following conditions:

1. there is no  $y^-$  nor  $z^-$  step,
2. there is no  $y^-$  step, but there are  $z^-$  steps and every step  $ijk$  satisfies  $k \geq i$ ,
3. there is no  $z^-$  step, but there are  $y^-$  steps and every step  $ijk$  satisfies  $j \geq i$ ,
4. there are  $y^-$  and  $z^-$  steps and every step  $ijk$  satisfies  $j \geq i$  and  $k \geq i$ .

Since exactly 11 of the 26 steps are neither  $y^-$  nor  $z^-$ , the generating function of models satisfying Condition 1 is  $(1+u)^{11} = [11]$ . For models satisfying Condition 2, there are also 11 admissible steps, among which 9 are not  $z^-$ . Hence the associated generating function is  $[11] - [9]$ . Of course, the argument and the series are the same for Condition 3. Finally, there are 13 admissible steps for Condition 4, among which 10 are not  $z^-$ , 10 are not  $y^-$  and 8 are neither  $y^-$  nor  $z^-$ . Hence the generating function of models satisfying Condition 4 is  $[13] - 2[10] + [8]$ . In total, this gives

$$[13] + 3[11] - 2[10] - 2[9] + [8]$$

for the generating function of models satisfying Lemma 3. We now want to subtract those that have unused steps. We use the notation  $A_x$  for the generating function of models that satisfy Lemma 3 and Condition  $(A_x)$  of Lemma 4. Similarly,  $C_z$  counts models that satisfy Lemma 3 and Condition  $(C_z)$  of Lemma 4, and so on. Observe that

$$A_y = A_{xy}, \quad BA_x = B, \quad BA_{yz} = A_{yz}, \quad C_x = 0 \quad \text{and} \quad A_x C_z = C_z.$$

Moreover,  $y$  and  $z$  play symmetric roles. Hence, the inclusion-exclusion formula reduces in this case to

$$K_x^{\text{id}} = [13] + 3[11] - 2[10] - 2[9] + [8] - A_x.$$

Let us determine  $A_x$ , that is, the generating function of models that contain  $x^-$  steps but no  $x^+$  steps, and satisfy one of the 4 conditions above. For those that satisfy Condition 1, we find the polynomial  $[7] - [3]$  (because there are 7 steps that are neither  $x^+$ , nor  $y^-$  nor  $z^-$ , among which 3 are not  $x^-$  either). For Condition 2, we obtain  $[9] - [7]$  and for Condition 3 as well, by symmetry. Finally, for Condition 4 we obtain  $[12] - 2[9] + [7]$ . Finally,

$$A_x = [12] - [3].$$

Hence

$$K_x^{\text{id}} = [13] - [12] + 3[11] - 2[10] - 2[9] + [8] + [3]. \quad (34)$$

**The generating function  $K_{xy}^{\text{id}}$ .** This polynomial counts models with no unused step that satisfy Lemma 3 and the counterpart of Lemma 3 with  $x$  replaced by  $y$ . Rather than proceeding by inclusion-exclusion as above, we find convenient to list all these models  $\mathcal{S}$ :

- Either  $\mathcal{S}$  only consists of steps from  $\{0, 1\}^3 \setminus \{000\}$ ; the generating function is then [7].
- If there is a  $z^-$  step in  $\mathcal{S}$ , then Lemma 3 and its  $y$ -counterpart imply that it must be  $\bar{1}\bar{1}\bar{1}$ . Since this step is not unused, there must be an  $x^+$  step  $1jk$ , but then Lemma 3 implies that it is  $111$ . There is no other  $x^+$  nor  $y^+$  step. All remaining steps  $ijk$  must satisfy  $i = j \leq k$ , and so must be taken in  $\{001, \bar{1}\bar{1}0, \bar{1}\bar{1}1\}$ . Hence the associated generating function is  $u^2[3]$ .
- Otherwise there is no  $z^-$  step, and there is, say, a  $y^-$  step. By Lemma 3, it must be of the form  $\bar{1}\bar{1}k$  with  $k = 0, 1$ . Since this step is not unused, there must be also an  $x^+$  step, which must be of the form  $11\ell$ , with  $\ell = 0, 1$ . The only other possible step is  $001$ . Hence the generating function for this case is  $([2] - 1)^2 [1]$ .

In total,

$$K_{xy}^{\text{id}} = [7] + u^2[3] + ([2] - 1)^2 [1].$$

**The generating function  $K_{xyz}^{\text{id}}$ .** This polynomial counts models with no unused step that satisfy Lemma 3 and the counterparts of Lemma 3 with  $x$  replaced by  $y$  and then by  $z$ . It suffices to select from the list established above for  $K_{xy}^{\text{id}}$  the models satisfying also the latter condition. One finds that only models with non-negative steps, and also  $\mathcal{S} = \{\bar{1}\bar{1}\bar{1}, 111\}$  satisfy the required conditions, so that

$$K_{xyz}^{\text{id}} = [7] + u^2.$$

Returning to (33), we obtain the generating function of models of dimension at most 1 having no unused steps:

$$K^{\text{id}} = 3[13] - 3[12] + 9[11] - 6[10] - 6[9] + 3[8] - 2[7] + 3[3] - 3u^2[3] - 3([2] - 1)^2 [1] + u^2. \quad (35)$$

**A.2.2. Small dimension,  $xy$ -symmetry: the series  $K^{(1,2)}$ .** We revisit the enumeration of Section A.2.1 and enforce now an  $xy$ -symmetry. The variables  $x$  and  $y$  still play the same role, but  $z$  plays a different role, and (33) becomes

$$K^{(1,2)} = 2K_x^{(1,2)} + K_z^{(1,2)} - K_{xy}^{(1,2)} - 2K_{xz}^{(1,2)} + K_{xyz}^{(1,2)}.$$

We note however that the  $xy$ -symmetry implies that

$$K_x^{(1,2)} = K_{xy}^{(1,2)} \quad \text{and} \quad K_{xz}^{(1,2)} = K_{xyz}^{(1,2)},$$

so that

$$K^{(1,2)} = K_{xy}^{(1,2)} + K_z^{(1,2)} - K_{xyz}^{(1,2)}. \quad (36)$$

**The generating function  $K_z^{(1,2)}$ .** Clearly,  $K_z^{(1,2)} = K_x^{(2,3)}$ . We revisit the determination of  $K_x^{\text{id}}$  made in Section A.2.1, but restricting the enumeration to models with a  $yz$ -symmetry. We begin with the models that satisfy Lemma 3 and have a  $yz$ -symmetry. With Condition 1 we find the generating function  $[5][[3]]$ . Conditions 2 and 3 do not satisfy  $yz$ -symmetry, so do not contribute. Condition 4 contributes  $[5][[4]] - [4][[2]]$ .

As in the determination of  $K_x^{\text{id}}$ , it remains to subtract the series  $\overline{A_x}$  corresponding to models that contain  $x^-$  steps, but no  $x^+$  step. With Condition 1 we find  $[3][[2]] - [1][[1]]$ , and with Condition 4,  $[4][[4]] - [3][[2]]$ . Hence

$$K_z^{(1,2)} = [5][[3]] + [5][[4]] - [4][[2]] + [1][[1]] - [4][[4]].$$

**The generating function  $K_{xy}^{(1,2)}$ .** We now revisit the list of models used to determine  $K_{xy}^{\text{id}}$  in Section A.2.1, now enforcing an  $xy$ -symmetry. The generating function of symmetric non-negative models is  $[3][[2]]$ . All listed models that include a negative step are  $xy$ -symmetric. Hence

$$K_{xy}^{(1,2)} = [3][[2]] + u^2[3] + ([2] - 1)^2[1].$$

**The generating function  $K_{xyz}^{(1,2)}$ .** We now revisit the determination of  $K_{xyz}^{\text{id}}$  by enforcing an  $xy$ -symmetry. Besides non-negative models, counted by  $[3][[2]]$ , we only have the model  $\{\bar{1}\bar{1}\bar{1}, 111\}$ . Hence

$$K_{xyz}^{(1,2)} = [3][[2]] + u^2.$$

Returning to (36), we obtain

$$K^{(1,2)} = [5][[3]] + [5][[4]] - [4][[2]] + [1][[1]] - [4][[4]] + u^2[3] + ([2] - 1)^2[1] - u^2. \quad (37)$$

**A.2.3. Small dimension, cyclic symmetry: the series  $K^{(1,2,3)}$ .** We have finally reached the last, and simplest step of our calculation. By symmetry, we have

$$K^{(1,2,3)} = K_{xyz}^{(1,2,3)}.$$

Hence we now revisit the determination of  $K_{xyz}^{\text{id}}$  by enforcing a cyclic symmetry. Besides non-negative models, counted by  $[1]\langle 2 \rangle$ , we only have the model  $\{\bar{1}\bar{1}\bar{1}, 111\}$ . Hence

$$K^{(1,2,3)} = [1]\langle 2 \rangle + u^2. \quad (38)$$

We can now conclude the

*Proof of Proposition 20.* Apply Burnside's formula (32) with  $K^{\text{id}}$ ,  $K^{(1,2)}$  and  $K^{(1,2,3)}$  respectively given by (35), (37) and (38).  $\square$

We have finally counted how many models we need to study.

*Proof of Proposition 5.* The series  $I$  is  $J - K$ , with  $J$  and  $K$  given by Propositions 19 and 20 respectively.  $\square$

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