Lattice Green's Functions of the Higher-Dimensional Face-Centered Cubic Lattices

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November 7
Séminaires Algorithms

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

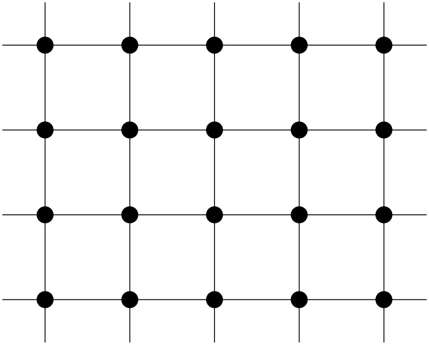
Study random walks on the *face-centered cubic (fcc) lattice*.

Consider random walks on the lattice points:

- In each step move to one of the nearest neighbors.
- All steps have the same probability.
- A point can be visited several times.
- Starting point is the origin $\mathbf{0}$.

The fcc Lattice in 2D

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



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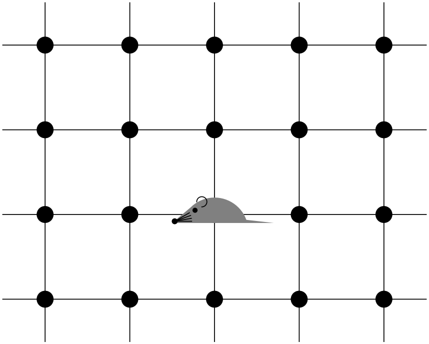

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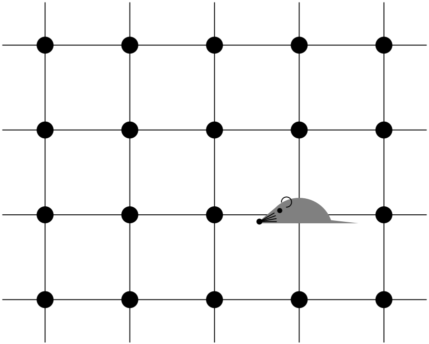

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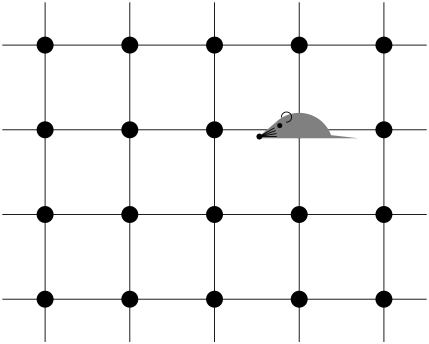

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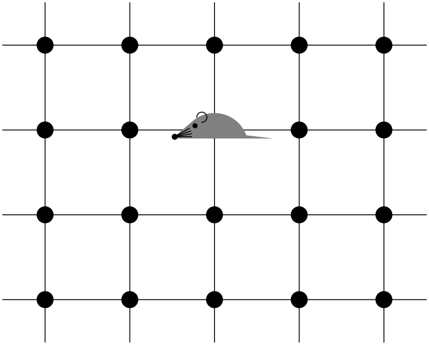

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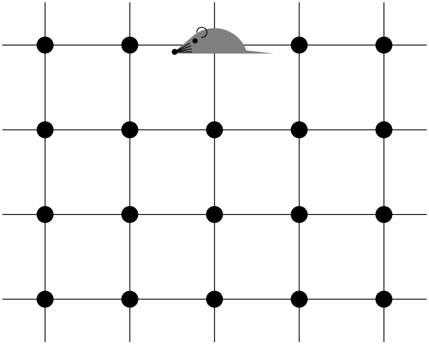

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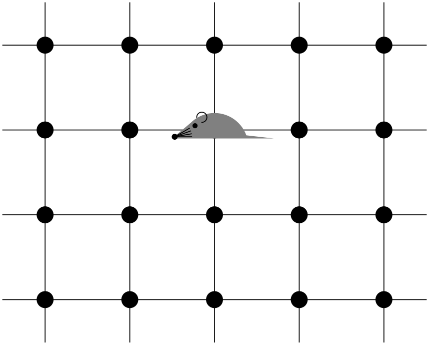

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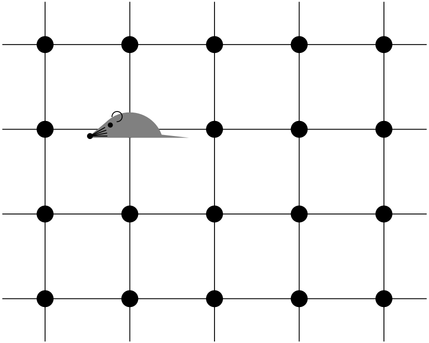

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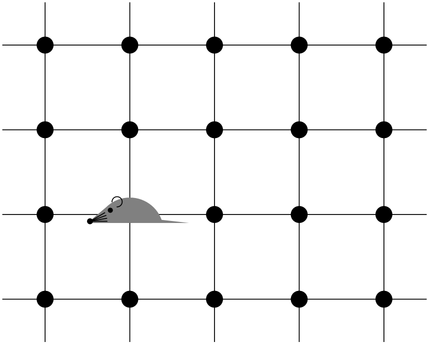

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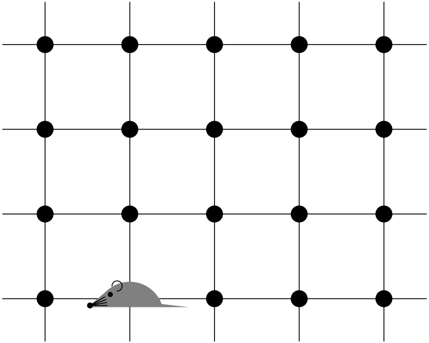

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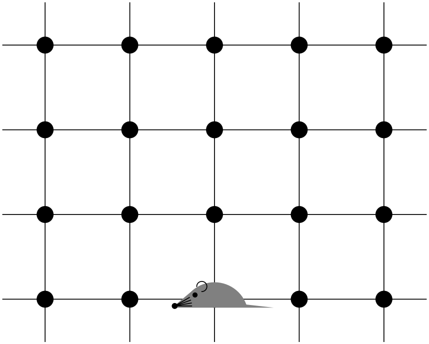

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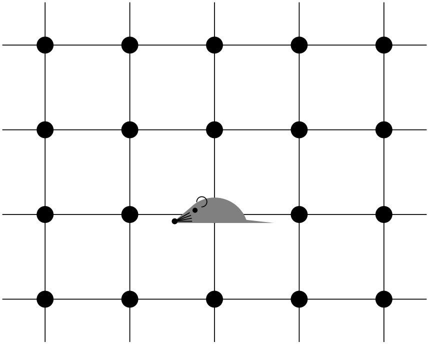

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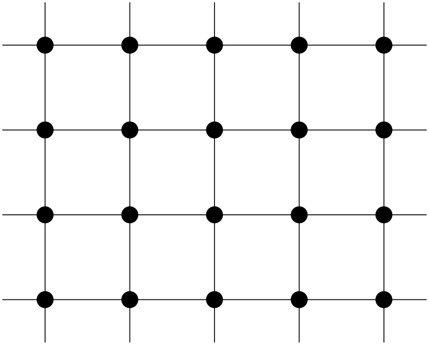

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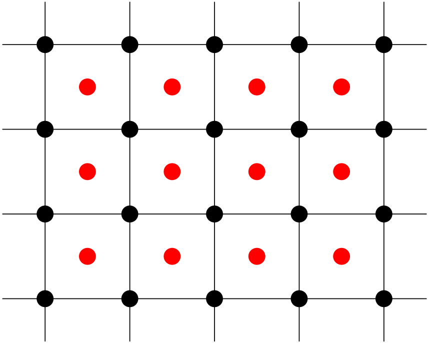

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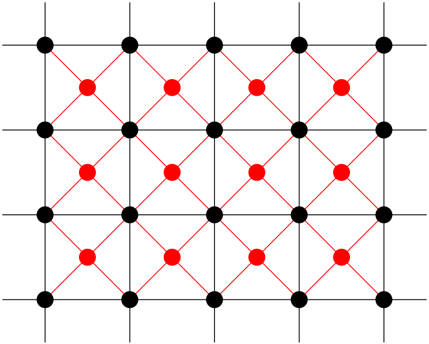

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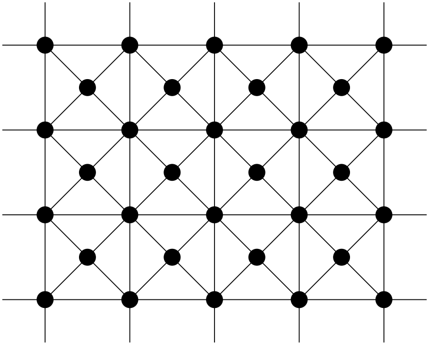

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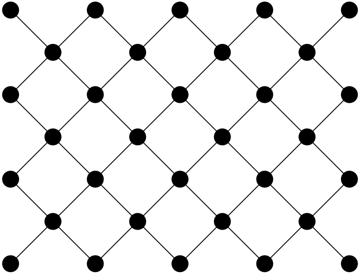

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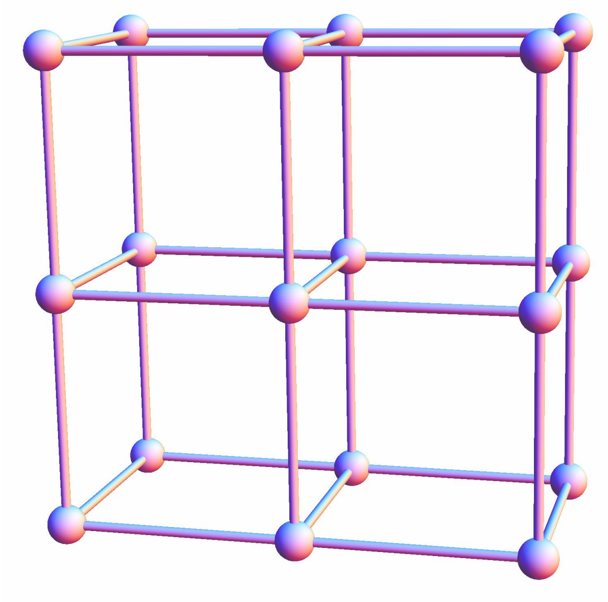

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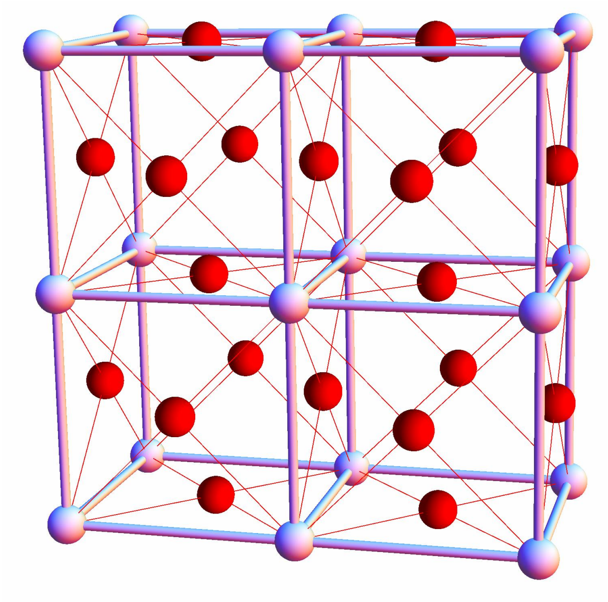

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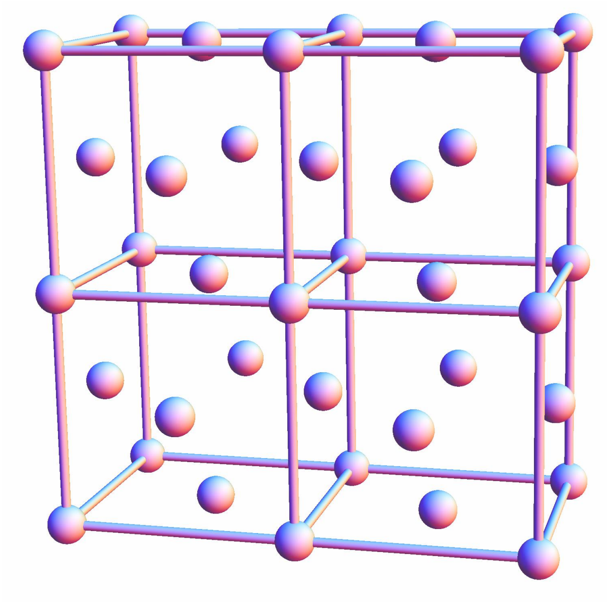

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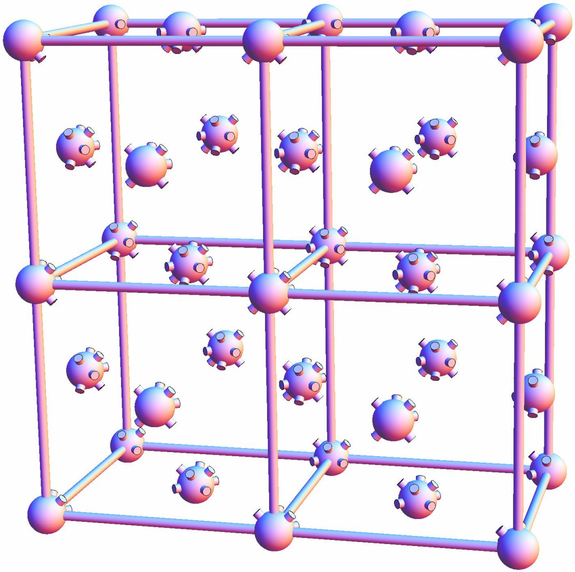

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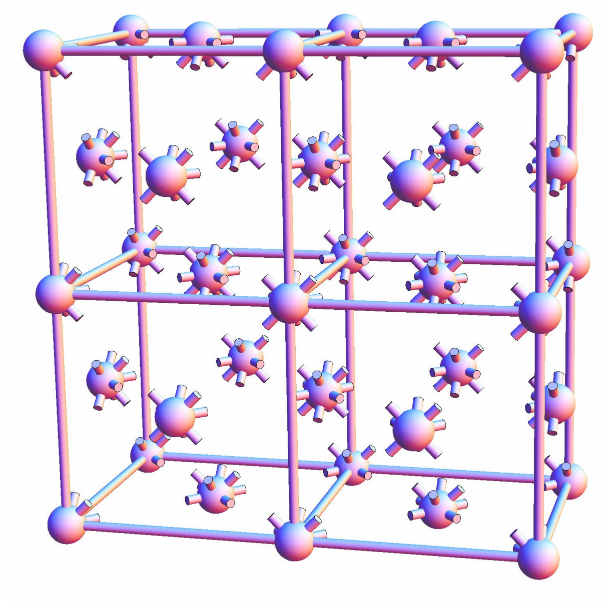

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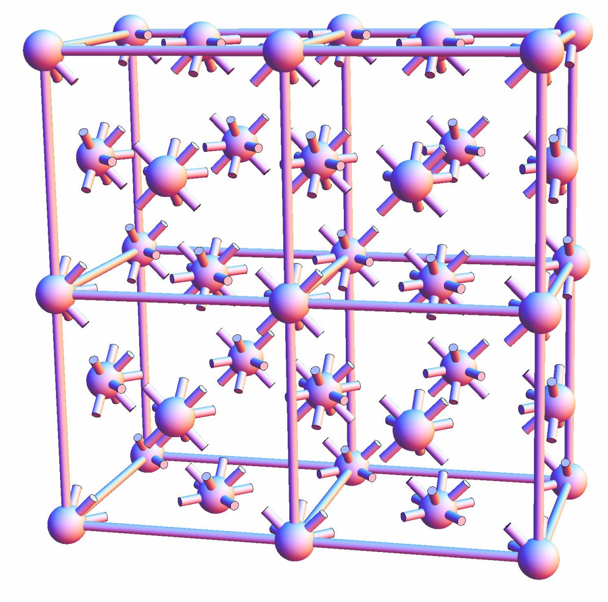

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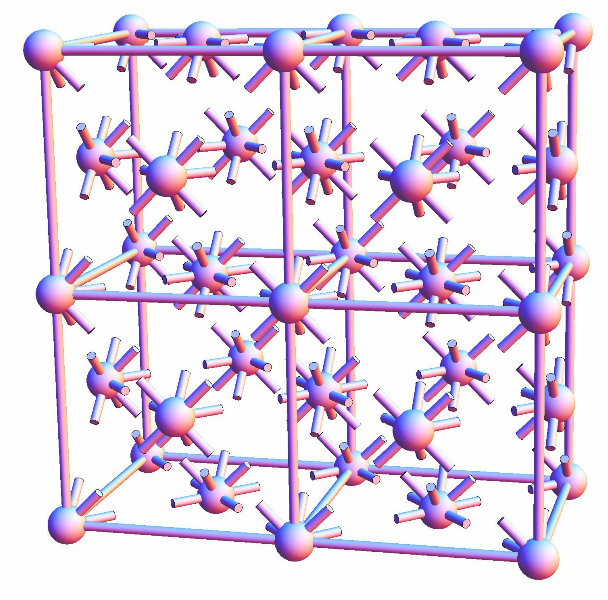

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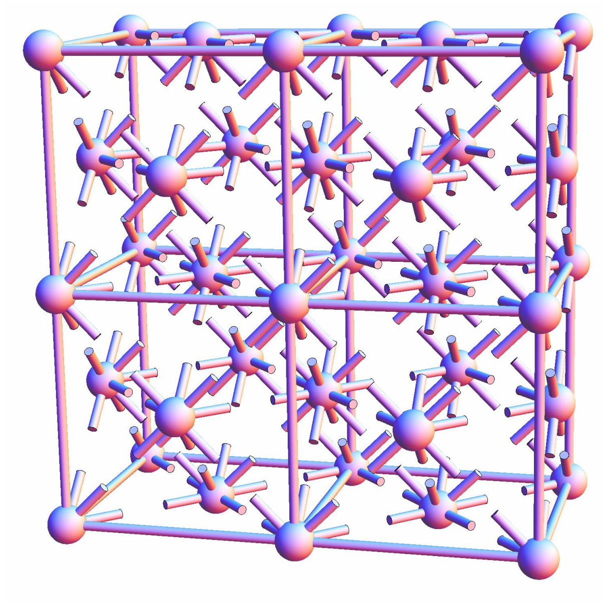

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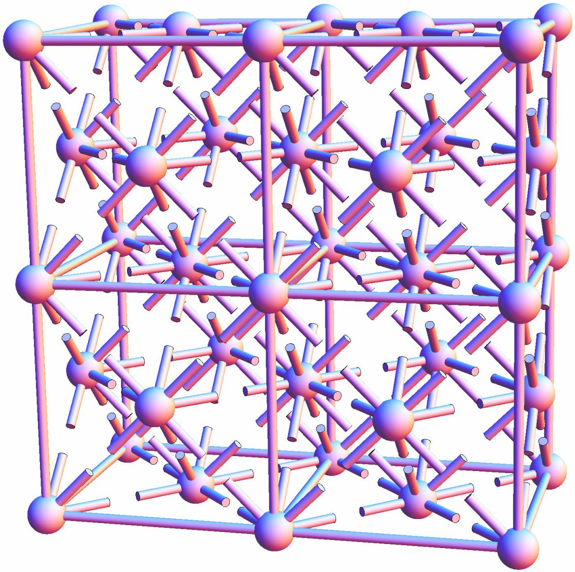

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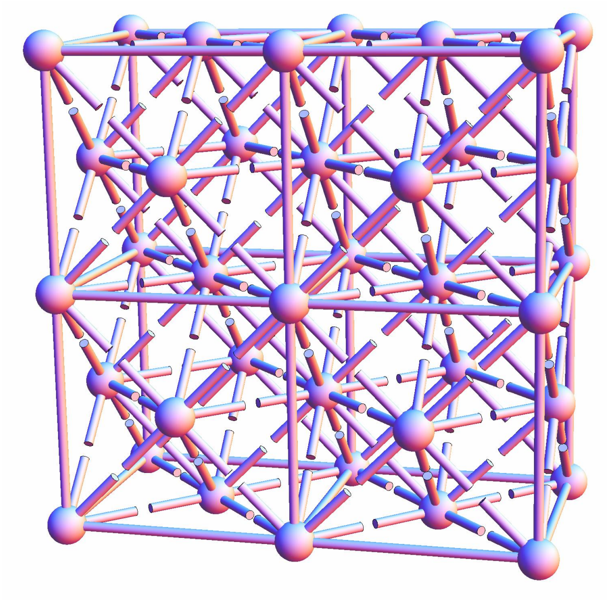

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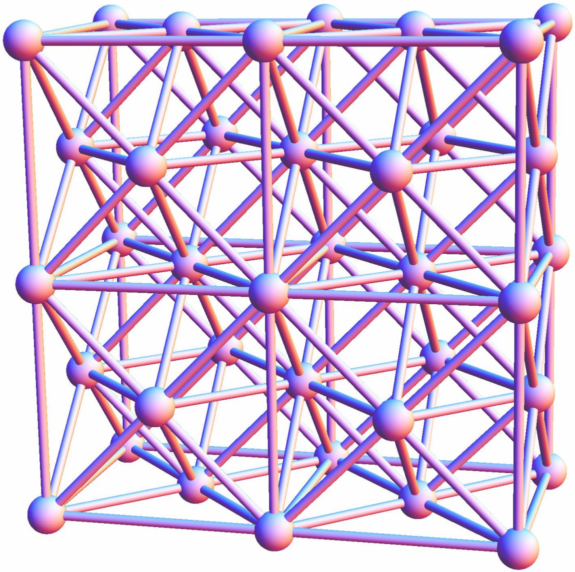

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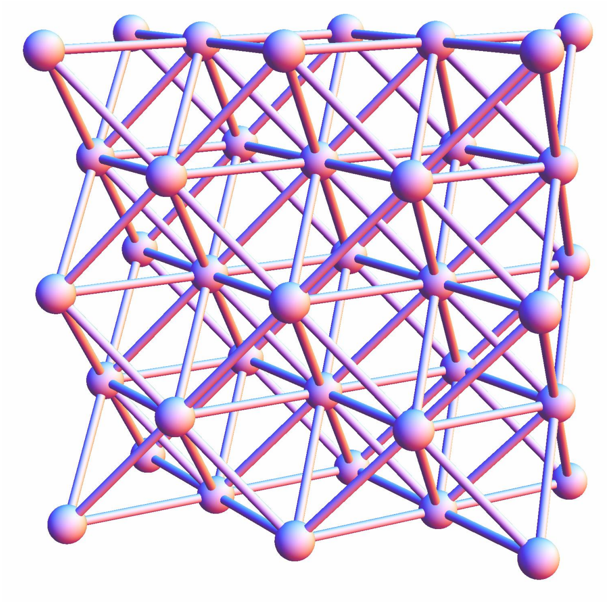

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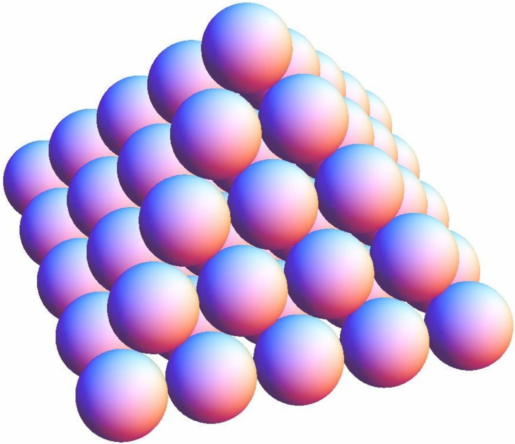
Densest possible packing: Kepler conjecture (Hales 2005)

$\longrightarrow$ 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

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

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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 Dimension

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 $p_n(\boldsymbol{x})$ = probability of being at position $\boldsymbol{x}$ 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 describes the return probabilities.

Here $\lambda(\boldsymbol{k})$ is the *structure function*, 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.

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:

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

  using the angle-sum identity $\cos(x\pm y)=\cos x\cos y\mp\sin x\sin y$.

- 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*:

$$R = 1 - \left(\frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{\mathrm{d}k_1 \, \mathrm{d}k_2 \, \mathrm{d}k_3}{1 - \frac{1}{3}(c_1 c_2 + c_1 c_3 + c_2 c_3)} \right)^{-1} = 1 - \frac{16 \sqrt[3]{4} \pi^4}{9 (\Gamma(\frac{1}{3}))^6}$$

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.

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

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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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$\longrightarrow$ 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 $(\binom{d}{2} - 1)$-fold sum.

Method 2: Naive Walk Enumeration

Proceed as follows:

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

- symmetry
- “return to the origin” property
- positions with odd coordinate sum cannot be reached

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.

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

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

The Differential Equation Detour

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

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

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

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

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*.

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 $\cos(k_i) \to x_i$:

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

Indeed, the integrand is annihilated by the operators:

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

Concrete Example: Creative Telescoping

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

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

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

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}+
7534597696291106962430400000z^{5}+39205436741982652114368000000z^{4}+
28783951431239861464320000000z^{3}+13480356439133473536000000000z^{2}+
2423069019610564608000000000z+192805230237696000000000000)P^{(8)}(z)z^{6}+2(z+
15)(800100086574208z^{36}+227389988057526336z^{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}+
3447189729571578013712505600000000000000z^{4}+3144130563959386258385101824000000000000z^{3}+
1403603566598885837201141760000000000000z^{2}+250840098120631904501760000000000000000z+
19733923803196565913600000000000000000)P^{(7)}(z)z^{5}+
$$

Result for the 6D fcc Lattice

$$(35882454730090752z^{37} + 1061260405161448665 6z^{36} + 1276532600942212775168z^{35} +$$
$$89393980129433032096320z^{34} + 4221606838983473228197008z^{33} + 145494567985766484898923048z^{32} +$$
$$3840828004490920060950969480z^{31} + 80160062388267727172211985080z^{30} +$$
$$1350855094398006902682870922050z^{29} + 18631082892630536824222949409585z^{28} +$$
$$211815796834464054711973645322142z^{27} + 1986708322085667572665525016037411z^{26} +$$
$$15263082383031406770429022758762048z^{25} + 94068732852089205756130773605094705z^{24} +$$
$$441055376229095921513357130918811338z^{23} + 1319636945498761264973744224282378779z^{22} -$$
$$1376268096732267953995912640790 41112z^{21} - 31072001737970299221405533198706303141z^{20} -$$
$$226886176666918560987240200768631693150z^{19} - 1033954017266382248984767586852072344191z^{18} -$$
$$3356732946224373601649087937349109785896z^{17} - 7573126212785007618891225542456994124245z^{16} -$$
$$9076459539413303184641722134776573895810z^{15} + 10278671248090335377408918358815408788425z^{14} +$$
$$85149274357043292385925033653294291853550z^{13} + 240689360358498296007939096187740586134000z^{12} +$$
$$429409878921957648790555775268242743350000z^{11} + 495779225046771906420255540348281344800000z^{10}$$
$$287121363379312616871562346484465378000000z^{9} - 119682652007548350954457856750250720000000z^{8} -$$
$$395683465592680867401293480616198000000000z^{7} - 327383462755042385949747691240824000000000z^{6} -$$
$$866425754505013910667872020195200000000000z^{5} + 597046839721706795489319772224000000000000z^{4} +$$
$$725116102774123909908393630720000000000000z^{3} + 338828967558720719568862617600000000000000z^{2} +$$
$$63111567713049173257666560000000000000000z + 51232302181375699968000000000000000000000)P^{(6)}(z)z^{4} +$$
$$3(13024002087218124 8z^{37} + 3807222047478676915 2z^{36} + 448027411720532102323 2z^{35} +$$
$$30598839345549153729024 0z^{34} + 14079224644087925329523520z^{33} + 472739613103493977658692800z^{32} +$$
$$12162402278802667065896636880z^{31} + 247501384020921867412586484240z^{30} +$$
$$4068564888973003880820853550310z^{29} + 54750340798147926328921245513135z^{28} +$$
$$607255705204278811351245801585018z^{27} + 5552646100941335755747908121811397z^{26} +$$
$$41511153616540066669903815109576752z^{25} + 247864598814302846690177415162792735z^{24} +$$
$$1112001535696035843878120629687073790z^{23} + 3006740720618245361400876608130182349z^{22} -$$
$$3066274907647801401815807099801425704z^{21} - 93149956267467504725225680596497523339z^{20} -$$
$$635954475887313295192241042199635547930z^{19} - 2858027882158570016919188514224326558185z^{18} -$$
$$9468529098949077023394535618861256937240z^{17} - 23191419391770985171480237991217872142915z^{16} -$$
$$38330478964162570556645949941637505810110z^{15} - 23459339067193287788165144055727575111225z^{14} +$$
$$87213988833696382614552027738719280959850z^{13} + 349803608265045461612489069936675179800000z^{12} +$$
$$696554593654757665866719966270600171130000z^{11} +$$

Result for the 6D fcc Lattice

$$865953342265454601104437816976581680000000z^{10}+586378944861718695144037906690882422000000z^{9}-$$
$$448918716637412377029136427636037600000000z^{8}-526332032930456915428235817813056400000000z^{7}-$$
$$518937227107573341964843985332680000000000z^{6}-226302972537833147253780811598400000000000z^{5}+$$
$$104974053097834899670129395840000000000000z^{4}+641357814865841417537072778240000000000000z^{3}+$$
$$347089467368149273535429836800000000000000z^{2}+699409221434846453300428800000000000000000z+$$
$$595812699442665547776000000000000000000000)P^{(5)}(z)z^{3}+15(1461877785299993\,60z^{37}+$$
$$4223268089848725120 0z^{36}+485766573409896369024 0z^{35}+32316579131970248403552 0z^{34}+$$
$$1446760113658410970765440 0z^{33}+472534466386674980533072704z^{32}+11827310475440684698801079376z$$
$$234205994182438943769949245108z^{30}+3746772515516029997311378363446z^{29}+$$
$$490565172884487019349669493992 01z^{28}+52896073753822096219923216572670 0z^{27}+$$
$$4693678127508685757329704793118274z^{26}+33925520928056707379949042245154948z^{25}+$$
$$194225784819376433418854177036400765z^{24}+815865984997630892337526061797547730z^{23}+$$
$$1820210924970374403477059898368292414z^{22}-5626714951506760337684784884293147302z^{21}-$$
$$87288636539051237531541938169181610997z^{20}-548617946604162829617617348998523187024z^{19}-$$
$$2396582727922965009354571656000074347578z^{18}-7949778754688875639594299226888542864672z^{17}-$$
$$20284887219829242010855806602752336703097z^{16}-38476335393060119379820741759126402451166z^{15}-$$
$$47185211186009106848535876331178061122490z^{14}-10222760436927155616364669208395729054260z^{13}+$$
$$107413528041921729529347960434391761302800z^{12}+279266241080334469793315941614102969564000z^{11}$$
$$379975092805467869163550626412993759200000z^{10}+276342679146887322412220759883497997600000z^{9}+$$
$$633792615980891821330869081670046400000 0z^{8}-2149651298091206908272829027314686400000 00z^{7}-$$
$$2424557018759285535178443324933024000000 00z^{6}-14026124741577288569154640743552000000000 0z^{5}-$$
$$36772706828360958944274523883520000000000z^{4}+77477283796273934947265452032000000000000z^{3}+$$
$$75225685122988247345321041920000000000000z^{2}+17760293941127209315703193600000000000000z+$$
$$1618181751862118404915200000000000000000)P^{(4)}(z)z^{2}+90(6910694985054515 2z^{37}+$$
$$1972812595897802803 2z^{36}+221566662927925099724 8z^{35}+14338736108436054355737 6z^{34}+$$
$$623580276394586806342435 2z^{33}+197763282456363307438541552z^{32}+4805890762274729535435673296z^{31}$$
$$923909991148149059073179743 92z^{30}+14344858211621752378880914720 86z^{29}+$$
$$18213230428133179674440523308931z^{28}+190122674553786922619563973540916z^{27}+$$
$$1627987793820686707319681442965532z^{26}+11283714208962998257330503635013918z^{25}+$$
$$61070425289478623056319494081223364z^{24}+232117491219054750436300759063832796z^{23}+$$
$$335162333006577190998078624832466745z^{22}-$$

Result for the 6D fcc Lattice

$$3212526847572548623801062566839102968z^{21} - 3392965866525625940881278435486638557z^{20} - 1951831789900573496432722754351267363 40z^{19} - 8185961182051286059853304788561116790 58z^{18} - 2671193766306193321259081077503739718922z^{17} - 6879647707640439013900747488611335523490z^{16} - 1379139225878289581995545399895510251754 8z^{15} - 2039504216816486273624834199179924314327 5z^{14} - 1855905114263490123161823006701124526173 0z^{13} + 3407638735402551318083430675030634548 00z^{12} + 3257326839237100365484129096668460631400 0z^{11} + 5466062732110740554093410787098386984000 0z^{10} + 4197072940270847392338662093562381480000 0z^{9} + 7577293239379519390446429293510400000 00z^{8} - 3465345486136948584706296425184552000000 0z^{7} - 4190926430444018560287676453660320000000 0z^{6} - 2764938702145552027676616654604800000000 0z^{5} - 9932878926912153370258947363840000000000 z^{4} - 1112041174659253407521806233600000000000 z^{3} + 2849114538408597196020019200000000000000 z^{2} + 1142306781314819226668236800000000000000 z + 1148615564955287298048000000000000000000)P^{(3)}(z)z +$$

$$90(4556502187948032z^{35} + 125450296082457292 8z^{34} + 13018547375127734988 8z^{33} + 7675748903189765748480z^{32} + 302276251598295683586240z^{31} + 8653460076869413651316640z^{30} + 189382045823502675349219920z^{29} + 3269391489631666671425989920z^{28} + 45371384308945745114138623620z^{27} + 510811439434664402615401586970z^{26} + 4663284432121091702260620852777z^{25} + 34047746401934351907977621763618z^{24} + 190773160991774404319508940400373z^{23} + 717575244018720111969771948822450z^{22} + 574602465936356660227512513519630z^{21} - 1637741546116042110308200542114644 4z^{20} - 1581950482369037259488002576985820 66z^{19} - 9246260014932568335203802331153828 26z^{18} - 4044657270312306250764976742472089595z^{17} - 14017460872371123201967056591950292270z^{16} - 39203789245543299948038211301310631735z^{15} - 88492994651041978105789511893808827410z^{14} - 158672230290697625052364901820833352540z^{13} - 217051701285403806039787021788244210200z^{12} - 204430925935804223158200138096719244000z^{11} - 83930464288781215080378386513083200000z^{10} + 98749247882439137822044179686396640000z^{9} + 234855990648514674287291744222356800000z^{8} + 252029928377053385449407192172320000000z^{7} + 165979815868291791006070607462400000000z^{6} + 52113850317609070332668882227200000000z^{5} - 9698100095942063765846249472000000000z^{4} - 12270310453108287668341923840000000000z^{3} - 3932207868973120630810214400000000000z^{2} - 578659365675271609712640000000000000z - 26986562465909833728000000000000000)P(z) +$$

$$45(8809237563366195 2z^{36} + 2454929977696474521 6z^{35} + 26193575275540078407 68z^{34} + 1596286114809884359065 60z^{33} + 6513463004865397861819008z^{32} + 193479386194110772817766720z^{31} + 4398883914180352580752205664z^{30} + 79010991647695967734365641136z^{29} +$$

Result for the 6D fcc Lattice

$$1143508859378085891069139805496z^{28} + 1347828522176737423743381389415 6z^{27} +$$
$$12967481859657838184170935236331 0z^{26} + 1010115611151696866102360444043867z^{25} +$$
$$6203408988166712509967367951961350z^{24} + 2782834220828526964581126761397575 1z^{23} +$$
$$6540406228719004529247350188237644 6z^{22} - 2329669581156953199668980714871155 50z^{21} -$$
$$3776626287411277314694612568191478460z^{20} - 2566599099502838134775728413297379008 6z^{19} -$$
$$12330432201735600084488496344721300430 2z^{18} - 461005100390610028275047960932687009761z^{17} -$$
$$1382954753973214192431623770039149437562z^{16} - 3351334353377309619203633178809010250269z^{15} -$$
$$6500636144955681369542005264067707999470z^{14} - 9808779912515181085311292716635118617340z^{13} -$$
$$10758301750323045400708026810527005985400z^{12} - 6955035214429661410040236974622315476000z^{11} +$$
$$6981140777757766718851536754637620800 00z^{10} + 7349743557503879010410921836212410400000z^{9} +$$
$$8691043975963666049447299379144001600000z^{8} + 5165781565021067274342996673450656000000z^{7} +$$
$$4013363318863177741077133187904000000 00z^{6} - 2226964464248713386006518356377600000000z^{5} -$$
$$186353476702189192213117998796800000000 0z^{4} - 655267817084534423521940643840000000000z^{3} -$$
$$12258850488317871618828533760000000000 0z^{2} - 8434528659189021937434624000000000000z +$$
$$186207281014777852723200000000000000 0)P'(z) + 45(180741253455271936z^{37} +$$
$$509807062676369848 32z^{36} + 5584340634105826525184z^{35} + 35101006700535148822425 6z^{34} +$$
$$148020804054836778239431 04z^{33} + 454875015831485400909097248z^{32} + 10707051961496414217407305536z$$
$$1992882916936004451670664714 88z^{30} + 29932647745401008160507081545 40z^{29} +$$
$$367074145552194684404472419039 70z^{28} + 369055333918742878506923895821094z^{27} +$$
$$3028085987873439981041316741040299z^{26} + 1990811820727714328084691755273863 8z^{25} +$$
$$9977135720587522014510946645010651 7z^{24} + 32204116185543506281453342072328248 2z^{23} -$$
$$374464592158210104407054773630095 0z^{22} - 858368654555170847175829121046069103 2z^{21} -$$
$$7029464735690152410102474097293305691 6z^{20} - 36969293487586269267877075661236045707 0z^{19} -$$
$$147214977976430391291070082511951312574 5z^{18} - 464622768606334736814026972110265692319 4z^{17} -$$
$$1175772146089121725315050743722297659096 3z^{16} - 2366752490571808731981420802294141008335 4z^{15} -$$
$$3674781432634711427037798715831161233826 0z^{14} - 4065296610031057621942283934585108515484 0z^{13} -$$
$$2419355326304235125911742553950270151840 0z^{12} + 9719645940829530820988532518598953424000z^{11} +$$
$$372973414525651557027878105163615336000 00z^{10} + 3476411901315617635383740361997011360000 0z^{9} +$$
$$674683108256279898237849563695795200000 0z^{8} - 206567614085456615808107511463276800000 00z^{7} -$$
$$296590785716996082563757344262144000000 00z^{6} - 209328340890338852707306503014400000000 00z^{5} -$$
$$778439230783972616865055592448000000000 00z^{4} - 142858314386426996076979077120000000000 0z^{3} -$$
$$8324112389233016688574464000000000000 00z^{2} + 148601506218532499423232000000000000000z +$$
$$161919374795459002368000000000000000 00)P''(z) = 0$$

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 $d = 5$: $\sim$ 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

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 behaviour of the solutions.

In particular, we got the following results:

- $d = 3$: $R_3 = 1 - \frac{16\sqrt[3]{4}\pi^4}{9(\Gamma(\frac{1}{3}))^6} = 0.2563182365\ldots$
- $d = 4$: $R_4 = 0.09571315417256289673531676490121018 5\ldots$
- $d = 5$: $R_5 = 0.04657695746384802419337442059480329 1\ldots$
- $d = 6$: $R_6 = 0.02699987828795612426936417542619638 0\ldots$

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