

Lattice Green Functions: the d -dimensional face-centred cubic lattice, $d = 8, 9, 10, 11, 12$

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Dedicated to A. J. Guttmann, for his 70th birthday.

Abstract. We previously reported on a recursive method to generate the expansion of the lattice Green function of the d -dimensional face-centred cubic lattice (fcc). The method was used to generate many coefficients for $d = 7$ and the corresponding linear differential equation has been obtained. In this paper, we show the strength and the limit of the method by producing the series and the corresponding linear differential equations for $d = 8, 9, 10, 11, 12$. The differential Galois groups of these linear differential equations are shown to be symplectic for $d = 8, 10, 12$ and orthogonal for $d = 9, 11$. The recursion relation naturally provides a 2-dimensional array $t_d(n, j)$ where only the coefficients $t_d(n, 0)$ correspond to the coefficients of the lattice Green function of the d -dimensional fcc. The coefficients $t_d(n, j)$ are associated to D -finite bivariate series annihilated by linear partial differential equations that we analyze.

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1. Introduction

The *lattice Green function* (LGF) of the d -dimensional face-centred cubic (fcc) lattice is given by a d -fold integral whose expansion around the origin is hard to obtain as the dimension goes higher [1, 2, 3, 4]. Only for $d = 3$ a closed form is known [5]. But since the integrand is of a very simple form—a rational function, after an appropriate variable transform—it follows from the theory of holonomic functions [6, 7] that those integrals are *D -finite* or *holonomic*, i.e. each of them satisfies a linear ordinary differential equation (ODE) with polynomial coefficients. For $d = 4$ the corresponding

linear ODE was obtained in [8], for $d = 5$ in [2], and for $d = 6$ in [4], by different methods. In a previous paper [9] we forwarded a *recursive method* that was efficient enough to allow us generate many series coefficients for $d = 7$ necessary to obtain the linear ODE. Since the recursion parameter in the method is the dimension d , we have obtained many short series for d as high as 45. From these data and the *Landau equations method* [10] on the integrals, we inferred many properties that we conjecture to be common to all the linear ODEs of d -dimensional fcc lattices. The order-eleven linear differential operator, corresponding to the linear differential equation, we have obtained [9] for the lattice Green function of the 7-dimensional face-centred cubic (fcc) has been found to verify a property recently forwarded [11]. This property is a canonical decomposition of irreducible linear differential operators with symplectic or orthogonal differential Galois groups and corresponds to the occurrence of a homomorphism of the operator and its adjoint. This property has been seen to occur [12, 13, 14] for many linear differential operators that emerge in lattice statistical physics and enumerative combinatorics.

In this paper, we show the strength and the limit of the method. With some technical improvements in the computations, we show how much high in dimension d we can go in generating sufficiently many terms of the LGF series in order to obtain the corresponding linear ODE. We find that the conjectures (especially on the singularities) given in [9] are all verified. We also find that the canonical decompositions of the operators follow the scheme given in [11].

Furthermore, the recursion relation gives a 2-dimensional array $t_d(n, j)$ where only the coefficients $t_d(n, 0)$ correspond to the coefficients of the lattice Green function of the d -dimensional fcc. We give the integrals whose expansion gives *bivariate series* with coefficients $t_d(n, j)$, and address the *D-finite systems* that annihilate these bivariate series.

The paper is organized as follows. Recalls are given in Section 2 where improvements of the method and some computational details are also given. Section 3 deals with our results on the differential equations annihilating the LGF of the d -dimensional fcc lattice for $d = 8, 9, 10, 11, 12$. The orders and singularities of all these linear ODEs are seen in agreement with our conjectures and computed *Landau singularities* in [9]. In Section 4, we show that the *differential Galois groups* of the operators are symplectic for $d = 8, d = 10, d = 12$ and orthogonal for $d = 9, d = 11$. We give for the operators corresponding to $d = 8$ and $d = 9$ the canonical decomposition that should [11] occur for the operators with symplectic or orthogonal differential Galois groups. In Section 5 we give the d -dimensional integrals depending on two variables (z, y) whose expansion around $(0, 0)$ (and integration) writes in terms of the coefficients $t_d(n, j)$. These coefficients generate a *D-finite bivariate series* $T_d(z, y)$ annihilated by a system of partial differential equations (PDE) that we give in Section 6 for the case $d = 2$. Switching to a system of *decoupled* PDE, we give in Section 7 the solutions that combine to match $T_2(z, y)$. Section 8 deals with $d = 3$, where we focus on one solution which, remarkably, is a modular form. We present some remarks in Section 9 and conclude in Section 10.

2. LGF generation of series

2.1. Recalls on the recursive method

The lattice Green function (LGF) of the d -dimensional face-centred cubic (fcc) lattice reads

$$LGF_d(x) = \frac{1}{\pi^d} \int_0^\pi \cdots \int_0^\pi \frac{dk_1 \cdots dk_d}{1 - x \cdot \lambda_d}, \quad (1)$$

where λ_d , called the structure function of the lattice, is given by:

$$\lambda_d = \binom{d}{2}^{-1} \cdot \sum_{i=1}^d \sum_{j=i+1}^d \cos(k_i) \cdot \cos(k_j). \quad (2)$$

The expansion around the origin of $LGF_d(x)$ is given by

$$LGF_d(z) = \sum_{n=0} z^n \cdot t_d(n, 0), \quad z = \frac{x}{4} \cdot \binom{d}{2}^{-1}, \quad (3)$$

where the array[‡] $t_d(n, j)$ is obtained with the recursive relation (see Section 2 in [9])

$$t_d(n, j) = \sum_{p=0}^n \sum_{q=q_1}^{q_2} \binom{n}{p} \binom{2j}{2q+p-n} \binom{2n+2j-2p-2q}{n+j-p-q} \cdot t_{d-1}(p, q), \quad (4)$$

$$q_1 = [(n-p+1)/2], \quad q_2 = [(n-p+2j)/2], \quad (5)$$

where $[x]$ is the integer part of x . To start the recursion, one needs:

$$t_2(n, j) = \sum_{p=p_1}^{p_2} \binom{2p}{p} \binom{2j}{2p-n} \binom{2n+2j-2p}{n+j-p}, \quad (6)$$

$$p_1 = [(n+1)/2], \quad p_2 = [(n+2j)/2]. \quad (7)$$

2.2. Computational details

The shape of the recurrence (4) suggests to start with the two-dimensional array $t_2(n, j)$, then compute $t_3(n, j)$, and so on. Once $t_3(n, j)$ is completed, the data of $t_2(n, j)$ is not any more needed since the recurrence (4) is of order 1 with respect to d . Also from the recurrence it is easy to see that for computing $t_d(n, 0)$, $0 \leq n \leq N$, the desired coefficients of the Taylor series, one needs the values of $t_{d-1}(n, j)$ for $0 \leq n \leq N$ and $0 \leq j \leq [(N-n)/2]$ (the same range applies to the arrays t_{d-2}, \dots, t_2). The advantage of such an implementation is that *it stores only $O(N^2)$ elements, which are integers*. The disadvantage is that one has to fix N at the very beginning, but the number of terms needed for constructing the linear differential operator is *not known in advance*.

If one looks at the recurrence (4) more closely, one discovers the remarkable fact that neither its coefficients, i.e. the product of the three binomials, nor its support, i.e. the summation bounds, depend on the parameter d . Hence, in the previous approach, the coefficients are the same in each step, but they are recomputed in each iteration $d = 3, 4, \dots$, which is clearly a waste of computational resources. In principle, we could collect all the coefficients in a big matrix A that maps the array t_{d-1} to t_d , so that $t_d = A^{d-2} \cdot t_2$. For this purpose the two-dimensional arrays $t_d(n, j)$, $0 \leq n \leq N$,

[‡] See Section 5 for the integral representation corresponding to $t_d(n, j)$.

$0 \leq j \leq [(N-n)/2]$, have to be represented as vectors of dimension $[(N/2+1)^2]$. So the whole computation then boils down to compute the power of some matrix, and then multiply it to the vector that corresponds to t_2 . The problem is that the matrix A has dimension $[(N/2+1)^2] \times [(N/2+1)^2]$, which already for the 8-dimensional fcc lattice (where we need at least $N = 704$ Taylor coefficients, see Table 1) means a 124609×124609 square matrix. Of course, A is not dense. A simple calculation reveals that it has $(N+2)(N+4)(N^2+4N+12)/96$ nonzero entries if N is even, and $(N+1)(N+3)(N^2+6N+17)/96$ nonzero entries when N is odd. It follows that A has sparsity $1/6$. Nevertheless it would require a considerable and impractical amount of memory to store the full matrix: for $d = 8$ it has about 2.6 billion nonzero entries (which themselves are big integers), and for $d = 11$, where we need $N = 2464$ terms, it has about 386 billion nonzero entries.

From the above discussion we are led to the following considerations: on the one hand, we would like to avoid recomputation of the coefficients, and on the other hand, we do not want to compute them all at once. Moreover, it is desirable to have a program that computes the Taylor coefficients one after the other, so that one does not have to fix N at the very beginning. The following algorithm satisfies all three requirements. The main loop is $n = 0, 1, 2, \dots$ and in each iteration the values $t_d(0, n/2), t_d(2, n/2 - 1), t_d(4, n/2 - 2), \dots, t_d(n, 0)$ if n is even (resp. $t_d(1, (n-1)/2), t_d(3, (n-3)/2), \dots, t_d(n, 0)$ for odd n) are computed in the given order, for all d between 2 and the dimension of the lattice. For sake of brevity, and without loss of generality, we will focus on the case of even n in the following. Note that in this way all the data that is required for $t_d(2k, n/2 - k)$ is already available. Similarly as before, we can obtain $t_d(2k, n/2 - k)$ as the scalar product $a \cdot t_{d-1}$, where a is a row vector and the two-dimensional array t_{d-1} , again, has to be interpreted as a single column vector. The vector a corresponds to a single row of the above-mentioned matrix A . Then $t_3(2k, n/2 - k), t_4(2k, n/2 - k), \dots$ are computed by using always the same vector a , so that any recomputation of coefficients is avoided. The only drawback of this approach is that one has to keep the whole three-dimensional array $t_d(n, j)$ in memory, and therefore this method is *more memory-intensive* than the naive approach (by a factor of approximately $d/2$).

The described computational scheme allows for lots of further (technical) improvements, some of which we want to mention briefly here. For example, *one does not need to compute* the vector a from scratch for each k , but reuse the previous one by adding and deleting a few entries, and apply the simple recurrences for binomial coefficients:

$$\binom{n+1}{k} = \frac{n+1}{n-k+1} \cdot \binom{n}{k} \quad \text{and} \quad \binom{n}{k+1} = \frac{n-k}{k+1} \cdot \binom{n}{k}. \quad (8)$$

Multiplying by a simple rational number is much cheaper than calculating a binomial coefficient.

With a little effort there is also the possibility to parallelize the computation. This can be done by splitting the sequence $t_d(0, n/2), t_d(2, n/2 - 1), \dots, t_d(n, 0)$ into parts, each of which is done by a single processor. The only caveat is the contribution of $t_d(0, n/2), \dots, t_d(2k-2, n/2 - k + 1)$ to the computation of $t_d(2k, n/2 - k)$, which has to be postponed until all processors have finished their task. This causes some synchronization overhead at each iteration of n , which prevents us from using an excessive amount of processors. For example, the computation time for the required $N = 999$ terms for the 9-dimensional fcc lattice dropped from 60 hours to 7.5 hours by using 10 parallel processors.

For the interested reader we also mention the timings for the other dimensions of the lattice considered here: in the 10-dimensional case we obtained the necessary $N = 1739$ terms in 3 days using 20 parallel processes, for $d = 11$ the same number of processes was running for 18 days to compute the 2464 terms mentioned in Table 1. For the 12-dimensional fcc lattice we only computed modulo $p = 2^{31} - 1$, and found that the minimal number of terms necessary for constructing the linear differential operator is 3618: these were obtained in 10 days using 25 parallel processes.

Table 1. The number of terms N_m (and N_0) needed to obtain the minimal-order linear ODE of order Q_{min} (and the optimal-order linear ODE of order Q_{opt}) annihilating $LGF_d(x)$.

d	N_m	N_0	$N_m - N_0$	$Q_{opt} - Q_{min}$
4	40	40	0	4-4 = 0
5	98	88	10	7-6 = 1
6	342	228	114	11-8 = 3
7	732	391	341	16-11 = 5
8	1740	704	1036	21-14 = 7
9	2964	999	1965	26-18 = 8
10	6509	1739	4770	36-22 = 14
11	10864	2464	8400	43-27 = 16
12	19503	3618	15885	53-32 = 21

3. The differential equations of the LGF of the d -dimensional fcc lattice, $d = 8, \dots, 12$

We obtain the corresponding linear ODE using an ansatz $\sum_{i,j} c_{i,j} x^j (x \frac{d}{dx})^i$ with undetermined coefficients $c_{i,j} \in \mathbb{Q}$. Substituting the generated series into this ansatz and equating the coefficients with respect to x to zero yields a linear system for the $c_{i,j}$. The result is very trustworthy once we use a sufficient amount of series data, i.e., such that the resulting linear system has more equations than unknowns. In the computer algebra literature this methodology is referred to as *guessing*, which somehow hides the fact that it is a completely algorithmic and constructive method. The linear ODE for $d = 8, 9, 10, 11$ are obtained in exact arithmetic and the linear ODE for $d = 12$ is obtained modulo one prime. These linear ODEs are given in electronic form in [15].

The linear differential operators corresponding to $d = 8, 9, 10, 11, 12$ are called, respectively, G_{14}^{8Dfcc} , G_{18}^{9Dfcc} , G_{22}^{10Dfcc} , G_{27}^{11Dfcc} , and G_{32}^{12Dfcc} , where the subscript refers to the order of the linear ODE. These orders are in agreement with the conjecture given in [9]:

$$q = \frac{d^2}{4} - \frac{d}{2} + \frac{17}{8} - \frac{(-)^d}{8}. \quad (9)$$

We have also agreement with the regular singularities x_s obtained by the *Landau equations method*, which read [9]

$$x_s = \binom{d}{2} \cdot \frac{1}{\xi(d, k, j)}, \quad (10)$$

where

$$\xi(d, k, j) = \frac{d^2 - (k + 4j + 1) \cdot d + 4j^2 + k + 4jk}{2 \cdot (1 - k)}, \quad (11)$$

with $k = 0, 2, 3, \dots, d - 1, \quad j = 0, \dots, [(d - k)/2],$

and where $[x]$ is the integer part of x .

The singularities as they occur in front of the head derivative of respectively $G_{14}^{8Dfcc}, G_{18}^{9Dfcc}, G_{22}^{10Dfcc}, G_{27}^{11Dfcc}, G_{32}^{12Dfcc}$ are given in Appendix A.

As far as the local exponents at the singularities are concerned, one remarks that the regular pattern seen [9] at $x = 0$ continues. Note that this is the pattern from which we inferred the order of the linear ODE. The local exponents, at each singularity, are given in Table 2. The singularities x_d , which read $x_3 = -3, x_5 = -5, x_6 = -15, x_7 = -7, x_8 = -14, x_9 = -9, x_{10} = -15, x_{11} = -11, x_{12} = -33/2$, seem to be given by:

$$x_d = -\frac{2d \cdot (d - 1)}{2d - 5 - 3 \cdot (-1)^d}. \quad (12)$$

For $d = 11$, there is also the singularity $x = -55$ not included in “others” (not shown in Table 2) with local exponents $9/2, 11/2$.

Table 2. The local exponents at the regular singularities. Only the exponents giving a singular behavior are shown.

d	$x = 0$	$x = \infty$	$x = 1$	x_d	others
3	0^3	$3/2$	$1/2$	0^3	
4	0^4	2^2	1^2		1^2
5	$0^5, 1$	$5/2$	$3/2$	$3/4, 5/4$	$3/2$
6	$0^6, 1^2$	3^2	2^2	$2^2, 3^2$	2^2
7	$0^7, 1^3, 2$	$7/2$	$5/2$	$3/2, 5/2, 2^3$	$5/2$
8	$0^8, 1^4, 2^2$	4^2	3^2	$3^2, 4^2$	3^2
9	$0^9, 1^5, 2^3, 3$	$9/2, 11/2$	$7/2$	$9/4, 11/4, 13/4, 15/4$	$7/2$
10	$0^{10}, 1^6, 2^4, 3^2$	5^2	4^2	$4^2, 5^2$	4^2
11	$0^{11}, 1^7, 2^5, 3^3, 4$	$11/2$	$9/2$	$7/2, 9/2, 3^2, 4^3, 5^2$	$9/2$
12	$0^{12}, 1^8, 2^6, 3^4, 4^2$	6^2	5^2	$5^2, 6^2$	5^2

4. The differential Galois groups of G_q^{dDfcc} , $d = 8, 9, 10, 11, 12$

The equivalence of two properties, namely the *homomorphism of the operator with its adjoint*, and either the occurrence of a *rational solution* for the *symmetric (or exterior) square* of that operator, or the drop of order of these squares, have been seen for many linear differential operators [12]. The operators with these properties are such that their *differential Galois groups* are included in the *symplectic or orthogonal differential groups*. We have also shown that such operators have a “canonical decomposition” [11], which means that they can be written in terms of “tower of intertwiners”. These properties hold also for the (non-Fuchsian) operators emerging in the square Ising model at the scaling limit [13].

For the linear differential operators annihilating $LGF_d(x)$, ($d = 5, 6, 7$), of the fcc lattice, these properties hold [9, 12]. For instance, the order-eleven operator G_{11}^{7Dfcc} (corresponding to $LF G_7(x)$) has the following canonical decomposition [9]

$$G_{11}^{7Dfcc} = (A_1 \cdot B_1 \cdot C_1 \cdot D_1 \cdot E_7 + A_1 \cdot B_1 \cdot E_7 + A_1 \cdot D_1 \cdot E_7 + A_1 \cdot B_1 \cdot C_1 + C_1 \cdot D_1 \cdot E_7 + E_7 + C_1 + A_1) \cdot r(x), \quad (13)$$

where $r(x)$ is a rational function, and the factors (the indices correspond to their orders) are all *self-adjoint* linear differential operators.

The decomposition (13) occurs because G_{11}^{7Dfcc} is *non-trivially homomorphic to its adjoint*, and the decomposition is obtained through a sequence of Euclidean right divisions (see Section 5 in [9]).

From this decomposition one understands easily why the *symmetric square* of G_{11}^{7Dfcc} is of order 65, instead of the generically expected order 66. The symmetric square of the self-adjoint order-seven linear differential operator E_7 is of order 27, instead of the generically expected order 28 (see [9, 11] for details). From the decomposition (13) one immediately deduces the decomposition of the adjoint of G_{11}^{7Dfcc} (because the factors are self-adjoints). The symmetric square of the adjoint G_{11}^{7Dfcc} will annihilate a rational solution which is the square of the solution of the order-one operator A_1 . The differential Galois group of G_{11}^{7Dfcc} is included in $SO(11, \mathbb{C})$.

In the sequel, we show that the operators G_{14}^{8Dfcc} , G_{18}^{9Dfcc} , G_{22}^{10Dfcc} , G_{27}^{11Dfcc} and G_{32}^{12Dfcc} verify the same properties as the operators G_{11}^{7Dfcc} (and G_6^{5Dfcc} for $d = 5$, see [2], G_8^{6Dfcc} for $d = 6$, see [4]). For d odd (resp. d even), one must consider the symmetric square (resp. exterior square) of the operator.

Note that to compute the homomorphism, for our purpose, between an operator and its adjoint, the operator should be irreducible (see Section 2.1 in [12]). We have shown in [9] that G_6^{5Dfcc} , G_8^{6Dfcc} , G_{11}^{7Dfcc} are irreducible. In the next section, we will assume that G_{14}^{8Dfcc} , G_{18}^{9Dfcc} , G_{22}^{10Dfcc} , G_{27}^{11Dfcc} and G_{32}^{12Dfcc} are irreducible \S .

4.1. The differential Galois group of G_{14}^{8Dfcc}

Producing the 14 formal solutions of the linear differential operator G_{14}^{8Dfcc} , it is easy to show that its *exterior square* is of order 90, instead of the generically expected order 91. The differential Galois group of the operator G_{14}^{8Dfcc} is included in $Sp(14, \mathbb{C})$.

The exterior square of the adjoint of G_{14}^{8Dfcc} either has the order 90, or annihilates a rational solution. We find that the exterior square of the adjoint of G_{14}^{8Dfcc} annihilates the following rational function

$$sol_R(ext^2(adjoint(G_{14}^{8Dfcc}))) = \frac{x^{21} \cdot P_{84}(x) \cdot S_8(x)^2}{P_{14}(x)}, \quad (14)$$

where $P_{14}(x)$ is the degree-95 *apparent polynomial* of G_{14}^{8Dfcc} , $S_8(x)$ is a degree-8 polynomial corresponding to the finite singularities given in Appendix A, and P_{84} is a degree-84 polynomial.

From these results, we should expect, in the “canonical decomposition” of G_{14}^{8Dfcc} , the factor equivalent to A_1 in (13) to be an order-two self-adjoint operator with (14) as the Wronskian. We should expect also the equivalent to E_7 in (13) to be self-adjoint

\S The results given in (16) and (20) show that G_{14}^{8Dfcc} and G_{18}^{9Dfcc} are, indeed, irreducible.

with even order greater than two. It is tempting to find the “canonical decomposition” of G_{14}^{8Dfcc} , and see whether the order of the “last” factor (i.e. the equivalent of E_7 in (13)) is equal to the dimension $d = 8$ as we conjectured in [9].

Indeed, the “canonical decomposition” [11] of G_{14}^{8Dfcc} is

$$G_{14}^{8Dfcc} = (A_2 \cdot B_2 \cdot C_2 \cdot D_8 + A_2 \cdot B_2 + C_2 \cdot D_8 + A_2 \cdot D_8 + 1) \cdot r(x), \quad (15)$$

where $r(x)$ is a rational function, and where all the factors are *self-adjoint*, with the indices indicating the order.

The starting relation to obtain this decomposition is the homomorphism that maps the solutions of G_{14}^{8Dfcc} to the solutions of the adjoint:

$$\text{adjoint}(L_{12}) \cdot G_{14}^{8Dfcc} = \text{adjoint}(G_{14}^{8Dfcc}) \cdot L_{12} \quad (16)$$

The sequence of Euclidean right divisions (the indices indicate the orders)

$$G_{14}^{8Dfcc} = A_2 \cdot L_{12} + L_{10}, \quad L_{12} = B_2 \cdot L_{10} + L_8, \quad L_{10} = C_2 \cdot L_8 + r(x), \quad (17)$$

and substitutions, give the decomposition (15). We have shown in [11] that the factors A_2 , B_2 , C_2 are automatically self-adjoint. The sequence ends when the rest of the last Euclidean right division is a rational function: one, then, obtains the order-8 self-adjoint operator $D_8 = L_8/r(x)$. If the exterior square of G_{14}^{8Dfcc} was of the generic order 91, and annihilated a rational function, the sequence of right divisions would continue, and the last Euclidean right division would be $L_4 = F_2 \cdot L_2 + r(x)$.

4.2. The differential Galois group G_{18}^{9Dfcc}

Similar calculations performed on the operator G_{18}^{9Dfcc} show that the symmetric square is of order 170, instead of the generically expected order 171. The differential Galois group of the operator G_{18}^{9Dfcc} is included in $SO(18, \mathbb{C})$.

The symmetric square of the adjoint of G_{18}^{9Dfcc} annihilates the rational function

$$\text{sol}_R(\text{sym}^2(\text{adjoint}(G_{18}^{9Dfcc}))) = \frac{x^{28} \cdot P_{260}(x) \cdot S_9(x)^2}{P_{18}(x)^2}, \quad (18)$$

where $P_{18}(x)$ is the apparent polynomial of the operator G_{18}^{9Dfcc} , $S_9(x)$ is a degree-9 polynomial corresponding to the finite singularities given in Appendix A, and P_{260} is a degree-260 polynomial.

Heavy calculations give the canonical decomposition [11] of G_{18}^{9Dfcc} as (again, the indices denote the order):

$$G_{18}^{9Dfcc} = (A_1 \cdot B_1 \cdot C_1 \cdot D_1 \cdot E_1 \cdot F_1 \cdot G_1 \cdot H_1 \cdot I_1 \cdot J_9 + \dots) \cdot r(x). \quad (19)$$

All the factors are self-adjoint. The decomposition contains 89 terms and is obtained through a sequence of nine Euclidean right divisions starting from the homomorphism that maps the solutions of G_{18}^{9Dfcc} to the solutions of the adjoint:

$$\text{adjoint}(L_{17}) \cdot G_{18}^{9Dfcc} = \text{adjoint}(G_{18}^{9Dfcc}) \cdot L_{17}. \quad (20)$$

Here also, we see that the conjecture of [9] is verified. The order of the last self-adjoint factor (i.e. J_9) is equal to the dimension of the lattice, $d = 9$.

4.3. The differential Galois groups of G_{22}^{10Dfcc} , G_{27}^{11Dfcc} and G_{32}^{12Dfcc}

The detailed calculations done for the decompositions of G_{14}^{8Dfcc} and G_{18}^{9Dfcc} are too huge to be performed on G_{22}^{10Dfcc} and G_{27}^{11Dfcc} . However, it is straightforward to obtain that the exterior square of G_{22}^{10Dfcc} is of order 230, instead of the generic order 231. The differential Galois group of the linear differential operator G_{22}^{10Dfcc} is included in $Sp(22, \mathbb{C})$. The symmetric square of G_{27}^{11Dfcc} is of order 377, instead of the generic order 378. The differential Galois group of the operator G_{27}^{11Dfcc} is included in $SO(27, \mathbb{C})$. Also, the exterior square of the known modulo a prime G_{32}^{12Dfcc} , is of order 495 instead of the generic order 496. The differential Galois group of the operator G_{32}^{12Dfcc} is included in $Sp(32, \mathbb{C})$.

5. Coupling of lattices

In Section 2.2, we mentioned that some recurrences on the coefficients $t_d(n, p)$ have been used to improve the efficiency of the computations. Recall that to obtain the recursion relation giving the coefficients $t_d(n, p)$, we introduced [9]

$$\zeta_d = \sum_{i=1}^d \sum_{j=i+1}^d \cos(k_i) \cdot \cos(k_j), \quad \sigma_d = \sum_{i=1}^d \cos(k_i), \quad (21)$$

in terms of which the coefficients $t_d(n, p)$ are given by

$$t_d(n, p) = 4^{n+p} \cdot \langle \zeta_d^n \cdot \sigma_d^{2p} \rangle \quad (22)$$

where the symbol $\langle \cdot \rangle$ means that the integration on the variables k_j , occurring in the integrand, has been performed (with the normalization π^d).

It is straightforward to see that the coefficients $t_d(n, p)$ correspond to the coefficients in the expansion around $(0, 0)$ of the d -dimensional integral

$$\begin{aligned} T_d(z, y) &= \frac{1}{\pi^d} \int_0^\pi \cdots \int_0^\pi \frac{dk_1 \cdots dk_d}{(1 - 4z \zeta_d) \cdot (1 - 4y \sigma_d^2)} \\ &= \sum_{n=0}^{\infty} \sum_{p=0}^{\infty} z^n \cdot y^p \cdot t_d(n, p), \end{aligned} \quad (23)$$

which gives the $LGF_d(z)$ of the d -dimensional fcc lattice for $y = 0$, and the $LGF_d(y)$ of the d -dimensional simple cubic lattice for $z = 0$. Note that for the simple cubic lattice, σ_d^2 should be σ_d . The expansion of the LGF of the simple cubic lattice corresponds to the expansion of (23) with $z = 0$ and $y = (x/d)^2/4$, where x is the expansion parameter.

From the computation of $t_d(n, p)$ for some values of d , we infer the first terms of the expansion around $(0, 0)$ of $T_d(z, y)$

$$\begin{aligned} T_d(z, y) &= 1 + 2d \cdot y + 2d \cdot (d-1) \cdot z^2 + 4d \cdot (d-1) \cdot zy + 6d \cdot (2d-1) \cdot y^2 \\ &\quad + 8d \cdot (d-1)(d-2) \cdot z^3 + 4d \cdot (d-1)(5d-7) \cdot z^2y + 48d \cdot (d-1)^2 \cdot zy^2 \\ &\quad + 20d \cdot (4 + 6d^2 - 9d) \cdot y^3 + \cdots \end{aligned} \quad (24)$$

Even if there is no obvious lattice corresponding to the Green function (23), we found that it might be worthy to analyze the bivariate series $T_d(z, y)$, *per se*.

In the sequel, we address || the *system of linear partial differential equations* (PDE) that annihilates the D -finite bivariate series $T_d(z, y)$ for $d = 2$.

|| See e.g. [16] for an introduction on partial differential equations.

6. Partial differential equations for $T_2(z, y)$

To find the PDEs that annihilate $T_2(z, y)$ we can either proceed as for the linear ODEs, i.e. by the guessing method, or apply the creative telescoping technique [17, 18, 19]; the latter is computationally more costly, but provides a certificate of correctness of the obtained differential equations. For example [4], it was powerful enough to find *and prove* the ODEs satisfied by the LGF for $d = 4, 5, 6$, but failed for $d \geq 7$. All the differential equations mentioned in this and the following sections are also available in electronic form [15].

In order to apply the guessing method we assume a partial differential equation of order Q in the homogeneous partial derivatives $z \cdot \partial / \partial z$ and $y \cdot \partial / \partial y$, with polynomials in z and y of degree D that annihilates $T_2(z, y)$:

$$\sum_{q=0}^Q \sum_{n=0}^D \sum_{p=0}^D a_{n,p}^{(q)} \cdot z^n \cdot y^p \cdot \left(z \cdot \frac{\partial}{\partial z} \right)^q \cdot \left(y \cdot \frac{\partial}{\partial y} \right)^{Q-q} \cdot T_2(z, y) = 0. \quad (25)$$

This linear system fixes the coefficients $a_{n,p}^{(q)}$, and leaves some of them free. The number of non-fixed coefficients is the number of PDEs with order Q and degree D . If all the coefficients are such that $a_{n,p}^{(q)} = 0$, we increase the order Q and/or the degree D .

For $Q = 1$, and various increasing values of D , all the coefficients are such that $a_{n,p}^{(q)} = 0$. For $Q = 2$ and $D = 2$, there is only one PDE, that we denote PDE_2 . For $Q = 3$ and $D = 1$, there are only two PDEs, called $PDE_3^{(1)}$ and $PDE_3^{(2)}$. Note that *there is no concept of "minimal order" for PDEs*, while there is one for ODEs. Instead, one can consider a *Gröbner basis* (see Appendix B) in the ring of partial differential operators, as is demonstrated in Section 6.4. It is obvious that there are as many PDEs that annihilate $T_2(z, y)$ as we wish (namely, all elements of the left ideal $\text{ann}(T_2)$, see Appendix B). For instance, for $Q = 4$ and $D = 1$, we obtain five PDEs, three of them are of order four and two of them are combinations of $PDE_3^{(1)}$ and $PDE_3^{(2)}$.

6.1. Two PDEs for $T_2(z, y)$

With the notation

$$D_{zy}^{(n,p)} = \frac{\partial^{n+p}}{\partial z^n \partial y^p}, \quad (26)$$

the system of two partial differential operators for $T_2(z, y)$ reads

$$\begin{aligned} PDE_3^{(1)} &= 2y^3 \cdot (16y - 1) \cdot D_{zy}^{(0,3)} + 3y^2z \cdot (16zy + 12y - 1) \cdot D_{zy}^{(1,2)} \\ &+ yz^2 \cdot (48zy + 12y - 1 - 2z) \cdot D_{zy}^{(2,1)} + 12yz^2 \cdot (4z + 1) \cdot D_{zy}^{(2,0)} \\ &+ 4yz \cdot (60zy + 24y - 1 - z) \cdot D_{zy}^{(1,1)} + 2y^2 \cdot (24zy + 80y - 3) \cdot D_{zy}^{(0,2)} \\ &+ 24yz \cdot (6z + 1) \cdot D_{zy}^{(1,0)} + 2y \cdot (68y - 1 + 72zy) \cdot D_{zy}^{(0,1)} \\ &+ 8y \cdot (6z + 1) \cdot D_{zy}^{(0,0)}, \end{aligned} \quad (27)$$

and:

$$\begin{aligned} PDE_3^{(2)} &= 2y^3 \cdot (16y - 1) \cdot D_{zy}^{(0,3)} + y^2z \cdot (24y + 32zy - 3 + 4z) \cdot D_{zy}^{(1,2)} \\ &+ yz^2 \cdot (32zy - 1 + 8y) \cdot D_{zy}^{(2,1)} + 8yz^2 \cdot (4z + 1) \cdot D_{zy}^{(2,0)} \end{aligned}$$

$$\begin{aligned}
& + 4yz \cdot (40zy + 16y - 1 + z) \cdot D_{zy}^{(1,1)} + 2y^2 \cdot (16zy + 80y - 3 + 2z) \cdot D_{zy}^{(0,2)} \\
& + 16yz \cdot (6z + 1) \cdot D_{zy}^{(1,0)} + 2y \cdot (68y + 2z + 48zy - 1) \cdot D_{zy}^{(0,1)} \\
& + 8y \cdot (4z + 1) \cdot D_{zy}^{(0,0)}. \tag{28}
\end{aligned}$$

These two operators annihilate (by construction) a finite truncation of the power series $T_2(z, y)$, where the truncation index has been chosen such that it is very likely that they also annihilate the infinite series $T_2(z, y)$. That they indeed annihilate $T_2(z, y)$ will be made rigorous in Section 6.4. In particular, it follows that $PDE_3^{(1)}$ and $PDE_3^{(2)}$ are compatible. By assuming a common solution of the form

$$\sum_{n=0} \sum_{p=0} b_{n,p} \cdot z^n \cdot y^p, \tag{29}$$

we find a unique solution to the system of PDEs that identifies with $T_2(z, y)$, up to an overall constant. Only one constant means that if we switch to recurrences on the coefficients we will need only one initial condition.

The recursions for $t_2(n, p) = U(n, p)$ are

$$\begin{aligned}
& - 4 \cdot (8p^2 + 17p + 9np + 9n + 8 + 3n^2) \cdot U(n + 1, p) \\
& + 2 \cdot n(n + 1) \cdot U(n, p + 1) + (n + p + 2)(2p + n + 3) \cdot U(n + 1, p + 1) \\
& - 48 \cdot (n + 1)(n + p + 1) \cdot U(n, p) = 0, \tag{30}
\end{aligned}$$

and

$$\begin{aligned}
& 8 \cdot (3 + 4p^2 + 7p + 3np + 3n + n^2) \cdot U(n + 1, p) \\
& + 4 \cdot (n + 1)(p + 1) \cdot U(n, p + 1) + (p - n + 2)(2p + n + 3) \cdot U(n + 1, p + 1) \\
& + 32 \cdot (n + 1)(n + p + 1) \cdot U(n, p) = 0, \tag{31}
\end{aligned}$$

with the auxiliary recurrence:

$$(p + 1)^2 \cdot U(0, p + 1) - 4 \cdot (2p + 1)^2 \cdot U(0, p) = 0. \tag{32}$$

With the coefficient $U(0, 0)$ given, these three recurrences generate all the $U(n, p)$.

6.2. One PDE for $T_2(z, y)$

There is only one *partial differential operator* of order $Q = 2$ and degree $D = 2$ that annihilates $T_2(z, y)$

$$\begin{aligned}
PDE_2 & = z^2 \cdot (4z - 1)(4z + 1)(4y - 1) \cdot D_{zy}^{(2,0)} \\
& + zy \cdot (64z^2y - 16z^2 - 4z - 20y + 3) \cdot D_{zy}^{(1,1)} \\
& - 2y^2 \cdot (16y - 1) \cdot D_{zy}^{(0,2)} + z(192z^2y - 48z^2 - 32zy - 12y + 1) \cdot D_{zy}^{(1,0)} \\
& + 2y \cdot (32z^2y - 8z^2 - 32y - 24zy - 2z + 1) \cdot D_{zy}^{(0,1)} \\
& - (16z^2 + 32zy + 8y - 64z^2y) \cdot D_{zy}^{(0,0)}, \tag{33}
\end{aligned}$$

which acting on the bivariate form (29) generates, remarkably, a unique solution that identifies with $T_2(z, y)$, up to an overall constant.

The coefficients $t_2(n, p) = U(n, p)$ are given by the recursion

$$\begin{aligned}
& - (20np + 72p + 40 + 24n + 32p^2 + 4n^2) \cdot U(n + 2, p) \\
& + 64(n + 1)(n + p + 1) \cdot U(n, p) - 4(p + 1)(n + 2) \cdot U(n + 1, p + 1) \\
& + (p + 3 + n)(2p + 4 + n) \cdot U(n + 2, p + 1) \\
& - (64 + 48p + 32n) \cdot U(n + 1, p) - 16 \cdot (n + 1)(n + 2 + p) \cdot U(n, p + 1) = 0, \tag{34}
\end{aligned}$$

with the auxiliary recursions:

$$\begin{aligned}
(n+2)^2 \cdot U(n+2, 0) - 16 \cdot (n+1)^2 \cdot U(n, 0) &= 0, & U(1, 0) &= 0, \\
(p+1)^2 \cdot U(0, p+1) - 4(2p+1)^2 \cdot U(0, p) &= 0, & & \\
(p+2)(2p+3) \cdot U(1, p+1) - 4(p+1)(5+8p) \cdot U(1, p) & & & \\
&= 16 \cdot (2+3p) \cdot U(0, p) + 4(p+1) \cdot U(0, p+1). & &
\end{aligned} \tag{35}$$

Here also, these recurrences generate all the coefficients starting with $U(0, 0)$.

6.3. On the logarithmic solutions

The system of PDEs given in (27, 28) has no logarithmic solution of the form

$$\sum_{n=0}^{\infty} \sum_{p=0}^{\infty} F_{n,p}(z, y) \cdot \ln(z)^n \cdot \ln(y)^{n-p}, \tag{36}$$

where $F_{n,p}(z, y)$ are analytic at $(0, 0)$ bivariate series.

In contrast, the PDE given in (33) *seems to have no bound in the summation on n* (we obtained logarithmic solutions up to $n = 17$). Furthermore, we find that the logarithms $\ln(z)$, and $\ln(y)$, appear in the solutions as:

$$\sum_{n=0}^{\infty} \sum_{p=0}^{\infty} F_{n,p}(z, y) \cdot (\ln(z) - \mu \cdot \ln(y))^p. \tag{37}$$

The number of logarithmic solutions depends now on the value of μ . For $\mu = 1$ and $\mu = 1/2$, we find no bound to n (in our calculations, we reached $n = 17$). For any other value of $\mu \neq 1, 1/2$, there is only one logarithmic solution i.e. $n = 1$. For generic μ the solutions are $T_2(z, y)$ and \clubsuit :

$$\begin{aligned}
&T_2(z, y) \cdot (\ln(z) - \mu \cdot \ln(y)) \\
&+ \left(\frac{1}{2} + 2\mu - 4\mu \cdot z + 2 \cdot (3 + 5\mu) \cdot z^2 + 4 \cdot (1 - \mu) \cdot zy \right. \\
&- (13 + 12\mu) \cdot y^2 - \frac{304}{9} \mu \cdot z^3 + \frac{2}{3} \cdot (33 - 16\mu) \cdot z^2 y + \frac{8}{15} \cdot (31 - 90\mu) \cdot zy^2 \\
&\left. - \frac{4}{9} \cdot (559 + 420\mu) \cdot y^3 + \dots \right). \tag{38}
\end{aligned}$$

Let us address the details of the computations on how the values $\mu = 1$, and $\mu = 1/2$ appear. Acting by PDE_2 on the form (37) rewritten as

$$F_{n,n}(z, y) \cdot (\ln(z) - \mu \cdot \ln(y))^n + \dots, \tag{39}$$

gives the choice of zeroing

$$a_{0,0} \cdot (\mu - 1/2)(\mu - 1) = 0, \tag{40}$$

where $a_{0,0}$ is the leading coefficient of the bivariate series $F_{n,n}(z, y)$. The choice $\mu = 1$ (or $\mu = 1/2$) allows $a_{0,0} \neq 0$, which permits n to be higher. The choice $a_{0,0} = 0$ will decrease the degree n , and the process continues with $n - 1$.

The choice (40) comes from the action of PDE_2 on (39), and the leading coefficient of the expansion to be cancelled is:

$$n \cdot (n-1) \cdot a_{0,0} \cdot (\mu - 1/2)(\mu - 1) \cdot (\ln(z) - \mu \cdot \ln(y))^{n-2} + O(z^1, y^1). \tag{41}$$

\clubsuit Note that the derivative with respect to μ of the logarithmic solution is also a solution.

6.4. Gröbner basis of PDEs for $T_2(z, y)$

A Gröbner basis for $\text{ann}(T_2)$, the annihilating ideal of PDEs for $T_2(z, y)$, can be obtained by applying Buchberger's algorithm to the input $\{PDE_3^{(1)}, PDE_3^{(2)}, PDE_2\}$ (some basics about Gröbner bases are given in Appendix B). Alternatively, we can compute the annihilating ideal *from scratch*, i.e. from the integral representation (23) of $T_2(z, y)$, by the method of creative telescoping. Both tasks can be performed with the HolonomicFunctions package [20] and yield the same result. The second approach, however, gives an independent proof that the guessed PDEs presented in the previous sections are correct.

The Gröbner basis of $\text{ann}(T_2)$ (with respect to degree-lexicographic order and $D_y \prec D_z$) consists of 3 operators, whose supports are given as follows:

$$\begin{aligned} & \{D_{zy}^{(2,0)}, D_{zy}^{(1,1)}, D_{zy}^{(0,2)}, D_{zy}^{(1,0)}, D_{zy}^{(0,1)}, D_{zy}^{(0,0)}\}, \\ & \{D_{zy}^{(0,3)}, D_{zy}^{(1,1)}, D_{zy}^{(0,2)}, D_{zy}^{(1,0)}, D_{zy}^{(0,1)}, D_{zy}^{(0,0)}\}, \\ & \{D_{zy}^{(1,2)}, D_{zy}^{(1,1)}, D_{zy}^{(0,2)}, D_{zy}^{(1,0)}, D_{zy}^{(0,1)}, D_{zy}^{(0,0)}\}. \end{aligned}$$

Note that the first basis element is exactly PDE_2 . By investigating the *leading monomials* $D_{zy}^{(2,0)}, D_{zy}^{(0,3)}, D_{zy}^{(1,2)}$ one immediately finds that there are 5 monomials under the stairs, namely the monomials $D_{zy}^{(1,1)}, D_{zy}^{(0,2)}, D_{zy}^{(1,0)}, D_{zy}^{(0,1)}, D_{zy}^{(0,0)}$, which cannot be reduced by either of the leading monomials. We say that $\text{ann}(T_2)$ has holonomic rank 5. Hence one could expect that 5 initial conditions have to be given to identify the particular solution $T_2(z, y)$. As discussed before, we remarkably need only one initial condition.

7. Ordinary differential equations for $T_2(z, y)$

The *bivariate series* $T_2(z, y)$ may be seen as depending on the variable z (or y) where y (or z) is a parameter. By derivation of the PDE system, and elimination of the unwanted derivatives, one obtains a linear ODE on the variable z (or y) that annihilates $T_2(z, y)$. Such elimination can be conveniently performed by using the Gröbner basis presented in Section 6.4.

7.1. ODE with the derivative on z for $T_2(z, y)$

The linear ODE with the variable z , that annihilates $T_2(z, y)$, is of order five, and we call the corresponding operator $L_5^{(z)}$, (with the derivative $D_z = \frac{\partial}{\partial z}$):

$$L_5^{(z)} = \sum_{n=0}^5 P_n(z, y) \cdot D_z^n. \quad (42)$$

The polynomial in front of the highest derivative is

$$z^2 \cdot (4z - 1) \cdot (4z + 1) \cdot (z - 4y) \cdot (16z^2y + y + 8zy - 4z^2) \cdot P_{app}, \quad (43)$$

where P_{app} carries apparent singularities:

$$\begin{aligned} P_{app} = & 192y \cdot (4y - 1) \cdot z^5 - (128y^2 + 32y - 12) \cdot z^4 + 4y(80y - 19) \cdot z^3 \\ & - (40y^2 + 4y - 1) \cdot z^2 + y \cdot (y - 1) \cdot z + y^2. \end{aligned} \quad (44)$$

The factorization of the order-five linear differential operator $L_5^{(z)}$ reads (the indices are the orders)

$$L_5^{(z)} = \left(L_1^{(2)} \cdot L_1^{(1)} \right) \oplus \left(L_1^{(3)} \cdot L_1^{(1)} \right) \oplus \left(L_2 \cdot L_1^{(1)} \right), \quad (45)$$

where the four factors are given in Appendix C.

The solution of $L_1^{(1)}$ reads:

$$\text{sol} \left(L_1^{(1)} \right) = \sqrt{\frac{z}{(z-4y) \cdot (4 \cdot (4y-1) \cdot z^2 + 8zy + y)}}. \quad (46)$$

The second solution of $L_1^{(2)} \cdot L_1^{(1)}$ reads:

$$\text{sol}(L_1^{(1)}) \cdot \int \frac{z^{-3/2}}{\sqrt{(z-4y)(4 \cdot (4y-1) \cdot z^2 + 8zy + y)}} \cdot dz. \quad (47)$$

The integral can be evaluated in terms of the incomplete elliptic integrals, so that the second solution of $L_1^{(2)} \cdot L_1^{(1)}$ reads

$$\text{sol}(L_1^{(1)}) \cdot \left(\frac{(4y - \sqrt{y})}{2y^2} \cdot E(z_1, z_2) - \frac{4 \cdot (8y - 1 - 2\sqrt{y})}{y \cdot (16y - 1)} \cdot F(z_1, z_2) \right) - \frac{2}{(z-4y)y},$$

with

$$z_1 = \sqrt{\frac{(4\sqrt{y}-1)^2 z}{z-4y}}, \quad z_2 = \sqrt{\frac{(4\sqrt{y}+1)^2}{(4\sqrt{y}-1)^2}} \quad (48)$$

and where E and F are the incomplete elliptic integrals:

$$E(z, k) = \int_0^z \frac{\sqrt{1-k^2 t^2}}{\sqrt{1-t^2}} \cdot dt, \quad F(z, k) = \int_0^z \frac{1}{\sqrt{1-k^2 t^2} \sqrt{1-t^2}} \cdot dt. \quad (49)$$

The second solution of $L_1^{(3)} \cdot L_1^{(1)}$ can be written as the general *Heun function*

$$f(z) \cdot \text{Heun} \left(a, q, \frac{1}{2}, 1, \frac{3}{2}, \frac{1}{2}, g(z) \right), \quad (50)$$

with

$$f(z) = \frac{z \cdot \sqrt{4z\sqrt{y} + \sqrt{y} - 2z}}{(16z^2y + y + 8zy - 4z^2) \cdot \sqrt{z-4y}},$$

$$g(z) = \frac{zy \cdot (64zy + 16y - 12z + 1) - 2z \cdot \sqrt{y} \cdot (z-4y)}{4y \cdot (16z^2y + y + 8zy - 4z^2)}, \quad (51)$$

and:

$$a = \frac{1}{2} + \frac{16y+1}{16\sqrt{y}}, \quad q = \frac{1+a}{4}. \quad (52)$$

The solution of $L_2 \cdot L_1^{(1)}$ which is not solution of $L_1^{(1)}$ can be written as

$$\text{sol}(L_1^{(1)}) \cdot \int \frac{\text{sol}L_2}{\text{sol}(L_1^{(1)})} \cdot dz, \quad (53)$$

where one of the solutions of L_2 reads

$$\text{sol}(L_2) = \frac{z \cdot (16z^2 - 1)(64z^3y - 80z^2y + 16z^2 - 36zy - 3y)}{3y(z-4y)(y+8zy+16z^2y-4z^2)} \cdot \frac{dH(z)}{dz}$$

$$+ 4 \cdot \frac{z \cdot (256z^4y + 112z^3 - 512z^3y - 224z^2y + z - 32zy - 3y)}{y \cdot (z-4y)(y+8zy+16z^2y-4z^2)} \cdot H(z), \quad (54)$$

where $H(z)$ is the hypergeometric function

$$H(z) = {}_2F_1 \left(\left[\frac{3}{2}, \frac{5}{2} \right], [1], 16z^2 \right). \quad (55)$$

7.2. ODE with the derivative on y for $T_2(z, y)$

The bivariate series $T_2(z, y)$, where z is a parameter, is annihilated by an order-five linear differential operator $N_5^{(y)}$ (with the derivative $D_y = \frac{\partial}{\partial y}$):

$$N_5^{(y)} = \sum_{n=0}^5 Q_n(z, y) \cdot D_y^n. \quad (56)$$

The polynomial, in front of the highest derivative, reads

$$y^2 \cdot (16y - 1) \cdot (z - 4y) \cdot (16z^2y + y + 8zy - 4z^2) \cdot P_{app}, \quad (57)$$

where P_{app} carries *apparent singularities*:

$$\begin{aligned} P_{app} = & -12 \cdot (4z + 1) \cdot (32z^2 - 12z - 1) \cdot y^3 \\ & + (1344z^3 - 8 + 20z^2 - 114z + 64z^4) \cdot y^2 \\ & - (1 + 12z - 20z^2 - 264z^3 + 48z^4) \cdot y + (32z^2 - 1 - 6z) \cdot z^2. \end{aligned} \quad (58)$$

The order-five operator $N_5^{(y)}$ has the following direct sum factorization

$$N_5^{(y)} = \left(N_1^{(2)} \cdot N_1^{(1)} \right) \oplus \left(N_1^{(3)} \cdot N_1^{(1)} \right) \oplus \left(N_2 \cdot N_1^{(1)} \right), \quad (59)$$

where the four factors are given in Appendix C.

The solution of $N_1^{(1)}$ reads:

$$\text{sol}(N_1^{(1)}) = \sqrt{\frac{y}{(z - 4y)(4 \cdot (4y - 1) \cdot z^2 + 8zy + y)}}. \quad (60)$$

The second solution of $N_1^{(2)} \cdot N_1^{(1)}$ reads:

$$\text{sol}(N_1^{(1)}) \cdot \int \frac{y^{-3/2} \cdot (16y + 1)}{\sqrt{(z - 4y) \cdot (4 \cdot (4y - 1)z^2 + 8zy + y)}} \cdot dy. \quad (61)$$

The integral can be evaluated in terms of the incomplete elliptic integrals and the second solution of $N_1^{(2)} \cdot N_1^{(1)}$ reads

$$\text{sol}(N_1^{(1)}) \cdot \left(\frac{(4z - 1)}{2z^{5/2}} \cdot E(z_1, z_2) + \frac{(80z^2 + 1 + 8z)}{2z^{5/2} \cdot (4z - 1)} \cdot F(z_1, z_2) \right) - \frac{1}{2z^3}, \quad (62)$$

with:

$$z_1 = \sqrt{-\frac{16z^2y + y + 8zy - 4z^2}{4z^2}}, \quad z_2 = \sqrt{-\frac{16z}{(4z - 1)^2}}. \quad (63)$$

The second solution of $N_1^{(3)} \cdot N_1^{(1)}$ is a general Heun function

$$\text{sol}(N_1^{(1)}) \cdot \sqrt{y} \cdot \text{Heun}\left(a, q, \frac{1}{2}, 1, \frac{3}{2}, \frac{1}{2}, \frac{4y}{z}\right), \quad (64)$$

with:

$$a = \frac{16z}{(4z + 1)^2}, \quad q = \frac{1 + a}{4}. \quad (65)$$

The solution of $N_2 \cdot N_1^{(1)}$ which is not solution of $N_1^{(1)}$ can be written as

$$\text{sol}(N_1^{(1)}) \cdot \int \frac{\text{sol}(N_2)}{\text{sol}(N_1^{(1)})} \cdot dy, \quad (66)$$

where one of the solutions of N_2 reads

$$\begin{aligned} \text{sol}(N_2) &= \frac{y \cdot (16y - 1) \cdot (64z^2y + 48zy + 16y - 20z^2 - 3z)}{3 \cdot z^5 \cdot (z - 4y) \cdot (y + 8zy + 16z^2y - 4z^2)} \cdot \frac{dH_y(y)}{dy} \\ &+ 2 \cdot \frac{256z^2y^2 + 384y^2z + 112y^2 - 112z^2y - 24zy + y - 2z^2}{z^5 \cdot (z - 4y) \cdot (y + 8zy + 16z^2y - 4z^2)} \cdot H_y(y), \end{aligned} \quad (67)$$

where $H_y(y)$ is the hypergeometric function:

$$H_y(y) = {}_2F_1\left(\left[\frac{3}{2}, \frac{5}{2}\right], [1], 16y\right). \quad (68)$$

7.3. The linear ODE on z and y as PDE for $T_2(z, y)$

The linear differential equations corresponding to the operators $L_5^{(z)}$ and $N_5^{(y)}$ act on $T_2(z, y)$ as a system of decoupled PDEs. Both ODEs annihilate (as it should) the bivariate series $T_2(z, y)$, and they generate a unique common bivariate series solution, analytic at $(0, 0)$, that identifies with $T_2(z, y)$.

As for the solutions of the three PDEs of the previous sections, one remarks that $\text{sol}(L_1^{(1)})$ and $\text{sol}(N_1^{(1)})$ have simple structures, and we can check that

$$\sqrt{\frac{yz}{(z - 4y) \cdot (y + 8zy + 4 \cdot (4y - 1) \cdot z^2)}}. \quad (69)$$

is *actually* a solution of the three PDEs, $PDE_3^{(1)}$, $PDE_3^{(2)}$ and PDE_2 . Unfortunately, the other solutions are too complicated to be used to fabricate more general common solutions of the three PDEs.

However, the bivariate series $T_2(z, y)$ can be written as a combination of the solutions of $L_5^{(z)}$. Let us call $S_1^{(z)}$, $S_2^{(z)}$ and $S_3^{(z)}$ the formal solutions analytic at $z = 0$ of (respectively) the operators $L_1^{(2)} \cdot L_1^{(1)}$, $L_1^{(3)} \cdot L_1^{(1)}$ and $L_2 \cdot L_1^{(1)}$. The first terms of these solutions are given in Appendix D.

The bivariate series $T_2(z, y)$ reads

$$T_2(z, y) = C_1^{(z)}(y) \cdot S_1^{(z)} + C_2^{(z)}(y) \cdot S_2^{(z)} + C_3^{(z)}(y) \cdot S_3^{(z)}, \quad (70)$$

where the combination coefficients $C_j^{(z)}(y)$ are given in Appendix D.

Similarly, one may consider the bivariate series $T_2(z, y)$ as a combination of the solutions of $N_5^{(y)}$. With $S_1^{(y)}$, $S_2^{(y)}$ and $S_3^{(y)}$ the formal solutions analytic at $y = 0$ of (respectively) the operators $N_1^{(2)} \cdot N_1^{(1)}$, $N_1^{(3)} \cdot N_1^{(1)}$ and $N_2 \cdot N_1^{(1)}$ (see Appendix E), the bivariate series $T_2(z, y)$ reads

$$T_2(z, y) = C_1^{(y)}(z) \cdot S_1^{(y)} + C_2^{(y)}(z) \cdot S_2^{(y)} + C_3^{(y)}(z) \cdot S_3^{(y)}, \quad (71)$$

where the combination coefficient $C_j^{(y)}(z)$ are given in Appendix E.

Note that we have used for the solutions $S_j^{(z)}$ (resp. $S_j^{(y)}$) the formal solutions of the corresponding operators since this is easier. Otherwise a full closed expression for $T_2(z, y)$ is given in Appendix F, which is obtained by integration of the double integral. One should note that the expression is a ‘‘partition’’ that does not reflect the factorization of (e.g.) $L_5^{(z)}$.

8. Partial differential equations for $T_3(z, y)$

Similar calculations can be performed for the bivariate series $T_3(z, y)$ corresponding to the expansion around $(0, 0)$ of the integral (23) with $d = 3$. In this instance, however, the creative telescoping method turned out to be too costly, and hence, all the PDEs presented below have been obtained by the guessing method.

We find that, for $Q = 3$ and $D = 3$, there is only one PDE (denoted PDE_3) and for $Q = 4$, $D = 2$ there are two PDEs (called $PDE_4^{(1)}$, $PDE_4^{(2)}$). Here also, and similarly to $T_2(z, y)$, both $PDE_4^{(1)}$, $PDE_4^{(2)}$ acting on the generic bivariate series (29) generate the unique $T_3(z, y)$, while PDE_3 is sufficient to generate a unique solution that identifies with $T_3(z, y)$.

As for the logarithmic solutions, there is no solution of the form (36) for the system $(PDE_4^{(1)}, PDE_4^{(2)})$. However, and similarly to what happened for $T_2(z, y)$, the number of logarithmic solutions for PDE_3 depends on the value of μ in the combination (37). For $\mu = 1$ and $\mu = 1/2$, there is non finite number of such solutions (we reached $n = 17$ in our calculations).

For generic values of $\mu \neq 1, 1/2$, one obtains three solutions, the bivariate series $T_3(z, y)$ and the logarithmic solutions

$$\begin{aligned} T_3(z, y) \cdot (\ln(z) - \mu \cdot \ln(y))^2 &+ T_3^{(1)} \cdot (\ln(z) - \mu \cdot \ln(y)) + T_3^{(0)}, \\ T_3(z, y) \cdot (\ln(z) - \mu \cdot \ln(y)) &+ \frac{1}{2} T_3^{(1)}, \end{aligned} \quad (72)$$

where:

$$\begin{aligned} T_3^{(1)} &= 4 \cdot (1 - 4\mu) \cdot z - 4 \cdot (7\mu - 1) \cdot y - 2 \cdot (24\mu - 17) \cdot z^2 \\ &+ 4 \cdot (13 - 40\mu) \cdot yz - 6 \cdot (87\mu - 7) \cdot y^2 + \dots \end{aligned} \quad (73)$$

$$\begin{aligned} T_3^{(0)} &= 8 \cdot \mu \cdot (1 - 5\mu) \cdot z + 2 \cdot (8\mu - 11) \cdot y - 2 \cdot (3\mu - 2 + 31\mu^2) \cdot z^2 \\ &- \frac{4}{3} \cdot (57\mu^2 + 41 - 9\mu) \cdot yz + \frac{1}{2} \cdot (700\mu + 392\mu^2 - 831) \cdot y^2 + \dots \end{aligned} \quad (74)$$

8.1. Decoupled linear differential equations for $T_3(z, y)$

For the PDE system $\{PDE_3, PDE_4^{(1)}, PDE_4^{(2)}\}$ annihilating $T_3(z, y)$, we used Buchberger's algorithm as implemented in the HolonomicFunctions program [20] and obtained immediately a Gröbner basis (given in electronic form in [15]). It allows us to derive two (order-nine) ordinary differential equations[‡] for $T_3(z, y)$, one involving only D_z , the other one only D_y :

$$L_9^{(z)} = \sum_{n=0}^9 P_n(z, y) \cdot D_z^n, \quad N_9^{(y)} = \sum_{n=0}^9 Q_n(z, y) \cdot D_y^n. \quad (75)$$

One factorization of $L_9^{(z)}$ reads[†] (the indices denote orders):

$$L_9^{(z)} = L_3 \cdot L_1^{(4)} \cdot L_1^{(3)} \cdot L_1^{(2)} \cdot L_1^{(1)} \cdot L_2. \quad (76)$$

The similar factorization of $N_9^{(y)}$ reads:

$$N_9^{(y)} = N_3 \cdot N_1^{(4)} \cdot N_1^{(3)} \cdot N_1^{(2)} \cdot N_1^{(1)} \cdot N_2. \quad (77)$$

[‡] Do not confuse the labels of some factors with those occurring for $T_2(z, y)$.

[†] The full factorization of $L_9^{(z)}$ as a *direct sum* is $L_9^{(z)} = \tilde{L}_3 \cdot L_2 \oplus L_1^{(1)} \cdot L_2 \oplus \tilde{L}_1^{(2)} \cdot L_2 \oplus \tilde{L}_1^{(3)} \cdot L_2 \oplus \tilde{L}_1^{(4)} \cdot L_2$.

The two order-two operators L_2 and N_2 are given in Appendix G. They are self-adjoint, up to a conjugation by their Wronskians $W(L_2)$ and $W(N_2)$ (see Appendix G):

$$L_2 \cdot W(L_2) = W(L_2) \cdot \text{adjoint}(L_2), \quad N_2 \cdot W(N_2) = W(N_2) \cdot \text{adjoint}(N_2). \quad (78)$$

We have been able to find one solution for $L_9^{(z)}$ (and $N_9^{(y)}$). Defining the hypergeometric function

$$S_{zy} = \frac{\sqrt{yz}}{\sqrt{P_{zy}}} \cdot {}_2F_1 \left(\left[\frac{1}{4}, \frac{3}{4} \right], [1], \frac{64 \cdot yz \cdot (z-3y)^3 \cdot (1+4z)^2}{P_{zy}^2} \right), \quad (79)$$

where

$$P_{zy} = 1728y^2z^3 - 432yz^3 + 16z^3 + 864z^2y^2 - 72z^2y + 108zy^2 + zy - 4y^2, \quad (80)$$

one checks that S_{zy} is solution of the *two most right order-two operators* L_2 and N_2

$$L_2(S_{zy}) = 0, \quad N_2(S_{zy}) = 0. \quad (81)$$

As was seen for the operators $L_5^{(z)}$ and $N_5^{(y)}$ corresponding to $T_2(z, y)$, with the solution (69), one can check that the solution (79) of $L_9^{(z)}$ (and $N_9^{(y)}$), is one solution to the whole PDE system:

$$PDE_3(S_{zy}) = 0, \quad PDE_4^{(1)}(S_{zy}) = 0, \quad PDE_4^{(2)}(S_{zy}) = 0. \quad (82)$$

This solution (79) of the whole PDE system is, in fact, quite remarkable. It corresponds to a *modular form* [21, 22, 23]. In order to see this modular form structure, let us recall various (non trivial) identities on hypergeometric functions.

The use of the identity

$${}_2F_1 \left(\left[\frac{1}{4}, \frac{3}{4} \right], [1], X \right) = \frac{1}{(1+3X)^{1/4}} \cdot {}_2F_1 \left(\left[\frac{1}{12}, \frac{5}{12} \right], [1], \frac{27X \cdot (1-X)^2}{(1+3X)^3} \right), \quad (83)$$

together with the identity

$${}_2F_1 \left(\left[\frac{1}{4}, \frac{3}{4} \right], [1], X \right) = \left(\frac{4}{4-3X} \right)^{1/4} \cdot {}_2F_1 \left(\left[\frac{1}{12}, \frac{5}{12} \right], [1], \frac{27X^2 \cdot (X-1)}{(3X-4)^3} \right), \quad (84)$$

implies the following identity on *the same* hypergeometric function

$${}_2F_1 \left(\left[\frac{1}{12}, \frac{5}{12} \right], [1], A_1 \right) = \sqrt{2} \cdot \left(\frac{1+3X}{4-3X} \right)^{1/4} \cdot {}_2F_1 \left(\left[\frac{1}{12}, \frac{5}{12} \right], [1], A_2 \right), \quad (85)$$

with the *two different arguments*†

$$A_1(X) = \frac{27 \cdot X \cdot (1-X)^2}{(1+3X)^3}, \quad A_2(X) = \frac{27 \cdot X^2 \cdot (X-1)}{(3X-4)^3} = A_1(1-X). \quad (86)$$

This enables to rewrite the solution S_{zy} of (82), where S_{zy} is given in (79), as a ${}_2F_1$ hypergeometric function with *two different pullbacks*, namely A_1 and A_2 given by (86) where X is given by (with P_{zy} given by (80)):

$$X = \frac{64 \cdot yz \cdot (z-3y)^3 \cdot (1+4z)^2}{P_{zy}^2}, \quad (87)$$

† Such non-trivial identity (85) is characteristic of *modular forms* [21, 22, 23].

and where $1 - X$ reads:

$$\frac{(144y^2z^2 + 96y^2z - 40yz^2 + 16y^2 - 8yz + z^2)(144yz^2 + 24yz - 16z^2 + y)^2}{P_{zy}^2}. \quad (88)$$

This shows that the solution S_{zy} , given in (79), corresponds to a *modular form*, seen as a function of z , or seen as a function of y .

The two pullbacks A_1 and A_2 are lying on the algebraic genus zero *modular curve*

$$\begin{aligned} & 1953125 \cdot A_1^3 A_2^3 - 187500 \cdot A_1^2 A_2^2 \cdot (A_1 + A_2) \\ & + 375 \cdot A_1 A_2 \cdot (16 A_1^2 - 4027 A_1 A_2 + 16 A_2^2) \\ & - 64 \cdot (A_1 + A_2) \cdot (A_1^2 + 1487 A_1 A_2 + A_2^2) + 110592 A_1 A_2 = 0. \end{aligned} \quad (89)$$

If one introduces Z such that $X = Z/(Z+64)$, one can see clearly that this *modular equation*† (89) is the same as the one corresponding to the *fundamental modular curve* X_0 , associated with the Landen transformation, and its well-known Hauptmodul rational parametrization [21, 22, 23]:

$$A_1 = \frac{1728 \cdot Z}{(Z+16)^3}, \quad A_2 = \frac{1728 \cdot Z^2}{(Z+256)^3}. \quad (90)$$

Remark: We have a quite remarkable result for the $X = \text{const.}$ foliation. When X is a constant, one finds that the curves $X = \text{const.}$, are genus zero curves.

9. Remarks and comments

We give here some miscellaneous remarks on the calculations presented in the previous sections.

Remark 1: The system of recurrence equations for $t_2(n, j)$ can be obtained by the creative telescoping method [17, 19]. For higher d , the computations get too heavy. But with the guessing method, the recurrences for $d = 5$ can be reached and this may yield an efficient implementation, since one could take $t_5(n, j)$ as initial values instead of $t_2(n, j)$ in (4).

Remark 2: In our calculations, (Sections 3 and 2.2), we have experienced that we do not gain anything by doing the computation modulo primes, and then using chinese remaindering to construct the true result in \mathbb{Z} . The reason is that here we do not encounter an intermediate expression swell, but rather the fact that the largest integers that occur during the computation are basically those that are given as the final result (when this is considered to be the list of Taylor coefficients). Of course, we are mostly interested in the linear differential operator, which, itself, has much smaller integer coefficients. Therefore the natural strategy would be to compute the Taylor coefficients modulo prime, and guess the operator modulo prime, and, only after this is done for sufficiently many primes, use chinese remaindering and rational reconstruction to get the true operator. Unfortunately, the operator also has quite large integers in its coefficients so that this strategy is unfavorable. However, we can still use homomorphic images for the purpose of prediction, e.g. how many terms are required for guessing the linear differential operator.

As an example, in the case ($d = 11$, 20 processes, 2464 terms), the timing is 18 days in exact arithmetic calculations. When we compute modulo the prime $2^{31} - 1$, our

† G.S. Joyce already noticed the emergence of *modular equations* on lattice Green functions [5].

implementation needs 58 hours, but the rational reconstruction of the linear differential operator requires 185 primes of this size.

Remark 3: With the emergence of the algebraic solution (69) for the system of $d = 2$ PDEs, and the emergence of the modular form solution (79) for the system of $d = 3$ PDEs, it is tempting to conjecture that similar solutions of two variables exist for all the system of PDEs for arbitrary value of d .

Remark 4: For one complex variable, the holonomic (or D-finite [6]) functions are solutions of linear ODEs with polynomial coefficients in the complex variable. The singularities (and apparent singularities) can be seen immediately as solutions of the head polynomial coefficient of the linear ODE. For partial differential equations system annihilating holonomic functions of several complex variables, the singular manifolds would be too complex or simply could not be well defined. By considering several Picard-Fuchs systems of two-variables “associated” to Calabi-Yau ODEs[†], we showed [24] that D-finite (holonomic) functions are actually a good framework for actually finding properly the singular manifolds. The singular algebraic varieties for some $T_d(z, y)$ are given in Appendix H.

10. Conclusion

A *recursive method* has been introduced in [9] to generate the expansion of the lattice Green function of the d -dimensional face-centred cubic lattice. The method has been used to generate many coefficients for $d = 7$ and the corresponding linear differential equation has been obtained [9].

We have shown, here, the strength and the limit of this recursive method. Some observations on the recursive method allow us to improve the computations and produce the series up to $d = 12$. The corresponding linear differential equations have been obtained (available online [15]) and show that the pattern (order, singularities, differential Galois group) seen for the lower d 's continues, as discussed in Sections 3 and 4.

In the recursive method, a two-dimensional array $t_d(n, j)$, defined in (4)–(7), is computed where only the coefficients $t_d(n, 0)$ correspond to the expansion of the lattice Green function. The two-dimensional array $t_d(n, j)$ gives the expansion of a “lattice” Green function $T_d(z, y)$ that depends on two variables. These D -finite bivariate series are studied, in Sections 6 and 7 for $d = 2$ and in Section 8 for $d = 3$, and the differential equations they are solution of, are addressed.

We have been able to produce some solutions of the partial differential equations annihilating the bivariate series $T_d(z, y)$. In Section 8 a remarkable *modular form* solution emerged for $d = 3$. The corresponding Hauptmodul pullback is a simple rational function of y and z . In terms of this Hauptmodul, the (y, z) -plane is a foliation of rational curves. Such kind of results are clearly a strong incentive to generalize the search of solutions of the D -finite systems corresponding to higher dimensions d .

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[†] Along the line of the relation between lattice Green functions and Calabi-Yau ODEs see for instance [8].

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Appendix A. Singularities of the ODEs for $d = 8, 9, 10, 11, 12$

The singularities, occurring at the head derivative of G_{14}^{8Dfcc} , are $x^{11}S_8(x) \cdot P_{14}(x)$. The roots of the degree-95 polynomial $P_{14}(x)$ are *apparent singularities*. The polynomial $S_8(x)$ corresponding to the finite singularities reads:

$$\begin{aligned} S_8(x) = & (14+x)^2 (x-1) (x-7) (x-2) (6+x) (7+x) (20+x) (28+x) \\ & (48+x) (21+2x) (4+3x) (28+3x) (32+3x) (16+5x) (28+5x) \\ & (28+11x) (112+11x) (224+13x) (112+19x). \end{aligned} \quad (\text{A.1})$$

The singularities of G_{18}^{9Dfcc} are $x^{14} \cdot S_9(x) P_{18}(x)$. The roots of the degree-133 polynomial $P_{18}(x)$ are *apparent singularities*. The polynomial $S_9(x)$ corresponding to the finite singularities reads:

$$\begin{aligned} S_9(x) = & (x+9)^4 (7x+9) (4x+9) (x+3) (2x+9) (7x+36) (5x+27) (x+12) \\ & (2x+27) (5x+72) (x+15) (x+18) (2x+45) (x+27) (x+36) (x+63) \\ & (2x-9) (5x-9) (x-1). \end{aligned} \quad (\text{A.2})$$

The singularities of G_{22}^{10Dfcc} are $x^{18} \cdot S_{10}(x) \cdot P_{22}(x)$. The roots of the degree-252 polynomial $P_{22}(x)$ are *apparent singularities*. The polynomial $S_{10}(x)$, corresponding to the finite singularities, reads:

$$\begin{aligned} S_{10}(x) = & (15+x)^2 (x-1) (4x+75) (19x+540) (x-15) (4x+15) (x+80) \\ & (2x+45) (22x+45) (2x+25) (7x+20) (7x+120) (2x+15) (23x+180) \\ & (13x+60) (29x+360) (17x+135) (x+45) (4x+45) (x+35) (3x-5) \\ & (4x+5) (11x+135) (x+20) (13x-45) (x+12) (x+9) (x+8) (x+5). \end{aligned} \quad (\text{A.3})$$

The singularities of G_{27}^{11Dfcc} are $x^{22}S_{11}(x)P_{27}(x)$. The roots of the degree-352 polynomial $P_{27}(x)$ are *apparent singularities*. The polynomial $S_{11}(x)$, corresponding to the finite singularities, reads:

$$\begin{aligned} S_{11}(x) = & (x+11)^6 (55+x)^2 (x-1) (8x+55) (29x+55) (4x+55) (2x+55) \\ & (4x+11) (7x+165) (7x-55) (2x+33) (17x+55) (x+44) (13x+275) \\ & (3x+55) (7x-11) (13x+55) (7x+110) (x+35) (3x+22) (x+99) \\ & (19x-55) (7x+33) (9x+11) (x+15) (9x+55) (17x+275) (3x+77) \\ & (23x+165). \end{aligned} \quad (\text{A.4})$$

The singularities of G_{32}^{12Dfcc} are $x^{27}S_{12}(x)P_{32}(x)$. The roots of the degree-580 polynomial $P_{32}(x)$ are *apparent singularities*. The polynomial $S_{12}(x)$, corresponding to the finite singularities, reads:

$$\begin{aligned} S_{12}(x) = & (2x+33)^2 (43x+264) (5x+6) (37x+66) (3x+8) (23x+66) \\ & (67x+264) (2x+9) (13x+66) (5x+33) (7x+48) (7x+66) (9x+88) \\ & (10x+99) (53x+528) (x+10) (x+11) (5x+66) (19x+264) (7x+99) \\ & (37x+528) (23x+330) (5x+72) (29x+528) (17x+330) (13x+264) \end{aligned}$$

$$\begin{aligned}
& (x + 21)(x + 22)(31x + 792)(8x + 231)(x + 32)(x + 33)(25x + 1056) \\
& (x + 54)(x + 66)(x + 120)(x - 33)(2x - 11) \\
& (13x - 33)(2x - 3)(x - 1).
\end{aligned} \tag{A.5}$$

Appendix B. Gröbner basis basics

The theory of Gröbner bases has been initiated by Bruno Buchberger in his Ph.D. thesis [25] in 1965. While originally it was formulated for commutative multivariate polynomial rings, we are interested in its generalization to noncommutative rings. Here we can only mention a few key facts that are important for the kind of applications that we have in mind. A very instructive introduction to Gröbner bases is given in [26].

Let D_z denote the operator $\partial/\partial z$. The motivation for using operator notation is that it turns ODEs and PDEs into (univariate resp. multivariate) polynomials. For example the PDEs appearing in Sections 6–8 can be represented by polynomials in the ring $\mathbb{O} = \mathbb{C}(z, y)[D_z, D_y]$, i.e., the ring of partial differential operators in z and y (it is an instance of an *Ore algebra*). Note that this ring is not commutative, because of the Leibniz rule $D_z a = a D_z + \partial a/\partial z$ for all $a \in \mathbb{C}(z, y)$.

Let f be a power series (or some other kind of “function”); we define

$$\text{ann}_{\mathbb{O}}(f) = \{P \in \mathbb{O} \mid P(f) = 0\},$$

called the *annihilating ideal* of f . It can be easily seen that this set is indeed a left ideal in \mathbb{O} , as for example, the left-multiplication of $P \in \mathbb{O}$ by D_z corresponds to differentiating the differential equation represented by P with respect to z . Since univariate polynomial rings are principal ideal domains, $\text{ann}(f)$ is generated by a single element if we consider only one derivation; this unique generator corresponds to the minimal-order ODE. In fact the Gröbner basis computation specializes to the *greatest common right divisor* in this setting. Of course, in the case of PDEs, an annihilating ideal in general is generated by several operators.

We need some notion of *leading term* for PDEs (in the case of ODEs it is clear). For this purpose one imposes a total order on the monomials in the ring under consideration, that is compatible with multiplication and that has 1 as the smallest monomial; such an ordering is called a *monomial order*. For example, the degree-lexicographic order on the ring $\mathbb{C}(z, y)[D_z, D_y]$ with $D_y \prec D_z$ is defined by

$$D_z^i D_y^j \prec D_z^k D_y^\ell \iff i + j < k + \ell \vee (i + j = k + \ell \wedge i < k). \tag{B.1}$$

Using this notion of leading term, it is straightforward to define a multivariate polynomial division (called *reduction*) of $P \in \mathbb{O}$ by some $Q_1, \dots, Q_r \in \mathbb{O}$. It works by subtracting, in each step, a suitable multiple of some Q_i such that the leading term of the dividend vanishes. In some steps of this process one may have the choice between several of the Q_i , and this has the consequence that the remainder of the multivariate polynomial division is not unique in general. Now, if I is an ideal, then a set G of generators of I is called a *Gröbner basis* if for each polynomial the remainder of the division by G is unique. In particular, we have that the division of P by G has remainder 0 if and only if $P \in I$; this property allows to decide the *ideal membership problem*. Gröbner bases are also a powerful tool for elimination purposes, i.e., for finding elements in an ideal that do not depend on some of the variables of the polynomial ring. There are several algorithms to compute, from an arbitrary set of generators of an ideal, a Gröbner basis, the most classic one being Buchberger’s algorithm [25].

Appendix C. The factorization of $L_5^{(z)}$ and $L_5^{(y)}$ for $T_2(z, y)$

The factors in the decomposition (45) of $L_5^{(z)}$ read

$$L_1^{(1)} = D_z + 2 \cdot \frac{8z^3y - 16z^2y^2 + 6z^2y - 2z^3 + y^2}{(16z^2y + y + 8zy - 4z^2)(z - 4y) \cdot z}, \quad (\text{C.1})$$

$$L_1^{(2)} = D_z + 2 \cdot \frac{32z^3y - 8z^3 - 96z^2y^2 + 36z^2y + zy - 32y^2z - 2y^2}{(16z^2y + y + 8zy - 4z^2)(z - 4y) \cdot z}, \quad (\text{C.2})$$

$$L_1^{(3)} = L_1^{(2)} - \frac{1}{z}, \quad (\text{C.3})$$

and

$$L_2 = D_z^2 + \frac{p_1(z, y)}{p_2(z, y)} \cdot D_z + \frac{p_0(z, y)}{p_2(z, y)}, \quad (\text{C.4})$$

where:

$$p_2(z, y) = z \cdot (4z - 1) \cdot (4z + 1) \cdot (y + 8yz + 16yz^2 - 4z^2) \cdot (z - 4y) \quad (\text{C.5}) \\ (256z^4y^2 - 64z^4y - 128z^3y^2 + 4z^3 + 64z^2y^2 - 20yz^2 + 40y^2z - 2yz + 3y^2),$$

$$p_1(z, y) = 2z \cdot \left(y^3 + 16y^4 - 3200z^4y^2 - 208z^4y + 816z^3y^2 + 84z^2y^2 + y^2z \right. \\ - 18z^3y + 576yz^5 - 40704z^5y^2 - 46080z^6y^2 + 8704yz^6 + 3584z^7y \\ - 98304z^8y^2 + 12288z^8y + 196608z^8y^3 - 217088z^4y^4 + 181248z^5y^3 \\ + 212992z^7y^3 - 24576z^6y^3 + 196608z^6y^4 - 524288z^7y^4 - 98304z^5y^4 \\ - 63488z^3y^4 + 89088z^4y^3 - 20480z^7y^2 - 1440z^2y^3 + 6080z^3y^3 \\ \left. - 116zy^3 - 3840z^2y^4 + 384zy^4 + 24z^5 - 896z^7 \right), \quad (\text{C.6})$$

$$p_0(z, y) = 144y^4 - 7296z^4y^2 - 112z^4y + 528z^3y^2 + 124z^2y^2 - 2y^2z \\ - 28z^3y + 1600yz^5 - 80896z^5y^2 - 107520z^6y^2 + 18176yz^6 + 8192z^7y \\ - 196608z^8y^2 + 24576z^8y + 393216z^8y^3 - 315392z^4y^4 + 347136z^5y^3 \\ + 49152z^7y^3 - 8192z^6y^3 + 458752z^6y^4 - 524288z^7y^4 - 229376z^5y^4 \\ - 88064z^3y^4 + 150016z^4y^3 + 20480z^7y^2 - 736z^2y^3 + 11840z^3y^3 \\ - 188zy^3 - 8960z^2y^4 + 384zy^4 + 16z^5 - 2048z^7. \quad (\text{C.7})$$

The factors in the decomposition (59) of $N_5^{(y)}$ read

$$N_1^{(1)} = D_y + 2 \cdot \frac{16z^2y^2 - z^3 + y^2 + 8y^2z}{(16z^2y + y + 8zy - 4z^2) \cdot (4y - z) \cdot y} \quad (\text{C.8})$$

$$N_1^{(2)} = D_y + 2 \cdot \frac{q_0(z, y)}{y \cdot (16z^2y + y + 8zy - 4z^2) (16y + 1) (z - 4y)}, \quad (\text{C.9})$$

where

$$q_0(z, y) = -2z^3 + zy + 24z^2y + 16z^3y - 6y^2 - 40y^2z + 96z^2y^2 \\ + 128z^3y^2 - 64y^3 - 512zy^3 - 1024z^2y^3, \quad (\text{C.10})$$

$$N_1^{(3)} = N_1^{(2)} - \frac{1}{(16y + 1) \cdot y}, \quad (\text{C.11})$$

and

$$N_2 = D_y^2 + \frac{\tilde{p}_1(z, y)}{\tilde{p}_2(z, y)} \cdot D_y + \frac{\tilde{p}_0(z, y)}{\tilde{p}_2(z, y)}, \quad (\text{C.12})$$

where:

$$\begin{aligned} \tilde{p}_2(z, y) = & y \cdot (16y - 1) \cdot (z - 4y) \cdot (y + 8zy + 16z^2y - 4z^2) \cdot (32z^4y \\ & - 8z^4 + 256z^3y^2 - 32z^2y^2 + 10z^2y - 32y^2z + zy - 2y^2), \end{aligned} \quad (\text{C.13})$$

$$\begin{aligned} \tilde{p}_1(z, y) = & -24y^4 + 15360y^5z + 102400y^5z^2 - 1310720y^5z^5 - 491520y^5z^4 \\ & + 163840y^5z^3 - 672z^4y^2 - 60z^3y^2 - 2z^2y^2 + 24yz^5 - 3456z^5y^2 \\ & - 20480z^6y^2 + 576yz^6 + 1920z^7y - 104448z^4y^4 + 41472z^5y^3 \\ & + 32768z^7y^3 + 94208z^6y^3 + 221184z^5y^4 - 82944z^3y^4 + 26112z^4y^3 \\ & - 15360z^7y^2 + 432z^2y^3 + 4672z^3y^3 + 18zy^3 - 14592z^2y^4 \\ & - 1056zy^4 - 32z^7 + 640y^5, \end{aligned} \quad (\text{C.14})$$

$$\begin{aligned} \tilde{p}_0(z, y) = & -8y^3 + 480y^4 + 96z^6 + 10240z^4y^2 - 104z^4y + 1320z^3y^2 \\ & + 152z^2y^2 + 8y^2z - 4z^3y - 672yz^5 + 34048z^5y^2 + 104448z^6y^2 \\ & - 11648yz^6 - 8704z^7y - 368640z^4y^4 + 2048z^5y^3 - 155648z^6y^3 \\ & - 983040z^5y^4 + 122880z^3y^4 - 64512z^4y^3 + 18432z^7y^2 - 8544z^2y^3 \\ & - 44288z^3y^3 - 568zy^3 + 76800z^2y^4 + 11520zy^4 - 8z^5 + 640z^7. \end{aligned} \quad (\text{C.15})$$

Appendix D. The matching of $T_2(z, y)$ with the solutions of $L_5^{(z)}$

$T_2(z, y)$ as a linear combination on the formal solutions of $L_5^{(z)}$ reads

$$T_2(z, y) = C_1^{(z)}(y) \cdot S_1^{(z)} + C_2^{(z)}(y) \cdot S_2^{(z)} + C_3^{(z)}(y) \cdot S_3^{(z)}, \quad (\text{D.1})$$

where

$$\begin{aligned} S_1^{(z)} = & 1 + \left(-\frac{16}{3} + 2y^{-1}\right) \cdot z^2 + \left(\frac{512}{15} - \frac{184}{15}y^{-1}\right) \cdot z^3 \\ & + \left(-\frac{18176}{105} + \frac{320}{7}y^{-1} + \frac{208}{35}y^{-2}\right) \cdot z^4 \\ & + \left(\frac{253952}{315} - \frac{2304}{35}y^{-1} - \frac{2816}{35}y^{-2} - \frac{4}{315}y^{-3}\right) \cdot z^5 + \dots \\ S_2^{(z)} = & z + \left(-\frac{16}{3} + \frac{1}{6}y^{-1}\right) \cdot z^2 + \left(\frac{368}{15} + \frac{22}{15}y^{-1} + \frac{1}{30}y^{-2}\right) \cdot z^3 \\ & + \left(-\frac{11264}{105} - \frac{2864}{105}y^{-1} + \frac{8}{35}y^{-2} + \frac{1}{140}y^{-3}\right) \cdot z^4 \\ & + \left(\frac{144128}{315} + \frac{79424}{315}y^{-1} + \frac{96}{35}y^{-2} + \frac{2}{45}y^{-3} + \frac{1}{630}y^{-4}\right) \cdot z^5 + \dots \\ S_3^{(z)} = & z^2 - 6z^3 + (36 + 3y^{-1}) \cdot z^4 - (180 + 40y^{-1}) \cdot z^5 \\ & + (900 + 370y^{-1} + 10y^{-2}) \cdot z^6 + \dots \\ C_1^{(z)}(y) = & \frac{1}{\sqrt{1-16y}} \cdot {}_2F_1\left(\left[\frac{1}{2}, \frac{1}{2}\right], [1], 16 \cdot \frac{y}{16y-1}\right), \end{aligned} \quad (\text{D.2})$$

$$C_2^{(z)}(y) = -\frac{8y}{(8y-1)^{3/2}} \cdot {}_2F_1\left(\left[\frac{3}{4}, \frac{5}{4}\right], [2], 64 \cdot \frac{y^2}{(1-8y)^2}\right), \quad (\text{D.3})$$

$$C_3^{(z)}(y) = -2y^{-1}. \quad (\text{D.4})$$

Appendix E. The matching of $T_2(z, y)$ with the solutions of $N_5^{(y)}$

$T_2(z, y)$ as linear combination on the formal solutions of $N_5^{(y)}$ reads

$$T_2(z, y) = C_1^{(y)}(z) \cdot S_1^{(y)} + C_2^{(y)}(z) \cdot S_2^{(y)} + C_3^{(y)}(z) \cdot S_3^{(y)}, \quad (\text{E.1})$$

where

$$\begin{aligned} S_1^{(y)} = & 1 - 16y - \left(\frac{128}{3} + \frac{208}{3}z^{-1} + \frac{16}{3}z^{-2} + \frac{1}{3}z^{-3}\right) \cdot y^2 \\ & - \left(\frac{2048}{15} + \frac{4096}{15}z^{-1} + \frac{1408}{5}z^{-2} + \frac{464}{15}z^{-3} + \frac{8}{3}z^{-4} + \frac{1}{15}z^{-5}\right) \cdot y^3 + \dots \end{aligned}$$

$$\begin{aligned} S_2^{(y)} = & y + \left(\frac{8}{3} + 4z^{-1} + \frac{1}{6}z^{-2}\right) \cdot y^2 \\ & + \left(\frac{128}{15} + 16z^{-1} + \frac{232}{15}z^{-2} + z^{-3} + \frac{1}{30}z^{-4}\right) \cdot y^3 + \dots \end{aligned}$$

$$S_3^{(y)} = y + (8 + 3z^{-1}) \cdot y^2 + (76 + 30z^{-1} + 10z^{-2}) \cdot y^3 + \dots$$

$$C_1^{(y)}(z) = \frac{1}{\sqrt{1-16z^2}} \cdot {}_2F_1\left(\left[\frac{1}{2}, \frac{1}{2}\right], [1], \frac{16z^2}{16z^2-1}\right), \quad (\text{E.2})$$

$$C_2^{(y)}(z) = \frac{2 \cdot (12z+1)}{z} \cdot H_z(z) + \frac{(4z+1)(4z-1)}{2z} \cdot \frac{d}{dz} H_z(z), \quad (\text{E.3})$$

$$\text{with: } H_z(z) = {}_2F_1\left(\left[\frac{1}{2}, \frac{1}{2}\right], [1], 16z^2\right), \quad (\text{E.4})$$

$$C_3^{(y)}(z) = -2z^{-1}. \quad (\text{E.5})$$

Appendix F. Closed form expression of $V_2(z, y)$

The bivariate series

$$V_2(z, y) = \frac{1}{\pi^2} \int_0^\pi \int_0^\pi \frac{dk_1 dk_2}{(1-z\zeta_2) \cdot (1-\frac{y}{2}\sigma_2)}, \quad (\text{F.1})$$

with

$$\zeta_2 = \cos(k_1) \cdot \cos(k_2), \quad \sigma_2 = \cos(k_1) + \cos(k_2), \quad (\text{F.2})$$

is related to the integral (23) with $d = 2$ by $T_2(z, y) = V_2(4z, \pm 4\sqrt{y})$. The integral $V_2(z, y)$ can be written in the closed form expression

$$\begin{aligned} V_2^{\text{closed}}(z, y) = & \frac{y}{zy+y-2z} \cdot K(y) + \frac{z}{\delta} \cdot \left(\Pi\left(\frac{(z-\delta)^2}{y^2}, z\right) - \Pi\left(\frac{(z+\delta)^2}{y^2}, z\right)\right) \\ & + \frac{y \cdot (1-y) \cdot \delta}{(z-y^2)(zy+y-2z)} \cdot \left(\Pi(\Delta_-, y) - \Pi(\Delta_+, y)\right), \quad (\text{F.3}) \end{aligned}$$

with

$$\delta = \sqrt{z^2 - zy^2}, \quad \Delta_{\pm} = \frac{2zy + y^2 - zy^2 - 2z \pm 2(1-y) \cdot \delta}{zy + y - 2z}, \quad (\text{F.4})$$

and where Π and K are the complete elliptic integrals of the third and first kind:

$$\Pi(\nu, k) = \int_0^{\pi} \frac{1}{(1 - \nu \cos(\phi)^2)} \cdot \frac{1}{\sqrt{1 - k^2 \cos(\phi)^2}} \cdot d\phi, \quad K(k) = \Pi(0, k). \quad (\text{F.5})$$

One has

$$V_2(z, y) = \text{Re}(V_2^{\text{closed}}(z, y)), \quad \text{for } |z| < 1, \quad |y| < 1, \quad (\text{F.6})$$

and

$$V_2(z, y) = V_2^{\text{closed}}(z, y), \quad \text{for } y \cdot (zy + y - 2z) > 0. \quad (\text{F.7})$$

Appendix G. The two right-most order-two operators L_2 and N_2 for $T_3(z, y)$

• The right-most order-two linear differential operator L_2 (see (76)) in the factorization of the order-nine operators $L_9^{(z)}$ reads:

$$L_2 = D_z^2 + z^2 \cdot \frac{p_1(z, y)}{p_2(z, y)} \cdot D_z + \frac{p_0(z, y)}{p_2(z, y)}, \quad (\text{G.1})$$

where:

$$\begin{aligned} p_2(z, y) &= z^2 \cdot (432y^2z^2 + 180zy^2 - 36z^2y + 12y^2 - 13yz + 2z^2) \\ &\quad \times (4z + 1) \cdot (3y - z) \cdot (144z^2y + 24yz - 16z^2 + y) \\ &\quad \times (144y^2z^2 + 96zy^2 - 40z^2y + 16y^2 - 8yz + z^2), \end{aligned} \quad (\text{G.2})$$

$$\begin{aligned} p_1(z, y) &= 512 \cdot (4y - 1) \cdot (36y - 1) \cdot (9y - 1) (216y^2 - 18y + 1) \cdot z^7 \\ &\quad - 32 \cdot (10077696y^6 - 10730880y^5 + 3050784y^4 - 361080y^3 + 20176y^2 - 481y + 3) \cdot z^6 \\ &\quad - 16y (25754112y^5 - 16422912y^4 + 3259008y^3 - 270672y^2 + 9518y - 103) \cdot z^5 \\ &\quad - 2y (103762944y^5 - 46033920y^4 + 6379200y^3 - 334704y^2 + 5464y - 1) \cdot z^4 \\ &\quad - 2y^2 \cdot (26065152y^4 - 8142336y^3 + 717600y^2 - 17920y + 13) \cdot z^3 \\ &\quad - y^3 (6816960y^3 - 1407888y^2 + 60196y - 99) \cdot z^2 \\ &\quad - 24y^4 (18288y^2 - 1960y + 3) \cdot z - 10944y^6 - 144y^5, \end{aligned} \quad (\text{G.3})$$

$$\begin{aligned} p_0(z, y) &= 256 (4y - 1) (36y - 1) (9y - 1) (216y^2 - 18y + 1) \cdot z^8 \\ &\quad - (107495424y^6 - 134369280y^5 + 41720832y^4 - 5163264y^3 + 284928y^2 - 6240y + 32) \cdot z^7 \\ &\quad - 8y (14556672y^5 - 10917504y^4 + 2372544y^3 - 202944y^2 + 6788y - 63) \cdot z^6 \\ &\quad - 16 (3032640y^4 - 1574640y^3 + 235404y^2 - 12305y + 178)y^2 \cdot z^5 \\ &\quad - 4y^2 (2519424y^4 - 883872y^3 + 81840y^2 - 1956y + 1) \cdot z^4 \\ &\quad - 16y^3 \cdot (75168y^3 - 15768y^2 + 746y - 3) \cdot z^3 \\ &\quad - 2 \cdot (49032y^2 - 5550y + 113) \cdot y^4 \cdot z^2 - 12 \cdot (456y - 35)y^5 \cdot z - 144y^6, \end{aligned} \quad (\text{G.4})$$

This order-two operator L_2 is self-adjoint up to a conjugation by its Wronskian $W(L_2)$

$$L_2 \cdot W(L_2) = W(L_2) \cdot \text{adjoint}(L_2), \quad (\text{G.5})$$

where this Wronskian $W(L_2)$ reads:

$$W(L_2) = \frac{432 y^2 z^2 + 180 y^2 z - 36 y z^2 + 12 y^2 - 13 y z + 2 z^2}{(4z+1) \cdot (z-3y) \cdot d_1 \cdot d_2} \quad (\text{G.6})$$

$$\text{where:} \quad d_1 = 144 y z^2 + 24 y z - 16 z^2 + y,$$

$$\text{and:} \quad d_2 = 144 y^2 z^2 + 96 y^2 z - 40 y z^2 + 16 y^2 - 8 y z + z^2.$$

• The right-most order-two linear differential operator N_2 (see (77)) in the factorization of the order-nine operators N_9^y reads:

$$N_2 = D_y^2 + y^2 \cdot \frac{q_1(z, y)}{q_2(z, y)} \cdot D_y + \frac{q_0(z, y)}{q_2(z, y)}, \quad (\text{G.7})$$

where:

$$\begin{aligned} q_2(z, y) &= y^2 \cdot (36 y z - 6 y + z) \cdot (3 y - z) \\ &\quad \times (144 y^2 z^2 + 96 y^2 z - 40 y z^2 + 16 y^2 - 8 y z + z^2) \\ &\quad \times (144 y z^2 + 24 y z - 16 z^2 + y), \end{aligned} \quad (\text{G.8})$$

$$\begin{aligned} q_1(z, y) &= 864 \cdot (6z-1) \cdot (3z+1)^2 \cdot (12z+1)^2 \cdot y^4 \\ &\quad - 96z \cdot (15552z^5 + 25920z^4 + 4428z^3 - 1098z^2 - 273z - 7) \cdot y^3 \\ &\quad + 6z^2 \cdot (38016z^4 + 7200z^3 - 8184z^2 - 1850z - 31) \cdot y^2 \\ &\quad + 2z^3 \cdot (8064z^3 + 6000z^2 + 944z + 11) \cdot y - 1360z^6 - 104z^5 - z^4, \end{aligned} \quad (\text{G.9})$$

$$\begin{aligned} q_0(z, y) &= 4z^6 + 16 \cdot (25z-4) \cdot z^5 \cdot y \\ &\quad - 2z^3 \cdot (2448z^3 + 24z^2 - 163z - 1) \cdot y^2 \\ &\quad + 12z^2 \cdot (432z^4 - 792z^3 - 669z^2 - 113z - 2) \cdot y^3 \\ &\quad - 12z \cdot (15552z^5 + 22032z^4 + 1188z^3 - 1989z^2 - 363z - 10) \cdot y^4 \\ &\quad + 216 \cdot (6z-1) \cdot (3z+1)^2 \cdot (12z+1)^2 \cdot y^5. \end{aligned} \quad (\text{G.10})$$

This order-two operator N_2 is self-adjoint up to a conjugation by its Wronskian $W(N_2)$

$$N_2 \cdot W(N_2) = W(N_2) \cdot \text{adjoint}(N_2), \quad (\text{G.11})$$

where this Wronskian $W(N_2)$ reads:

$$\begin{aligned} W(N_2) &= \frac{36 y z - 6 y + z}{z \cdot (z - 3 y) \cdot d_1 \cdot d_2} \quad \text{where:} \quad d_1 = 144 y z^2 + 24 y z - 16 z^2 + y, \\ \text{and:} \quad d_2 &= 144 y^2 z^2 + 96 y^2 z - 40 y z^2 + 16 y^2 - 8 y z + z^2. \end{aligned} \quad (\text{G.12})$$

Appendix H. Singularities of the $T_d(z, y)$

Based on the singularities of the ODEs in one variable (the other being a parameter) or Landau conditions methods [10], we have the following results. The bivariate series have singularities bearing on the variable z , these singularities are those of the linear ODEs of the LGF of the d -dimensional fcc lattice. Similarly, the singularities corresponding to the simple lattice appear as singularities in the variable y . Besides

these obvious and expected singularities, one obtains algebraic curves on (z, y) as singular varieties. For $d = 2$, $d = 3$ and $d = 4$, they read:

$$\begin{aligned}
 d = 2, \quad & 4y - z = 0, \quad 4z^2 \cdot (4y - 1) + 8yz + y = 0, \\
 d = 3, \quad & 3y - z = 0, \quad 16z^2 \cdot (9y - 1) + 24yz + y = 0, \\
 & 16y^2 \cdot (3z + 1)^2 - z \cdot (40yz + 8y - z) = 0, \\
 d = 4, \quad & 8y - 3z = 0, \quad 36z^2 \cdot (16y - 1) + 48yz + y = 0, \\
 & 4z^2 \cdot (16y - 1) + 16yz + y = 0, \quad 16yz + 4y - z = 0.
 \end{aligned} \tag{H.1}$$

One may infer from the first two varieties of each d , the expressions in function of the dimension

$$y - \frac{d-1}{2d} \cdot z = 0, \quad y - \frac{4 \cdot (d-1)^2 \cdot z^2}{(1 + 2 \cdot d \cdot (d-1) \cdot z)^2} = 0. \tag{H.2}$$

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