Pushing forward the dimension of fcc lattices

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(joint work with Jean-Marie Maillard)

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Motivation: statistical physics, crystallography, atomic structure

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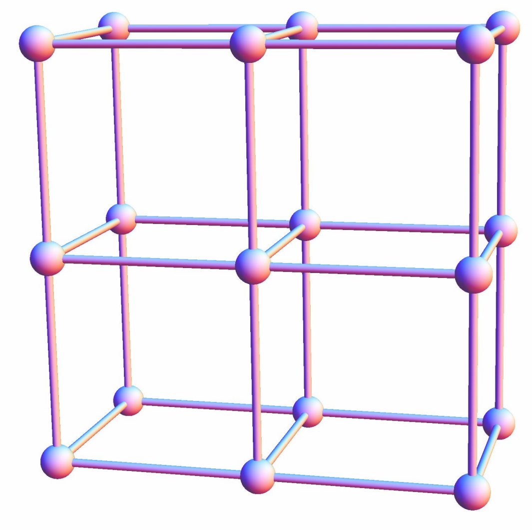

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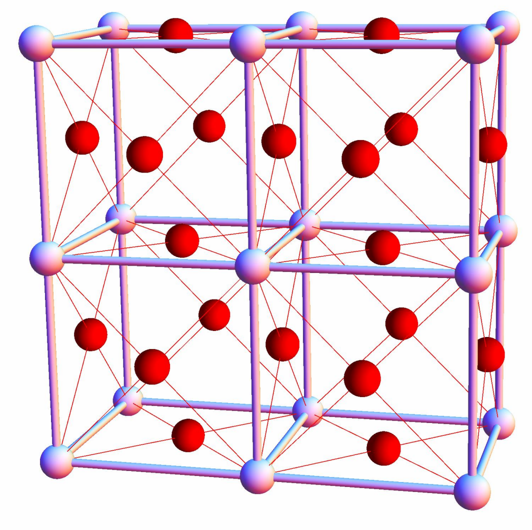

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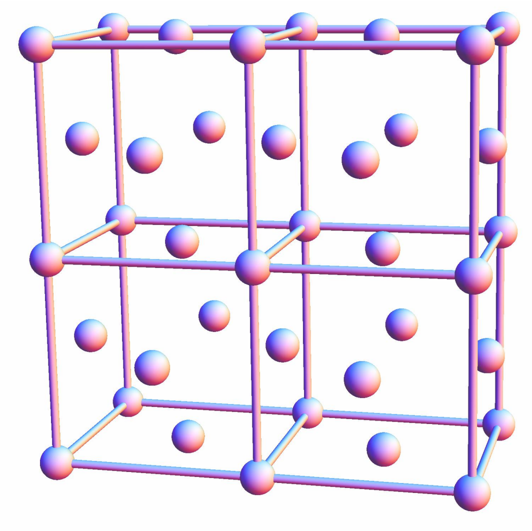

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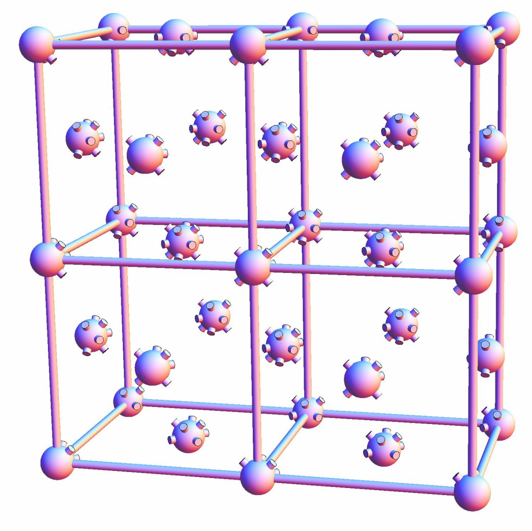

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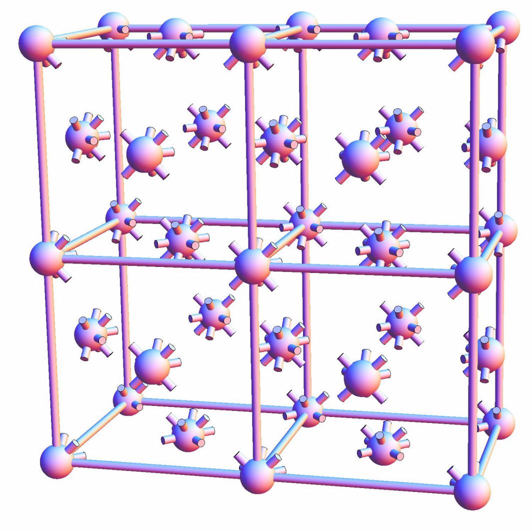

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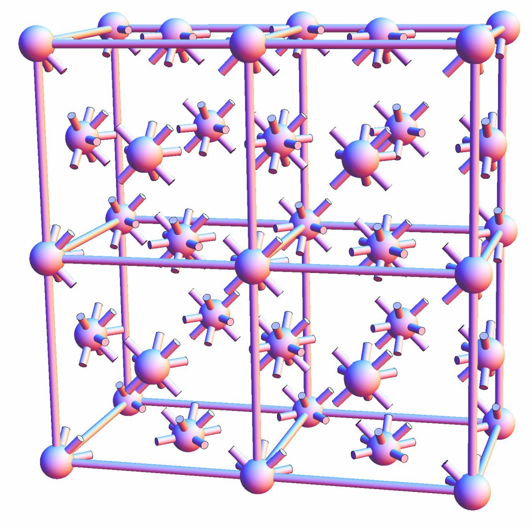

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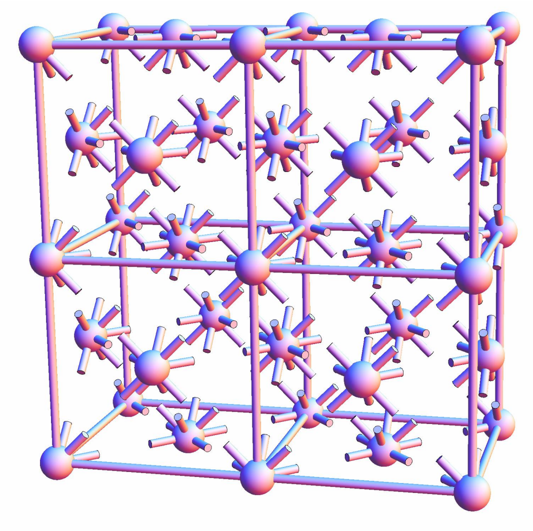

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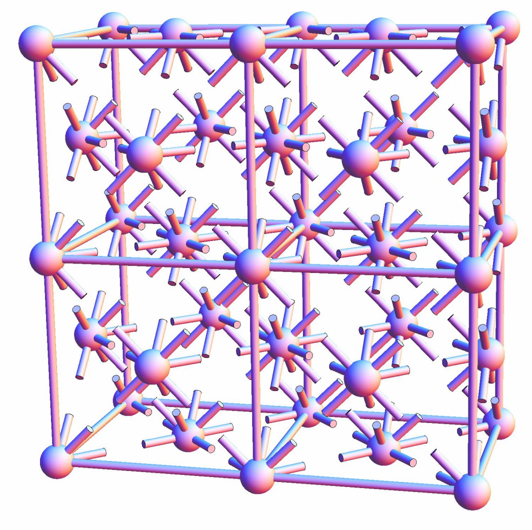

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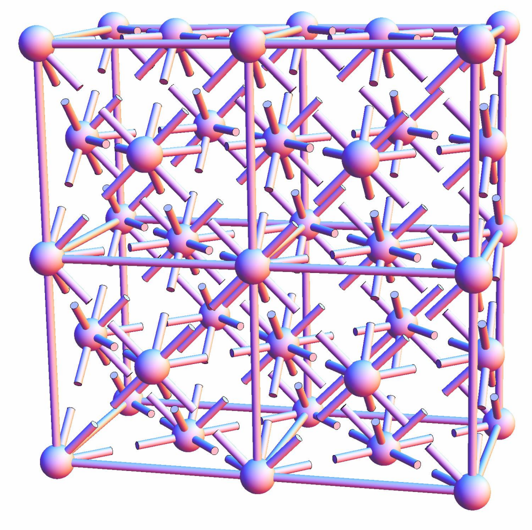

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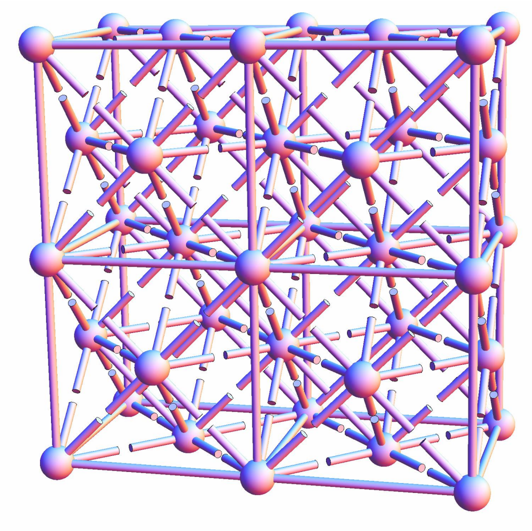

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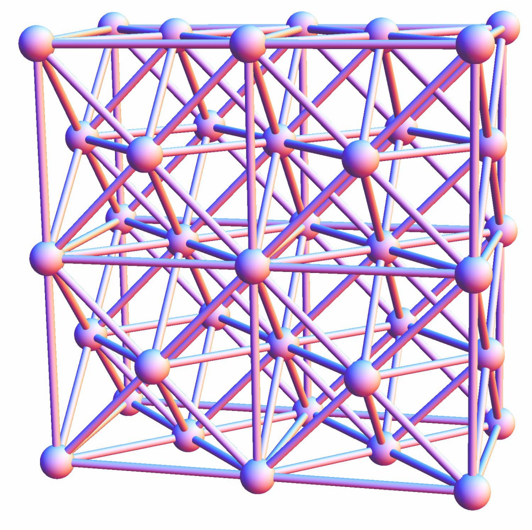

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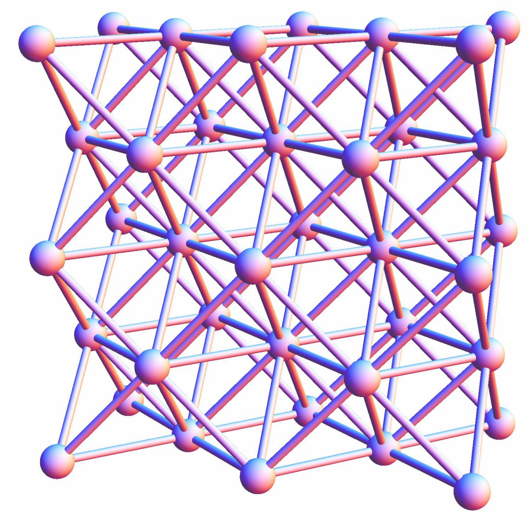

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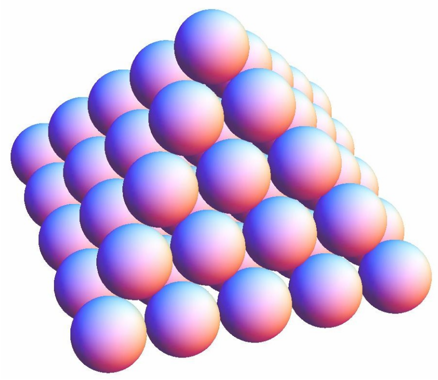

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The d-dimensional fcc lattice is composed of $1 + \binom{d}{2}$ translated copies of $\mathbb{Z}^d$:

$$\mathbb{Z}^d + \sum_{1 \le i < j \le d} \left(\tfrac{1}{2}(\boldsymbol{e}_i + \boldsymbol{e}_j) + \mathbb{Z}^d \right).$$

Random Walks

We consider random walks on the lattice points:

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

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

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

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

Lattice Green's Function

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

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

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

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Its multivariate generating function

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

is rational (S is the step set).

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We are particularly interested in

$$P(\mathbf{0}; z) = \sum_{n=0}^{\infty} p_n(\mathbf{0}) z^n = \langle y_1^0 \dots y_d^0 \rangle F(\boldsymbol{y}; z) = \frac{1}{\pi^d} \int_0^{\pi} \dots \int_0^{\pi} \frac{\mathrm{d}k_1 \dots \mathrm{d}k_d}{1 - z\lambda(\boldsymbol{k})}$$

that encodes the return probabilities. It is D-finite.

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

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In the case of the fcc lattice:

$$\lambda(\boldsymbol{k}) = \binom{d}{2}^{-1} \sum_{1 \le i < j \le d} \cos(k_i) \cos(k_j).$$

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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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3. WZ proof theory (creative telescoping)

Previous results

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7	11	68	$\lambda^7(\lambda-1)^3(\lambda-2)$

Expansion of the integrand

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

Expand the integrand in a geometric series:

$$\frac{1}{1 - \frac{z}{3}(c_1 c_2 + c_1 c_3 + c_2 c_3)} = \sum_n \left(\frac{z}{3}\right)^n (c_1 c_2 + c_1 c_3 + c_2 c_3)^n$$

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Use the multinomial theorem:

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

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Use Wallis's integration formula:

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

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The n-th Taylor coefficient can be computed by a recursive method.

The Recursive Method

Define

$$T_d(n,j) := \frac{4^{n+j}}{\pi^d} \int_0^{\pi} \cdots \int_0^{\pi} \left(\sum_{1 \le i < j \le d} \cos(k_i)\cos(k_j) \right)^n \left(\sum_{i=1}^{d} \cos(k_i) \right)^{2j} \mathrm{d}\boldsymbol{k}.$$

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A straightforward calculation leads to the recurrence:

$$T_d(n,j) = \sum_{p=0}^{n} \sum_{q=q_1}^{q_2} \binom{n}{p} \binom{2j}{2q+p-n} \binom{2n+2j-2p-2q}{n+j-p-q} T_{d-1}(p,q)$$

with $q_1 = [(n-p+1)/2]$ and $q_2 = [(n-p+2j)/2]$.

Initial condition:

$$T_2(n,j) = \sum_{p=p_1}^{p_2} \binom{2p}{p} \binom{2j}{2p-n} \binom{2n+2j-2p}{n+j-p}$$

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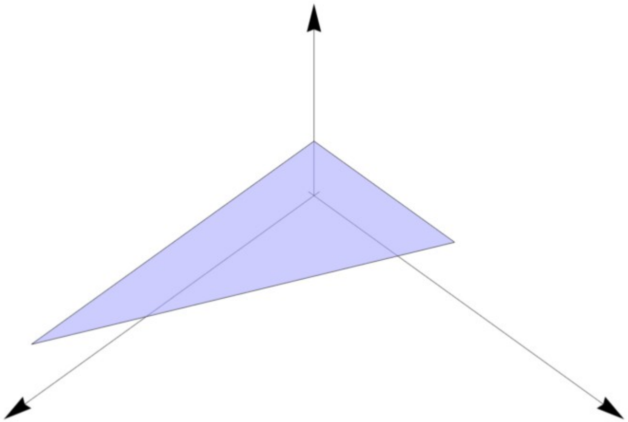
Computational Scheme

$$T_d(n,j) = \sum_{p=0}^{n} \sum_{q=q_1}^{q_2} \binom{n}{p} \binom{2j}{2q+p-n} \binom{2n+2j-2p-2q}{n+j-p-q} T_{d-1}(p,q)$$



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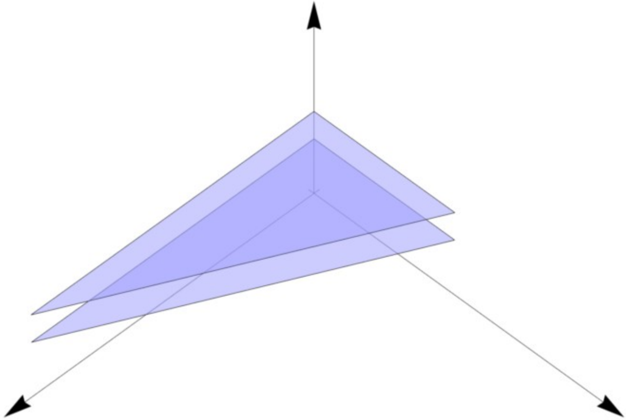

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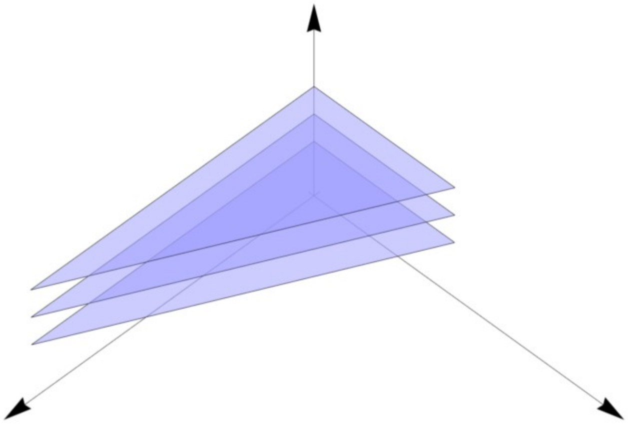

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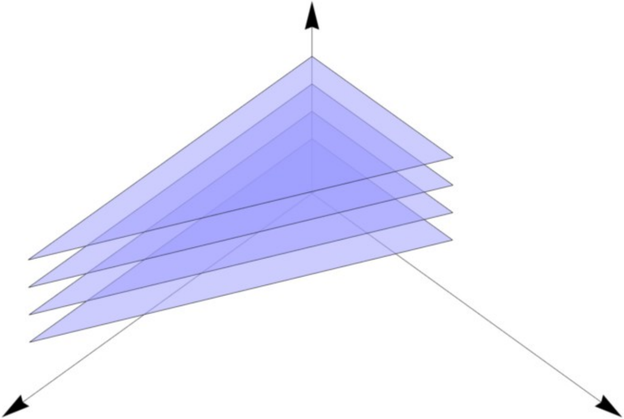

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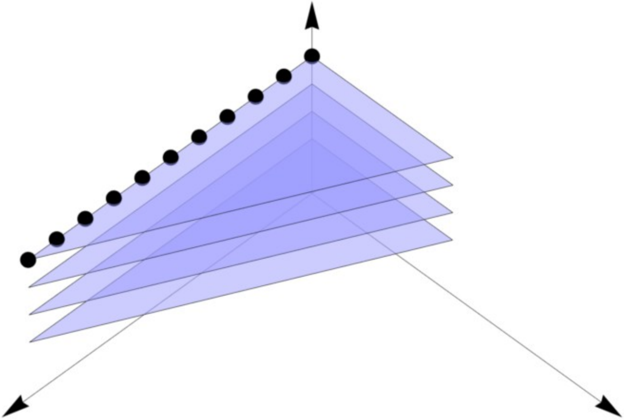

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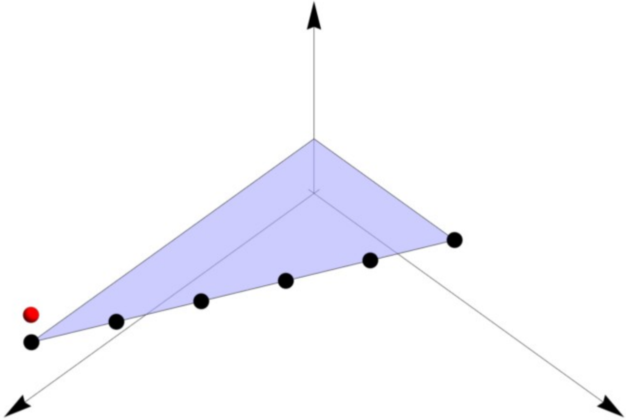

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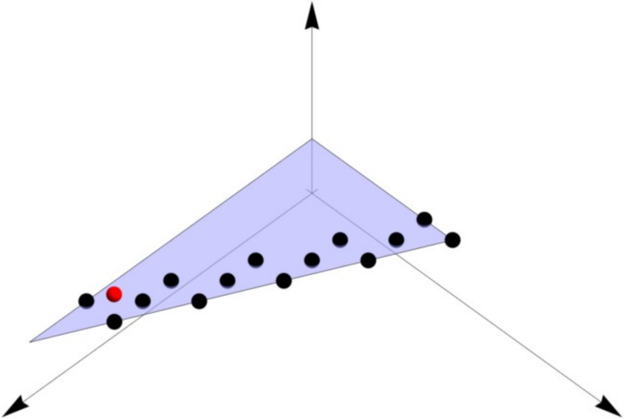

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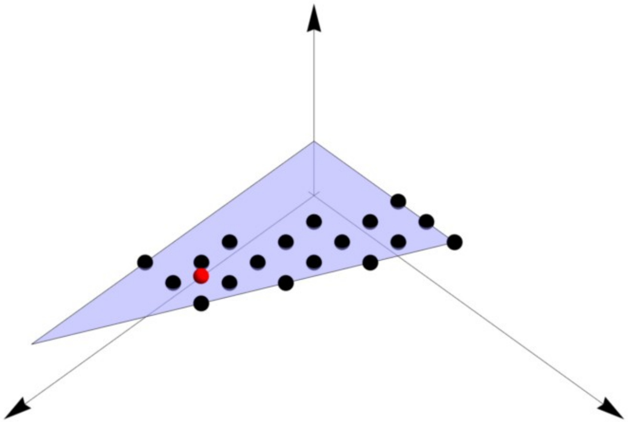

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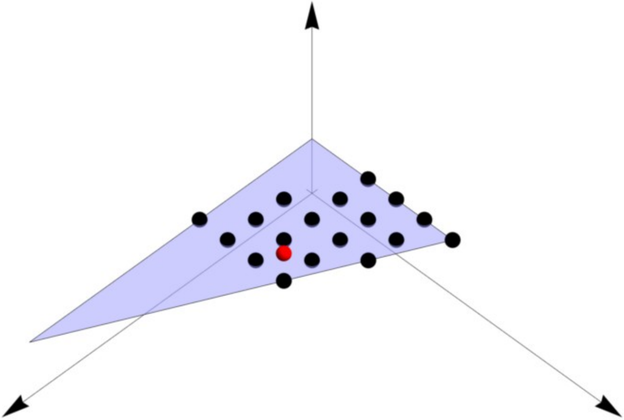

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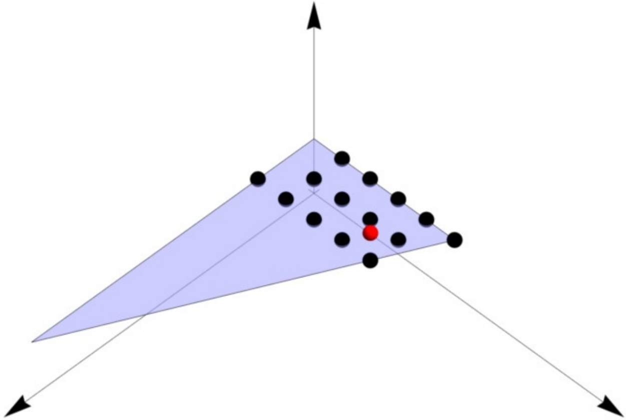

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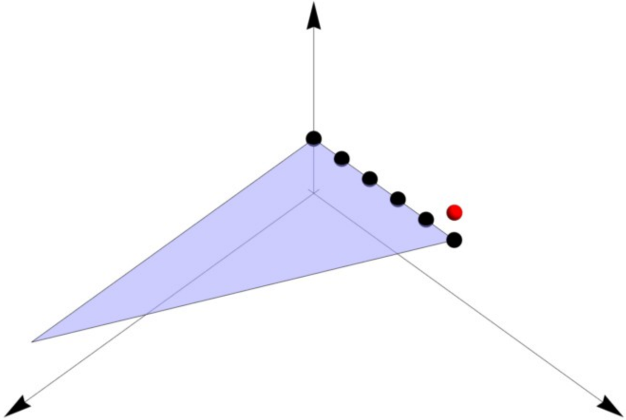

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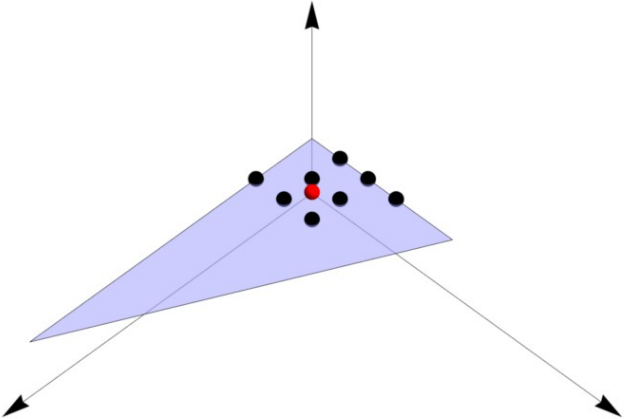

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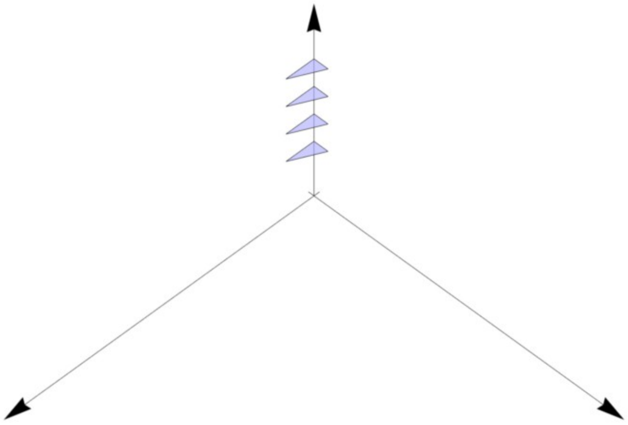

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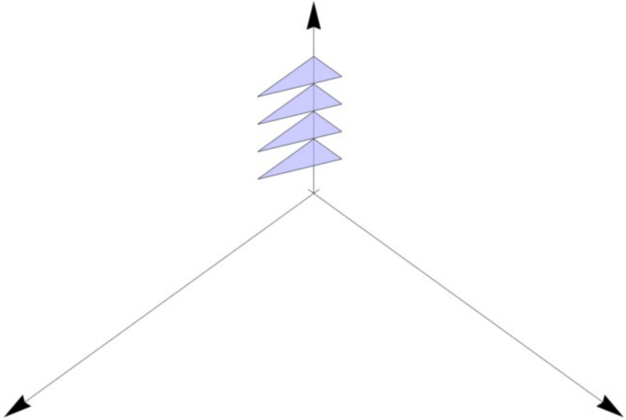

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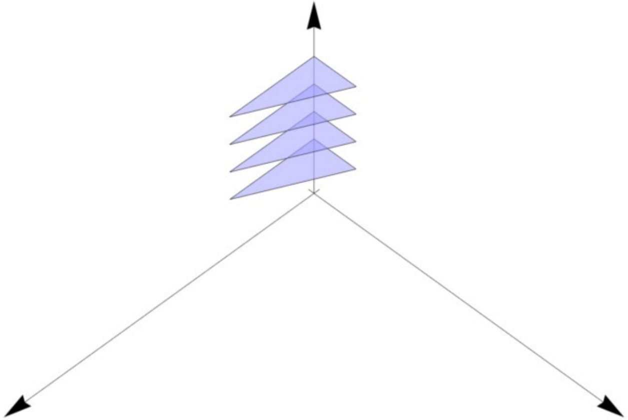

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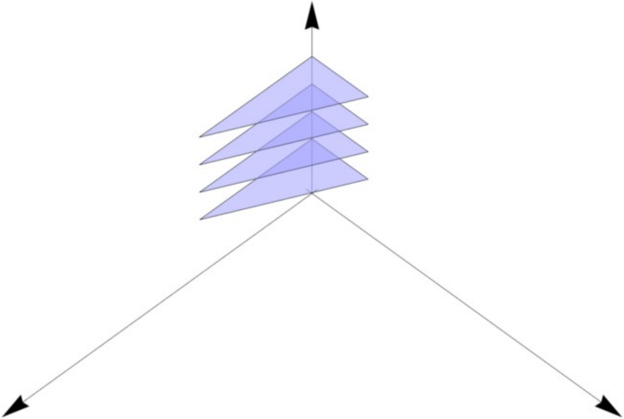

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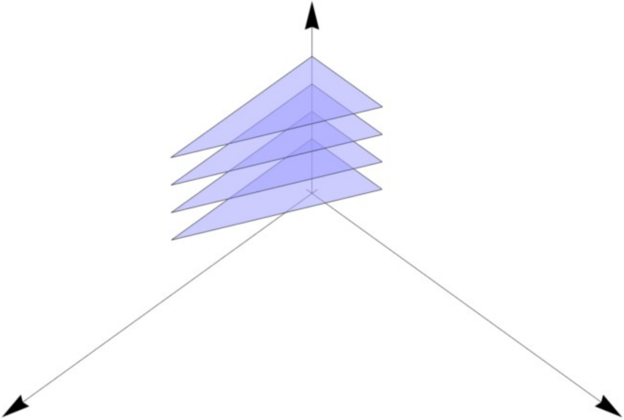

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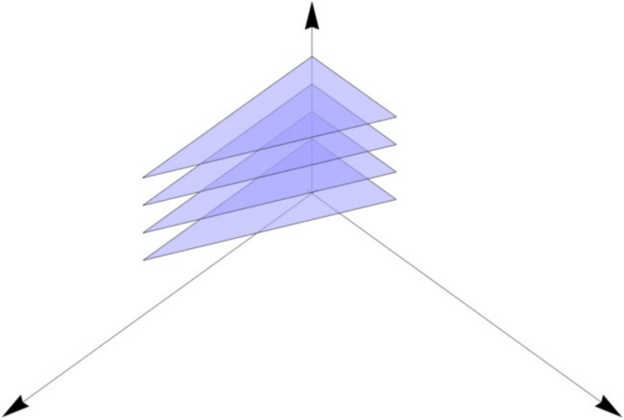

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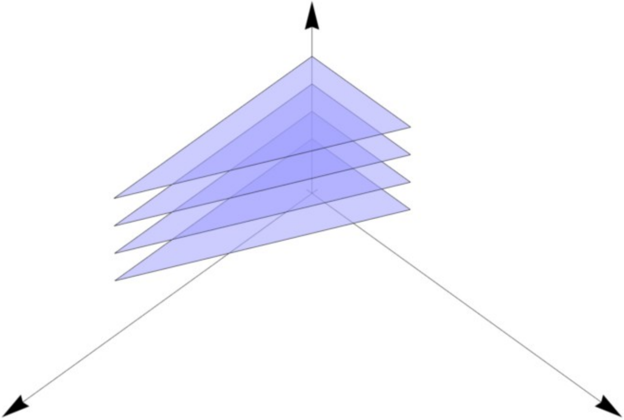

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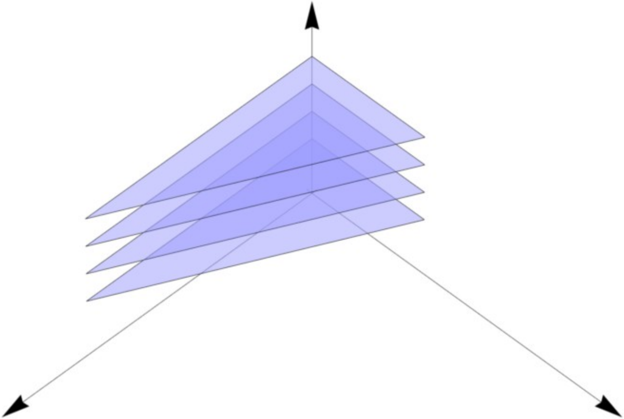

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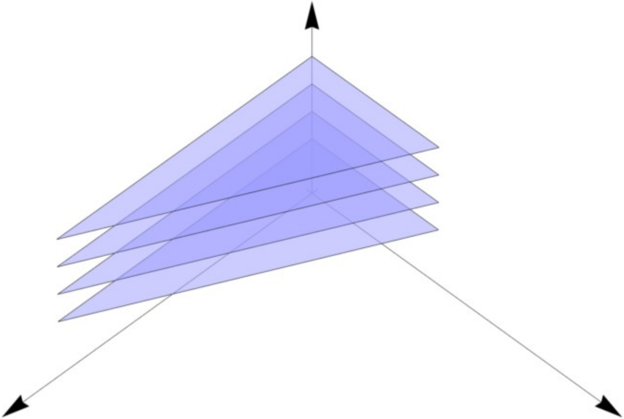

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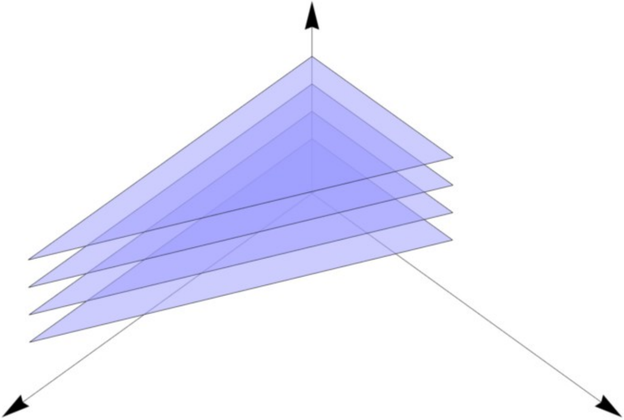

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1. Main loop over d:
   - Have to fix the number of Taylor coefficients $T_d(n,0)$ a priori.
   - Recompute the coefficients in each iteration.
2. Main loop over n:
   - No knowledge about the necessary expansion order is needed.
   - Recomputation is avoided.
   - One needs to keep the full 3-dimensional array.

New Results

d	order	degree	terms	ind. pol. at $z = 0$
3	3	5	20	λ^3
4	4	10	40	λ^4
5	6	17	88	$\lambda^5(\lambda - 1)$
6	8	43	228	$\lambda^6(\lambda - 1)^2$
7	11	68	391	$\lambda^7(\lambda - 1)^3(\lambda - 2)$

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12*	32	617	3618	$\lambda^{12}(\lambda - 1)^8(\lambda - 2)^6(\lambda - 3)^4(\lambda - 4)^2$

* modulo prime

Landau Singularities

Leading coefficient of the order-6 operator for $d = 5$:

$$16(-5+z)(-1+z)z^4(5+z)^2(10+z)(15+z)(5+3z)$$
$$\times(-675000+3465000z-1053375z^2+933650z^3$$
$$+449735z^4+144776z^5+15678z^6)$$

Landau Singularities:

- Singularities of a function defined by a multiple integral
- Can be found by imposing conditions on the integrand.
- For $P(\mathbf{0}; z)$ one obtains

$$\binom{d}{2}\frac{2(1-k)}{d^2-(k+4j+1)d+4j^2+k+4jk}$$

  for $k = 0, 2, 3, \ldots, d-1$ and $j = 0, 1, \ldots, [(d-1)/2]$.
- Can be used as a consistency check.

Landau Singularities for $d = 11$

The leading coefficient of the differential operator is

$$x^{22}\,(x+11)^6\,(55+x)^2\,(x-1)\,(8\,x+55)\,(29\,x+55)$$
$$(4\,x+55)\,(2\,x+55)\,(4\,x+11)\,(7\,x+165)\,(7\,x-55)$$
$$(2\,x+33)\,(17\,x+55)\,(x+44)\,(13\,x+275)\,(3\,x+55)$$
$$(7\,x-11)\,(13\,x+55)\,(7\,x+110)\,(x+35)\,(3\,x+22)$$
$$(x+99)\,(19\,x-55)\,(7\,x+33)\,(9\,x+11)\,(x+15)$$
$$(9\,x+55)\,(17\,x+275)\,(3\,x+77)\,(23\,x+165)$$
$$\times\ \langle\text{irreducible polynomial of degree } 352\rangle$$

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3. For even dimension d:
   - Exterior square has a drop of order by 1.
   - Galois group is included in $Sp(r, \mathbb{C})$.
4. There exists a nontrivial homomorphism that maps the solutions of the operator L to the solutions of its adjoint:

   $$\exists L_{\text{hom}} : \quad \operatorname{adj}(L_{\text{hom}}) \cdot L = \operatorname{adj}(L) \cdot L_{\text{hom}}$$

   This gives rise to a "canonical decomposition".

Canonical Decomposition

Perform successive Euclidean right divisions of L and L_{hom}:

$$L_0 := L$$
$$L_1 := L_{\text{hom}}$$
$$L_i := U_{i+1} L_{i+1} + L_{i+2}$$

- The quarks U_i are self-adjoint.
- Tower of intertwiners: $\text{adj}(L_{i+1}) \cdot L_i = \text{adj}(L_i) \cdot L_{i+1}$
- Also the L_i have special Galois groups.
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Example: $(d = 7, r = 11)$

$$L = \big(U_1U_2U_3U_4U_5 + U_1U_2U_5 + U_1U_4U_5 + U_1U_2U_3 + U_3U_4U_5 + U_5 + U_3 + U_1\big) \cdot r$$

where U_1, U_2, U_3, U_4 have order 1, the order of U_5 is 7, and r is a rational function.

Pushing forward the dimension of fcc lattices

Christoph Koutschan
(joint work with Jean-Marie Maillard)

Johann Radon Institute for Computational and Applied Mathematics (RICAM)
Austrian Academy of Sciences

August 10, 2015
DART-VI, ICIAM'2015, Beijing, China