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

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Introduction

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

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

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

$\longrightarrow$ 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

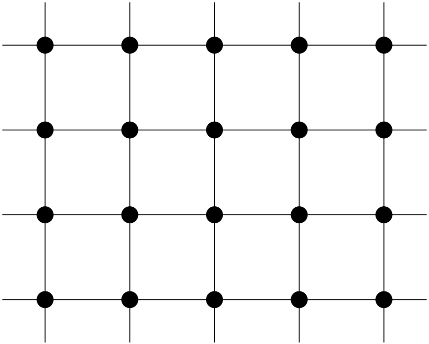
Study random walks on the *face-centered cubic (fcc) lattice*.

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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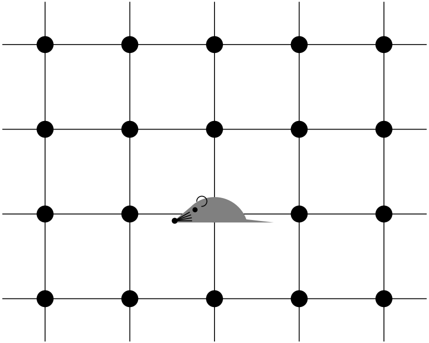

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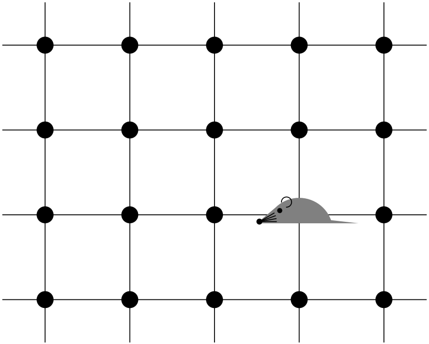

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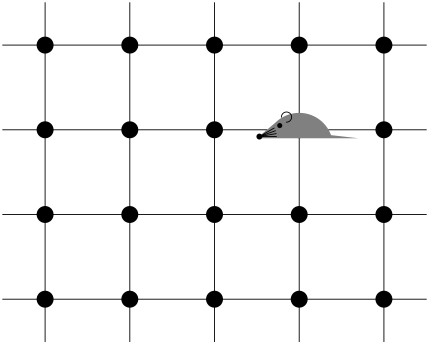

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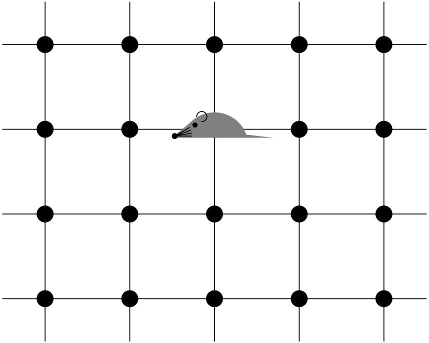

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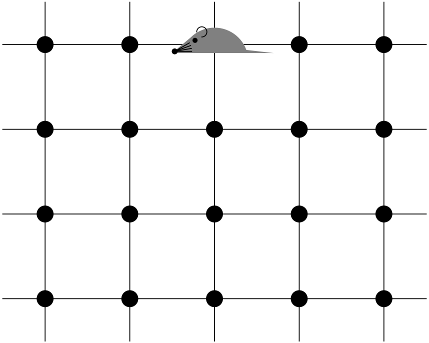

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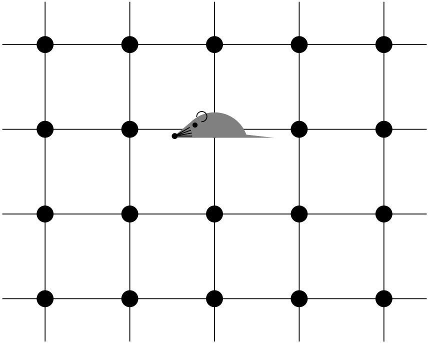

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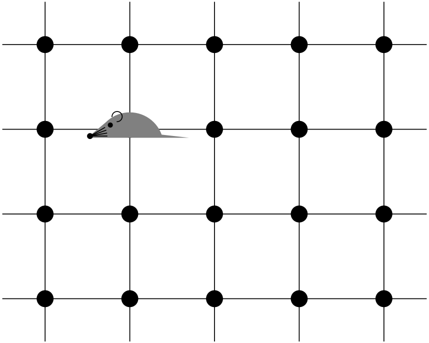

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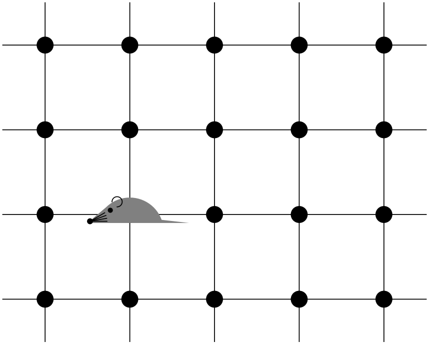

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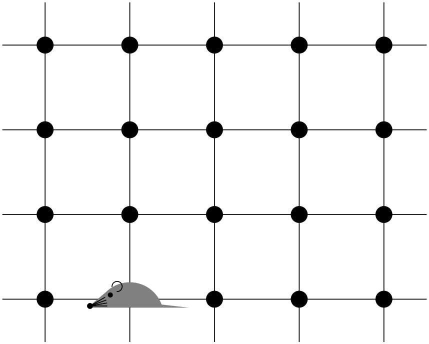

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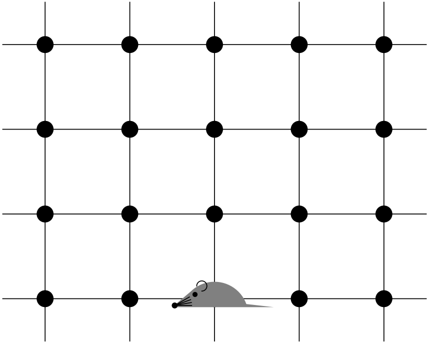

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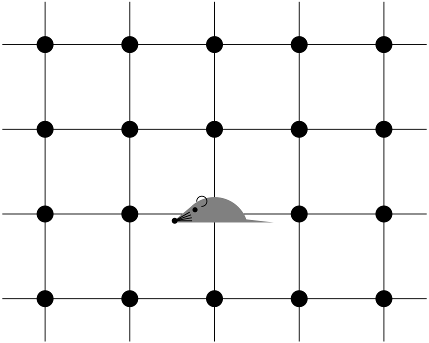

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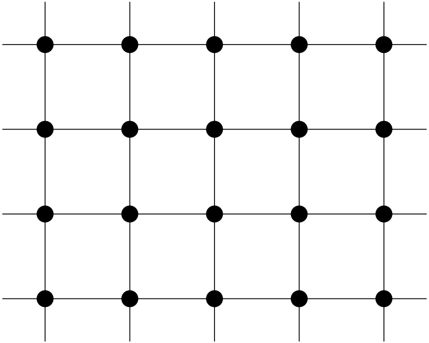

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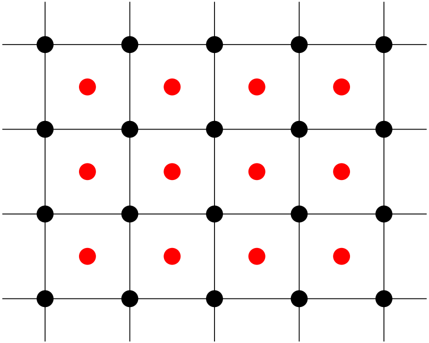

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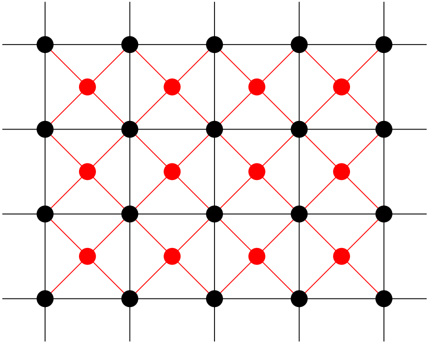

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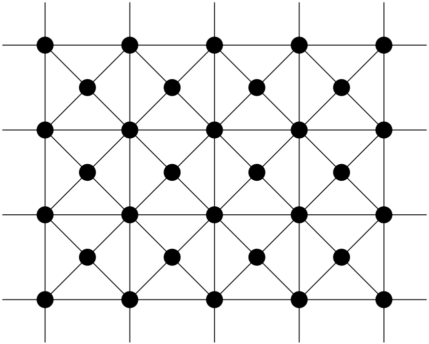

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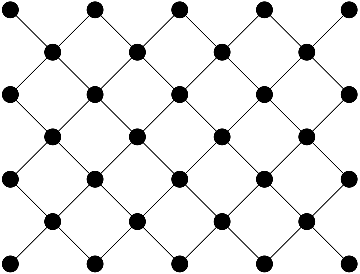

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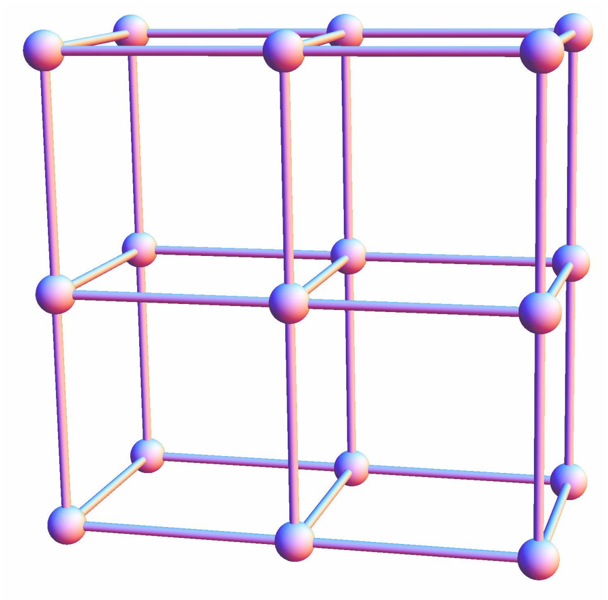

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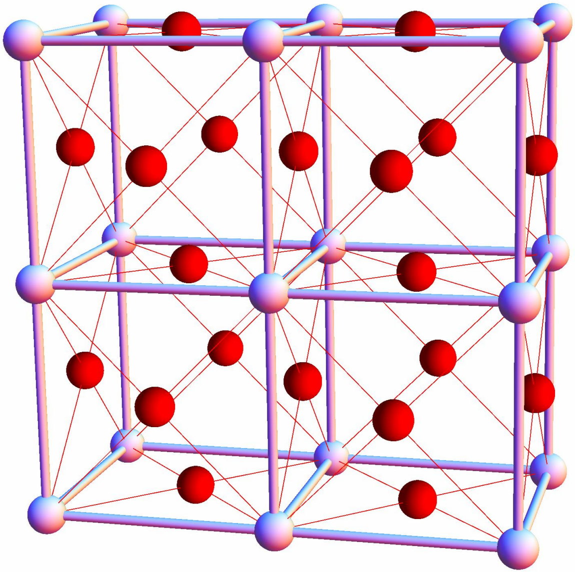

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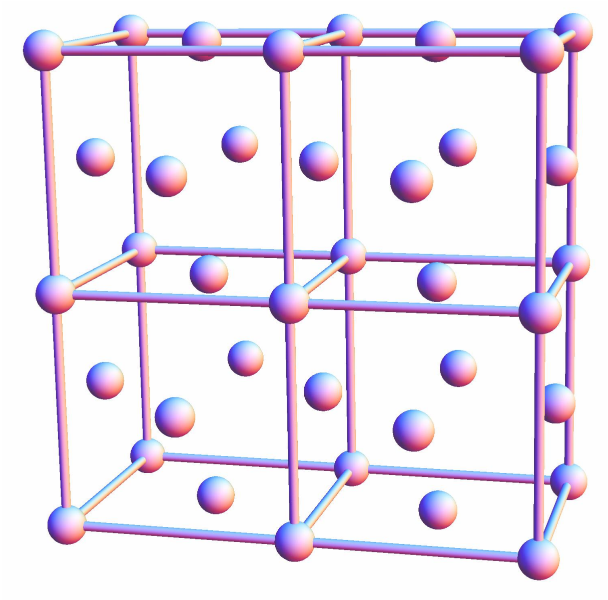

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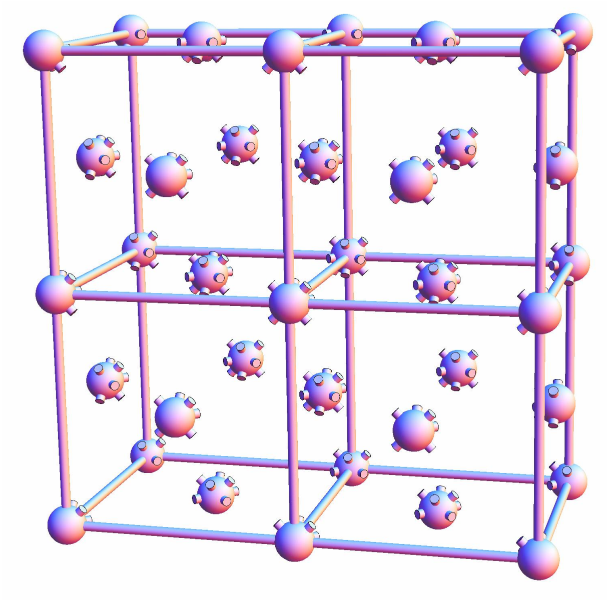

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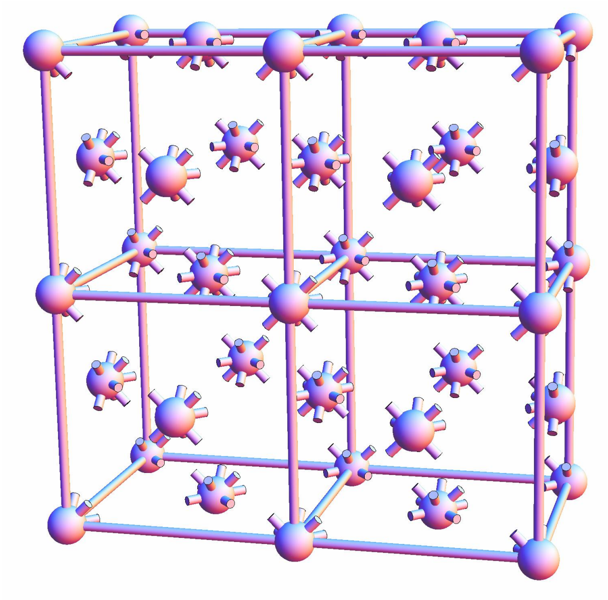

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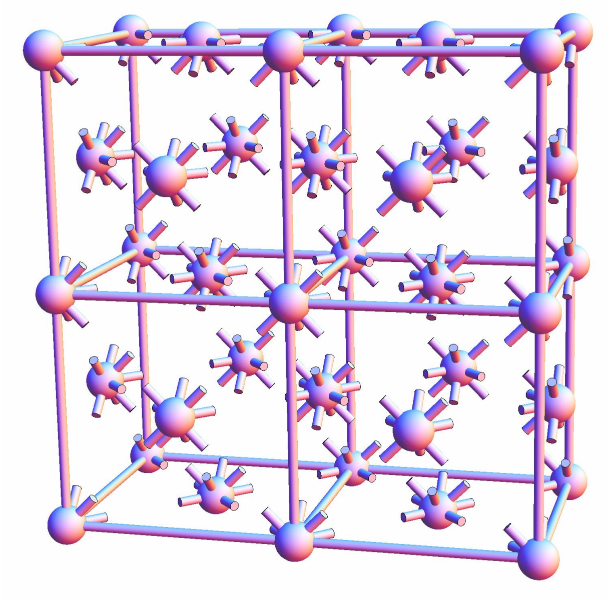

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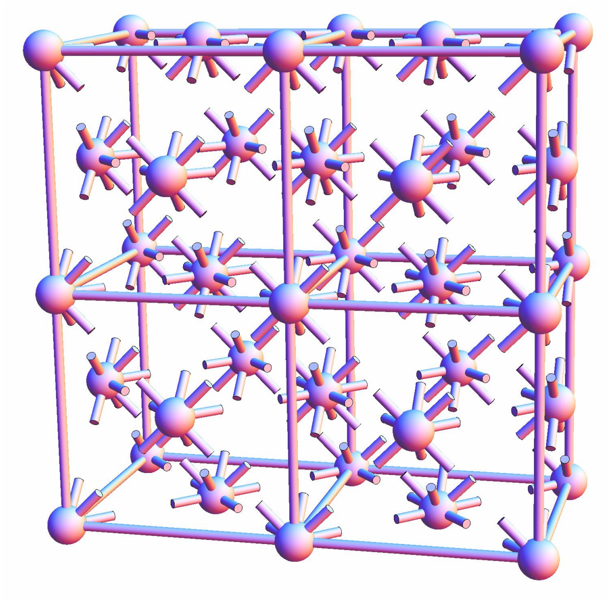

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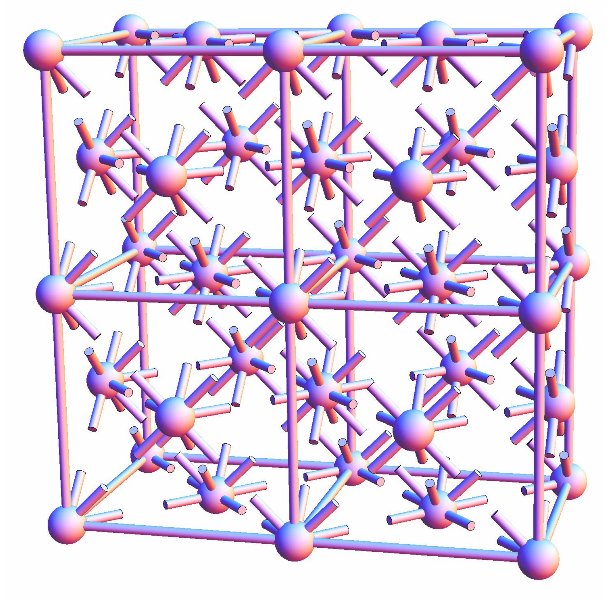

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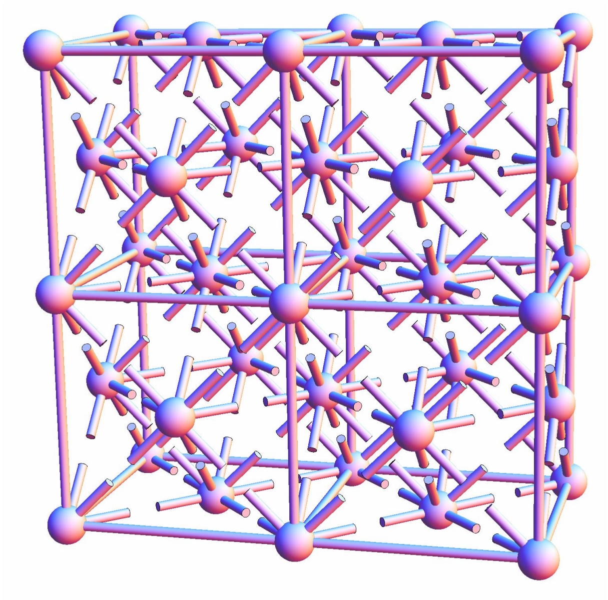

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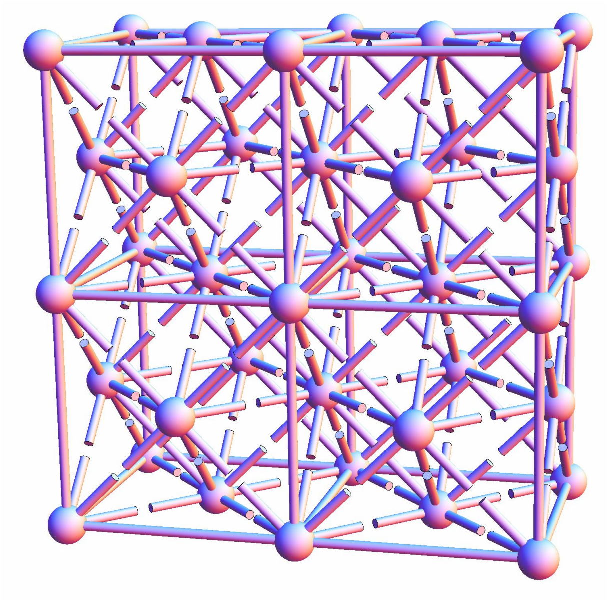

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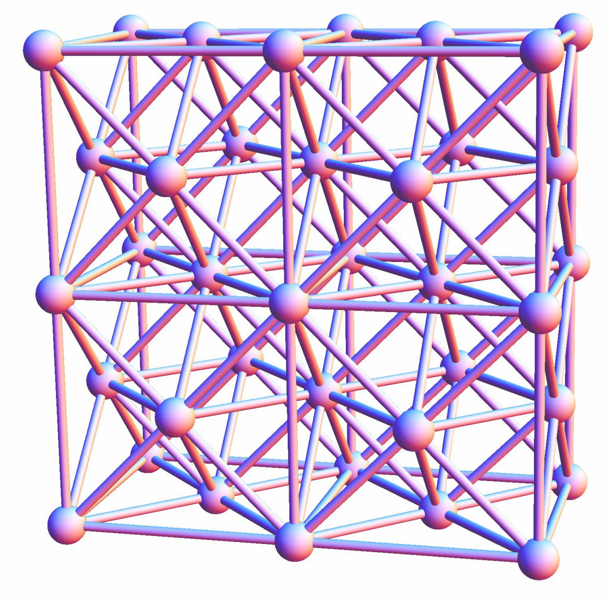

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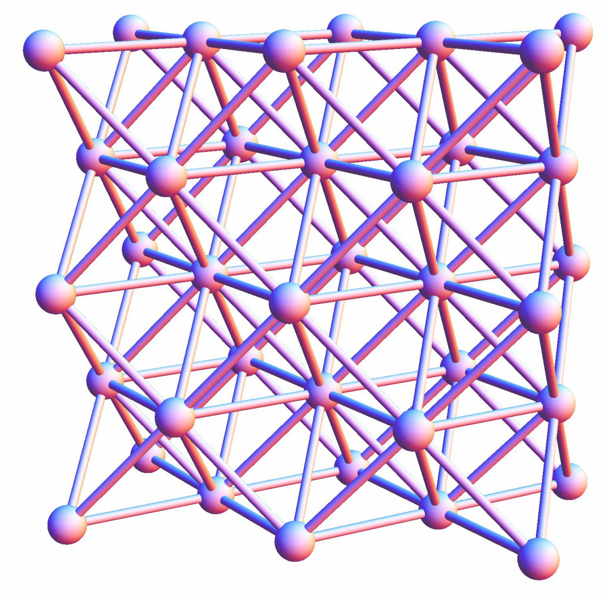
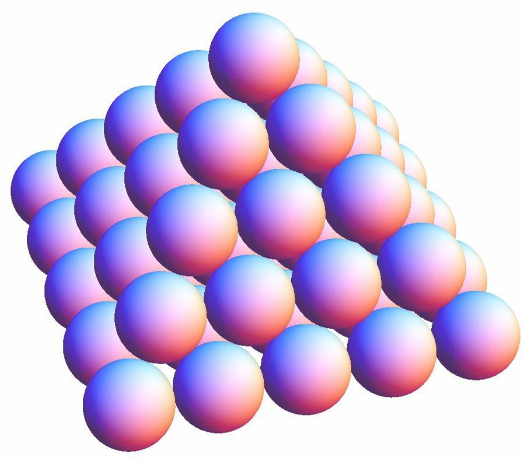


The fcc Lattice in 3D

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 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 returning to 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 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!

Differential Equation Approach

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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

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

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

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

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

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

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*.

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

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

Indeed, the integrand is annihilated by the operators:

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

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

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

Result for the 6D fcc Lattice

$$
\begin{gathered}
(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)P^{(8)}(z)z^{6}+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}+3144130563959386258385101824000000000000z^{3}+ \\
1403603566598885837201141760000000000000z^{2}+2508400981206319045017600000000000000000z+ \\
1973392380319656591360000000000000000000)P^{(7)}(z)z^{5}+
\end{gathered}
$$

Result for the 6D fcc Lattice

$$
\begin{aligned}
&(35882454730090752z^{37} + 1061260405161448665 6z^{36} + 127653260094221277516 8z^{35} + \\
&89393980129433032096320z^{34} + 4221606838983473228197008z^{33} + 14549456798576648489892304 8z^{32} + \\
&384082800449092006095096948 0z^{31} + 801600623882677271722119850 80z^{30} + \\
&135085509439800690268287092205 0z^{29} + 186310828926305368242229494095 85z^{28} + \\
&211815796834464054711973645322142z^{27} + 198670832208566757266552501603741 1z^{26} + \\
&152630823830314067704290227587620 48z^{25} + 940687328520892057561307736050947 05z^{24} + \\
&441055376229095921513357130918811338z^{23} + 131963694549876126497374422428237877 9z^{22} - \\
&137626809673226795399591264079041112z^{21} - 310720017379702992214055331987063031 41z^{20} - \\
&226886176666918560987240200768631693150z^{19} - 103395401726638224898476758685207234419 1z^{18} - \\
&335673294622437360164908793734910978589 6z^{17} - 757312621278500761889122554245699412424 5z^{16} - \\
&907645953941330318464172213477657389581 0z^{15} + 102786712480903353774089183588154087884 25z^{14} + \\
&851492743570432923859250336532942918535 50z^{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)P^{(6)}(z)z^{4} \\
&3(13024002087218124 8z^{37} + 3807222047478676915 2z^{36} + 4480274117205321023232z^{35} + \\
&305988393455491537290240z^{34} + 14079224644087925329523520z^{33} + 47273961310349397765869280 0z^{32} + \\
&121624022788026670658966368 80z^{31} + 247501384020921867412586484240z^{30} + \\
&406856488897300388082085355031 0z^{29} + 547503407981479263289212455131 35z^{28} + \\
&607255705204278811351245801585018z^{27} + 555264610094133575574790812181139 7z^{26} + \\
&415111536165400666990381510957675 2z^{25} + 247864598814302846690177415162792735z^{24} + \\
&111200153569603584387812062968707379 0z^{23} + 300674072061824536140087660813018234 9z^{22} - \\
&306627490764780140181580709980142570 4z^{21} - 931499562674675047252256805964975233 39z^{20} - \\
&635954475887313295192241042199635547930z^{19} - 285802788215857001691918851422432655818 5z^{18} - \\
&946852909894907702339453561886125693724 0z^{17} - 231914193917709851714802379912178721429 15z^{16} - \\
&383304789641625705566459499416375058101 10z^{15} - 234593390671932877881651440557275751112 25z^{14} + \\
&872139888336963826145520277387192809598 50z^{13} + 349803608265045461612489069936675179800000z^{12} + \\
&696554593654757665866719966270600171130000z^{11} +
\end{aligned}
$$

Result for the 6D fcc Lattice

$$865953342265454601104437816976581680000000z^{10}+586378944861718695144037906690882422000000z^{9}-$$
$$448918716637412377029136427636037600000000z^{8}-526332032930456915428235817813056400000000z^{7}-$$
$$5189372271075733419648439853326800000000000z^{6}-2263029725378331472537808115984000000000000z^{5}+$$
$$104974053097834899670129395840000000000000z^{4}+641357814865841417537072778240000000000000z^{3}+$$
$$347089467368149273535429836800000000000000z^{2}+6994092214348464533004288000000000000000000z+$$
$$595812699442665547776000000000000000000000)P^{(5)}(z)z^{3}+15(14618777852999360z^{37}+$$
$$42232680898487251200z^{36}+48576657340989636902400z^{35}+32316579131970248403552 0z^{34}+$$
$$1446760113658410970765440 0z^{33}+4725344663866749805330727 04z^{32}+11827310475440684698801079376z$$
$$23420599418243894376994924 5108z^{30}+374677251551602999731137836 3446z^{29}+$$
$$4905651728844870193496694939920 1z^{28}+5289607375382209621992321657267 00z^{27}+$$
$$4693678127508685757329704793118274z^{26}+3392552092805670737994904224515494 8z^{25}+$$
$$1942257848193764334188541770364007 65z^{24}+8158659849976308923375260617975477 30z^{23}+$$
$$182021092497037440347705989836829241 4z^{22}-562671495150676033768478488429314730 2z^{21}-$$
$$87288636539051237531541938169181610997z^{20}-54861794660416282961761734899852318702 4z^{19}-$$
$$2396582727922965009354571656000074347578z^{18}-79497787546888756395942992268885428646 72z^{17}-$$
$$20284887219829242010855806602752336703097z^{16}-38476335393060119379820741759126402451166z^{15}-$$
$$47185211186009106848535876331178061122490z^{14}-102227604369271556163646692083957290542 60z^{13}+$$
$$107413528041921729529347960434391761302800z^{12}+279266241080334469793315941614102969564000z^{11}$$
$$379975092805467869163550626412993759200000z^{10}+2763426791468873224122207598834979976000 00z^{9}+$$
$$633379261598089182133086908167004640000000z^{8}-214965129809120690827282902731468640000000z^{7}-$$
$$2424557018759285535178443324933024000000000z^{6}-1402612474157728856915464074355200000000000z^{5}-$$
$$367727068283609589442745238835200000000000z^{4}+774772837962739349472654520320000000000000z^{3}+$$
$$752256851229882473453210419200000000000000z^{2}+1776029394112720931570319360000000000000000z+$$
$$161818175186211840491520000000000000000000)P^{(4)}(z)z^{2}+90(6910694985054515 2z^{37}+$$
$$19728125958978028032z^{36}+2215666629279250997248z^{35}+143387361084360543557376z^{34}+$$
$$6235802763945868063424352z^{33}+197763282456363307438541552z^{32}+4805890762274729535435673296z^{31}$$
$$92390999114814905907317974392z^{30}+1434485821162175237888091472086z^{29}+$$
$$18213230428133179674440523308931z^{28}+190122674553786922619563973540916z^{27}+$$
$$1627987793820686707319681442965532z^{26}+11283714208962998257330503635013918z^{25}+$$
$$61070425289478623056319494081223364z^{24}+232117491219054750436300759063832796z^{23}+$$
$$335162333006577190998078624832466745z^{22}-$$

Result for the 6D fcc Lattice

$$3212526847572548623801062566839102968z^{21} - 3392965866525625940881278435486638557z^{20} - 1951831789900573496432722754351267363 40z^{19} - 8185961182051286059853304788561116790 58z^{18} - 2671193766306193321259081077503739718922z^{17} - 6879647707640439013900747488611335523490z^{16} - 1379139225878289581995545399895510251 7548z^{15} - 2039504216816486273624834199179924314 3275z^{14} - 1855905114263490123161823006701124526 1730z^{13} + 3407638735402551318083430675030634548 00z^{12} + 3257326839237100365484129096668460631 4000z^{11} + 5466062732110740554093410787098386984 0000z^{10} + 4197072940270847392338662093562381480 0000z^{9} + 7577293239379519390446429293510400000 00z^{8} - 3465345486136948584706296425184552000 0000z^{7} - 4190926430444018560287676453660320000 0000z^{6} - 2764938702145552027676616654604800000 00000z^{5} - 9932878926912153370258947363840000000 00z^{4} - 1112041174659253407521806233600000000 000z^{3} + 2849114538408597196020019200000000000 000z^{2} + 1142306781314819226668236800000000000 000z + 1148615564955287298048000000000000000 000)P^{(3)}(z)z + 90(455650218794803 2z^{35} + 1254502960824572928z^{34} + 13018547375127734 9888z^{33} + 767574890318976574 8480z^{32} + 302276251598295683586240z^{31} + 865346007686941365131 6640z^{30} + 1893820458235026753492199 20z^{29} + 32693914896316666714259899 20z^{28} + 45371384308945745114138623620z^{27} + 510811439434664402615401586970z^{26} + 4663284432121091702260620852777z^{25} + 34047746401934351907977621763618z^{24} + 190773160991774404319508940400373z^{23} + 717575244018720111969771948822450z^{22} + 5746024659363566602275125135196 30z^{21} - 16377415461160421103082005421146444z^{20} - 15819504823690372594880025769858 2066z^{19} - 92462600149325683352038023311538 2826z^{18} - 40446572703123062507649767424720 89595z^{17} - 14017460872371123201967056591950 292270z^{16} - 39203789245543299948038211301310 631735z^{15} - 88492994651041978105789511893808 827410z^{14} - 15867223029069762505236490182083 3352540z^{13} - 21705170128540380603978702178824 4210200z^{12} - 20443092593580422315820013809671 9244000z^{11} - 83930464288781215080378386513083 200000z^{10} + 98749247882439137822044179686396 640000z^{9} + 23485599064851467428729174422235 6800000z^{8} + 25202992837705338544940719217232 0000000z^{7} + 16597981586829179100607060746240 0000000z^{6} + 52113850317609070332668882227200 000000z^{5} - 96981000959420637658462494720000 00000z^{4} - 12270310453108287668341923840000 000000z^{3} - 39322078689731206308102144000000 000000z^{2} - 57865936567527160971264000000000 000000z - 26986562465909833728000000000000 000000)P(z) + 45(8809237563366195 2z^{36} + 245492997769647452 16z^{35} + 261935752755400784 0768z^{34} + 1596286114809884359065 60z^{33} + 6513463004865397861819008z^{32} + 193479386194110772817766720z^{31} + 4398883914180352580752205664z^{30} + 79010991647695967734365641136z^{29} +$$

Result for the 6D fcc Lattice

$$1143508859378085891069139805496z^{28} + 1347828522176737423743381389415 6z^{27} +$$

$$12967481859657838184170935236331 0z^{26} + 1010115611151696866102360444043867z^{25} +$$

$$6203408988166712509967367951961350z^{24} + 2782834220828526964581126761397575 1z^{23} +$$

$$6540406228719004529247350188237644 6z^{22} - 2329669581156953199668980714871155 50z^{21} -$$

$$37766262874112773146946125681914784 60z^{20} - 2566599099502838134775728413297379008 6z^{19} -$$

$$12330432201735600084488496344721300430 2z^{18} - 46100510039061002827504796093268700976 1z^{17} -$$

$$13829547539732141924316237700391494375 62z^{16} - 33513343533773096192036331788090102502 69z^{15} -$$

$$65006361449556813695420052640677079994 70z^{14} - 98087799125151810853112927166351186173 40z^{13} -$$

$$10758301750323045400708026810527005985400z^{12} - 6955035214429661410040236974622315476000z^{11} +$$

$$6981140777757766718851536754637620800 00z^{10} + 7349743557503879010410921836212410400000z^{9} +$$

$$8691043975963666049447299379144001600000z^{8} + 5165781565021067274342996673450656000000z^{7} +$$

$$4013363318863177741077133187904000000 00z^{6} - 2226964464248713386006518356377600000000z^{5} -$$

$$1863534767021891922131179987968000000000z^{4} - 655267817084534423521940643840000000000z^{3} -$$

$$1225885048831787161882853376000000000000z^{2} - 843452865918902193743462400000000000000z +$$

$$1862072810147778527232000000000000000)P'(z) + 45(1807412534552719 36z^{37} +$$

$$509807062676369848 32z^{36} + 5584340634105826525184z^{35} + 35101006700535148822425 6z^{34} +$$

$$14802080405483677823943104z^{33} + 45487501583148540090909724 8z^{32} + 10707051961496414217407305536$$

$$1992882916936004451670664714 88z^{30} + 29932647745401008160507081545 40z^{29} +$$

$$367074145552194684404472419039 70z^{28} + 3690553339187428785069238958210 94z^{27} +$$

$$30280859878734399810413167410402 99z^{26} + 19908118207277143280846917552738638z^{25} +$$

$$99771357205875220145109466450106517z^{24} + 322041161855435062814533420723282482z^{23} -$$

$$374464592158210104407054773630095 0z^{22} - 8583686545555170847175829121046069103 2z^{21} -$$

$$70294647356901524101024740972933056916z^{20} - 3696929348758626926787707566123604570 70z^{19} -$$

$$14721497797643039129107008251195131257 45z^{18} - 4646227686063347368140269721102656923194z^{17} -$$

$$11757721460891217253150507437222976590963z^{16} - 23667524905718087319814208022941410083354z^{15} -$$

$$36747814326347114270377987158311612338260z^{14} - 40652966100310576219422839345851085154840z^{13} -$$

$$24193553263042351259117425539502701518400z^{12} + 9719645940829530820988532518598953424000z^{11} +$$

$$3729734145256515570278781051636153360000 0z^{10} + 3476411901315617635383740361997011360000 0z^{9} +$$

$$6746831082562798982378495636957952000000z^{8} - 2065676140854566158081075114632768000000 0z^{7} -$$

$$2965907857169960825637573442621440000000 0z^{6} - 2093283408903388527073065030144000000000 0z^{5} -$$

$$7784392307839726168650555924480000000000z^{4} - 14285831438642699607697907712000000000000z^{3} -$$

$$8324112389233016688574464000000000000000z^{2} + 1486015062185324994232320000000000000000z +$$

$$161919374795459002368000000000000000000)P''(z) = 0$$

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 $d = 6$: $\sim$ 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).

Our 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:

- $d = 3$: $R_3 = 1 - \frac{16\sqrt[3]{4}\pi^4}{9(\Gamma(\frac{1}{3}))^6} = 0.2563182365\ldots$
- $d = 4$: $R_4 = 0.09571315417256289673531676490121018 5\ldots$
- $d = 5$: $R_5 = 0.046576957463848024193374420594803291\ldots$
- $d = 6$: $R_6 = 0.026999878287956124269364175426196380\ldots$

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