

# Random Walks in Multidimensional Lattices

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February 28, 2013

# Introduction

We consider lattices in  $\mathbb{R}^d$

$$\left\{ \sum_{i=1}^d n_i \mathbf{a}_i : n_1, \dots, n_d \in \mathbb{Z} \right\} \subseteq \mathbb{R}^d$$

for some linearly independent vectors  $\mathbf{a}_1, \dots, \mathbf{a}_d \in \mathbb{R}^d$ .

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for some linearly independent vectors  $\mathbf{a}_1, \dots, \mathbf{a}_d \in \mathbb{R}^d$ .

→ Simplest instance is the integer lattice  $\mathbb{Z}^d$

(choose  $\mathbf{a}_i = \mathbf{e}_i$ , the  $i$ -th unit vector):

- $d = 2$ : “square lattice”
- $d = 3$ : “cubic lattice”
- $d > 3$ : “hypercubic lattice”

The study of such lattices was inspired by crystallography in as much as the atomic structure of crystals forms such regular lattices.

## Topic of this Talk

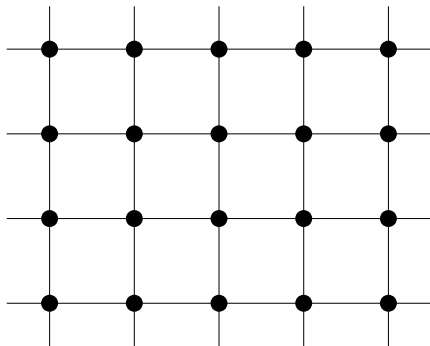
Study random walks on the *face-centered cubic (fcc) lattice*.

Consider random walks on the lattice points:

- Move to one of the nearest neighbors in each step.
- All steps have the same probability.
- A lattice point can be visited arbitrarily often.
- Starting point is the origin  $\mathbf{0}$ .

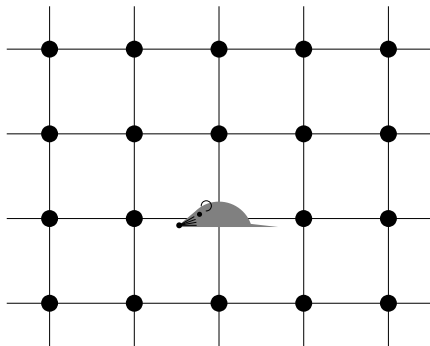
## A Random Walk in 2D

Square lattice (= integer lattice  $\mathbb{Z}^2$ )



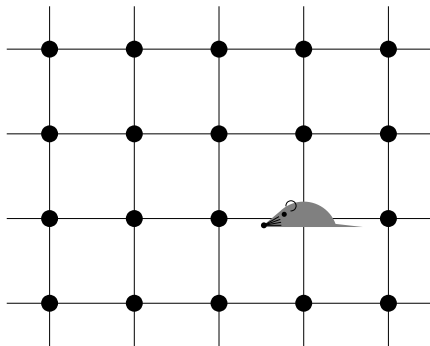
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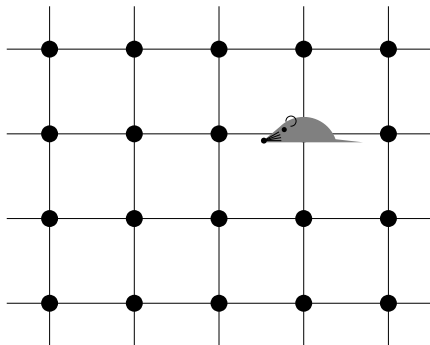
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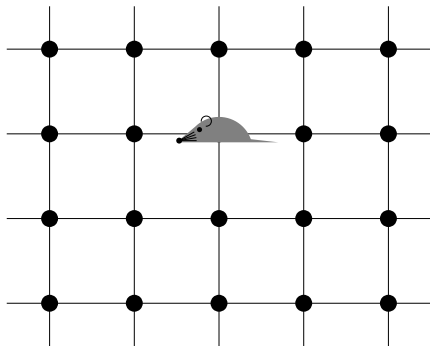
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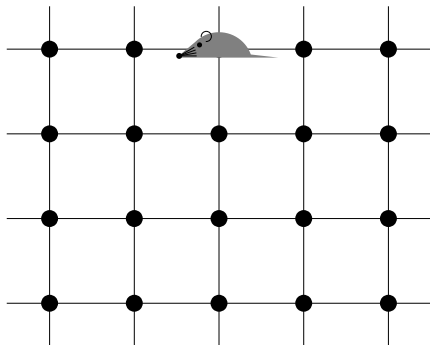
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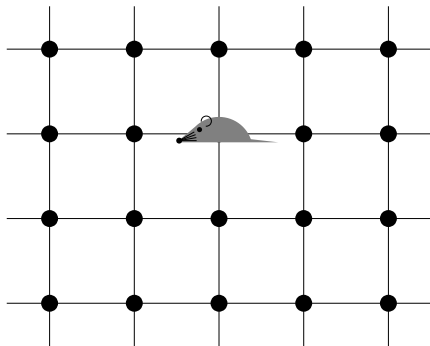
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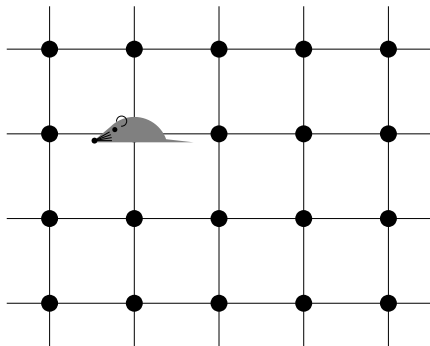
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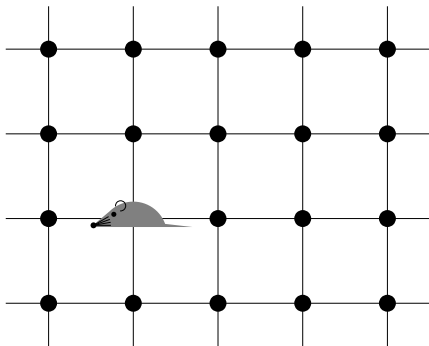
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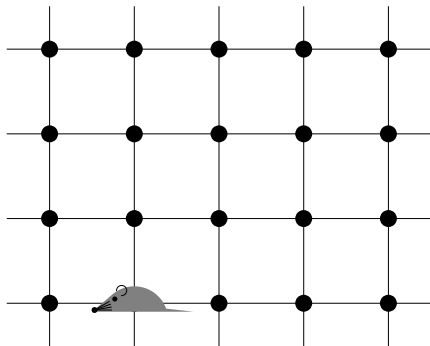
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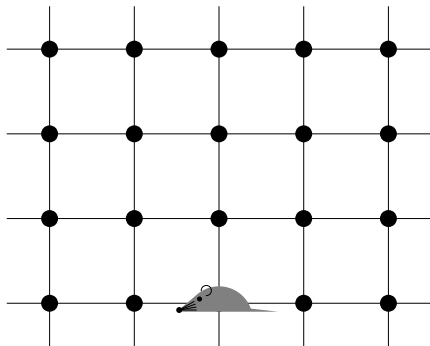
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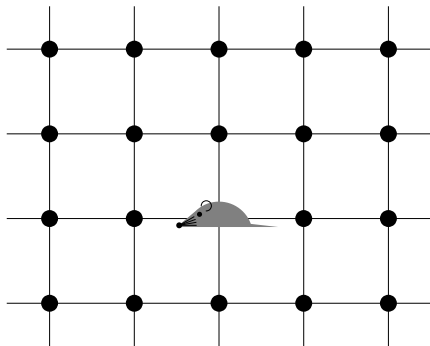
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## Lattice Green's Functions

The *lattice Green's function* is the probability generating function

$$P(\mathbf{x}; z) = \sum_{n=0}^{\infty} p_n(\mathbf{x}) z^n$$

where  $p_n(\mathbf{x})$  is the probability of being at point  $\mathbf{x}$  after  $n$  steps.

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→ Note that  $c^n p_n(\mathbf{x})$  is an integer and gives the total number of such (unrestricted) walks, where  $c$  is the coordination number of the lattice.

## Lattice Green's Functions

Of particular interest is

$$P(\mathbf{0}; z) = \sum_{n=0}^{\infty} p_n(\mathbf{0}) z^n = \frac{1}{\pi^d} \int_0^\pi \cdots \int_0^\pi \frac{dk_1 \dots dk_d}{1 - z\lambda(\mathbf{k})}.$$

that encodes the return probabilities.

Here  $\lambda(\mathbf{k})$  is called the *structure function* of the lattice; it is given by the discrete Fourier transform of the single-step probabilities:

$$\lambda(\mathbf{k}) = \sum_{\mathbf{x} \in \mathbb{R}^d} p_1(\mathbf{x}) e^{i\mathbf{x} \cdot \mathbf{k}}$$

(a finite sum, actually).

## Example

Square lattice  $\mathbb{Z}^2$  with step set  $\{(-1, 0), (1, 0), (0, -1), (0, 1)\}$

The structure function is

$$\lambda(k_1, k_2) = \frac{1}{4} \left( e^{-ik_1} + e^{ik_1} + e^{-ik_2} + e^{ik_2} \right) = \frac{1}{2} (\cos k_1 + \cos k_2).$$

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$$P(0, 0; z) = \frac{1}{\pi^2} \int_0^\pi \int_0^\pi \frac{dk_1 dk_2}{1 - \frac{z}{2} (\cos k_1 + \cos k_2)} = \frac{2}{\pi} \mathbf{K}(z^2)$$

where  $\mathbf{K}(z)$  is the complete elliptic integral of the first kind:

$$\mathbf{K}(z) = \int_0^1 \frac{dt}{\sqrt{(1-t^2)(1-z^2t^2)}}.$$

## Return Probability

**Question:** What is the probability that a walker ever returns to the origin?

The *return probability*  $R$  (Pólya number) is given by

$$R = 1 - \frac{1}{\sum_{n=0}^{\infty} p_n(\mathbf{0})} = 1 - \frac{1}{P(\mathbf{0}; 1)}.$$

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In our 2D example:

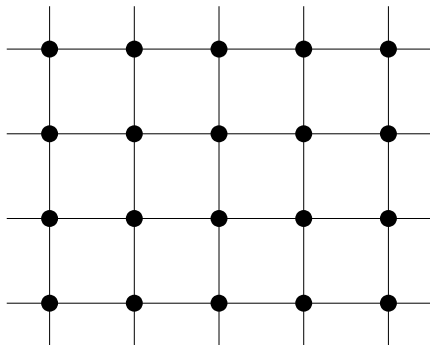
$$R = 1 - \frac{1}{\frac{2}{\pi} \mathbf{K}(1)} = 1$$

since  $\mathbf{K}(z)$  diverges for  $z = 1$ .

→ It is well known that in 2D the return is certain!

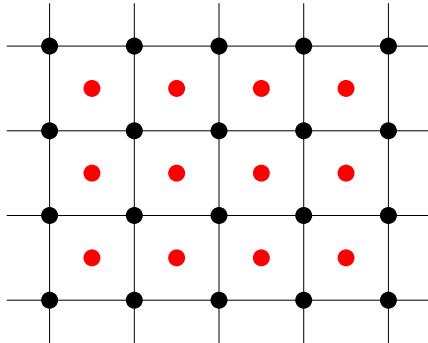
## The fcc Lattice in 2D

square lattice (= integer lattice  $\mathbb{Z}^2$ )



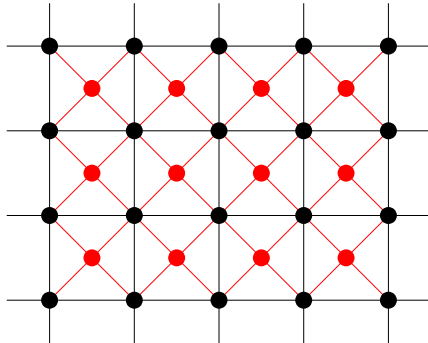
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face-centered square lattice



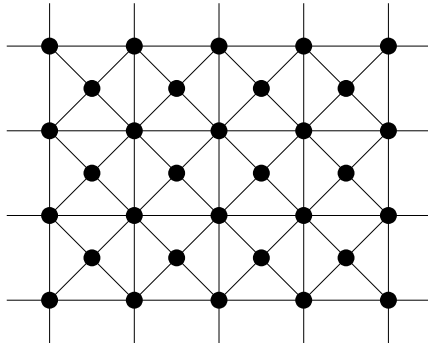
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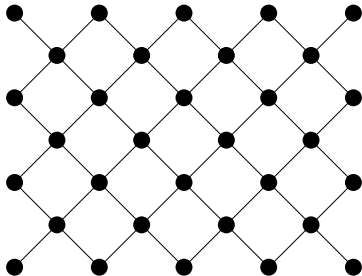
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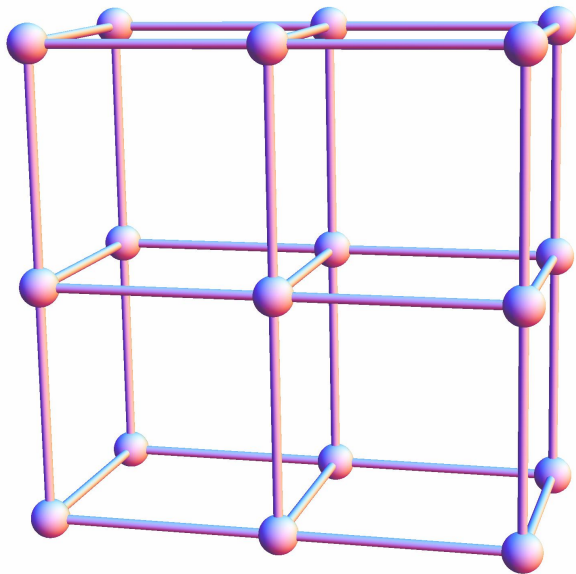


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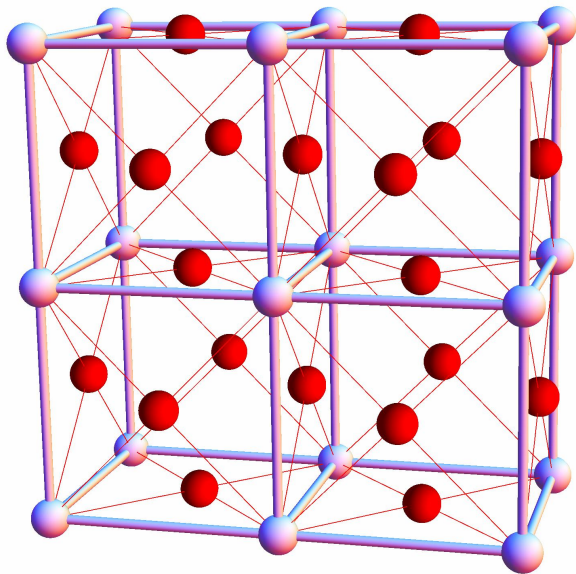
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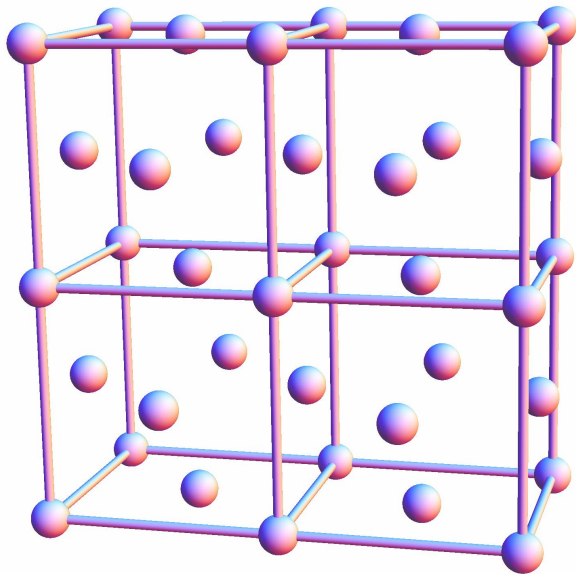
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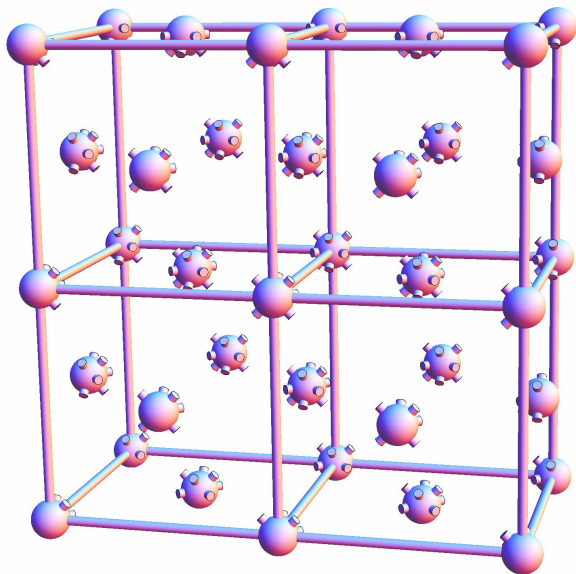
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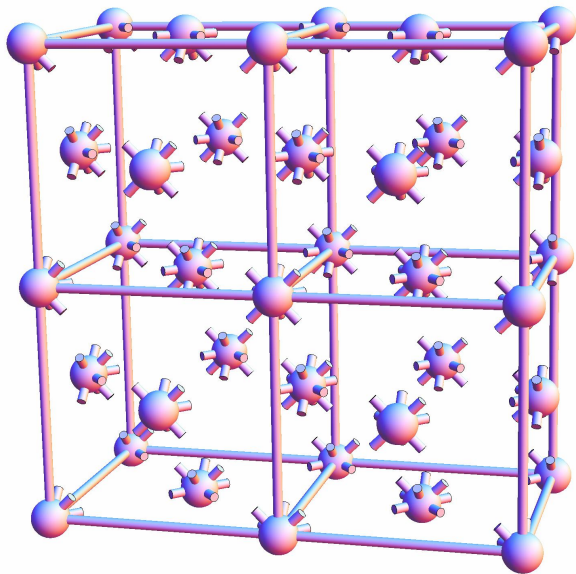
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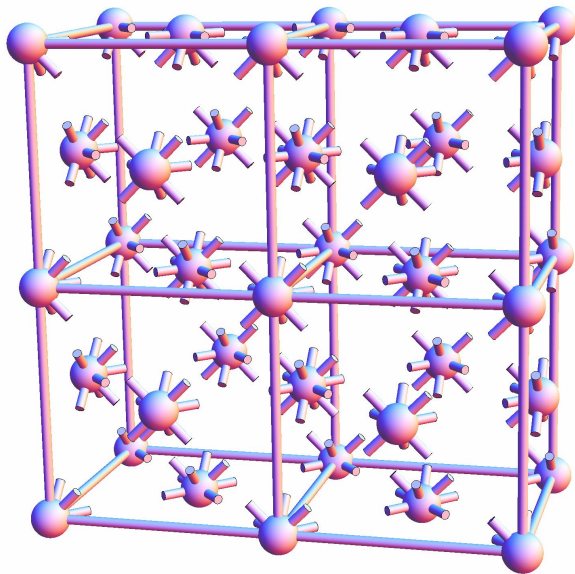
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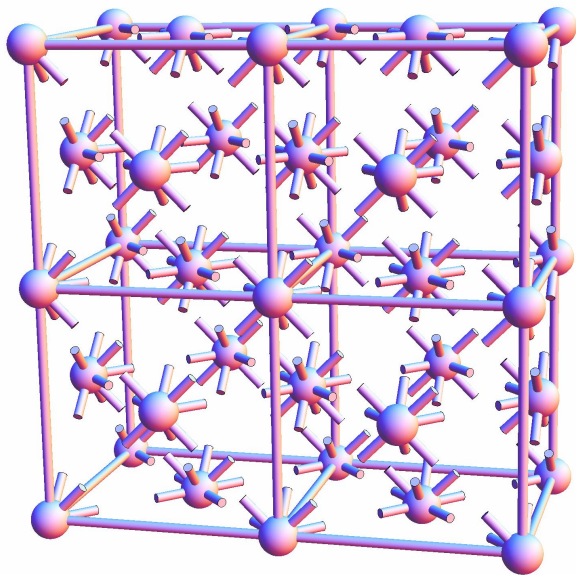
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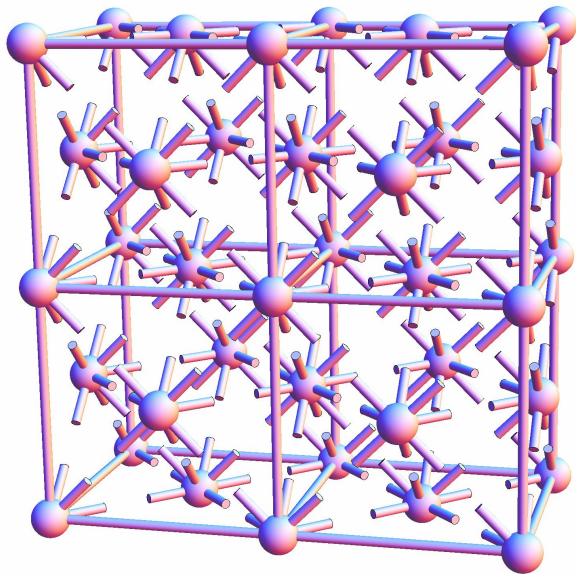
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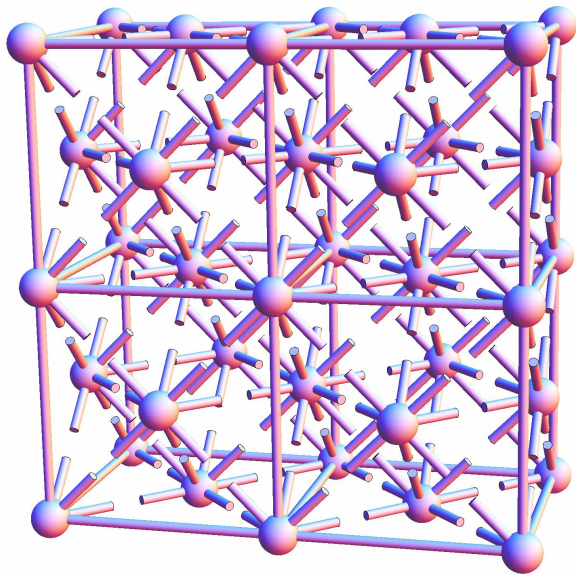
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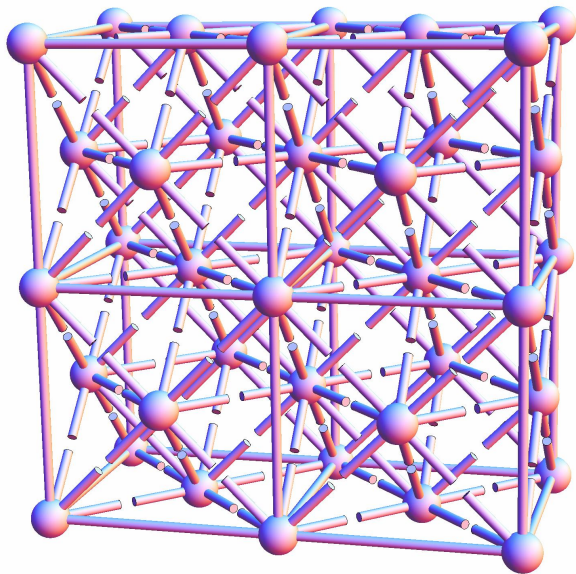
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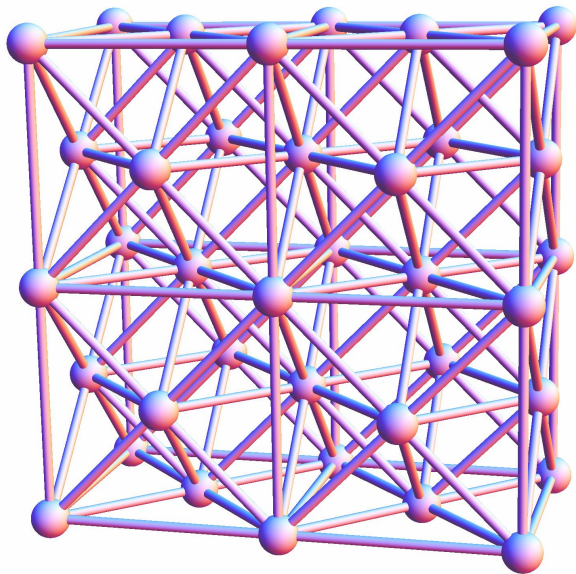
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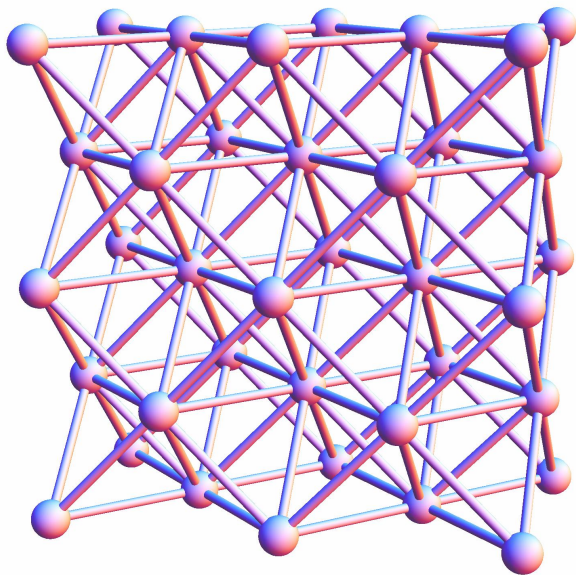
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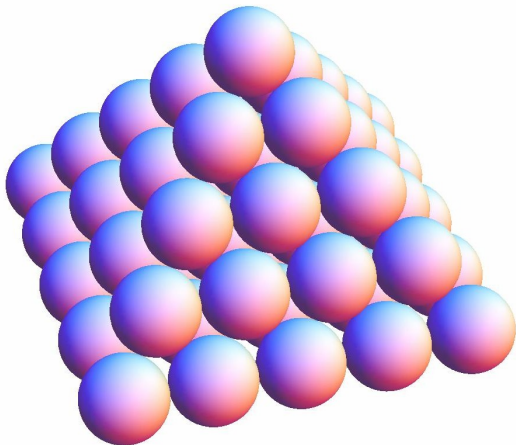
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Densest possible packing: Kepler conjecture (Hales 2005)

→ This arrangement is often encountered in nature, e.g., in aluminium, copper, silver, and gold.



## The fcc Lattice in 3D

It is not difficult to see that the 3D fcc lattice consists of four copies of  $\mathbb{Z}^3$ , namely

$$\mathbb{Z}^3 \cup \left( \mathbb{Z}^3 + \left( \frac{1}{2}, \frac{1}{2}, 0 \right) \right) \cup \left( \mathbb{Z}^3 + \left( \frac{1}{2}, 0, \frac{1}{2} \right) \right) \cup \left( \mathbb{Z}^3 + \left( 0, \frac{1}{2}, \frac{1}{2} \right) \right).$$

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**From now on:** Stretch the lattice by a factor 2 to avoid fractions.

Then the admissible steps (nearest neighbor rule) are:

$$\begin{aligned} &\{(-1, -1, 0), (-1, 1, 0), (1, -1, 0), (1, 1, 0), \\ &\quad (-1, 0, -1), (-1, 0, 1), (1, 0, -1), (1, 0, 1), \\ &\quad (0, -1, -1), (0, -1, 1), (0, 1, -1), (0, 1, 1)\} \end{aligned}$$

## The fcc Lattice in Arbitrary Dimensions

The  $d$ -dimensional fcc lattice is composed of  $1 + \binom{d}{2}$  translated copies of  $\mathbb{Z}^d$ .

The set of permitted steps in the  $d$ -dimensional fcc lattice is

$$\left\{ (s_1, \dots, s_d) \in \{0, -1, 1\}^d : |s_1| + \dots + |s_d| = 2 \right\},$$

i.e., there are  $4\binom{d}{2}$  steps (called the *coordination number*).

## Back to the fcc Lattice

The trivial (but illuminating) 2D case:

- step set:  $\{(-1, -1), (-1, 1), (1, -1), (1, 1)\}$
- structure function:

$$\begin{aligned}\lambda(k_1, k_2) &= \frac{1}{4} \left( e^{-i(k_1+k_2)} + e^{-i(k_1-k_2)} + e^{i(k_1-k_2)} + e^{i(k_1+k_2)} \right) \\ &= \frac{1}{2} \left( \cos(k_1 + k_2) + \cos(k_1 - k_2) \right) = \cos k_1 \cos k_2\end{aligned}$$

- lattice Green's function:

$$P(0, 0, z) = \frac{1}{\pi^2} \int_0^\pi \int_0^\pi \frac{dk_1 dk_2}{1 - z \cos k_1 \cos k_2} = \frac{2}{\pi} \mathbf{K}(z^2).$$

→ LGF is the same as for the square lattice (as expected), but not at all obvious from the integral representation!

## fcc Lattices for $d > 2$

The structure function is  $\lambda(\mathbf{k}) = \binom{d}{2}^{-1} \sum_{m=1}^d \sum_{n=m+1}^d \cos k_m \cos k_n$ .

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For  $d = 3$ , the return probability is one of *Watson's integrals*:

$$R = 1 - \left( \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{dk_1 dk_2 dk_3}{1 - \frac{1}{3}(c_1 c_2 + c_1 c_3 + c_2 c_3)} \right)^{-1} = 1 - \frac{16 \sqrt[3]{4} \pi^4}{9(\Gamma(\frac{1}{3}))^6}$$

where  $c_i = \cos(k_i)$ .

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A closed form for the LGF has been found by Joyce (1998), in terms of  $\mathbf{K}(z)$  and some fairly complicated algebraic functions.

→ For  $d > 3$  no such closed forms are known!

## Differential Equation Approach

**From now on:** Try to compute a differential equation for the LGF, instead of a closed form!

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A conjecture (“guess”) for such an equation can be made when the first terms of the Taylor expansion are known.

These can be obtained by different methods, e.g.

1. rewrite and expand the  $d$ -fold integral into a multisum (Guttmann and Broadhurst)
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→ However, any result obtained in this way is just a *conjecture*!

## Method 1 (Guttman and Broadhurst)

Example for  $d = 3$  ( $c_i$  denotes  $\cos k_i$ )

Expand the integrand in a geometric series:

$$\frac{1}{1 - \frac{z}{3}(c_1c_2 + c_1c_3 + c_2c_3)} = \sum_n \left(\frac{z}{3}\right)^n (c_1c_2 + c_1c_3 + c_2c_3)^n$$

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Use the multinomial theorem:

$$(c_1c_2 + c_1c_3 + c_2c_3)^n = \sum_{n_1+n_2+n_3=n} \binom{n}{n_1, n_2, n_3} (c_1c_2)^{n_1} (c_1c_3)^{n_2} (c_2c_3)^{n_3}$$

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Use Wallis's integration formula:

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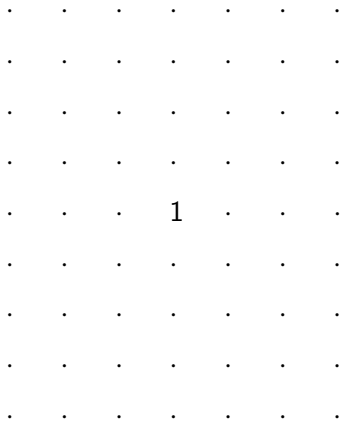
The  $n$ -th Taylor coefficient can be computed by a  $\left(\binom{d}{2} - 1\right)$ -fold sum.

## Method 2: Naive Walk Enumeration

Proceed as follows:

- Compute all values in the  $(d + 1)$ -dimensional array (a cube of side length  $2n$ , basically).
- The Taylor coefficients sit on the  $n$ -coordinate axis.

## Method 2: Naive Walk Enumeration



$$(n = 0)$$

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$$(n = 1)$$

## Method 2: Naive Walk Enumeration

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.	.	.	1	.	.	.
.	.	2	.	2	.	.
.	1	.	4	.	1	.
.	.	2	.	2	.	.
.	.	.	1	.	.	.
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$$(n = 2)$$

## Method 2: Naive Walk Enumeration

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.	.	.	1	.	.	.
.	.	3	.	3	.	.
.	3	.	9	.	3	.
1	.	9	.	9	.	1
.	3	.	9	.	3	.
.	.	3	.	3	.	.
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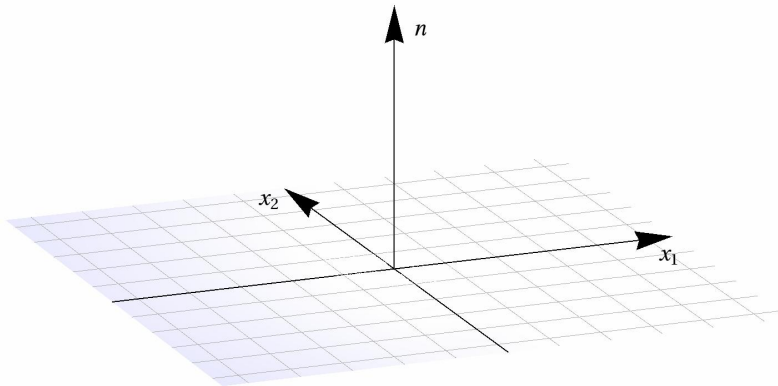
$$(n = 3)$$

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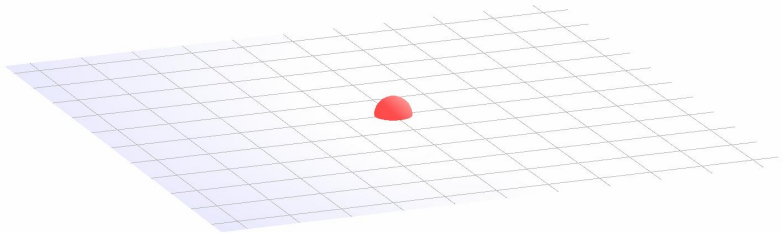
.	.	.	1	.	.	.
.	.	4	.	4	.	.
.	6	.	16	.	6	.
4	.	24	.	24	.	4
.	16	.	36	.	16	.
4	.	24	.	24	.	4
.	6	.	16	.	6	.
.	.	4	.	4	.	.
.	.	.	1	.	.	.

$$(n = 4)$$

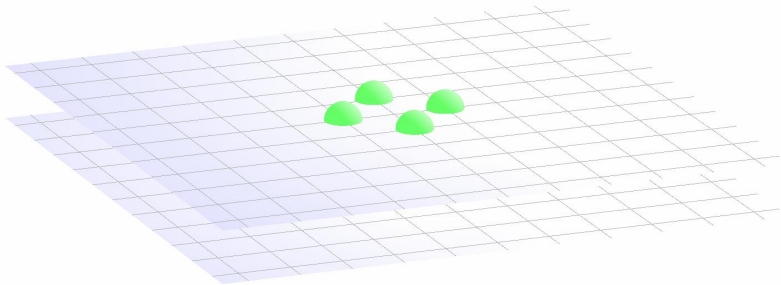
## Method 2: Naive Walk Enumeration



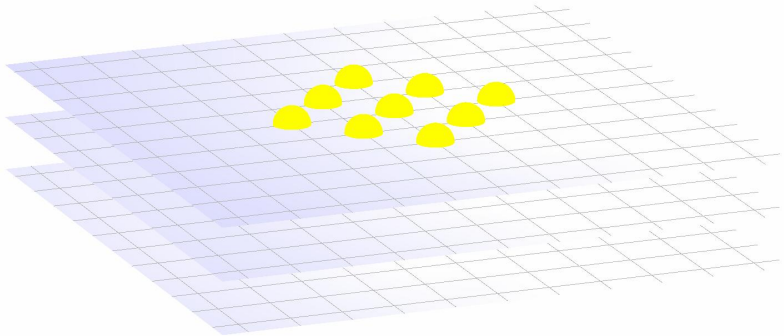
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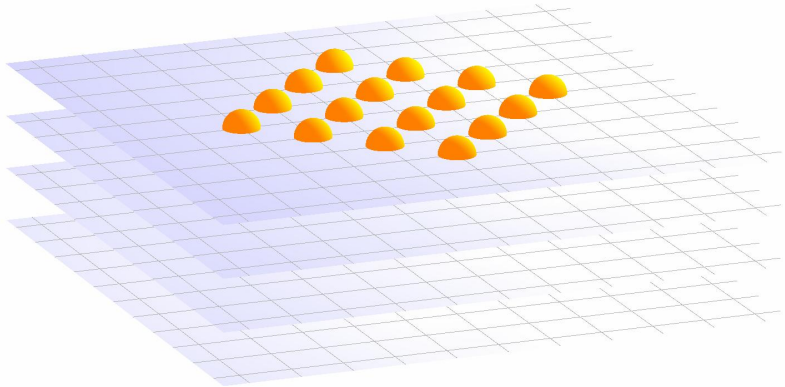
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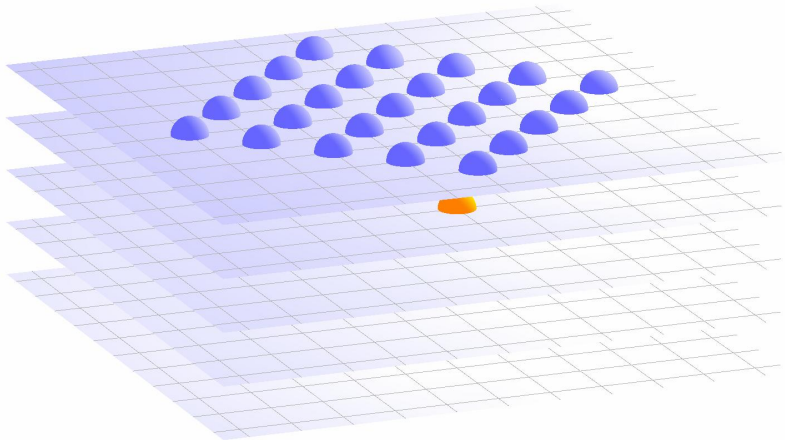
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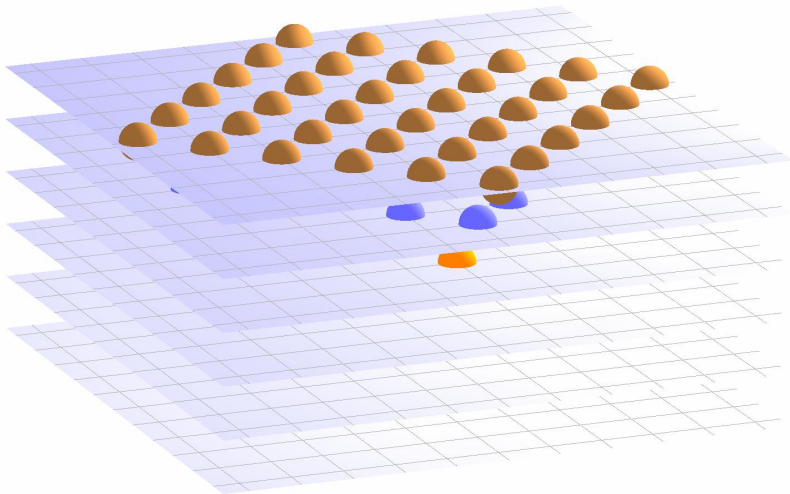
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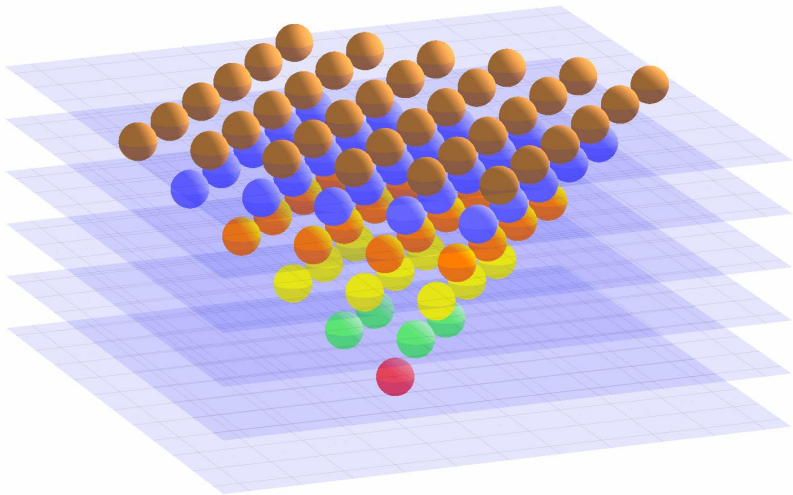
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- Compute all values in the  $(d + 1)$ -dimensional array (a cube of side length  $2n$ , basically).
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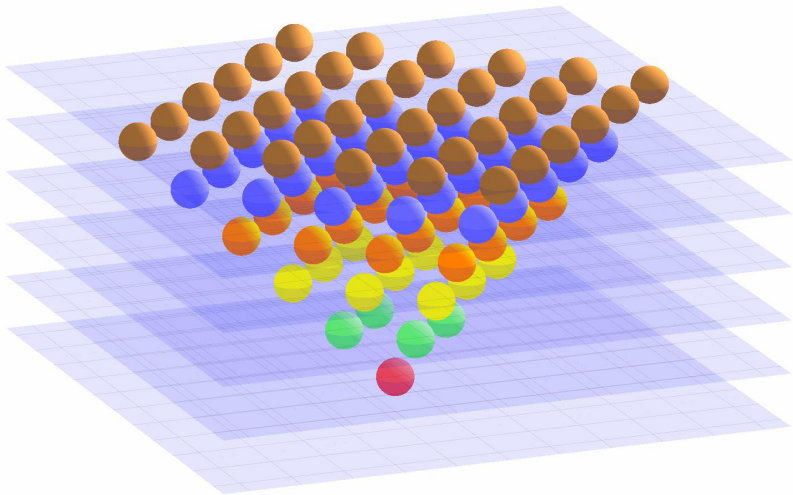
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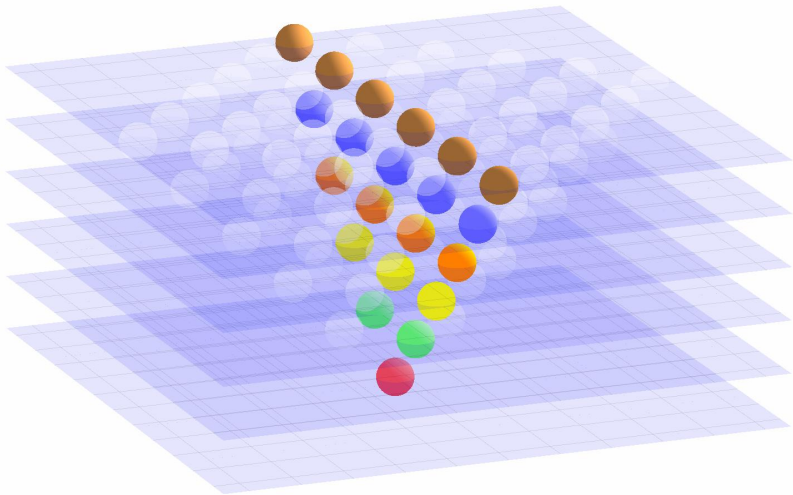
Some optimizations can reduce the effort:

- discard “empty” regions
- exploit symmetry
- cut at “points of no return”
- positions with odd coordinate sum cannot be reached

## Method 3: Multistep Guessing



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Example for  $d = 5$ .

- Crank out a moderate number of values for the 6-dimensional sequence  $a_n(x_1, \dots, x_5)$ , namely in the box  $[0, 15]^6$ .
- Pick the values  $a_n(x_1, x_2, x_3, 0, 0)$  which constitute a 4-dimensional sequence  $b_n(x_1, x_2, x_3)$ .
- Guess a recurrence for  $b_n(x_1, x_2, x_3)$ :

$$\begin{aligned} & (n+1)b_n(x_1, x_2+3, x_3+1) - (n+1)b_n(x_1, x_2+1, x_3+3) + \\ & (n+1)b_n(x_1+1, x_2, x_3+3) - (n+1)b_n(x_1+1, x_2+3, x_3) + \\ & (n+1)b_n(x_1+1, x_2+3, x_3+4) - (n+1)b_n(x_1+1, x_2+4, x_3+3) - \\ & (n+1)b_n(x_1+3, x_2, x_3+1) + (n+1)b_n(x_1+3, x_2+1, x_3) - \\ & (n+1)b_n(x_1+3, x_2+1, x_3+4) + (n+1)b_n(x_1+3, x_2+4, x_3+1) + \\ & (n+1)b_n(x_1+4, x_2+1, x_3+3) - (n+1)b_n(x_1+4, x_2+3, x_3+1) + \\ & (x_2+2)b_{n+1}(x_1+1, x_2+2, x_3+3) - (x_3+2)b_{n+1}(x_1+1, x_2+3, x_3+2) - \\ & (x_1+2)b_{n+1}(x_1+2, x_2+1, x_3+3) + (x_1+2)b_{n+1}(x_1+2, x_2+3, x_3+1) + \\ & (x_3+2)b_{n+1}(x_1+3, x_2+1, x_3+2) - (x_2+2)b_{n+1}(x_1+3, x_2+2, x_3+1) = 0 \end{aligned}$$

- Use this recurrence to produce more values for  $b_n(x_1, x_2, x_3)$  (problem: singularities!).
- Guess a recurrence for  $b_n(x_1, x_2, 0) =: c_n(x_1, x_2)$  and so on.

## A Different Approach to the LGF

Let's consider a lattice in  $\mathbb{Z}^d$  with some finite step set  $S \subset \mathbb{Z}^d$ .

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$$\sum_{n=0}^{\infty} \sum_{\mathbf{x} \in \mathbb{Z}^d} p_{n+1}(\mathbf{x}) \mathbf{y}^{\mathbf{x}} z^n = \frac{1}{|S|} \sum_{n=0}^{\infty} \sum_{\mathbf{x} \in \mathbb{Z}^d} \sum_{\mathbf{s} \in S} p_n(\mathbf{x} - \mathbf{s}) \mathbf{y}^{\mathbf{x}} z^n$$

$$\frac{1}{z} \sum_{n=1}^{\infty} \sum_{\mathbf{x} \in \mathbb{Z}^d} p_n(\mathbf{x}) \mathbf{y}^{\mathbf{x}} z^n = \frac{1}{|S|} \sum_{\mathbf{s} \in S} \sum_{n=0}^{\infty} \sum_{\mathbf{x} \in \mathbb{Z}^d} p_n(\mathbf{x}) \mathbf{y}^{\mathbf{x} + \mathbf{s}} z^n$$

$$\frac{1}{z} (F(\mathbf{y}; z) - 1) = \frac{1}{|S|} \sum_{\mathbf{s} \in S} \mathbf{y}^{\mathbf{s}} F(\mathbf{y}; z)$$

Thus we obtain  $F(\mathbf{y}; z) = \frac{1}{1 - \frac{z}{|S|} \sum_{\mathbf{s} \in S} \mathbf{y}^{\mathbf{s}}}$ .

## A Different Approach to the LGF

$$\text{Recall: } F(\mathbf{y}; z) = \sum_{n=0}^{\infty} \sum_{\mathbf{x} \in \mathbb{Z}^d} p_n(\mathbf{x}) \mathbf{y}^{\mathbf{x}} z^n = \frac{1}{1 - \frac{z}{|S|} \sum_{\mathbf{s} \in S} \mathbf{y}^{\mathbf{s}}}$$

$$\text{Connection to LGF: } P(\mathbf{0}; z) = \sum_{n=0}^{\infty} p_n(\mathbf{0}) z^n = \langle y_1^0 \dots y_d^0 \rangle F(\mathbf{y}; z)$$

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Therefore: if the differential operator

$A(z, D_z) + D_{y_1} B_1 + \dots + D_{y_d} B_d$  annihilates  $F(\mathbf{y}; z)/(y_1 \dots y_d)$ ,

where  $B_i = B_i(y_1, \dots, y_d, z, D_{y_1}, \dots, D_{y_d}, D_z)$  then  $A(z, D_z)$

annihilates  $P(\mathbf{0}; z)$ :

$$\underbrace{\langle y_1^{-1} \dots y_d^{-1} \rangle A(z, D_z) \left( \frac{F(\mathbf{y}, z)}{y_1 \dots y_d} \right)}_{=A(z, D_z)P(\mathbf{0}; z)} + \sum_{j=1}^d \underbrace{\langle y_1^{-1} \dots y_d^{-1} \rangle D_{y_j} B_j \left( \frac{F(\mathbf{y}, z)}{y_1 \dots y_d} \right)}_{=0} = 0$$

## Connection with the Integral Representation

$$\begin{aligned} P(\mathbf{0}; z) &= \langle y_1^0 \cdots y_d^0 \rangle \frac{1}{1 - \frac{z}{|S|} \sum_{\mathbf{s} \in S} \mathbf{y}^{\mathbf{s}}} \\ &= \frac{1}{\pi^d} \int_0^\pi \cdots \int_0^\pi \frac{dk_1 \cdots dk_d}{1 - z \sum_{\mathbf{s} \in S} p_1(\mathbf{s}) e^{i\mathbf{s} \cdot \mathbf{k}}} \end{aligned}$$

In the holonomic systems approach, the operator

$$A(z, D_z) + D_{y_1} B_1 + \cdots + D_{y_d} B_d$$

is called a *creative telescoping operator*.

## Excursion: The Holonomic Systems Approach

Consider the class of  $\partial$ -finite/holonomic functions (functions and sequences that satisfy “sufficiently many” linear differential equations and recurrences).

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→ All these operations can be executed algorithmically.

### **Example:**

Given a function  $f(x, y)$ , satisfying two ODEs (in  $x$  and  $y$ ). We can derive a differential equation for the definite integral  $\int_0^1 f(x, y) dx$  by means of a creative telescoping operator.

## Concrete Example: Creative Telescoping

The lattice Green's function of the 2D fcc lattice is given by

$$P(z) = \frac{1}{\pi^2} \int_0^\pi \int_0^\pi \frac{dk_1 dk_2}{1 - z \cos(k_1) \cos(k_2)}.$$

Unfortunately, the integrand is not  $\partial$ -finite/holonomic (no ODE w.r.t.  $k_1$  for example).

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Unfortunately, the integrand is not  $\partial$ -finite/holonomic (no ODE w.r.t.  $k_1$  for example).

But this is easily repaired by the substitutions  $\cos(k_i) \mapsto x_i$ :

$$P(z) = \frac{1}{\pi^2} \int_0^1 \int_0^1 \frac{dx_1 dx_2}{(1 - zx_1x_2)\sqrt{1-x_1^2}\sqrt{1-x_2^2}}.$$

Indeed, the integrand is annihilated by the operators:

$$\begin{aligned} & (x_1x_2z - 1)D_z + x_1x_2, \\ & (x_2^2 - 1)(x_1x_2z - 1)D_{x_2} + (2x_1x_2^2z - x_1z - x_2), \\ & (x_1^2 - 1)(x_1x_2z - 1)D_{x_1} + (2x_1^2x_2z - x_1 - x_2z). \end{aligned}$$

## Concrete Example: Creative Telescoping

$$P(z) = \int_0^1 \int_0^1 \frac{1}{(1 - zx_1x_2)\sqrt{1 - x_1^2}\sqrt{1 - x_2^2}} dx_1 dx_2.$$

The creative telescoping operator

$$\underbrace{(z^3 - z)D_z^2 + (3z^2 - 1)D_z + z + D_{x_1}}_{A(z, D_z)} \underbrace{\frac{x_2(1 - x_1^2)}{x_1x_2z - 1}}_{B_1} + D_{x_2} \underbrace{\frac{x_2z(1 - x_2^2)}{x_1x_2z - 1}}_{B_2}$$

which annihilates the integrand, certifies that  $P(z)$  satisfies the differential equation

$$(z^3 - z)P''(z) + (3z^2 - 1)P'(z) + zP(z) = 0.$$

## Creative Telescoping in General

In general, a creative telescoping operator has the form

$$A(\mathbf{v}, \partial_{\mathbf{v}}) + \Delta_1 B_1(\mathbf{v}, \mathbf{w}, \partial_{\mathbf{v}}, \partial_{\mathbf{w}}) + \cdots + \Delta_m B_m(\mathbf{v}, \mathbf{w}, \partial_{\mathbf{v}}, \partial_{\mathbf{w}})$$

where  $\Delta_i = S_{w_i} - 1$  or  $\Delta_i = D_{w_i}$  (depending on the problem).

- corresponds to an  $m$ -fold summation/integration problem
- $\mathbf{w} = w_1, \dots, w_m$  are the summation/integration variables
- $\mathbf{v} = v_1, v_2, \dots$  are the surviving parameters
- $A(\mathbf{v}, \partial_{\mathbf{v}})$  is called the *principal part* or the *telescoper*
- the  $B_i(\mathbf{v}, \mathbf{w}, \partial_{\mathbf{v}}, \partial_{\mathbf{w}})$  are called the *delta parts*
- they can be viewed as certificates for the correctness of the principal part

## Our Ansatz with Specific Denominators

For finding CT operators, we proposed an ansatz of the form

$$\sum_{\alpha} c_{\alpha}(\mathbf{v}) \partial_{\mathbf{v}}^{\alpha} + \sum_{i=1}^m \Delta_i \sum_{j=1}^{|\mathfrak{U}|} \frac{\sum_{\alpha} c_{i,j,\alpha}(\mathbf{v}) \mathbf{w}^{\alpha}}{d_{i,j}(\mathbf{v}, \mathbf{w})} U_j$$

with unknowns  $c_{\alpha}$  and  $c_{i,j,\alpha}$ , and with specific denominators  $d_{i,j}$ .

- input: a (non-commutative) Gröbner basis of the annihilating operators of the integrand
- denote by  $\mathfrak{U} = \{U_1, U_2, \dots\}$  the (finitely many) monomials under its stairs
- reduce the ansatz with this Gröbner basis and equation coefficients to zero
- coefficient comparison w.r.t.  $\mathbf{w}$  leads to a linear system of equations
- the denominators  $d_{i,j}$  can be predicted from the leading coefficients of the Gröbner basis
- implemented in `HolonomicFunctions` (Mathematica)

## Result for the 4D fcc Lattice

With this machinery, we find (and prove!) that the LGF  $P(z)$  of the 4D fcc lattice satisfies the differential equation

$$\begin{aligned} & (z-1)(z+2)(z+3)(z+6)(z+8)(3z+4)^2 z^3 P^{(4)}(z) + \\ & 2(3z+4)(21z^6 + 356z^5 + 2079z^4 + 4920z^3 + 3676z^2 - \\ & \quad 2304z - 3456)z^2 P^{(3)}(z) + \\ & 6(81z^7 + 1286z^6 + 7432z^5 + 19898z^4 + 25286z^3 + 11080z^2 - \\ & \quad 5248z - 5376)z P''(z) + \\ & 12(45z^7 + 604z^6 + 2939z^5 + 6734z^4 + 7633z^3 + 3716z^2 + \\ & \quad 224z - 384)P'(z) + \\ & 12(9z^5 + 98z^4 + 382z^3 + 702z^2 + 632z + 256)zP(z) = 0. \end{aligned}$$

## Result for the 5D fcc Lattice

$$\begin{aligned} & 16(z-5)(z-1)(z+5)^2(z+10)(z+15)(3z+5)(15678z^6 + 144776z^5 + 449735z^4 + 933650z^3 - \\ & 1053375z^2 + 3465000z - 675000)z^4 P^{(6)}(z) + 8(z+5)(3057210z^{12} + 97471734z^{11} + \\ & 1048560285z^{10} + 3939663705z^9 - 4878146975z^8 - 87265479875z^7 - 304623830625z^6 - \\ & 266627903125z^5 + 254876515625z^4 - 1289447109375z^3 - 503550000000z^2 + 1774828125000z - \\ & 354375000000)z^3 P^{(5)}(z) + 10(27279720z^{13} + 923795772z^{12} + 11725276842z^{11} + \\ & 68439921540z^{10} + 148313757125z^9 - 382134335775z^8 - 3351125770500z^7 - 7801785421250z^6 - \\ & 3779011321875z^5 - 7716298734375z^4 - 39702348750000z^3 + 3393646875000z^2 + \\ & 23905125000000z - 5568750000000)z^2 P^{(4)}(z) + 5(255864960z^{13} + 7892060544z^{12} + \\ & 92744995638z^{11} + 524857986060z^{10} + 1350059072325z^9 - 465440555100z^8 - 13545524756500z^7 - \\ & 26918293320000z^6 - 3649915059375z^5 - 77498059625000z^4 - 190176960000000z^3 + \\ & 40530375000000z^2 + 45343125000000z - 13162500000000)z P^{(3)}(z) + 5(496679040z^{13} + \\ & 13819981248z^{12} + 149186684934z^{11} + 810956145330z^{10} + 2287368823475z^9 + 1646226060075z^8 - \\ & 8282515456375z^7 - 6199228765625z^6 + 13367806743750z^5 - 110925736437500z^4 - \\ & 133825053750000z^3 + 44457862500000z^2 + 5055750000000z - 3240000000000)P''(z) + \\ & 10(167064768z^{12} + 4143853440z^{11} + 40678130502z^{10} + 209673119160z^9 + 607021304825z^8 + \\ & 689643286650z^7 - 135661728250z^6 + 3711617481250z^5 + 2664478321875z^4 - 21210430812500z^3 - \\ & 7268326875000z^2 + 4816462500000z - 189000000000)P'(z) + 30(7525440z^{11} + 163913184z^{10} + \\ & 1443544710z^9 + 6925739310z^8 + 19123388575z^7 + 21336230625z^6 + 36477006875z^5 + \\ & 187923165625z^4 - 55567000000z^3 - 346865625000z^2 + 84037500000z + 27000000000)P(z) = 0 \end{aligned}$$

# Result for the 6D fcc Lattice

$$\begin{aligned} & (z - 3)(z - 1)(z + 4)(z + 5)(z + 9)(z + 15)^2(z + 24)(2z + 3)(2z + 15)(4z + \\ & 15)(7z + 60)(242161043152z^{25} + 51659233261888z^{24} + 3764987488054392z^{23} + \\ & 149102740118852712z^{22} + 3823803744461234343z^{21} + 69321047461074869130z^{20} + \\ & 931032563834500230663z^{19} + 9465736161794804567892z^{18} + 72864795413899911011922z^{17} + \\ & 412843760981101392072948z^{16} + 1557656993073750677220582z^{15} + 2189507486524206284827296z^{14} - \\ & 16970927000980381863663141z^{13} - 152346950611719661239440526z^{12} - \\ & 693159300555093708939611829z^{11} - 2157072153972513398276826924z^{10} - \\ & 4872861027995366524279994100z^9 - 7971869741181425686355371200z^8 - \\ & 8883487977021576719907033600z^7 - 5337917399156522389289280000z^6 + \\ & 753459769629110696243040000z^5 + 3920543674198265211436800000z^4 + \\ & 2878395143123986146432000000z^3 + 1348035643913347353600000000z^2 + \\ & 242306901961056460800000000z + 19280523023769600000000000)z^6 P^{(8)}(z) + 2(z + \\ & 15)(800100086574208z^{36} + 227389988057526336z^{35} + 25996840572204888512z^{34} + \\ & 1719342411627828757728z^{33} + 76318086060490791960792z^{32} + 2462288021152606885358700z^{31} + \\ & 60618715038937670473018584z^{30} + 1175154434178119041671700740z^{29} + \\ & 18309889884984684630822323370z^{28} + 23211567168185433422158633858z^{27} + \\ & 2406227015296631910854902756563z^{26} + 20337622679657217515316342764256z^{25} + \\ & 138105907223379522203625428215332z^{24} + 724749378242590885585485419445843z^{23} + \\ & 2620577206027992337931632885352217z^{22} + 3221036141212186087856769990927054z^{21} - \\ & 35907063701591969077649893288537878z^{20} - 331259809437872111827650003935308209z^{19} - \\ & 1638945569143497023502201509481372411z^{18} - 5466573829106434312238352307226140764z^{17} - \\ & 11704453530273493922795299130700457200z^{16} - 7977590414255123112276744122571399783z^{15} + \\ & 51498237061832672183443454747804923575z^{14} + 253995260187409794081727430934766869450z^{13} + \\ & 661181529544504134786063620152764386400z^{12} + 1138666598560461678104890857545212608000z^{11} + \\ & 1251150937075501602577084871183562120000z^{10} + 564704048394845939194551470638922400000z^9 - \\ & 682640121106346995555734719308248000000z^8 - 1460286146960184444033629739148560000000z^7 - \\ & 1074498717874767393664900393675200000000z^6 - 145021874608394651059638847488000000000z^5 + \\ & 344718972957157801371250560000000000000z^4 + 314413056395938625838510182400000000000z^3 + \\ & 140360356659888583720114176000000000000z^2 + 2508400981206319045017600000000000000z + \\ & 197339238031965659136000000000000000)z^5 P^{(7)}(z) + \end{aligned}$$

# Result for the 6D fcc Lattice

$$\begin{aligned} & (35882454730090752z^{37} + 10612604051614486656z^{36} + 1276532600942212775168z^{35} + \\ & 893939801294330320696320z^{34} + 4221606838983473228197008z^{33} + 145494567985766484898923048z^{32} + \\ & 38408280044909200650969480z^{31} + 80160062388267727172211985080z^{30} + \\ & 1350855094398006902682870922050z^{29} + 18631082892630536824222949409585z^{28} + \\ & 211815796834464054711973645322142z^{27} + 1986708322085667572665525016037411z^{26} + \\ & 15263082383031406770429022758762048z^{25} + 94068732852089205756130773605094705z^{24} + \\ & 441055376229095921513357130918811338z^{23} + 1319636945498761264973744224282378779z^{22} - \\ & 137626809673226795399591264079041112z^{21} - 31072001737970299221405533198706303141z^{20} - \\ & 226886176666918560987240200768631693150z^{19} - 1033954017266382248984767586852072344191z^{18} - \\ & 3356732946224373601649087937349109785896z^{17} - 7573126212785007618891225542456994124245z^{16} - \\ & 9076459539413303184641722134776573895810z^{15} + 10278671248090335377408918358815408788425z^{14} + \\ & 85149274357043292385925033653294291853550z^{13} + 240689360358498296007939096187740586134000z^{12} + \\ & 429409878921957648790555775268242743350000z^{11} + 495779225046771906420255540348281344800000z^{10} + \\ & 287121363379312616871562346484465378000000z^9 - 119682652007548350954457856750250720000000z^8 - \\ & 395683465592680867401293480616198000000000z^7 - 327383462755042385949747691240824000000000z^6 - \\ & 86642575450501391066787202019520000000000z^5 + 5970468397217067954893197722240000000000z^4 + \\ & 7251161027741239099083936307200000000000z^3 + 3388289675587207195688626176000000000000z^2 + \\ & 6311156771304917325766656000000000000000z + 51232302181375699968000000000000000)z^4 P^{(6)}(z) + \\ & 3(130240020872181248z^{37} + 38072220474786769152z^{36} + 4480274117205321023232z^{35} + \\ & 305988393455491537290240z^{34} + 14079224644087925329523520z^{33} + 472739613103493977658692800z^{32} + \\ & 12162402278802667065896636880z^{31} + 247501384020921867412586484240z^{30} + \\ & 406856488897300388082085355030z^{29} + 54750340798147926328921245513135z^{28} + \\ & 607255705204278811351245801585018z^{27} + 5552646100941335755747908121811397z^{26} + \\ & 41511153616540066669903815109576752z^{25} + 247864598814302846690177415162792735z^{24} + \\ & 1112001535696035843878120629687073790z^{23} + 3006740720618245361400876608130182349z^{22} - \\ & 3066274907647801401815807099801425704z^{21} - 93149956267467504725225680596497523339z^{20} - \\ & 635954475887313295192241042199635547930z^{19} - 2858027882158570016919188514224326558185z^{18} - \\ & 9468529098949077023394535618861256937240z^{17} - 23191419391770985171480237991217872142915z^{16} - \\ & 38330478964162570556645949941637505810110z^{15} - 23459339067193287788165144055727575111225z^{14} + \\ & 87213988833696382614552027738719280959850z^{13} + 349803608265045461612489069936675179800000z^{12} + \\ & 696554593654757665866719966270600171130000z^{11} + \end{aligned}$$

# Result for the 6D fcc Lattice

$$\begin{aligned} & 865953342265454601104437816976581680000000z^{10} + 586378944861718695144037906690882422000000z^9 - \\ & 44891871663741237702913642763603760000000z^8 - 526332032930456915428235817813056400000000z^7 - \\ & 51893722710757334196484398533268000000000z^6 - 22630297253783314725378081159840000000000z^5 + \\ & 104974053097834899670129395840000000000z^4 + 6413578148658414175370727782400000000000z^3 + \\ & 3470894673681492735354298368000000000000z^2 + 69940922143484645330042880000000000000z + \\ & 5958126994426655477760000000000000000z^3 P^{(5)}(z) + 15(146187778529999360z^{37} + \\ & 42232680898487251200z^{36} + 4857665734098963690240z^{35} + 323165791319702484035520z^{34} + \\ & 14467601136584109707654400z^{33} + 472534466386674980533072704z^{32} + 11827310475440684698801079376z^{31} + \\ & 23420599418243894376994245108z^{30} + 3746772515516029997311378363446z^{29} + \\ & 49056517288448701934966949399201z^{28} + 528960737538220962199232165726700z^{27} + \\ & 4693678127508685757329704793118274z^{26} + 33925520928056707379949042245154948z^{25} + \\ & 194225784819376433418854177036400765z^{24} + 815865984997630892337526061797547730z^{23} + \\ & 1820210924970374403477059898368292414z^{22} - 5626714951506760337684784884293147302z^{21} - \\ & 87288636539051237531541938169181610997z^{20} - 548617946604162829617617348998523187024z^{19} - \\ & 2396582727922965009354571656000074347578z^{18} - 7949778754688875639594299226888542864672z^{17} - \\ & 20284887219829242010855806602752336703097z^{16} - 38476335393060119379820741759126402451166z^{15} - \\ & 47185211186009106848535876331178061122490z^{14} - 10222760436927155616364669208395729054260z^{13} + \\ & 107413528041921729529347960434391761302800z^{12} + 279266241080334469793315941614102969564000z^{11} + \\ & 379975092805467869163550626412993759200000z^{10} + 276342679146887322412220759883497997600000z^9 + \\ & 6337926159808918213308690816700464000000z^8 - 21496512980912069082728290273146864000000z^7 - \\ & 24245570187592855351784433249330240000000z^6 - 14026124741577288569154640743552000000000z^5 - \\ & 3677270682836095894427452388352000000000z^4 + 774772837962739349472654520320000000000z^3 + \\ & 752256851229882473453210419200000000000z^2 + 17760293941127209315703193600000000000z + \\ & 16181817518621184049152000000000000000z^2 P^{(4)}(z) + 90(69106949850545152z^{37} + \\ & 19728125958978028032z^{36} + 2215666629279250997248z^{35} + 143387361084360543557376z^{34} + \\ & 6235802763945868063424352z^{33} + 197763282456363307438541552z^{32} + 4805890762274729535435673296z^{31} + \\ & 9239099114814905907317974392z^{30} + 1434485821162175237888091472086z^{29} + \\ & 18213230428133179674440523308931z^{28} + 190122674553786922619563973540916z^{27} + \\ & 1627987793820686707319681442965532z^{26} + 11283714208962998257330503635013918z^{25} + \\ & 61070425289478623056319494081223364z^{24} + 232117491219054750436300759063832796z^{23} + \\ & 335162333006577190998078624832466745z^{22} - \end{aligned}$$

# Result for the 6D fcc Lattice

$$\begin{aligned} & 3212526847572548623801062566839102968z^{21} - 33929658665256259408812784354866385557z^{20} - \\ & 195183178990057349643272275435126736340z^{19} - 818596118205128605985330478856111679058z^{18} - \\ & 2671193766306193321259081077503739718922z^{17} - 6879647707640439013900747488611335523490z^{16} - \\ & 13791392258782895819955453998955102517548z^{15} - 20395042168164862736248341991799243143275z^{14} - \\ & 18559051142634901231618230067011245261730z^{13} + 340763873540255131808343067503063454800z^{12} + \\ & 32573268392371003654841290966684606314000z^{11} + 54660627321107405540934107870983869840000z^{10} + \\ & 419707294027084739233866209356623814800000z^9 + 757729323937951939044642929351040000000z^8 - \\ & 34653454861369485847062964251845520000000z^7 - 41909264304440185602876764536603200000000z^6 - \\ & 27649387021455520276766166546048000000000z^5 - 9932878926912153370258947363840000000000z^4 - \\ & 1112041174659253407521806233600000000000z^3 + 28491145384085971960200192000000000000z^2 + \\ & 114230678131481922666823680000000000000z + 114861556495528729804800000000000000zP^{(3)}(z) + \\ & 45(180741253455271936z^{37} + 50980706267636984832z^{36} + 5584340634105826525184z^{35} + \\ & 351010067005351488224256z^{34} + 14802080405483677823943104z^{33} + 454875015831485400909097248z^{32} + \\ & 10707051961496414217407305536z^{31} + 199288291693600445167066471488z^{30} + \\ & 2993264774540100816050708154540z^{29} + 36707414555219468440447241903970z^{28} + \\ & 369055333918742878506923895821094z^{27} + 3028085987873439981041316741040299z^{26} + \\ & 19908118207277143280846917552738638z^{25} + 99771357205875220145109466450106517z^{24} + \\ & 32204116185543506281453342072328248z^{23} - 3744645921582101044070547736300950z^{22} - \\ & 8583686545551708471758291210460691032z^{21} - 70294647356901524101024740972933056916z^{20} - \\ & 36969293487586269267870756612360457070z^{19} - 1472149779764303912910700825119513125745z^{18} - \\ & 4646227686063347368140269721102656923194z^{17} - 11757721460891217253150507437222976590963z^{16} - \\ & 23667524905718087319814208022941410083354z^{15} - 36747814326347114270377987158311612338260z^{14} - \\ & 40652966100310576219422839345851085154840z^{13} - 24193553263042351259117425539502701518400z^{12} + \\ & 9719645940829530820988532518598953424000z^{11} + 37297341452565155702787810516361533600000z^{10} + \\ & 34764119013156176353837403619970113600000z^9 + 6746831082562798982378495636957952000000z^8 - \\ & 206567614085456615808107511463276800000000z^7 - 29659078571699608256375734426214400000000z^6 - \\ & 20932834089033885270730650301440000000000z^5 - 778439230783972616865055592448000000000z^4 - \\ & 1428583143864269960769790771200000000000z^3 - 8324112389233016688574464000000000000z^2 + \\ & 14860150621853249942323200000000000000z + 161919374795459002368000000000000000)P''(z) + \\ & 45(88092375633661952z^{36} + 24549299776964745216z^{35} + 2619357527554007840768z^{34} + \\ & 159628611480988435906560z^{33} + 6513463004865397861819008z^{32} + 193479386194110772817766720z^{31} + \end{aligned}$$

# Result for the 6D fcc Lattice

$$\begin{aligned} & 4398883914180352580752205664z^{30} + 79010991647695967734365641136z^{29} + \\ & 1143508859378085891069139805496z^{28} + 13478285221767374237433813894156z^{27} + \\ & 129674818596578381841709352363310z^{26} + 1010115611151696866102360444043867z^{25} + \\ & 6203408988166712509967367951961350z^{24} + 27828342208285269645811267613975751z^{23} + \\ & 65404062287190045292473501882376446z^{22} - 232966958115695319966898071487115550z^{21} - \\ & 3776626287411277314694612568191478460z^{20} - 25665990995028381347757284132973790086z^{19} - \\ & 12330432201735600084488496344721300430z^{18} - 461005100390610028275047960932687009761z^{17} - \\ & 1382954753973214192431623770039149437562z^{16} - 3351334353377309619203633178809010250269z^{15} - \\ & 6500636144955681369542005264067707999470z^{14} - 9808779912515181085311292716635118617340z^{13} - \\ & 10758301750323045400708026810527005985400z^{12} - 6955035214429661410040236974622315476000z^{11} + \\ & 698114077775776671885153675463762080000z^{10} + 7349743557503879010410921836212410400000z^9 + \\ & 8691043975963666049447299379144001600000z^8 + 5165781565021067274342996673450656000000z^7 + \\ & 401336331886317774107713318790400000000z^6 - 2226964464248713386006518356377600000000z^5 - \\ & 1863534767021891922131179987968000000000z^4 - 655267817084534423521940643840000000000z^3 - \\ & 122588504883178716188285337600000000000z^2 - 843452865918902193743462400000000000z + \\ & 186207281047778527232000000000000)P'(z) + 90(455650218794803z^{35} \\ & 1254502960824572928z^{34} + 130185473751277349888z^{33} + 767548903189765748480z^{32} + \\ & 302276251598295683586240z^{31} + 8653460076869413651316640z^{30} + 189382045823502675349219920z^{29} + \\ & 3269391489631666671425989920z^{28} + 45371384308945745114138623620z^{27} + \\ & 510811439434664402615401586970z^{26} + 4663284432121091702260620852777z^{25} + \\ & 34047746401934351907977621763618z^{24} + 190773160991774404319508940400373z^{23} + \\ & 71755244018220111969771948822450z^{22} + 574602465936356660227512513519630z^{21} - \\ & 16377415461160421103082005421146444z^{20} - 158195048236903725948800257698582066z^{19} - \\ & 924626001493256833520380233115382826z^{18} - 40446572703123062507649767424272089595z^{17} - \\ & 14017460872371123201967056591950292270z^{16} - 39203789245543299948038211301310631735z^{15} - \\ & 88492994651041978105789511893808827410z^{14} - 158672230290697625052364901820833352540z^{13} - \\ & 217051701285403806039787021788244210200z^{12} - 204430925935804223158200138096719244000z^{11} - \\ & 83930464288781215080378386513083200000z^{10} + 9874924788243913782204419686396640000z^9 + \\ & 23485599064851467428791744222356800000z^8 + 252029928377053385449407192172320000000z^7 + \\ & 165979815868291791006070607462400000000z^6 + 52113850317609070332668882227200000000z^5 - \\ & 9698100095942063765846249472000000000z^4 - 12270310453108287668341923840000000000z^3 - \\ & 3932207868973120630810214400000000000z^2 - 57865936567527160971264000000000000z - \\ & 2698656246590983372800000000000000)P(z) = 0. \end{aligned}$$

## Some Timings

Timings with our new approach to creative telescoping:

- for  $d = 3$ :  $\sim 2$  seconds
- for  $d = 4$ :  $\sim 3$  minutes
- for  $d = 5$ :  $\sim 4$  hours
- for  $d = 6$ :  $\sim 5$  days

## Some Timings

Timings with our new approach to creative telescoping:

- for  $d = 3$ :  $\sim 2$  seconds
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- for  $d = 6$ :  $\sim 5$  days

→ With traditional methods (Chyzak's algorithm, Takayama's algorithm), the computations are not at all feasible (at least the cases  $d = 5$  and  $d = 6$ ).

→ We do not believe that  $d = 7$  can be done with our method (at least at the moment).

## Results for Return Probabilities

Recall the formula for the return probability:

$$R = 1 - \frac{1}{\sum_{n=0}^{\infty} p_n(\mathbf{0})} = 1 - \frac{1}{P(1)}.$$

We have computed a differential equation for

$$P(z) = \sum_{n=0}^{\infty} p_n(\mathbf{0}) z^n.$$

Derive a recurrence for the partial sums:

$$\begin{aligned} \frac{P(z)}{1-z} &= (p_0 + p_1 z + p_2 z^2 + \dots)(1 + z + z^2 + \dots) \\ &= p_0 + (p_0 + p_1)z + (p_0 + p_1 + p_2)z^2 + \dots \\ &= \sum_{N=0}^{\infty} \left( \sum_{n=0}^N p_n \right) z^N. \end{aligned}$$

→ Wimp-Zeilberger method delivers the asymptotic behavior.

## Results for Return Probabilities

In each case, the result is a linear ODE in  $z$ , which gives rise to recurrences for the series coefficients and their partial sums.

From this we can compute the return probability

$$R = 1 - \frac{1}{\sum_{n=0}^{\infty} p_n(\mathbf{0})}$$

to very high accuracy using the asymptotic behavior of the solutions.

In particular, we got the following results:

- $d = 3$ :  $R_3 = 1 - \frac{16 \sqrt[3]{4}\pi^4}{9(\Gamma(\frac{1}{3}))^6} = 0.2563182365\dots$
- $d = 4$ :  $R_4 = 0.095713154172562896735316764901210185\dots$
- $d = 5$ :  $R_5 = 0.046576957463848024193374420594803291\dots$
- $d = 6$ :  $R_6 = 0.026999878287956124269364175426196380\dots$

**Outlook:** We have no idea how to express them as closed forms!