

# $\partial$ -finite functions revisited

Christoph Koutschan

Research Institute for Symbolic Computation  
Johannes Kepler Universität Linz, Austria

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# What is this talk about?

Starting point: Algorithmic framework for the automatic treatment of  $\partial$ -finite functions, as described in Frédéric Chyzak's PhD thesis

Now: some new ideas, exemplified on two applications:

- ▶ Part I: Simulation of electromagnetic waves
- ▶ Part II: TSPP



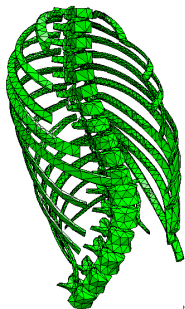
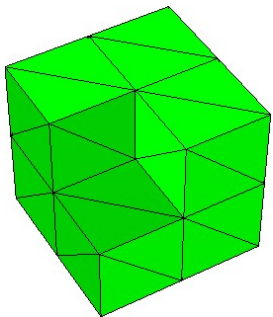
# Simulation of electromagnetic waves

- ▶ joint work by Joachim Schöberl (RWTH Aachen), Peter Paule and CK
- ▶ wide range of applications in constructing antennas, mobile phones, etc.
- ▶ merchandised by the company CST (Computer Simulation Technology)
- ▶ simulation with finite element methods
- ▶ significant contributions from Symbolic Computation using CK's package `HolonomicFunctions`
- ▶ symbolically derived formulae allow a considerable speed-up



# Finite Element Method (FEM)

Numerical method for finding approximate solutions to partial differential equations on non-trivial domains:



Hetgen 4,4

- ▶ divide the domain into small finite elements (triangles in 2D, tetrahedra in 3D)
- ▶ approximate the solution by certain basis functions that are defined on each finite element
- ▶ locally supported piecewise polynomial basis functions



## Our problem setting

Simulate the propagation of electromagnetic waves using the Maxwell equations

$$\frac{dH}{dt} = \text{curl } E, \quad \frac{dE}{dt} = -\text{curl } H$$

where  $H$  and  $E$  are the magnetic and the electric field respectively. Define basis functions (in 2D) in order to approximate the solution:

$$\varphi_{i,j}(x, y) := (1-x)^i P_j^{(2i+1,0)}(2x-1) P_i\left(\frac{2y}{1-x} - 1\right)$$

**Problem:** need to represent the partial derivatives of  $\varphi_{i,j}(x, y)$  in the basis (i.e., as linear combinations of shifts of the  $\varphi_{i,j}(x, y)$  itself)



## Recall: $\partial$ -finite functions

**Definition:** A function  $f(x_1, \dots, x_n)$  is called  $\partial$ -finite w.r.t. an Ore algebra  $\mathbb{O} = \mathbb{K}(x_1, \dots, x_n)[\partial_1; \sigma_1, \delta_1] \cdots [\partial_n; \sigma_n, \delta_n]$  if  $\mathbb{O}/\text{Ann}_{\mathbb{O}} f$  is a finite-dimensional  $\mathbb{K}(x_1, \dots, x_n)$ -vector space.

In other words,  $f$  is  $\partial$ -finite if all its “derivatives” span a finite-dimensional  $\mathbb{K}(x_1, \dots, x_n)$ -vector space.

**Example:** All derivatives (w.r.t.  $x$  and  $y$ ) of  $\sin\left(\frac{x+y}{x-y}\right)$  are of the form

$$r_1(x, y) \sin\left(\frac{x+y}{x-y}\right) + r_2(x, y) \cos\left(\frac{x+y}{x-y}\right), \quad r_1, r_2 \in \mathbb{Q}(x, y)$$

e.g.,

$$\begin{aligned} D_x^3 D_y^2 \bullet \sin\left(\frac{x+y}{x-y}\right) &= \frac{32(3x^4 + 12yx^3 - 30y^2x^2 - 4y^3x + 9y^4)}{(x-y)^9} \sin\left(\frac{x+y}{x-y}\right) \\ &\quad - \frac{16(6x^5 - 33yx^4 + 80y^3x^2 - 54y^4x + 3y^5)}{(x-y)^{10}} \cos\left(\frac{x+y}{x-y}\right) \end{aligned}$$



## First try

```
phi[i_,j_,x_,y_] :=  
  LegendreP[i,2*y/(1-x)-1]*(1-x)^i*JacobiP[j,2*i+1,0,2*x-1]  
ann = Annihilator[phi[i,j,x,y], {Der[x], S[i], S[j]}]  
      ⟨quite big output⟩
```

In order to see better the structure of the output, we look only at the support of each operator:

Support[ann]

$$\{\{S_j^2, S_j, 1\}, \{S_i S_j, D_x, S_i, S_j, 1\}, \{S_i^2, D_x, S_i, S_j, 1\}, \\ \{D_x S_j, D_x, S_i, S_j, 1\}, \{D_x S_i, D_x, S_i, S_j, 1\}, \{D_x^2, D_x, S_i, S_j, 1\}\}$$

→ second and third operator match exactly our needs!



## Second try

**BUT:** The numerists need a relation that is free of  $x$  and  $y$ ! In change, they allow also shifted derivatives.

- ▶ “switch” to the Ore algebra

$$\mathbb{Q}(i, j)[x, y][D_x; 1, D_x][S_i; S_i, 0][S_j; S_j, 0]$$

- ▶ compute Gröbner basis in order to eliminate  $x$  and  $y$
- ▶ takes very long, interrupt as soon as a desired operator is found
- ▶ result is quite big (2 pages of output)
- ▶ because of “extension/contraction” we can not be sure that we obtain the smallest operator



## Third try

Recall: We are looking for a relation of the following form

$$\sum_{(k,l) \in A} a_{k,l}(i,j) \frac{d}{dx} \varphi_{i+k,j+l}(x,y) = \sum_{(m,n) \in B} b_{m,n}(i,j) \varphi_{i+m,j+n}(x,y),$$

where  $A, B \subset \mathbb{N}^2$  are finite index sets.

- ▶ make an ansatz!
- ▶ let  $\mathbb{O} = \mathbb{Q}(i, j, x, y)[D_x; 1, D_x][S_i; S_i, 0][S_j; S_j, 0]$
- ▶ choose index sets  $A$  and  $B$
- ▶ reduce the ansatz with the Gröbner basis of  $\text{Ann}_{\mathbb{O}} \varphi$
- ▶ do coefficient comparison w.r.t.  $x$  and  $y$
- ▶ solve the resulting linear system for  $a_{k,l}, b_{m,n} \in \mathbb{Q}(i, j)$



## Result

With this method, we find in short time a (similar) relation:

$$\begin{aligned} & (2i + j + 5)(2i + 2j + 7) \frac{d}{dx} \varphi_{i,j+1}(x, y) \\ & + 2(2i + 1)(i + j + 3) \frac{d}{dx} \varphi_{i,j+2}(x, y) \\ & - (j + 3)(2i + 2j + 7) \frac{d}{dx} \varphi_{i,j+3}(x, y) \\ & + (j + 1)(2i + 2j + 5) \frac{d}{dx} \varphi_{i+1,j}(x, y) \\ & - 2(2i + 3)(i + j + 3) \frac{d}{dx} \varphi_{i+1,j+1}(x, y) \\ & + (2i + j + 5)(2i + 2j + 7) \frac{d}{dx} \varphi_{i+1,j+2}(x, y) = \\ & 2(i + j + 3)(2i + 2j + 5)(2i + 2j + 7) \varphi_{i,j+2}(x, y) \\ & - 2(i + j + 3)(2i + 2j + 5)(2i + 2j + 7) \varphi_{i+1,j+1}(x, y) \end{aligned}$$

Joachim Schöberl's answer: "jetzt bin ich echt beeindruckt...  
Genau so eine Relation brauche ich!"

→ these formulae caused a speed-up of 20 percent (!) in the  
numerical simulations



## 3D case

We would like to do the same thing in 3D.

### Problems:

- ▶ now the basis functions

$$\varphi(i, j, k, x, y, z) := P_i \left( \frac{2z}{(1-x)(1-y)} - 1 \right) (1-x)^i (1-y)^i \\ P_j^{(2i+1,0)} \left( \frac{2y}{1-x} - 1 \right) (1-x)^j \\ P_k^{(2i+2j+2,0)} (2x-1)$$

contain 6 variables

- ▶ computations become too big and too slow
- ▶ need some optimizations



# Optimizations (1)

Of course,

$$\text{nf} \left( \sum_k a_k \partial^{\alpha_k} \right) = \sum_k a_k \text{nf} (\partial^{\alpha_k})$$

- ▶ reduce each monomial  $\partial^{\alpha_k}$  separately
- ▶ use previously computed normal forms



## Optimizations (2)

**Idea:** Can we use homomorphic images for finding a good ansatz?

- ▶ surely we can compute in

$$\mathbb{Z}_p(i, j, x, y)[D_x; 1, D_x][S_i; S_i, 0][S_j; S_j, 0]$$

- ▶ this does not help much
- ▶ better: try to reduce polynomial arithmetic
- ▶ have to keep  $x$ ,  $y$  and  $z$  symbolically (coefficient comparison)
- ▶ what about  $i$ ,  $j$  and  $k$ ?



## Recall: normal form computation

**Input:**  $p \in \mathbb{O}$ , a Gröbner basis  $G = \{g_1, \dots, g_n\} \subseteq \mathbb{O}$

**Output:** normal form of  $p$  modulo  $\mathbb{O}\langle G \rangle$

while exists  $1 \leq i \leq n$  such that  $\text{lm}(g_i) \mid \text{lm}(p)$

$$g := (\text{lm}(p)/\text{lm}(g_i)) \cdot g_i$$

$$p := p - (\text{lc}(p)/\text{lc}(g)) \cdot g$$

end while



# Modular normal form computation

**Input:**  $p \in \mathbb{O}$ , a Gröbner basis  $G = \{g_1, \dots, g_n\} \subseteq \mathbb{O}$

**Output:** normal form of  $p$  modulo  $\mathbb{O}\langle G \rangle$

while exists  $1 \leq i \leq n$  such that  $\text{lm}(g_i) \mid \text{lm}(p)$

$$g := h((\text{lm}(p)/\text{lm}(g_i)) \cdot g_i)$$

$$p := p - (\text{lc}(p)/\text{lc}(g)) \cdot g$$

end while

where  $h$  is an insertion homomorphism, in our example

$$h : \mathbb{Q}(i, j, k, x, y, z) \rightarrow \mathbb{Q}(x, y, z)$$

$$f(i, j, k, x, y, z) \mapsto f(i_0, j_0, k_0, x, y, z), \quad \text{for } i_0, j_0, k_0 \in \mathbb{Z}$$



## A first result for 3D

One of the supports looks as follows:

$$\{S_j S_k^4, S_j^2 S_k^3, S_j^3 S_k^2, S_j^4 S_k, D_x S_j S_k^3, D_x S_j^2 S_k^2, D_x S_j^3 S_k, D_x S_j^4, S_j S_k^5, S_j^2 S_k^4, S_j^3 S_k^3, S_j^4 S_k^2, S_i S_k^5, S_i S_j S_k^4, S_i S_j^2 S_k^3, S_i S_j^3 S_k^2, D_x S_j S_k^4, D_x S_j^2 S_k^3, D_x S_j^3 S_k^2, D_x S_j^4 S_k, D_x S_i S_k^4, D_x S_i S_j S_k^3, D_x S_i S_j^2 S_k^2, D_x S_i S_j^3 S_k, S_j S_k^6, S_j^2 S_k^5, S_j^3 S_k^4, S_j^4 S_k^3, S_i S_k^6, S_i S_j S_k^5, S_i S_j^2 S_k^4, S_i S_j^3 S_k^3, D_x S_j S_k^5, D_x S_j^2 S_k^4, D_x S_j^3 S_k^3, D_x S_j^4 S_k^2, D_x S_i S_k^5, D_x S_i S_j S_k^4, D_x S_i S_j^2 S_k^3, D_x S_i S_j^3 S_k^2, S_j S_k^7, S_j^2 S_k^6, S_j^3 S_k^5, S_j^4 S_k^4, S_i S_k^7, S_i S_j S_k^6, S_i S_j^2 S_k^5, S_i S_j^3 S_k^4, D_x S_j S_k^6, D_x S_j^2 S_k^5, D_x S_j^3 S_k^4, D_x S_j^4 S_k^3, D_x S_i S_k^6, D_x S_i S_j S_k^5, D_x S_i S_j^2 S_k^4, D_x S_i S_j^3 S_k^3, S_j S_k^8, S_j^2 S_k^7, S_j^3 S_k^6, S_j^4 S_k^5, D_x S_j S_k^7, D_x S_j^2 S_k^6, D_x S_j^3 S_k^5, D_x S_j^4 S_k^4, D_x S_i S_k^7, D_x S_i S_j S_k^6, D_x S_i S_j^2 S_k^5, D_x S_i S_j^3 S_k^4, D_x S_j S_k^8, D_x S_j^2 S_k^7, D_x S_j^3 S_k^6, D_x S_j^4 S_k^5, D_x S_i S_k^8, D_x S_i S_j S_k^7, D_x S_i S_j^2 S_k^6, D_x S_i S_j^3 S_k^5, D_x S_j S_k^9, D_x S_j^2 S_k^8, D_x S_j^3 S_k^7, D_x S_j^4 S_k^6\}$$

Joachim Schöberl was impressed but not too happy about these results...



# Divide

**Next idea:** Write  $\varphi = u \cdot v \cdot w$  with

$$\begin{aligned}u &= P_i \left( \frac{2z}{(1-x)(1-y)} - 1 \right) (1-x)^i (1-y)^i \\v &= P_j^{(2i+1,0)} \left( \frac{2y}{1-x} - 1 \right) (1-x)^j \\w &= P_k^{(2i+2j+2,0)} (2x-1)\end{aligned}$$

and use the product rule

$$\frac{d\varphi}{dx} = \frac{du}{dx}vw + u\frac{dv}{dx}w + uv\frac{dw}{dx}$$

We now want to find a relation between e.g.  $uvw$  and  $\frac{du}{dx}vw$ .



...

**Task:** find relation between  $uvw$  and  $\frac{du}{dx}vw$

How does this fit into our framework?

Usually we have something like

$$\text{op} \bullet f = 0.$$

Now we search for a relation of the form

$$\text{op}_1 \bullet f = \text{op}_2 \bullet g.$$

Trivial solution:  $\text{op}_1 \in \text{Ann } f$  and  $\text{op}_2 \in \text{Ann } g$ . But since  $f$  and  $g$  are closely related we expect that there exists something “better”.



## and conquer

The natural way to express a relation like

$$\text{op}_1 \bullet f = \text{op}_2 \bullet g$$

is by using operator vectors in  $M = \mathbb{O} \times \mathbb{O}$  which we let act on  $\mathcal{F} \times \mathcal{F}$  by

$$P \bullet F = (P_1, P_2) \bullet (f, g) := P_1 \bullet f + P_2 \bullet g, \quad \text{where } P \in M, F \in \mathcal{F} \times \mathcal{F}$$

But how to compute a Gröbner basis for the ideal of relations between  $f$  and  $g$ , i.e. the annihilator  $\text{Ann}_M(f, g)$ ?



# Closure properties

Let  $f = uvw$  and  $g = \frac{du}{dx}vw$ .

We start with  $u$  and  $u' = \frac{du}{dx}$ :

$\text{Ann}_M(u, u') =$

$$\circlearrowleft \left\langle \{(p, 0) \mid p \in \text{Ann}_{\circlearrowleft} u\} \cup \{(0, p) \mid p \in \text{Ann}_{\circlearrowleft} u'\} \cup \{(D_x, -1)\} \right\rangle$$

After computing a Gröbner basis of the above, we can perform the closure property “multiplication by  $vw$ ” in a very similar fashion as usual (using an FGLM-like approach).



## Result

Finally we can use the ansatz technique as before in order to find an  $\{x, y, z\}$ -free operator:

$$\begin{aligned} & -2(1+2i)(2+j)(3+2i+j)(7+2i+2j)(5+i+j+k) \\ & (7+i+j+k)(8+i+j+k)(8+2i+2j+k)(9+2i+2j+k) \\ & (11+2i+2j+2k)(15+2i+2j+2k)f(i, j+1, k+3)+ \\ & \quad \vdots \\ & \quad \langle 31 \text{ similar terms} \rangle \\ & \quad \vdots \\ & -2(4+2i+j)(5+2i+j)(5+2i+2j)(5+i+j+k) \\ & (6+i+j+k)(8+i+j+k)(10+2i+2j+k) \\ & (11+2i+2j+k)(11+2i+2j+2k)(15+2i+2j+2k) \\ & g(i+1, j+2, k+3) = 0 \end{aligned}$$

where  $f = uvw$  and  $g = \frac{du}{dx}vw$ .



# Part II

## Totally Symmetric Plane Partitions

(joint work with M. Kauers and D. Zeilberger)



# Plane Partitions

**Definition:** A *plane partition*  $\pi$  is an array

$$\pi = (\pi_{ij}), \quad i, j \geq 1, \quad \pi_{ij} \geq 1$$

with finite sum  $|\pi| = \sum \pi_{ij}$ , which is weakly decreasing in rows and columns, i.e.,

$$\pi_{i+1,j} \leq \pi_{ij} \quad \text{and} \quad \pi_{i,j+1} \leq \pi_{ij} \quad \text{for all } i, j \geq 1.$$

**Example:**

5	4	1
3	2	1
1		



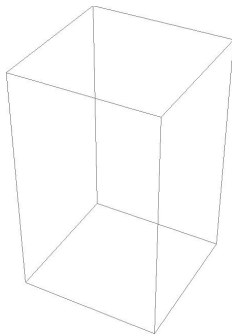
# 3D Ferrers diagram

By stacking  $\pi_{ij}$  unit cubes on top of the  $ij$  location, one gets the corresponding 3D Ferrers diagram, which is a left-, up-, and bottom-justified structure of unit cubes, and we can refer to the locations  $(i, j, k)$  of the individual unit cubes.



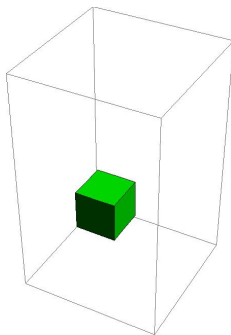
# 3D Ferrers diagram

5	4	1
3	2	1
1		



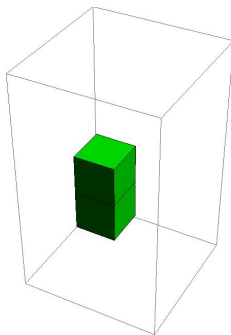
# 3D Ferrers diagram

5	4	1
3	2	1
1		



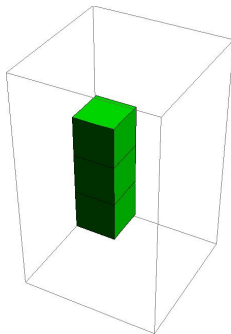
# 3D Ferrers diagram

5	4	1
3	2	1
1		



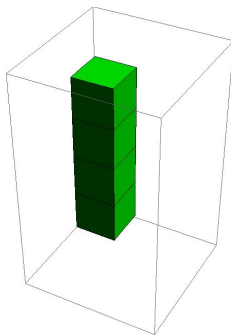
# 3D Ferrers diagram

5	4	1
3	2	1
1		



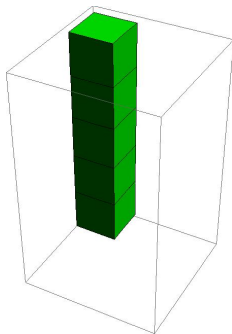
# 3D Ferrers diagram

5	4	1
3	2	1
1		



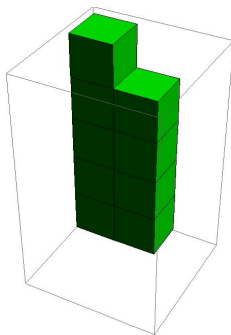
# 3D Ferrers diagram

5	4	1
3	2	1
1		



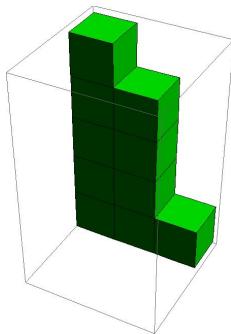
# 3D Ferrers diagram

5	4	1
3	2	1
1		



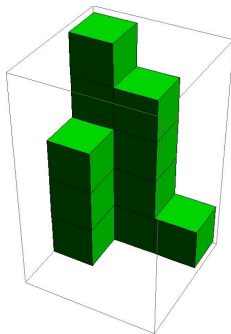
# 3D Ferrers diagram

5	4	1
3	2	1
1		



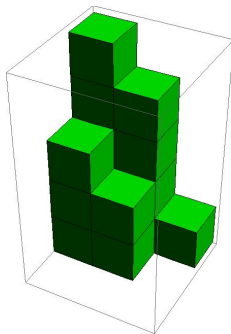
# 3D Ferrers diagram

5	4	1
3	2	1
1		



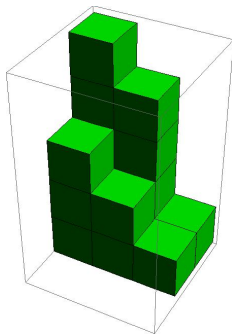
# 3D Ferrers diagram

5	4	1
3	2	1
1		



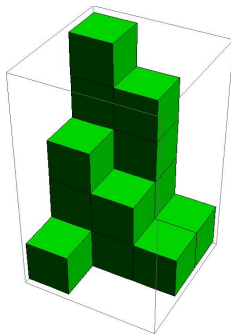
# 3D Ferrers diagram

5	4	1
3	2	1
1		



# 3D Ferrers diagram

5	4	1
3	2	1
1		

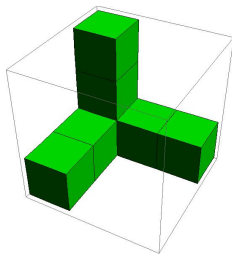


# Totally Symmetric Plane Partitions (1)

**Definition:** A plane partition is *totally symmetric* iff whenever  $(i, j, k)$  is occupied (i.e.  $\pi_{ij} \geq k$ ), it follows that all its (up to 5) permutations:  $\{(i, k, j), (j, i, k), (j, k, i), (k, i, j), (k, j, i)\}$  are also occupied.

**Example:**

3	1	1
1		
1		



# The TSPP Problem

**Conjecture:** (Ian Macdonald)

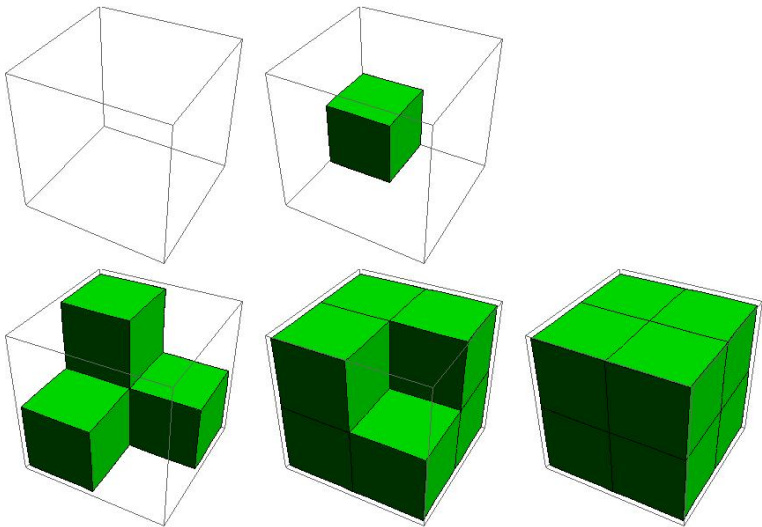
The number of totally symmetric plane partitions (TSPPs) whose 3D Ferrers diagram is bounded inside the cube  $[0, n]^3$  is given by the nice product-formula

$$\prod_{1 \leq i \leq j \leq k \leq n} \frac{i + j + k - 1}{i + j + k - 2}.$$



## Totally Symmetric Plane Partitions (2)

**Example:** All TSPPs for  $n = 2$ :



# The TSPP Problem

Ian Macdonald's conjecture was proven in 1995 by John Stembridge.

Ten years later George Andrews, Peter Paule, and Carsten Schneider came up with a computer-assisted proof, that, however required lots of human ingenuity and ad hoc tricks, in addition to a considerable amount of computer time.

We aim at a complete computer proof (which works analogously for the  $q$ -version of TSPP).



# The qTSP Problem

**Conjecture:** (independently by George Andrews and Dave Robbins, around 1983)

A  $q$ -analogue of the TSP problem leads to the nice formula

$$\prod_{1 \leq i \leq j \leq k \leq n} \frac{1 - q^{i+j+k-1}}{1 - q^{i+j+k-2}}.$$

This conjecture is still open.



# Okada's Determinant (1)

Soichi Okada reduced the problem to a determinant evaluation: He proved that the  $q$ -TSPP conjecture is true if

$$\det (\bar{a}(i, j))_{1 \leq i, j \leq n} = \prod_{1 \leq i \leq j \leq k \leq n} \left( \frac{1 - q^{i+j+k-1}}{1 - q^{i+j+k-2}} \right)^2 .$$

Analogously, in the  $q = 1$  case we have to show

$$\det (a(i, j))_{1 \leq i, j \leq n} = \prod_{1 \leq i \leq j \leq k \leq n} \left( \frac{i + j + k - 1}{i + j + k - 2} \right)^2 .$$



## Okada's Determinant (2)

where

$$\begin{aligned}\bar{a}(i, j) &= q^{i+j-1} \left( \begin{bmatrix} i+j-2 \\ i-1 \end{bmatrix} + q \begin{bmatrix} i+j-1 \\ i \end{bmatrix} \right) \\ &\quad + (1+q^i)\delta(i, j) - \delta(i, j+1)\end{aligned}$$

where

$$\begin{bmatrix} a \\ b \end{bmatrix} = \frac{(1-q^a)(1-q^{a-1})\cdots(1-q^{a-b+1})}{(1-q^b)(1-q^{b-1})\cdots(1-q)}.$$

**Remark:** In the ordinary TSPP case ( $q = 1$ ) we have

$$a(i, j) = \binom{i+j-2}{i-1} + \binom{i+j-1}{i} + 2\delta(i, j) - \delta(i, j+1)$$



# Zeilberger's Ansatz (1)

In his article

“The HOLONOMIC ANSATZ II. Automatic DISCOVERY(!) and PROOF(!!) of Holonomic Determinant Evaluations”,

Doron Zeilberger proposes the following method:

We want to prove for all  $n \geq 0$  that

$$\det(a(i, j))_{1 \leq i, j \leq n} = \text{Nice}(n),$$

for some explicit expressions  $a(i, j)$  and  $\text{Nice}(n)$ .



## Zeilberger's Ansatz (2)

Now a magician's trick is used: Pull out of the hat another "explicit" discrete function  $B(n, j)$ :



## Zeilberger's Ansatz (3)

Check the identities

$$\sum_{j=1}^n B(n, j)a(i, j) = 0, \quad (1 \leq i < n < \infty),$$

$$B(n, n) = 1, \quad (1 \leq n < \infty).$$

Then by uniqueness, it follows that  $B(n, j)$  equals the co-factor of the  $(n, j)$  entry of the  $n \times n$  determinant divided by the  $(n - 1) \times (n - 1)$  determinant.

Finally one has to check the identity

$$\sum_{j=1}^n B(n, j)a(n, j) = \text{Nice}(n)/\text{Nice}(n - 1) \quad (1 \leq n < \infty).$$



## Zeilberger's Ansatz (4)

If the suggested function  $B(n, j)$  does satisfy all these identities then the determinant identity follows as a consequence. So in a sense, the explicit description of  $B(n, j)$  plays the role of a certificate for the determinant identity.



# Some results on TSPP

**Result of guessing:** 65 recurrences for  $B(n, j)$ , their total size being about 5MB.

**$\partial$ -finite description:** We succeeded to compute a Gröbner basis of the annihilating ideal of  $B(n, j)$  (using CK's noncommutative OreGroebnerBasis implementation).

The Gröbner basis consists of 5 polynomials (their total size being about 1.6MB). Their leading monomials  $S_j^4, S_j^3 S_n, S_j^2 S_n^2, S_j S_n^3, S_n^4$  form a staircase of regular shape.



## How to proceed

We want to prove

$$\sum_{j=1}^n B(n, j) a(n, j) = \text{Nice}(n) / \text{Nice}(n-1)$$

where

$$a(n, j) = \binom{n+j-2}{n-1} + \binom{n+j-1}{n} + 2\delta(n, j) - \delta(n, j+1).$$

Hence we can consider the expression

$$\sum_{j=1}^n B(n, j) a'(n, j) + 2B(n, n) - B(n, n-1)$$

with  $a'(n, j) = \binom{n+j-2}{n-1} + \binom{n+j-1}{n}$  being hypergeometric.



# Several approaches

We unsuccessfully tried

- ▶ Gröbner basis elimination
- ▶ Takayama's algorithm
- ▶ Chyzak's algorithm

Finally, we succeeded by using the ansatz technique with an ansatz of the form

$$\sum_i \eta_i(n) S_n^i + (S_j - 1) \sum_{k,l,m} \varphi_{k,l,m}(n) j^k S_j^l S_n^m$$

**Note:** With this type of ansatz, it can happen that  $\eta_i = 0$  for all  $i$ .

(The computations just came to an end on Friday evening.)

