

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

Christoph Koutschan

Research Institute for Symbolic Computation
Johannes Kepler Universität Linz, Austria

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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*.

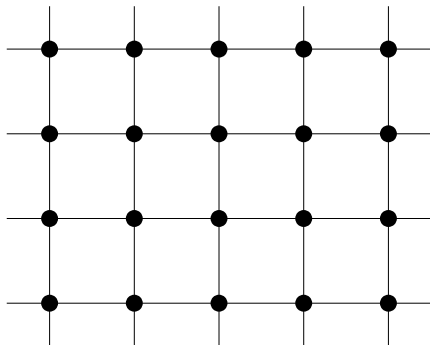
Consider random walks on the lattice points:

- 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 $\mathbf{0}$.



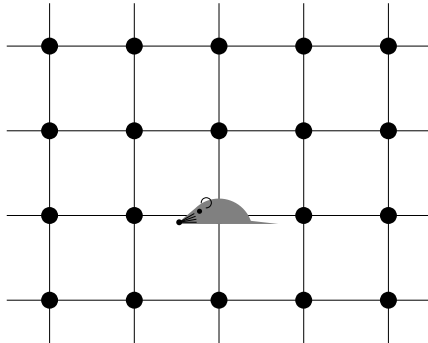
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square lattice (= integer lattice \mathbb{Z}^2)



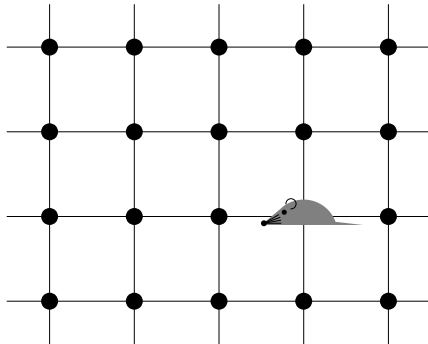
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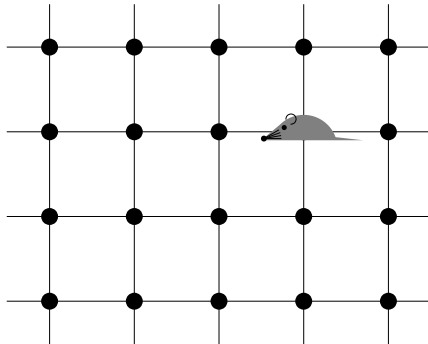
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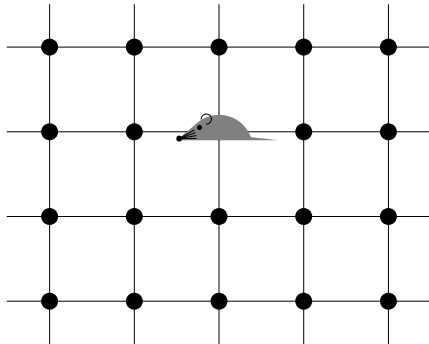
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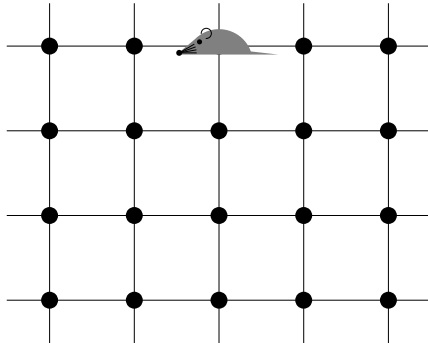
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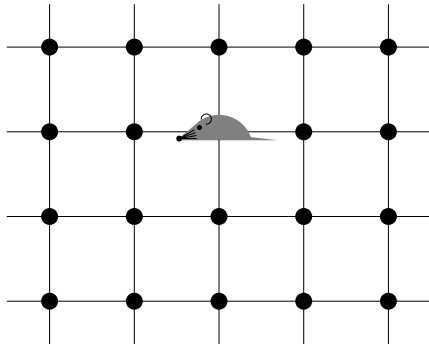
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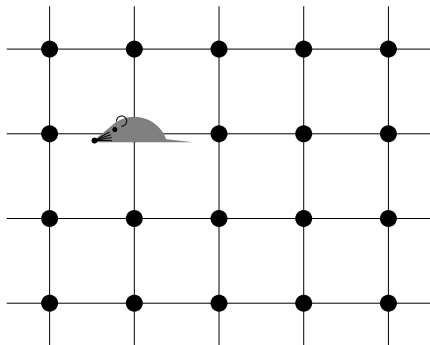
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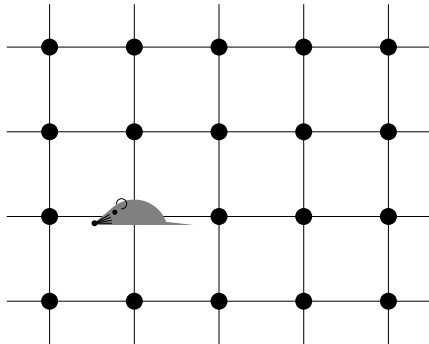
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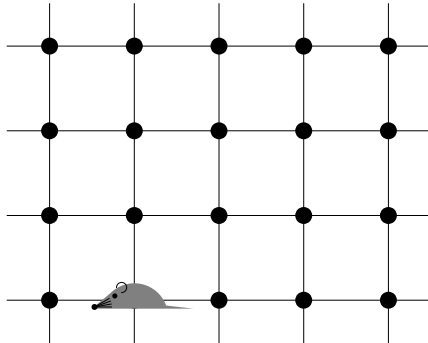
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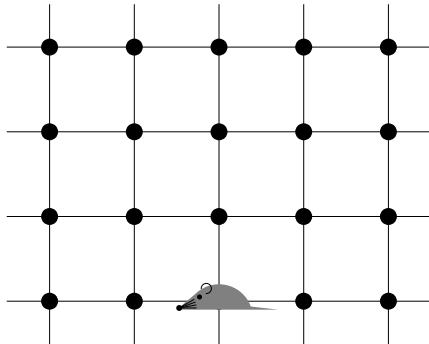
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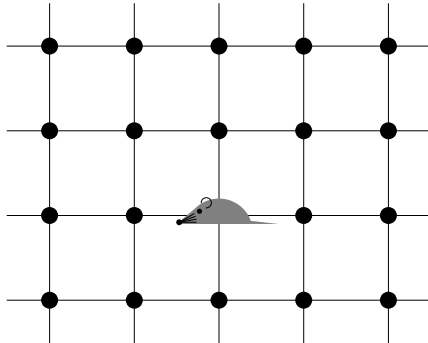
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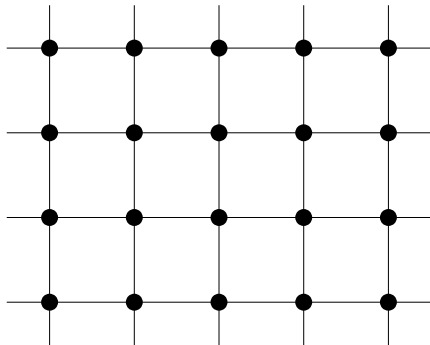
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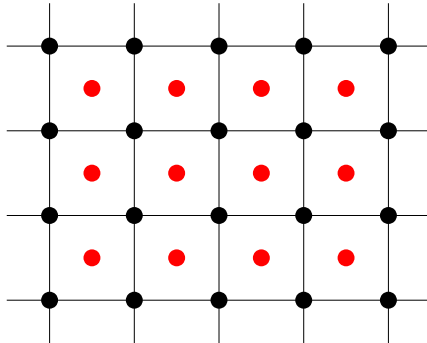
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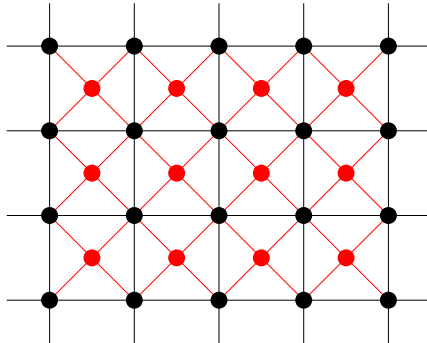
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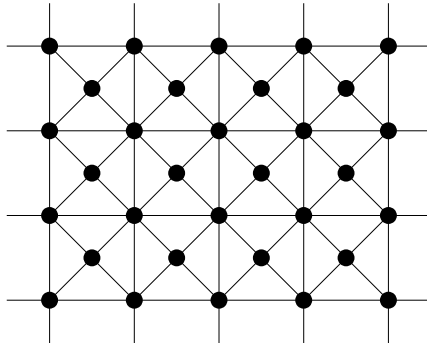
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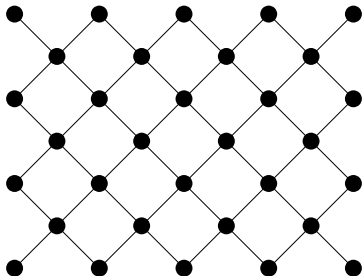
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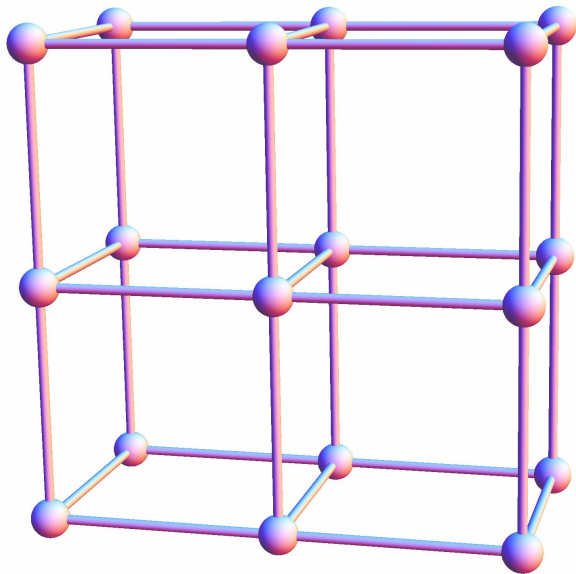


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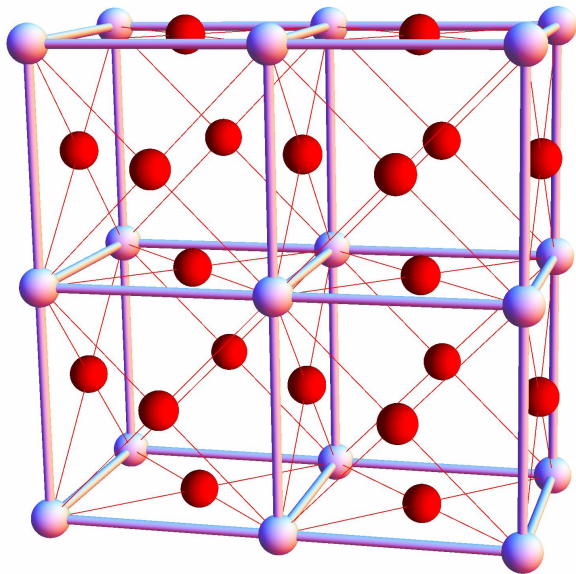
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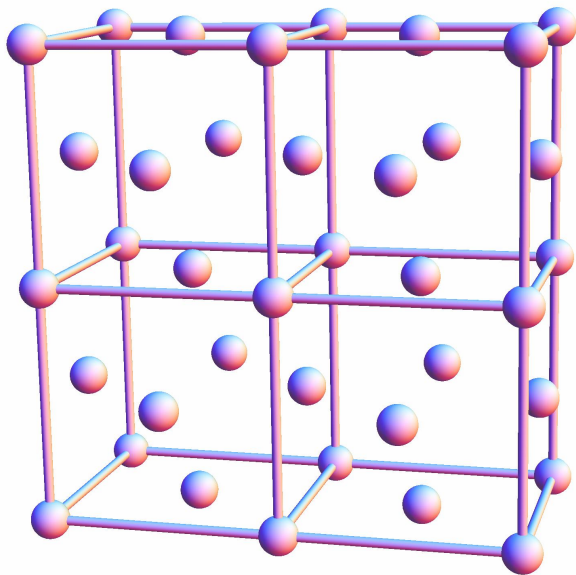
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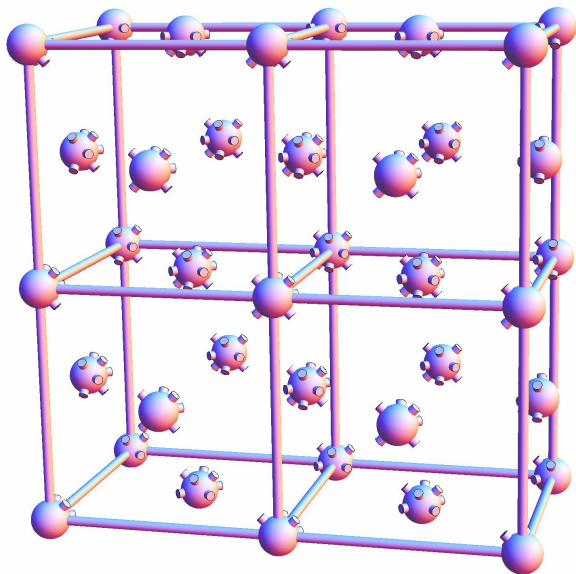
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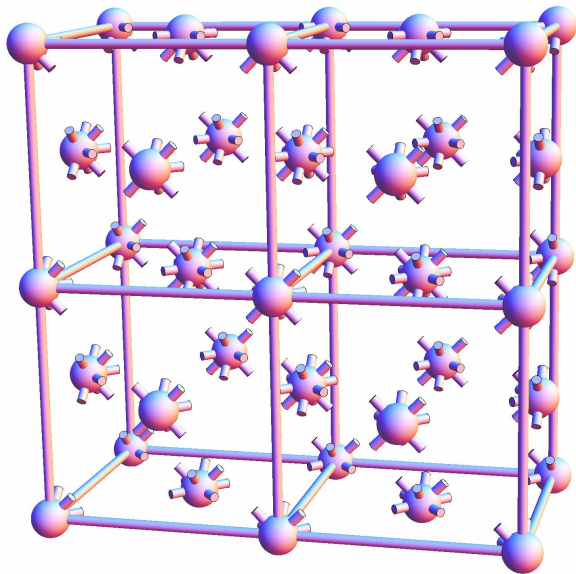
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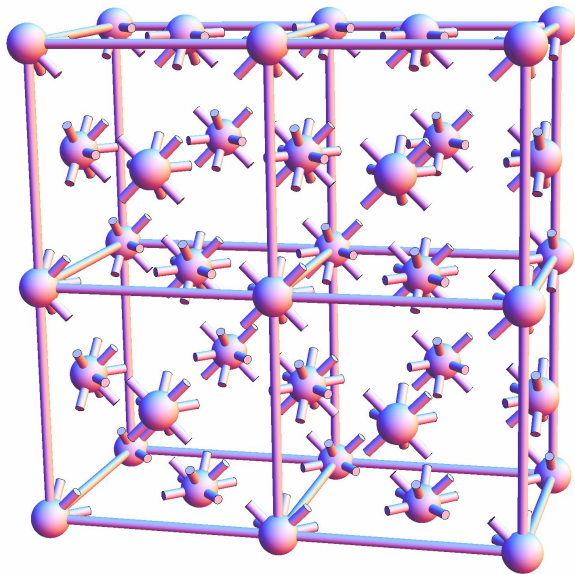
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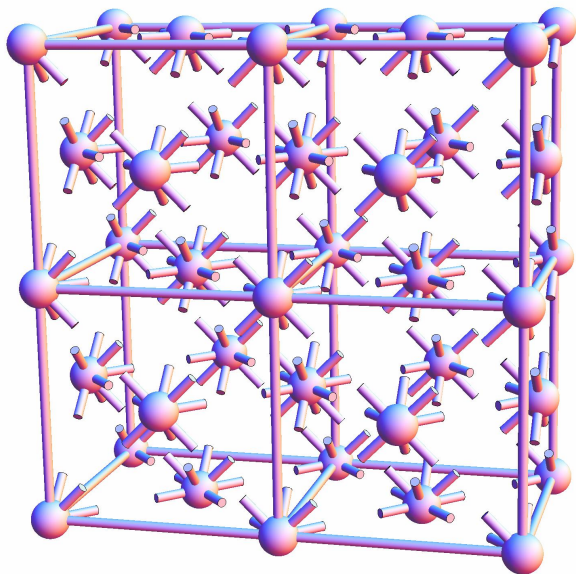
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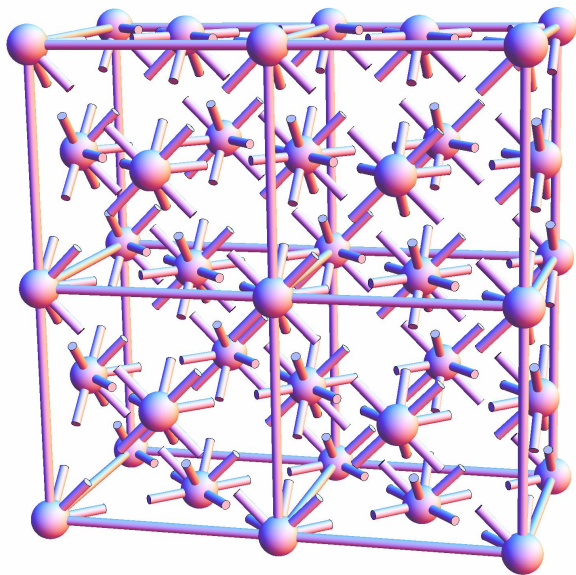
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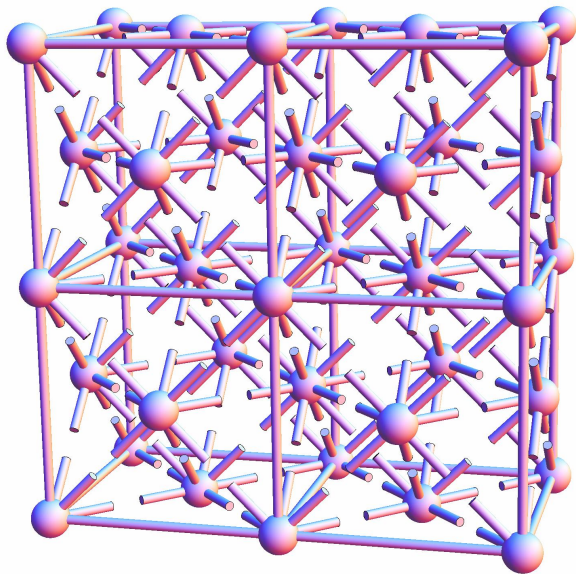
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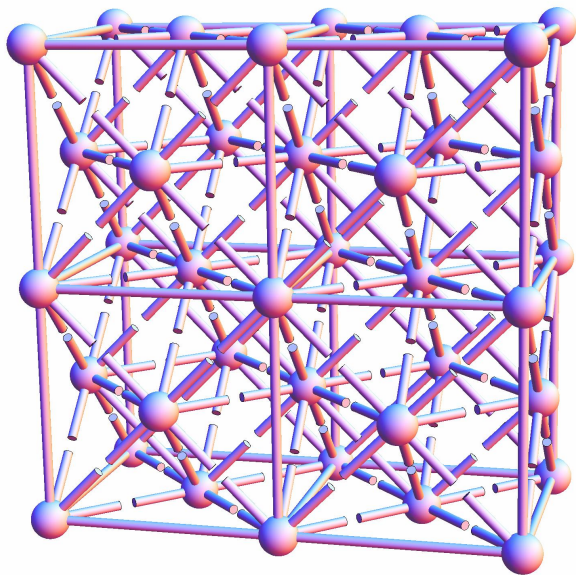
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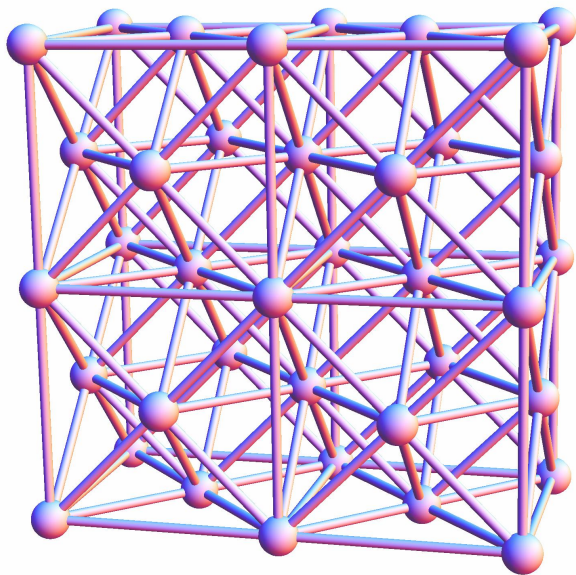
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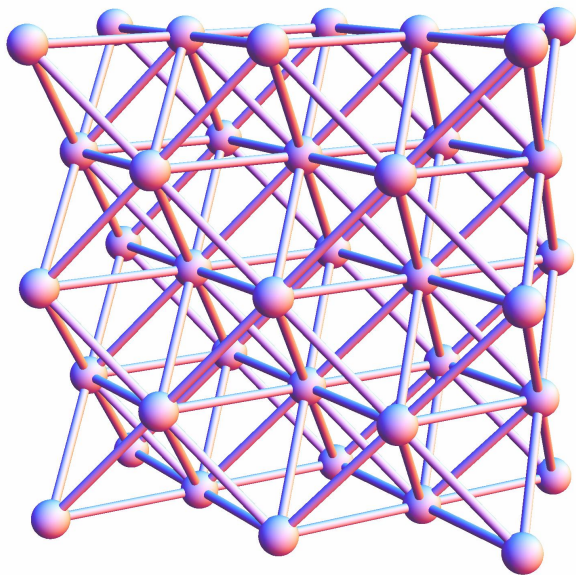
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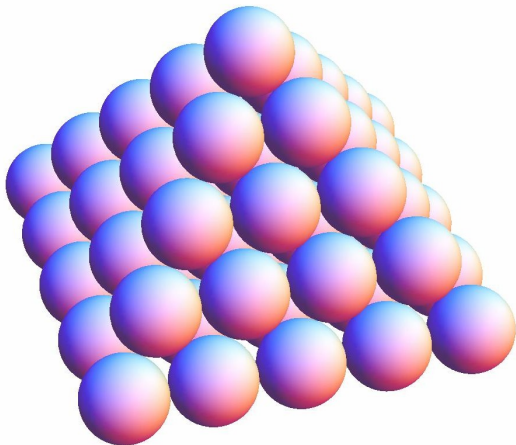
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The fcc Lattice in 3D

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 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

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

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



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

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

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

The lattice Green's function is

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

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



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!



Back to the fcc Lattice

The trivial (but illuminating) 2D case:

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

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

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

- lattice Green's function:

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

→ 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!



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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

- rewriting and expanding the d -fold integral into a multisum (Guttman and Broadhurst)
- counting all possible walks on the lattice
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→ However, any result obtained in this way is just a *conjecture*!



A Different Approach to the LGF

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Define the generating function $F(\mathbf{y}; z) = \sum_{n=0}^{\infty} \sum_{\mathbf{x} \in \mathbb{Z}^d} p_n(\mathbf{x}) \mathbf{y}^{\mathbf{x}} z^n$.



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



The Differential Equation Detour

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

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



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



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

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



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*.



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 ∂ -finite/holonomic (no ODE w.r.t. k_1 for example).



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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 ∂ -finite/holonomic (no ODE w.r.t. k_1 for example).

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

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

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

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



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 + \\ & 2423069019610564608000000000z + 19280523023769600000000000)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 - 146028614696018444033629739148560000000z^7 - \\ & 107449871787476739366490039367520000000z^6 - 14502187460839465105963884748800000000z^5 + \\ & 34471897295715780137125056000000000000z^4 + 31441305639593862583851018240000000000z^3 + \\ & 140360356659888583720114176000000000000z^2 + 250840098120631904501760000000000000z \\ & 19733923803196565913600000000000000)P^{(7)}(z)z^5 + \end{aligned}$$



Result for the 6D fcc Lattice

$$\begin{aligned} & (35882454730090752z^{37} + 10612604051614486656z^{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} - \\ & 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 + 338828967558720719568862617600000000000z^2 + \\ & 63111567713049173257666560000000000000z + 51232302181375699968000000000000000)P^{(6)}(z)z^4 \\ & 3(130240020872181248z^{37} + 38072220474786769152z^{36} + 4480274117205321023232z^{35} + \\ & 305988393455491537290240z^{34} + 14079224644087925329523520z^{33} + 472739613103493977658692800z^{32} + \\ & 12162402278802667065896636880z^{31} + 247501384020921867412586484240z^{30} + \\ & 4068564888973003880820853550310z^{29} + 54750340798147926328921245513135z^{28} + \\ & 607255705204278811351245801585018z^{27} + 5552646100941335755747908121811397z^{26} + \\ & 4151115361654006669903815109576752z^{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} + 58637894486171869514403790669088242200000z^9 \\ & 44891871663741237702913642763603760000000z^8 - 526332032930456915428235817813056400000000z^7 - \\ & 5189372271707573341964843985332680000000000z^6 - 22630297253783314725378081159840000000000z^5 + \\ & 1049740530978348996701293958400000000000z^4 + 6413578148658414175370727782400000000000z^3 + \\ & 3470894673681492735354298368000000000000z^2 + 6994092214348464533004288000000000000z + \\ & 59581269944266554777600000000000000000P^{(5)}(z)z^3 + 15(146187778529999360z^{37} + \\ & 42232680898487251200z^{36} + 4857665734098963690240z^{35} + 323165791319702484035520z^{34} + \\ & 14467601136584109707654400z^{33} + 472534466386674980533072704z^{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 + \\ & 6337926159808918213308690816700464000000z^8 - 21496512980912069082728290273146864000000z^7 - \\ & 242455701875928553517844332493302400000000z^6 - 140261247415772885691546407435520000000000z^5 - \\ & 36772706828360958944274523883520000000000z^4 + 774772837962739349472654520320000000000z^3 + \\ & 7522568512298824734532104192000000000000z^2 + 177602939411272093157031936000000000000z + \\ & 161818175186211840491520000000000000000P^{(4)}(z)z^2 + 90(69106949850545152z^{37} + \\ & 19728125958978028032z^{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} - \end{aligned}$$



Result for the 6D fcc Lattice

$$\begin{aligned} & 1143508859378085891069139805496z^{28} + 13478285221767374237433813894156z^{27} + \\ & 129674818596578381841709352363310z^{26} + 1010115611151696866102360444043867z^{25} + \\ & 6203408988166712509967367951961350z^{24} + 27828342208285269645811267613975751z^{23} + \\ & 65404062287190045292473501882376446z^{22} - 232966958115695319966898071487115550z^{21} - \\ & 3776626287411277314694612568191478460z^{20} - 25665990995028381347757284132973790086z^{19} - \\ & 123304322017356000844884963447213004302z^{18} - 461005100390610028275047960932687009761z^{17} - \\ & 1382954753973214192431623770039149437562z^{16} - 3351334353377309619203633178809010250269z^{15} - \\ & 6500636144955681369542005264067707999470z^{14} - 9808779912515181085311292716635118617340z^{13} - \\ & 10758301750323045400708026810527005985400z^{12} - 6955035214429661410040236974622315476000z^{11} + \\ & 69811407705776671885153675463762080000z^{10} + 734974355703879010410921836212410400000z^9 + \\ & 8691043975963666049447299379144001600000z^8 + 5165781565021067274342996673450656000000z^7 + \\ & 40133633188631777410771331879040000000z^6 - 2226964464248713386006518356377600000000z^5 - \\ & 1863534767021891922131179987968000000000z^4 - 655267817084534423521940643840000000000z^3 - \\ & 122588504883178716188285337600000000000z^2 - 843452865918902193743462400000000000z + \\ & 18620728101477785272320000000000000)P'(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} - 858368654555170847175829121046091032z^{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 - 2093283408903388527073065030144000000000z^5 - \\ & 7784392307839726168650555924480000000000z^4 - 1428583143864269960769790771200000000000z^3 - \\ & 8324112389233016688574464000000000000z^2 + 1486015062185324994232320000000000000z + \\ & 161919374795459002368000000000000000)P''(z) = 0 \end{aligned}$$



Some Timings

Timings with our new approach to creative telescoping:

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



Some Timings

Timings with our new approach to creative telescoping:

- for $d = 3$: ~ 2 seconds
- for $d = 4$: ~ 3 minutes
- for $d = 5$: ~ 4 hours
- for $d = 6$: ~ 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

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:

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

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

