The Face-Centered Cubic Lattice

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Introduction

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

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

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

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

$\longrightarrow$ Simplest instance is the integer lattice $\mathbb{Z}^d$
(choose $\boldsymbol{a}_i = \boldsymbol{e}_i$, 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

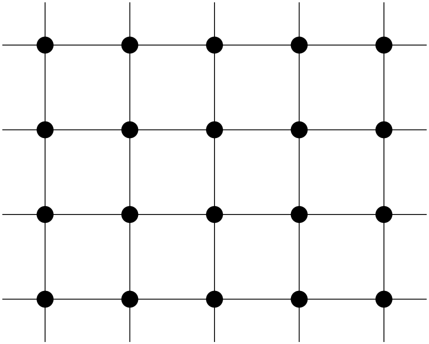
Study random walks on the *face-centered cubic (fcc) lattice*.

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 $\mathbf{0}$.

The fcc Lattice in 2D

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



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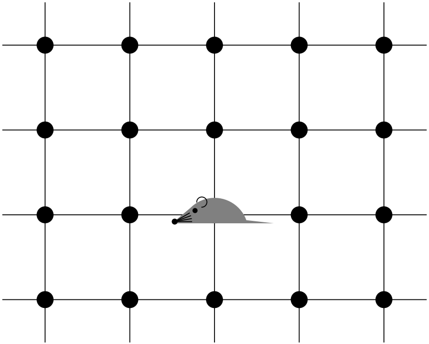

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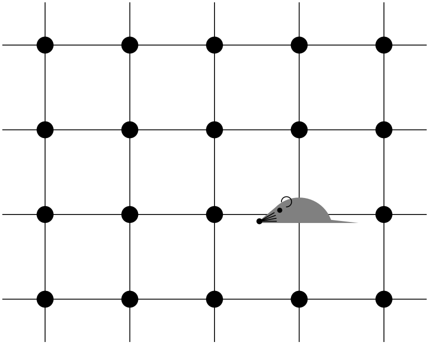

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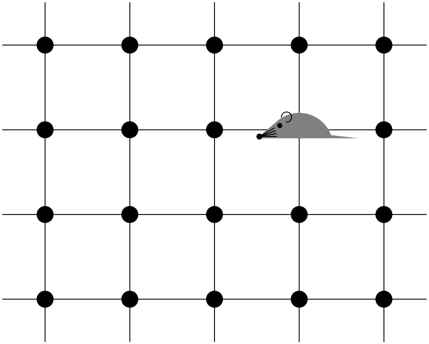

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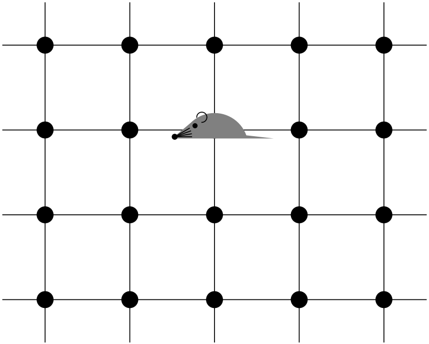

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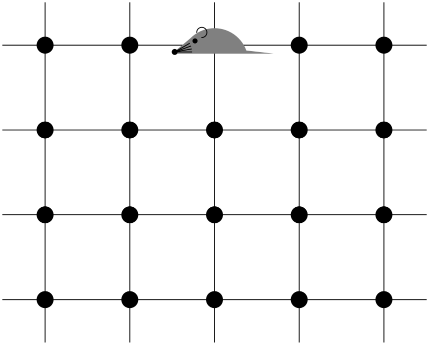

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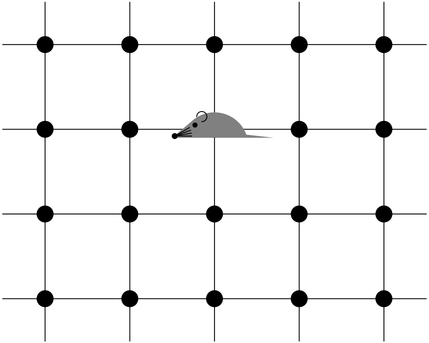

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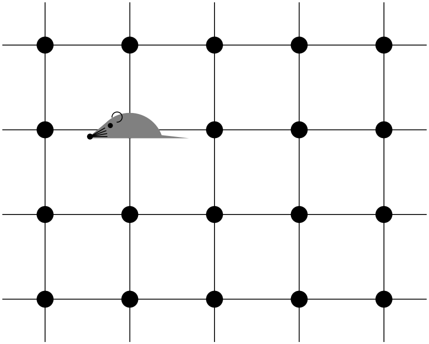

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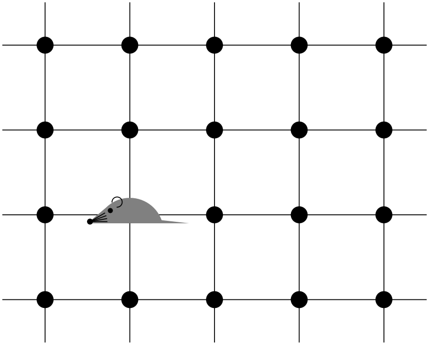

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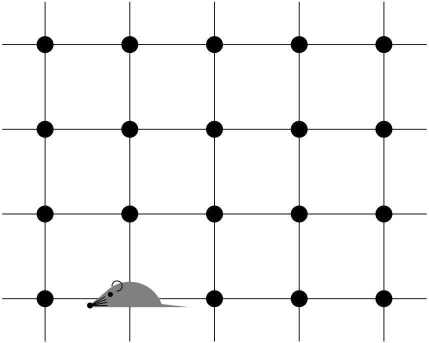

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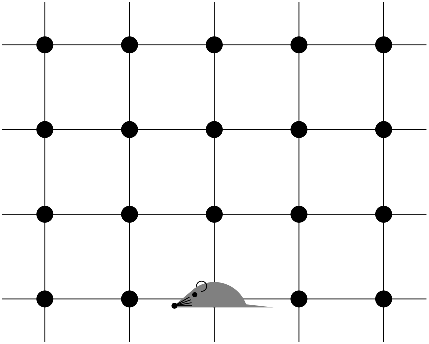

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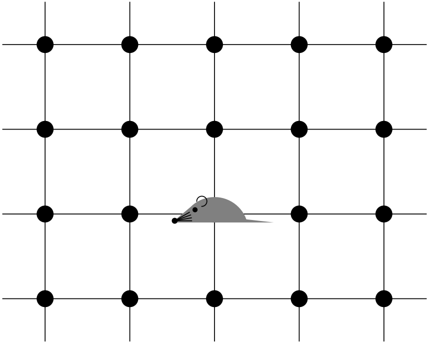

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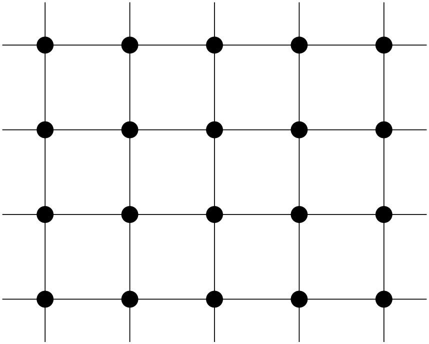

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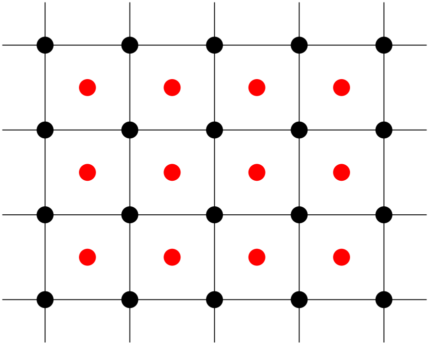
face-centered square lattice



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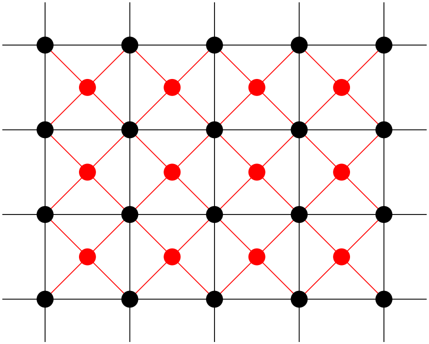

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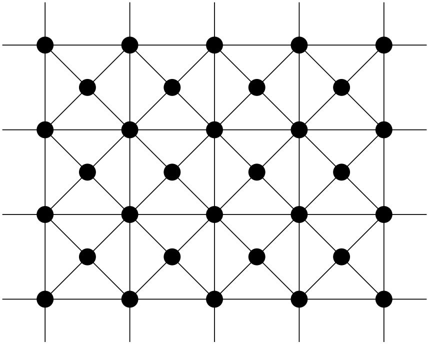

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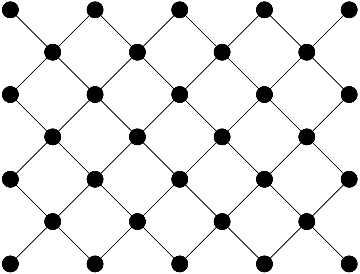

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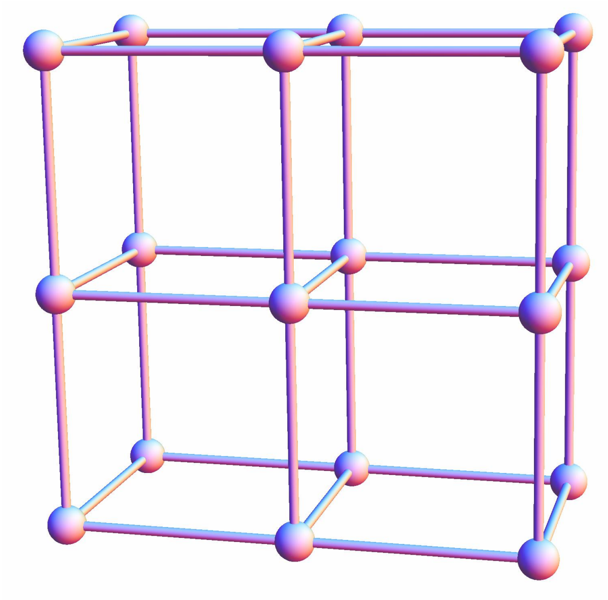

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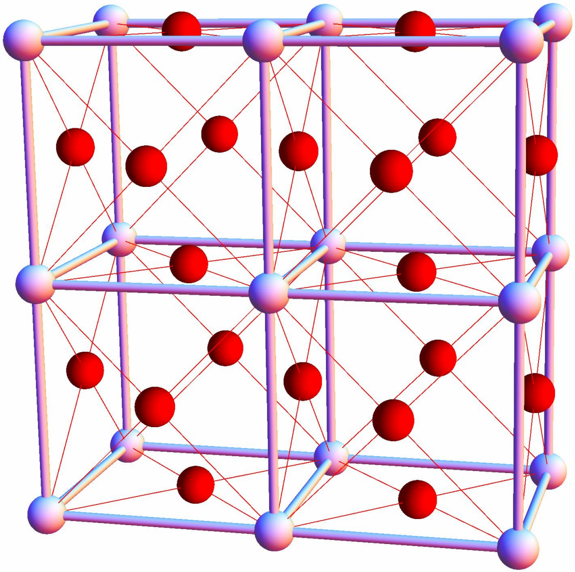

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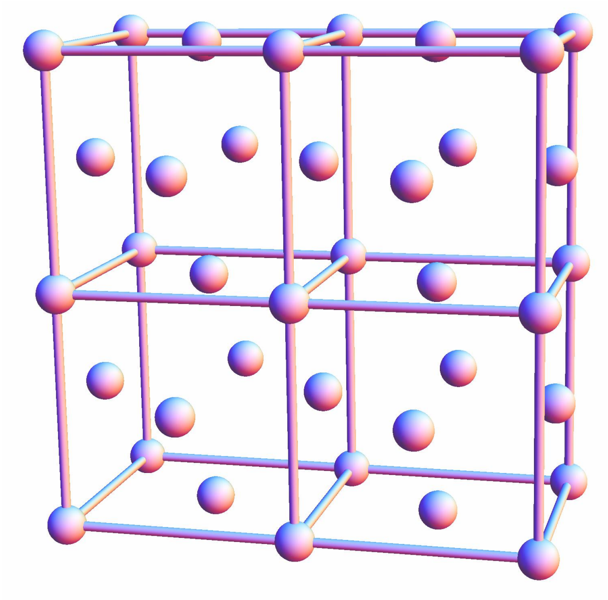

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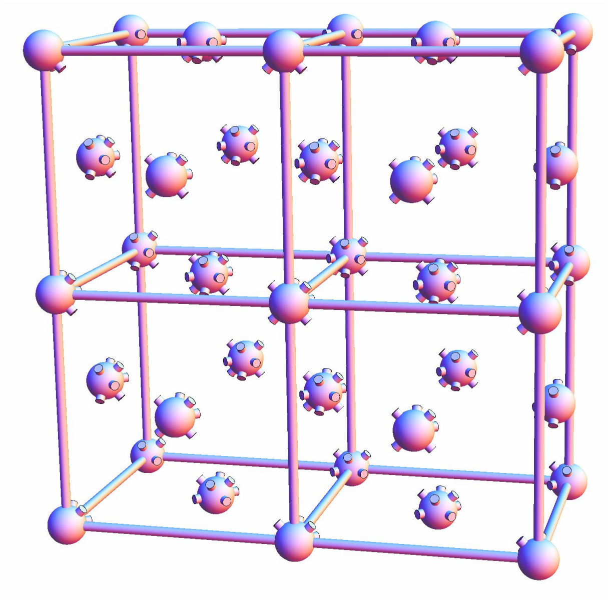

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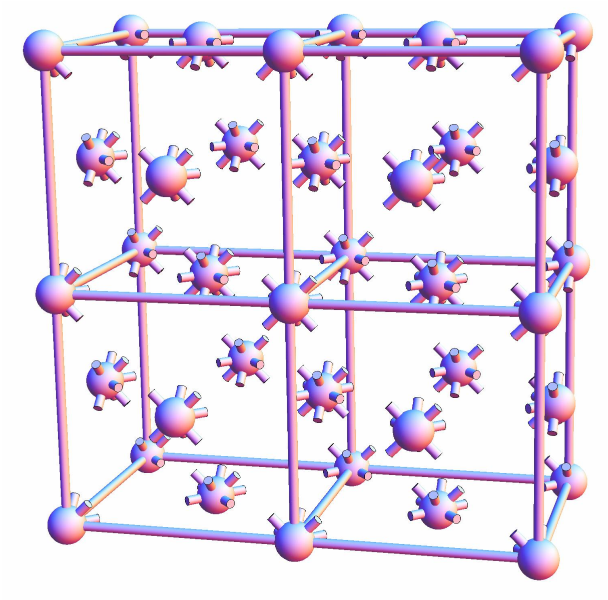

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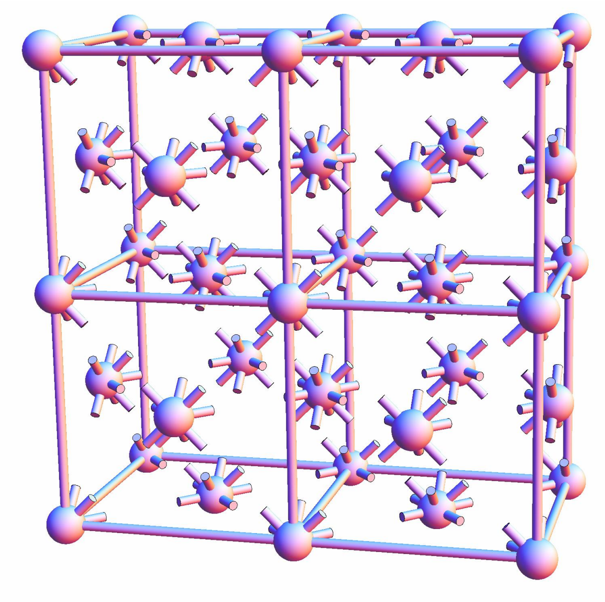

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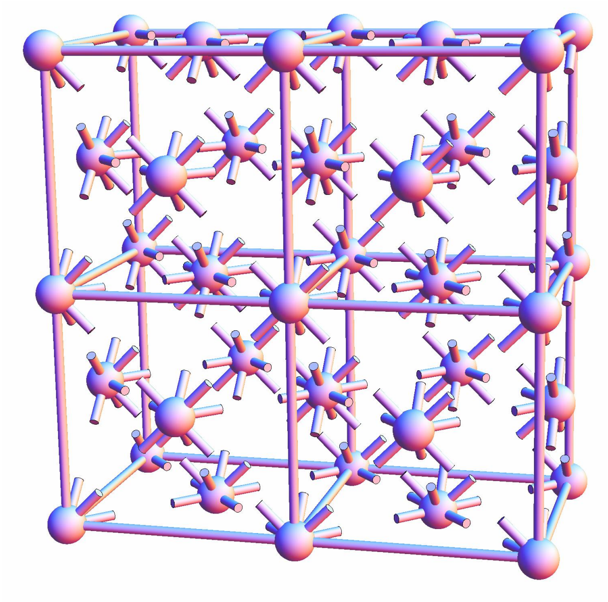

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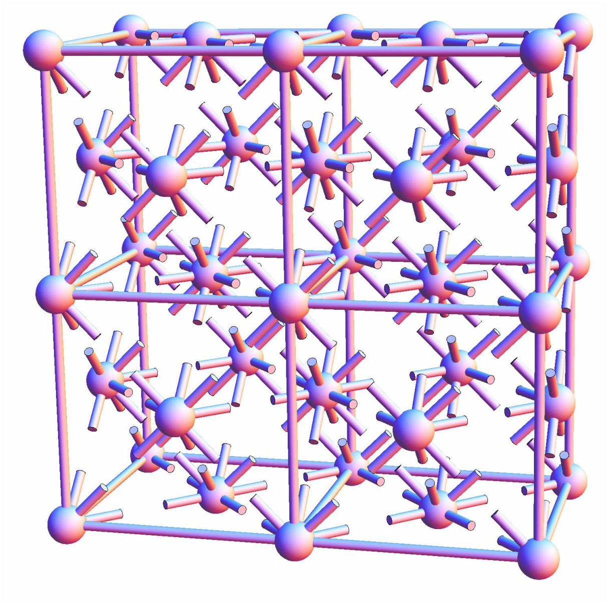

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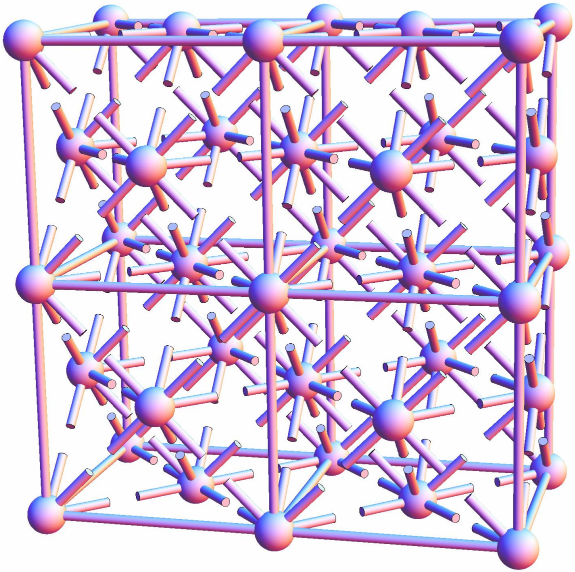

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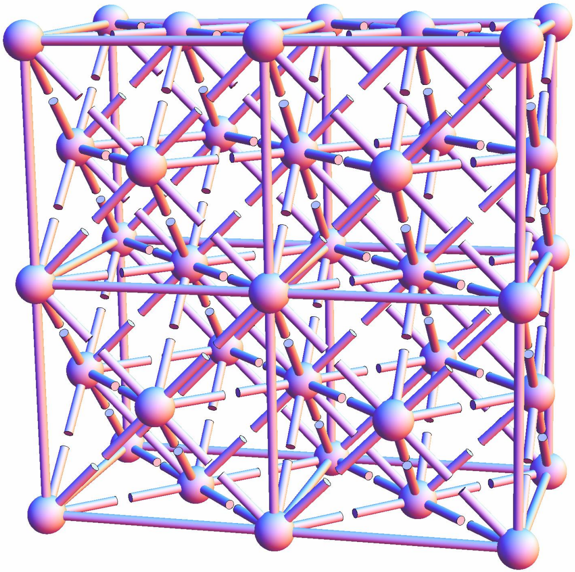

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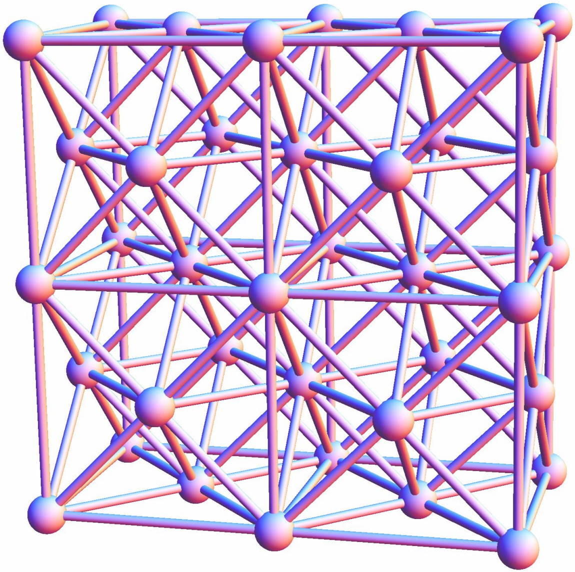

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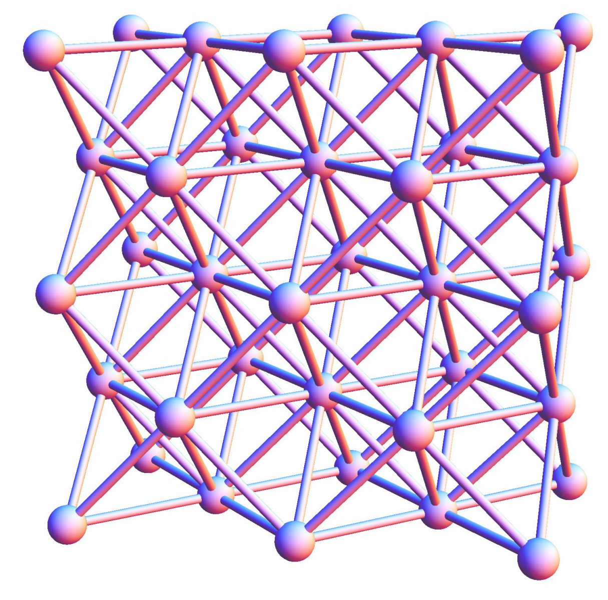

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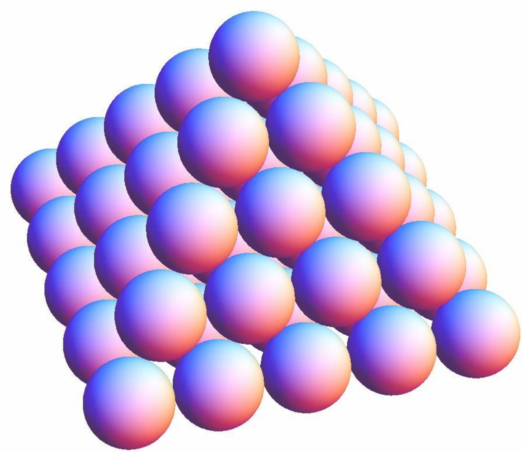
Densest possible packing: Kepler conjecture (Hales 2005)

$\longrightarrow$ 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

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

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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:

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

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

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

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

Lattice Green's Functions

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

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

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

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$\longrightarrow$ Note that $c^n p_n(\boldsymbol{x})$ 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

$$P(\mathbf{0}; z) = \sum_{n=0}^{\infty} p_n(\mathbf{0}) z^n = \frac{1}{\pi^d} \int_0^{\pi} \cdots \int_0^{\pi} \frac{\mathrm{d}k_1 \ldots \mathrm{d}k_d}{1 - z\lambda(\boldsymbol{k})}.$$

that encodes the return probabilities.

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

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

(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

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

The lattice Green's function is

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

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

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

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 $z = 1$.

$\longrightarrow$ It is well known that in 2D the return is certain!

Back to the fcc Lattice

The trivial (but illuminating) 2D case:

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

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

- lattice Green's function:

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

$\longrightarrow$ 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 $\lambda(\boldsymbol{k}) = \binom{d}{2}^{-1} \sum_{m=1}^{d} \sum_{n=m+1}^{d} \cos k_m \cos k_n$.

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

$$R = 1 - \left(\frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{\mathrm{d}k_1\,\mathrm{d}k_2\,\mathrm{d}k_3}{1 - \frac{1}{3}(c_1c_2 + c_1c_3 + c_2c_3)} \right)^{-1} = 1 - \frac{16\sqrt[3]{4}\pi^4}{9(\Gamma(\frac{1}{3}))^6}$$

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.

$\longrightarrow$ 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)
2. count all possible walks on the lattice
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2. count all possible walks on the lattice
3. count the excursions using "multi-step guessing"

$\longrightarrow$ However, any result obtained in this way is just a *conjecture*!

Method 1 (Guttmann 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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$$\frac{1}{\pi}\int_0^\pi \cos^{2n} k \, \mathrm{d}k = 4^{-n}\binom{2n}{n}$$

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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

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$(n = 0)$

Method 2: Naive Walk Enumeration

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$(n = 1)$

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·	·	2	·	2	·	·
·	·	·	1	·	·	·
·	·	·	·	·	·	·
·	·	·	·	·	·	·

$(n = 2)$

Method 2: Naive Walk Enumeration

·	·	·	·	·	·	·
·	·	·	1	·	·	·
·	·	3	·	3	·	·
·	3	·	9	·	3	·
1	·	9	·	9	·	1
·	3	·	9	·	3	·
·	·	3	·	3	·	·
·	·	·	1	·	·	·
·	·	·	·	·	·	·

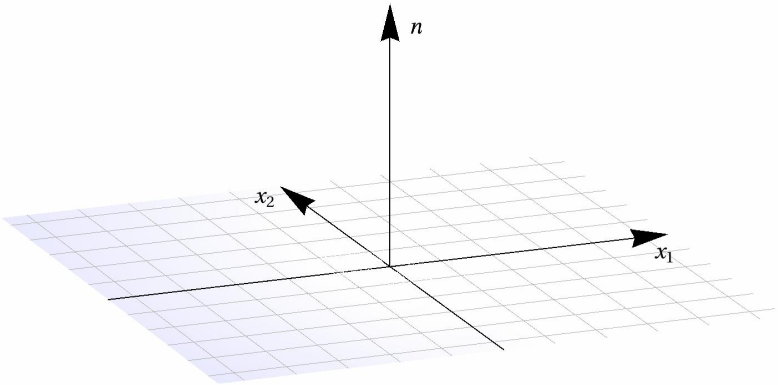
$(n = 3)$

Method 2: Naive Walk Enumeration

·	·	·	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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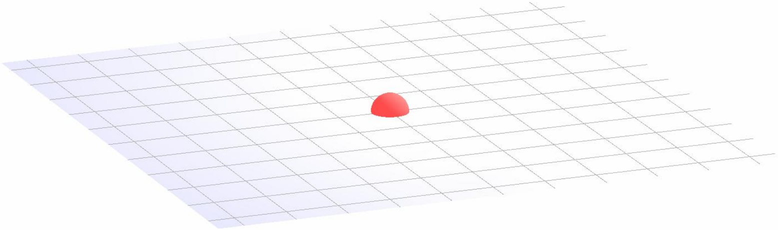

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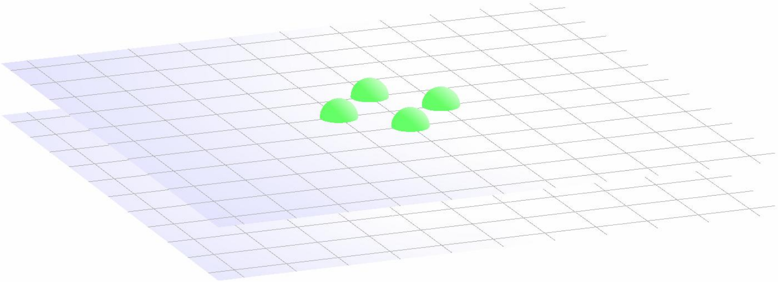

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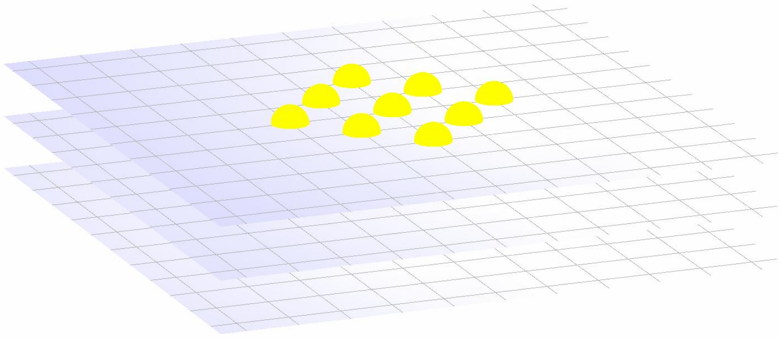

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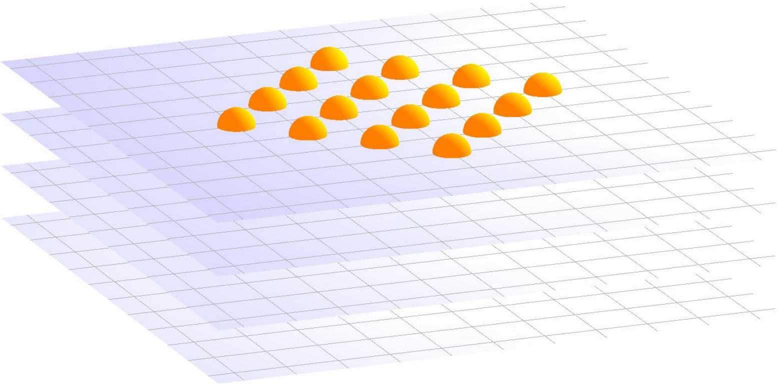

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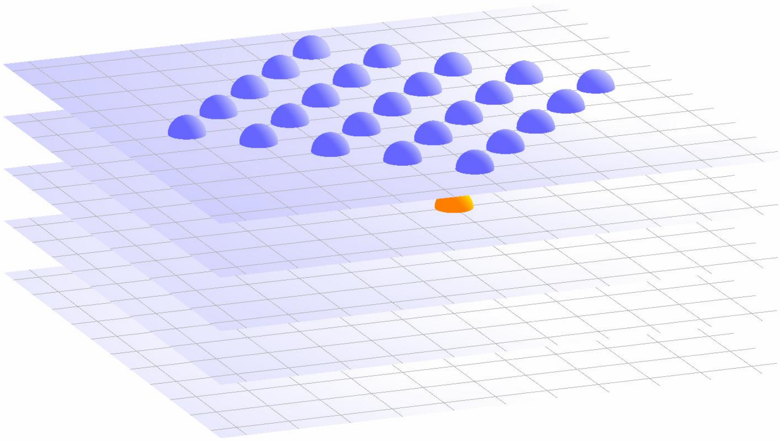

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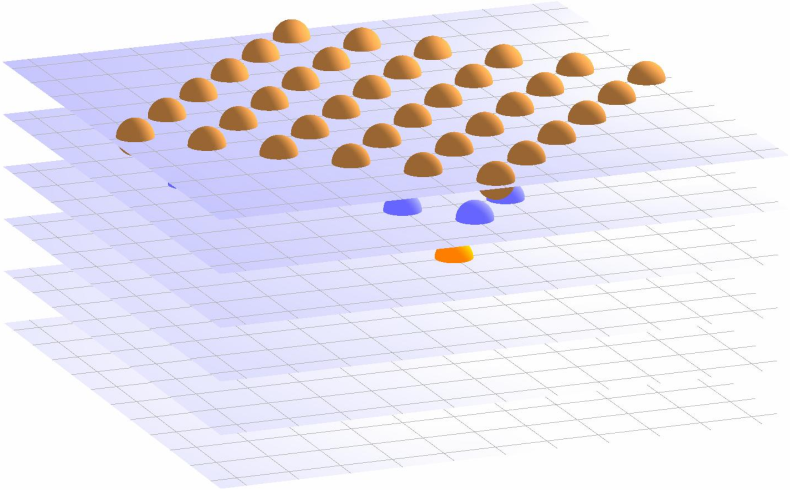

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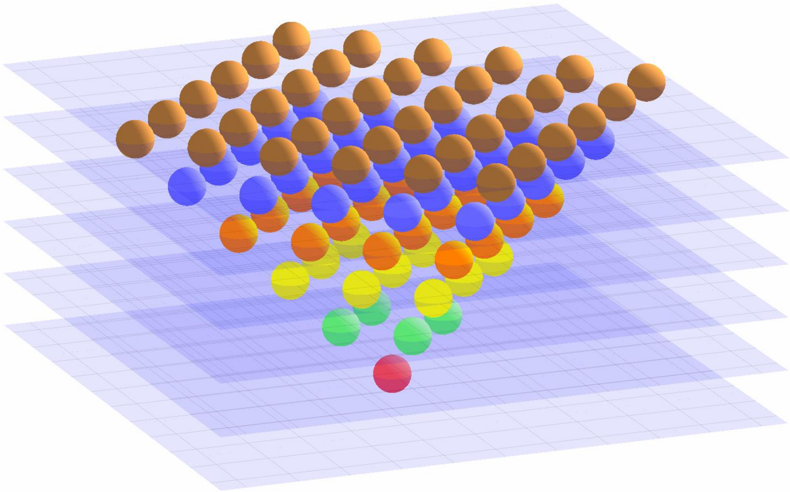

Method 2: Naive Walk Enumeration

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.

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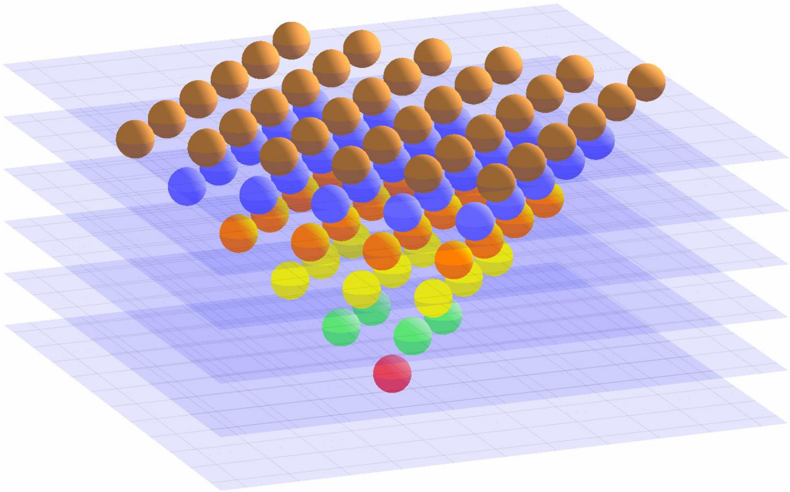
- Compute all values in the $(d+1)$-dimensional array (a cube of side length $2n$, basically).
- The Taylor coefficients sit on the n-coordinate axis.

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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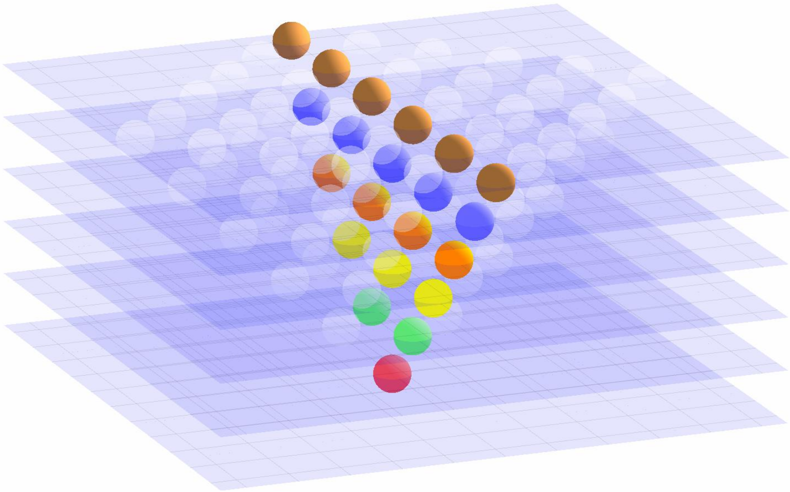

Method 3: Multistep Guessing

Example for $d = 5$.

- Crank out a moderate number of values for the 6-dimensional sequence $a_n(x_1, \ldots, x_5)$, 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.

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

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$$
\begin{aligned}
\sum_{n=0}^{\infty} \sum_{\boldsymbol{x} \in \mathbb{Z}^d} p_{n+1}(\boldsymbol{x}) \boldsymbol{y}^{\boldsymbol{x}} z^n &= \frac{1}{|S|} \sum_{n=0}^{\infty} \sum_{\boldsymbol{x} \in \mathbb{Z}^d} \sum_{\boldsymbol{s} \in S} p_n(\boldsymbol{x} - \boldsymbol{s}) \boldsymbol{y}^{\boldsymbol{x}} z^n \\
\frac{1}{z} \sum_{n=1}^{\infty} \sum_{\boldsymbol{x} \in \mathbb{Z}^d} p_n(\boldsymbol{x}) \boldsymbol{y}^{\boldsymbol{x}} z^n &= \frac{1}{|S|} \sum_{\boldsymbol{s} \in S} \sum_{n=0}^{\infty} \sum_{\boldsymbol{x} \in \mathbb{Z}^d} p_n(\boldsymbol{x}) \boldsymbol{y}^{\boldsymbol{x}+\boldsymbol{s}} z^n \\
\frac{1}{z} (F(\boldsymbol{y}; z) - 1) &= \frac{1}{|S|} \sum_{\boldsymbol{s} \in S} \boldsymbol{y}^{\boldsymbol{s}} F(\boldsymbol{y}; z)
\end{aligned}
$$

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

A Different Approach to the LGF

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

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

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Key observation: $\langle y^{-1} \rangle D_y G(y) = 0$ for any $G(y) = \sum_{n=-\infty}^{\infty} g_n y^n$.

Therefore: if the differential operator
$A(z, D_z) + D_{y_1} B_1 + \cdots + D_{y_d} B_d$ annihilates $F(\boldsymbol{y};z)/(y_1 \dots y_d)$,
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 $P(\mathbf{0};z)$:

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

Connection with the Integral Representation

$$\begin{aligned} P(\mathbf{0}; z) &= \langle y_1^0 \dots y_d^0 \rangle \frac{1}{1 - \frac{z}{|S|} \sum_{\boldsymbol{s} \in S} \boldsymbol{y}^{\boldsymbol{s}}} \\ &= \frac{1}{\pi^d} \int_0^\pi \dots \int_0^\pi \frac{\mathrm{d}k_1 \dots \mathrm{d}k_d}{1 - z \sum_{\boldsymbol{s} \in S} p_1(\boldsymbol{s}) e^{i \boldsymbol{s} \cdot \boldsymbol{k}}} \end{aligned}$$

In the holonomic systems approach, the operator

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

is called a *creative telescoping operator*.

Excursion: The Holonomic Systems Approach

Consider the class of ∂-finite/holonomic functions (functions and sequences that satisfy "sufficiently many" linear differential equations and recurrences).

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$\longrightarrow$ 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 $\int_0^1 f(x,y)\,\mathrm{d}x$ by means of a creative telescoping operator.

Concrete Example: Creative Telescoping

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

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

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

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

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

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

Indeed, the integrand is annihilated by the operators:

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

Concrete Example: Creative Telescoping

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

The creative telescoping operator

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

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

$$A(\boldsymbol{v}, \boldsymbol{\partial_v}) + \Delta_1 B_1(\boldsymbol{v}, \boldsymbol{w}, \boldsymbol{\partial_v}, \boldsymbol{\partial_w}) + \cdots + \Delta_m B_m(\boldsymbol{v}, \boldsymbol{w}, \boldsymbol{\partial_v}, \boldsymbol{\partial_w})$$

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
- $\boldsymbol{w} = w_1, \ldots, w_m$ are the summation/integration variables
- $\boldsymbol{v} = v_1, v_2, \ldots$ are the surviving parameters
- $A(\boldsymbol{v}, \boldsymbol{\partial_v})$ is called the *principal part* or the *telescoper*
- the $B_i(\boldsymbol{v}, \boldsymbol{w}, \boldsymbol{\partial_v}, \boldsymbol{\partial_w})$ 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

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

with unknowns $c_{\boldsymbol{\alpha}}$ and $c_{i,j,\boldsymbol{\alpha}}$, 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. $\boldsymbol{w}$ 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

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

Result for the 5D fcc Lattice

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

Result for the 6D fcc Lattice

$$(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^6P^{(8)}(z)+2(z+15)(800100086574208z^{36}+22738998805752633 6z^{35}+25996840572204888512z^{34}+1719342411627828757728z^{33}+76318086060490791960792z^{32}+2462288021152606885358700z^{31}+60618715038937670473018584z^{30}+1175154434178119041671700740z^{29}+18309889884984684630822323370z^{28}+232115671681854334221586338585z^{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}-1450218746083946510596388474880000000000z^{5}+344718972957157801371250560000000000000z^{4}+314413056395938625838510182400000000000z^{3}+140360356659888583720114176000000000000z^{2}+25084009812063190450176000000000000000z+1973392380319656591360000000000000000000)z^5P^{(7)}(z)+$$

Result for the 6D fcc Lattice

$$
\begin{aligned}
&(3588245473009075 2z^{37} + 1061260405161448665 6z^{36} + 127653260094221277516 8z^{35} + \\
&89393980129433032096320z^{34} + 422160683898347322819700 8z^{33} + 14549456798576648489892304 8z^{32} + \\
&384082800449092006095096948 0z^{31} + 8016006238826772717221198508 0z^{30} + \\
&135085509439800690268287092205 0z^{29} + 1863108289263053682422294940958 5z^{28} + \\
&211815796834464054711973645322142z^{27} + 1986708322085667572665525016037411z^{26} + \\
&15263082383031406770429022758762048z^{25} + 94068732852089205756130773605094705z^{24} + \\
&441055376229095921513357130918811338z^{23} + 1319636945498761264973744224282378779z^{22} - \\
&1376268096732267953995912640790411 12z^{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} - \\
&866425754505013910667872020195200000000000z^{5} + 597046839721706795489319772224000000000000z^{4} + \\
&725116102774123909908393630720000000000000z^{3} + 338828967558720719568862617600000000000000z^{2} + \\
&631115677130491732576665600000000000000000z + 512323021813756999680000000000000000000000)z^{4}P^{(6)}(z) + \\
&3(130240020872181248z^{37} + 3807222047478676915 2z^{36} + 448027411720532102323 2z^{35} + \\
&30598839345549153729024 0z^{34} + 1407922464408792532952352 0z^{33} + 4727396131034939776586928 00z^{32} + \\
&1216240227880266706589663688 0z^{31} + 2475013840209218674125864842 40z^{30} + \\
&406856488897300388082085355031 0z^{29} + 5475034079814792632892124551313 5z^{28} + \\
&607255705204278811351245801585018z^{27} + 5552646100941335755747908121811397z^{26} + \\
&41511153616540066669903815109576752z^{25} + 247864598814302846690177415162792735z^{24} + \\
&1112001535696035843878120629687073790z^{23} + 3006740720618245361400876608130182349z^{22} - \\
&30662749076478014018158070998014257 04z^{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

$$865953342265454601104437816976581680000000z^{10}+586378944861718695144037906690882422000000z^{9}-$$
$$448918716637412377029136427636037600000000z^{8}-526332032930456915428235817813056400000000z^{7}-$$
$$518937227107573341964843985332680000000000z^{6}-226302972537833147253780811598400000000000z^{5}+$$
$$104974053097834899670129395840000000000000z^{4}+641357814865841417537072778240000000000000z^{3}+$$
$$347089467368149273535429836800000000000000z^{2}+699409221434846453300428800000000000000000z+$$
$$595812699442665547776000000000000000000000)z^{3}P^{(5)}(z)+15(146187778529999360z^{37}+$$
$$422326808984872512 00z^{36}+48576657340989636902 40z^{35}+323165791319702484035520z^{34}+$$
$$1446760113658410970765 4400z^{33}+4725344663866749805330727 04z^{32}+11827310475440684698801079376z^{31}$$
$$234205994182438943769949245108z^{30}+3746772515516029997311378363446z^{29}+$$
$$49056517288448701934966949399201z^{28}+528960737538220962199232165726700z^{27}+$$
$$4693678127508685757329704793118274z^{26}+33925520928056707379949042245154948z^{25}+$$
$$194225784819376433418854177036400765z^{24}+815865984997630892337526061797547730z^{23}+$$
$$1820210924970374403477059898368292414z^{22}-5626714951506760337684784884293147302z^{21}-$$
$$87288636539051237531541938169181610997z^{20}-548617946604162829617617348998523187024z^{19}-$$
$$2396582727922965009354571656000074347578z^{18}-7949778754688875639594299226888542864672z^{17}-$$
$$20284887219829242010855806602752336703097z^{16}-38476335393060119379820741759126402451166z^{15}-$$
$$47185211186009106848535876331178061122490z^{14}-10222760436927155616364669208395729054260z^{13}+$$
$$107413528041921729529347960434391761302800z^{12}+279266241080334469793315941614102969564000z^{11}+$$
$$379975092805467869163550626412993759200000z^{10}+276342679146887322412220759883497997600000z^{9}+$$
$$63379261598089182133086908167004640000000z^{8}-214965129809120690827282902731468640000000z^{7}-$$
$$242455701875928553517844332493302400000000z^{6}-140261247415772885691546407435520000000000z^{5}-$$
$$36772706828360958944274523883520000000000z^{4}+77477283796273934947265452032000000000000z^{3}+$$
$$7522568512298824734532104192000000000000z^{2}+1776029394112720931570319360000000000000z+$$
$$161818175186211840491520000000000000000)z^{2}P^{(4)}(z)+90(691069498505451 52z^{37}+$$
$$197281259589780280 32z^{36}+2215666629279250997248z^{35}+143387361084360543557376z^{34}+$$
$$6235802763945868063424352z^{33}+197763282456363307438541552z^{32}+4805890762274729535435673296z^{31}+$$
$$92390999114814905907317974392z^{30}+1434485821162175237888091472086z^{29}+$$
$$18213230428133179674440523308931z^{28}+190122674553786922619563973540916z^{27}+$$
$$1627987793820686707319681442965532z^{26}+11283714208962998257330503635013918z^{25}+$$
$$61070425289478623056319494081223364z^{24}+232117491219054750436300759063832796z^{23}+$$
$$335162333006577190998078624832466745z^{22}-$$

Result for the 6D fcc Lattice

$$
\begin{aligned}
&3212526847572548623801062566839102968z^{21} - 3392965866525625940881278435486638557z^{20} - \\
&1951831789900573496432722754351267363 40z^{19} - 8185961182051286059853304788561116790 58z^{18} - \\
&2671193766306193321259081077503739718922z^{17} - 6879647707640439013900747488611335523490z^{16} - \\
&13791392258782895819955453998955102517548z^{15} - 20395042168164862736248341991799243143275z^{14} - \\
&1855905114263490123161823006701124526173 0z^{13} + 3407638735402551318083430675030634548 00z^{12} + \\
&32573268392371003654841290966684606314000z^{11} + 54660627321107405540934107870983869840000z^{10} + \\
&419707294027084739233866209356238148 00000z^{9} + 757729323937951939044642929351040000000z^{8} - \\
&3465345486136948584706296425184552 0000000z^{7} - 4190926430444018560287676453660320000000 0z^{6} - \\
&2764938702145552027676616654604800000000 0z^{5} - 99328789269121533702589473638400000000 0z^{4} - \\
&1112041174659253407521806233600000000000z^{3} + 2849114538408597196020019200000000000000z^{2} + \\
&11423067813148192266682368000000000000000z + 114861556495528729804800000000000000000000) z P^{(3)}(z) + \\
&45(180741253455271936z^{37} + 5098070626763698 4832z^{36} + 558434063410582652518 4z^{35} + \\
&35101006700535148822425 6z^{34} + 14802080405483677823943104z^{33} + 45487501583148540090909724 8z^{32} + \\
&107070519614964142174073055 36z^{31} + 199288291693600445167066471488z^{30} + \\
&2993264774540100816050708154540z^{29} + 36707414555219468440447241903970z^{28} + \\
&369055333918742878506923895821094z^{27} + 3028085987873439981041316741040299z^{26} + \\
&19908118207277143280846917552738638z^{25} + 99771357205875220145109466450106517z^{24} + \\
&322041161855435062814533420723282482z^{23} - 374464592158210104407054773630095 0z^{22} - \\
&8583686545551708471758291210460691032z^{21} - 70294647356901524101024740972933056916z^{20} - \\
&369692934875862692678770756612360457070z^{19} - 1472149779764303912910700825119513125745z^{18} - \\
&4646227686063347368140269721102656923194z^{17} - 11757721460891217253150507437222976590963z^{16} - \\
&23667524905718087319814208022941410083354z^{15} - 36747814326347114270377987158311612338260z^{14} - \\
&40652966100310576219422839345851085154840z^{13} - 24193553263042351259117425539502701518400z^{12} + \\
&9719645940829530820988532518598953424000z^{11} + 37297341452565155702787810516361533600000z^{10} + \\
&34764119013156176353837403619970113600000z^{9} + 6746831082562798982378495636957952000000z^{8} - \\
&20656761408545661580810751146327680000000z^{7} - 29659078571699608256375734426214400000000z^{6} - \\
&20932834089033885270730650301440000000000z^{5} - 7784392307839726168650555924480000000000z^{4} - \\
&1428583143864269960769790771200000000000z^{3} - 8324112389233016688574464000000000000000z^{2} + \\
&14860150621853249942323200000000000000000z + 161919374795459002368000000000000000000000) P''(z) + \\
&45(8809237563366 1952z^{36} + 2454929977696474521 6z^{35} + 261935752755400784076 8z^{34} + \\
&1596286114809884359065 60z^{33} + 6513463004865397861819008z^{32} + 193479386194110772817766720z^{31} +
\end{aligned}
$$

Result for the 6D fcc Lattice

$$
\begin{aligned}
&4398883914180352580752205664z^{30} + 7901099164769596773436564 1136z^{29} + \\
&1143508859378085891069139805496z^{28} + 1347828522176737423743381389 4156z^{27} + \\
&1296748185965783818417093523633 10z^{26} + 1010115611151696866102360444043867z^{25} + \\
&6203408988166712509967367951961350z^{24} + 27828342208285269645811267613975751z^{23} + \\
&65404062287190045292473501882376446z^{22} - 232966958115695319966898071487115550z^{21} - \\
&377662628741127731469461256819147846 0z^{20} - 2566599099502838134775728413297379008 6z^{19} - \\
&12330432201735600084488496344721300430 2z^{18} - 46100510039061002827504796093268700976 1z^{17} - \\
&138295475397321419243162377003914943756 2z^{16} - 335133435337730961920363317880901025026 9z^{15} - \\
&650063614495568136954200526406770799947 0z^{14} - 980877991251518108531129271663511861734 0z^{13} - \\
&107583017503230454007080268105270059854 00z^{12} - 695503521442966141004023697462231547600 0z^{11} + \\
&698114077775776671885153675463762080000z^{10} + 734974355750387901041092183621241040000 0z^{9} + \\
&869104397596366604944729937914400160000 0z^{8} + 516578156502106727434299667345065600000 0z^{7} + \\
&401336331886317774107713318790400000000z^{6} - 222696446424871338600651835637760000000 0z^{5} - \\
&186353476702189192213117998796800000000 0z^{4} - 655267817084534423521940643840000000000z^{3} - \\
&122588504883178716188285337600000000000 0z^{2} - 843452865918902193743462400000000000000z + \\
&1862072810147778527232000000000000000)P'(z) + 90(4556502187948032z^{35} + \\
&1254502960824572928z^{34} + 130185473751277349888z^{33} + 7675748903189765748480z^{32} + \\
&302276251598295683586240z^{31} + 8653460076869413651316640z^{30} + 189382045823502675349219920z^{29} + \\
&3269391489631666671425989920z^{28} + 45371384308945745114138623620z^{27} + \\
&510811439434664402615401586970z^{26} + 4663284432121091702260620852777z^{25} + \\
&34047746401934351907977621763618z^{24} + 190773160991774404319508940400373z^{23} + \\
&717575244018720111969771948822450z^{22} + 574602465936356660227512513519630z^{21} - \\
&16377415461160421103082005421146444z^{20} - 158195048236903725948800257698582066z^{19} - \\
&924626001493256833520380233115382826z^{18} - 4044657270312306250764976742472089595z^{17} - \\
&14017460872371123201967056591950292270z^{16} - 39203789245543299948038211301310631735z^{15} - \\
&88492994651041978105789511893808827410z^{14} - 158672230290697625052364901820833352540z^{13} - \\
&217051701285403806039787021788244210200z^{12} - 204430925935804223158200138096719244000z^{11} - \\
&83930464288781215080378386513083200000z^{10} + 98749247882439137822044179686396640000z^{9} + \\
&234855990648514674287291744222356800000z^{8} + 252029928377053385449407192172320000000z^{7} + \\
&165979815868291791006070607462400000000z^{6} + 52113850317609070332668882227200000000z^{5} - \\
&9698100095942063765846249472000000000z^{4} - 12270310453108287668341923840000000000z^{3} - \\
&3932207868973120630810214400000000000z^{2} - 578659365675271609712640000000000000z - \\
&26986562465909833728000000000000000)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
- for $d = 4$: $\sim$ 3 minutes
- for $d = 5$: $\sim$ 4 hours
- for $d = 6$: $\sim$ 5 days

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

$\longrightarrow$ 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:

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

$\longrightarrow$ 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:

- $d = 3$: $R_3 = 1 - \frac{16\sqrt[3]{4}\pi^4}{9\left(\Gamma\left(\frac{1}{3}\right)\right)^6} = 0.2563182365\ldots$
- $d = 4$: $R_4 = 0.09571315417256289673531676490121018\ldots$
- $d = 5$: $R_5 = 0.04657695746384802419337442059480329\ldots$
- $d = 6$: $R_6 = 0.02699987828795612426936417542619638\ldots$

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