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

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March 12, 2013

Abstract

We study the face-centered cubic lattice (fcc) in up to six dimensions. In particular, we are concerned with lattice Green's functions (LGF) and return probabilities. Computer algebra techniques, such as the method of creative telescoping, are used for deriving an ODE for a given LGF. For the four- and five-dimensional fcc lattices, we give rigorous proofs of the ODEs that were conjectured by Guttmann and Broadhurst. Additionally, we find the ODE of the LGF of the six-dimensional fcc lattice, a result that was not believed to be achievable with current computer hardware.

Keywords: bravais lattice, random walk, lattice Green's function, return probability, differential equation, symbolic integration, holonomic system, creative telescoping

MSC classification: 82B41, 06B05, 33F10, 68W30, 05A15

1 Introduction

Random walks on lattices, such as the face-centered cubic lattice, are an important concept in various applications in physics, chemistry, ecology, economics, and computer science, when lattice vibration problems (phonons), diffusion models, luminescence, Markov processes and other random processes are studied. A fundamental object to investigate is the probability generating function of a lattice, called the lattice Green's function (LGF). For example, the return probability of a lattice can be expressed in terms of the LGF. The LGFs of three-dimensional lattices have been computed and analyzed in [1, 2], for higher-dimensional lattices see [3, 4]. We present a completely different approach to LGFs that is based on computer algebra techniques, with which we are not only able to confirm independently the previously known results, but also go beyond. We believe that this methodology can be applied successfully to many other, yet unsolved problems of similar flavor, and therefore should be popularized in the community.

This article appeared in J. Phys. A: Math. Theor. **46** (2013) 125005.
DOI: 10.1088/1751-8113/46/12/125005, http://iopscience.iop.org/1751-8121/46/12/125005

The paper is organized as follows. In Section 1 we explain the general setting in which we work and introduce basic notions, such as Bravais lattice (Section 1.1), random walk (Section 1.2), and lattice Green's function (Section 1.3); in Section 1.4 an approach to LGFs via differential equations is motivated. We derive the integral representation of the LGF and show how a differential equation is connected to it. Section 2 is dedicated to different methods how to compute the ODE of a LGF in a nonrigorous way: Section 2.1 reviews the method for computing Taylor coefficients used in [3, 4] and Sections 2.2 and 2.3 count random walks in order to obtain sufficient data to construct the ODE. The main contribution of our work is contained in Section 3. The method of creative telescoping is described in Section 3.1; it enables us to compute the desired ODEs in a mathematical rigorous way, including correctness certificates. Applying this method to the LGF of the fcc lattice confirms the results of [3, 4] in dimensions four and five, and yields an ODE for the LGF of the six-dimensional fcc lattice that was not known previously (see Section 3.2).

1.1 Bravais Lattices

We consider lattices in $\mathbb{R}^d$ that are given as infinite sets of points

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

for some linearly independent vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_d \in \mathbb{R}^d$ (throughout this paper, vectors are denoted by bold letters). In three dimensions such lattices are called *Bravais lattices*. The simplest instance of such a lattice is obtained by choosing $\boldsymbol{a}_i = \boldsymbol{e}_i$, the i-th unit vector; the result is the integer lattice $\mathbb{Z}^d$ which is also called the *square lattice* (for $d = 2$), or the *cubic lattice* (for $d = 3$), or the *hypercubic lattice* (for $d \geqslant 4$).

The *face-centered (hyper-) cubic lattice* (fcc lattice) is obtained from the (hyper-) cubic lattice by adding the center point of each (two-dimensional) face to the set of lattice points. In two dimensions this operation is trivial: the faces of the square lattice $\mathbb{Z}^2$ are all unit squares with corners $(m, n), (m+1, n), (m+1, n+1), (m, n+1)$ for integers $m, n \in \mathbb{Z}$. Their center points are $\mathbb{Z}^2 + (\frac{1}{2}, \frac{1}{2})$ which together with $\mathbb{Z}^2$ again yields a square lattice, more precisely a copy of $\mathbb{Z}^2$ which is rotated by 45 degrees and shrunk by a factor of $\sqrt{2}$. The situation becomes more interesting in higher dimensions. For example, in three dimensions there are 6 faces of the unit cube, and their center points together with all integral translates have to be included. It is not difficult to see that the three-dimensional fcc lattice consists of four copies of $\mathbb{Z}^3$, namely

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

Similarly the fcc lattice in four dimensions consists of 7 copies of $\mathbb{Z}^4$, and in general the d-dimensional fcc lattice is composed of $1 + \binom{d}{2}$ translated copies of $\mathbb{Z}^d$.

The study of Bravais lattices was inspired by crystallography in as much as the atomic structure of crystals forms such regular lattices. While the cubic lattice is quite rarely found in nature (e.g., in polonium) due to its small *atomic packing factor* (the proportion of space that is filled when a sphere of maximal radius is put on each lattice point, in a way that these spheres do not overlap), the fcc lattice is more often encountered, for example, in aluminium, copper, silver, and gold. The atomic packing factor of the fcc lattice is $\sqrt{2}\pi/6$, the highest possible value as was shown by Hales in his famous proof of the Kepler conjecture [5].

1.2 Random Walks

For the sake of simplicity, the fcc lattice as introduced in the previous section, is stretched by a factor of 2 in all coordinate directions so that all lattice points have integral coordinates. This convention is kept throughout the paper as it does not change the relevant quantities that we are interested in (e.g., the return probability, see below).

The aim of this paper is to study random walks on the fcc lattice in several dimensions. We consider walks that allow only steps to the nearest neighbors of a point (with respect to the Euclidean metric). Furthermore it is assumed that all steps are taken with the same probability. For example, consider a point (k, m, n) in the three-dimensional cubic lattice $(2\mathbb{Z})^3$. It is the common corner point of 8 cubes. The nearest neighbors in the 3D fcc lattice are then the center points of some of those faces which have (k, m, n) as a corner point. Note that they all have distance $\sqrt{2}$ whereas the other corner and face-center points are farther away (their distance is $\geqslant 2$) and hence not reachable in a single step. Thus the number of possible steps is $8 \cdot 3/2 = 12$ (number of adjacent cubes times the number of adjacent faces per cube, divided by two since each face belongs to two cubes). The same situation is encountered at the center point of some face and hence every point in the 3D fcc lattice has exactly 12 nearest neighbors; this number is called the *coordination number* of the lattice.

The above considerations can be generalized to arbitrary dimensions in a straightforward manner; one finds that the set of permitted steps in the d-dimensional fcc lattice is given by

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

and thus its coordination number is $4\binom{d}{2}$.

1.3 Lattice Green's Function

Let $p_n(\boldsymbol{x})$ denote the probability that a random walk which started at the origin $\mathbf{0}$ ends at point $\boldsymbol{x}$ after n steps. Note that in our setting of unrestricted walks, $c^n p_n(\boldsymbol{x})$ is an integer and gives the total number of walks that end at location $\boldsymbol{x}$ after n steps, where c is the coordination number of the lattice.

In order to achieve information about random walks on the fcc lattice, the following multivariate generating function is introduced:

$$P(\boldsymbol{x}; z) = \sum_{n=0}^{\infty} p_n(\boldsymbol{x}) z^n. \tag{2}$$

This function is called the *lattice Green's function* (LGF). By defining the *structure function* $\lambda(\boldsymbol{k}) = \lambda(k_1, \ldots, k_d)$ of a lattice to be the discrete Fourier transform

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

of the single-step probability function $p_1(\boldsymbol{x})$, the generating function (2) can be expressed as the d-dimensional integral

$$P(\boldsymbol{x}; z) = \frac{1}{\pi^d} \int_0^\pi \ldots \int_0^\pi \frac{e^{i\boldsymbol{x}\cdot\boldsymbol{k}}}{1 - z\lambda(\boldsymbol{k})} \,\mathrm{d}k_1 \ldots \,\mathrm{d}k_d.$$

We shall be interested in walks which return to the origin and which we therefore call *excursions*. The LGF for excursions is given by

$$P(\mathbf{0}; z) = \sum_{n=0}^{\infty} p_n(\mathbf{0}) z^n = \frac{1}{\pi^d} \int_0^\pi \ldots \int_0^\pi \frac{\mathrm{d}k_1 \ldots \mathrm{d}k_d}{1 - z\lambda(\boldsymbol{k})}. \tag{3}$$

In the following, we will only refer to this special instance when talking about LGFs. This function allows one to calculate the *return probability* R, sometimes also referred to as the *Pólya number*, of the lattice. It signifies the probability that a random walk that started at the origin will eventually return to the origin. It can be computed via the formula

$$R = 1 - \frac{1}{P(\mathbf{0}; 1)} = 1 - \frac{1}{\sum_{n=0}^{\infty} p_n(\mathbf{0})}. \tag{4}$$

Example 1. Consider the square lattice $\mathbb{Z}^2$ which admits the steps $(-1, 0)$, $(1, 0)$, $(0, -1)$, and $(0, 1)$. Its structure function is

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

and therefore its LGF is (see, e.g., [4])

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

where $\mathbf{K}(z)$ is the complete elliptic integral of the first kind. The fact that the above integral diverges for $z = 1$ immediately implies that the return probability $R = 1$; in other words that every random walk will eventually return to the origin, a result that was already proven in 1921 by Pólya [6]. □

Example 2. We have already remarked that the two-dimensional fcc lattice is nothing else but a rotated and stretched version of the square lattice. Nevertheless let's have a look at the LGF when the step set $\{(-1, -1), (-1, 1), (1, -1), (1, 1)\}$ is taken. Its structure function is

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

using the well-known angle-sum identity $\cos(x \pm y) = \cos x \cos y \mp \sin x \sin y$. Although the structure function differs from that in Example 1 the LGF is the same:

$$P(0,0,z) = \frac{1}{\pi^2} \int_0^\pi \int_0^\pi \frac{\mathrm{d}k_1\,\mathrm{d}k_2}{1 - z \cos k_1 \cos k_2} = \frac{2}{\pi} \mathbf{K}(z^2) \tag{5}$$

as shown in Equation (6) of [4]. Note also that the different distances between nearest-neighboring lattice points—1 in Example 1 and $\sqrt{2}$ in Example 2—carry no weight since only excursions (and not walks with arbitrary end points) are investigated. □

It is now an easy exercise to compute the structure function $\lambda(\boldsymbol{k})$ for the d-dimensional fcc lattice:

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

The LGF is then given as the d-fold integral (3) and the return probability can be computed by integrating over $1/(1 - \lambda(\boldsymbol{k}))$

1.4 The Differential Equation Detour

The return probability in the fcc lattice in three dimensions was first computed by Watson [7] as one of the three integrals which were later named after him, and which give the return probabilities in different three-dimensional lattices. These probabilities can be expressed in terms of algebraic numbers, π, and values of the Gamma function at rational arguments. For example, the probability of returning to the origin in the 3D fcc lattice is given by

$$1 - \frac{16\sqrt[3]{4}\pi^4}{9\left(\Gamma\left(\frac{1}{3}\right)\right)^6}.$$

For the three-dimensional fcc lattice, Joyce expressed the lattice Green's function also in terms of complete elliptic integrals [1], but the expression is fairly complicated and for the higher-dimensionsal fcc lattices no such evaluation is known at all. Similarly we don't know of any closed-form representation of the return probabilities in higher dimensions.

Instead we will derive differential equations for the corresponding LGFs. Although less explicit than the previously mentioned closed-form results, such an implicit representation of the LGF provides considerable insight. It allows one to compute the number of excursions efficiently for any fixed number of steps, as well as the return probability with very high precision (see Section 3). But also the differential equations themselves reveal very interesting properties that are worth investigation.

To motivate our approach and to illuminate the origin of Equation (3), consider an arbitrary lattice in $\mathbb{Z}^d$ with some finite set $S \subset \mathbb{Z}^d$ of permitted steps. Then clearly the probability function $p_n(\boldsymbol{x})$ satisfies the constant-coefficient recurrence

$$p_{n+1}(\boldsymbol{x}) = \frac{1}{|S|} \sum_{\boldsymbol{s} \in S} p_n(\boldsymbol{x} - \boldsymbol{s}). \tag{6}$$

Let $F(\boldsymbol{y};z)$ denote the multivariate generating function

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

Multiplying both sides of (6) by $\boldsymbol{y}^{\boldsymbol{x}} z^n$ and summing with respect to n and $\boldsymbol{x}$ gives

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

Thus we obtain

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

and the LGF $P(\mathbf{0};z)$ is nothing else but the constant term $\langle \boldsymbol{y}^{\mathbf{0}} \rangle F(\boldsymbol{y};z)$. A differential equation for this expression can be derived from an operator of the form

$$A(z, D_z) + D_{y_1} B_1 + \cdots + D_{y_d} B_d \tag{7}$$

that annihilates the expression $F(\boldsymbol{y};z)/(y_1 \cdots y_d)$. Here the symbol D_x denotes the partial derivative w.r.t. x and the B_j are differential operators that may involve $y_1, \ldots, y_d, z$ as well as $D_{y_1}, \ldots, D_{y_d}, D_z$. The fact that A may only depend on z and D_z is crucial and therefore explicitly indicated. In Section 3 we will discuss how to find such an operator. From

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

and the fact that the coefficient of y^{-1} in an expression of the form $D_y \sum_{n=-\infty}^{\infty} a_n y^n$ is always zero, it follows that $A\big(\langle \boldsymbol{y}^{\mathbf{0}} \rangle F(\boldsymbol{y};z)\big) = A\big(P(\mathbf{0};z)\big) = 0$. Also in Section 3 we will demonstrate how the operator (7) is used to derive a differential equation for the d-fold integral

$$\int \cdots \int \frac{d\boldsymbol{y}}{(y_1 \cdots y_d)(1 - \frac{z}{|S|} \sum_{\boldsymbol{s}\in S} \boldsymbol{y}^{\boldsymbol{s}})} = \int \cdots \int \frac{d\boldsymbol{k}}{1 - z\lambda(\boldsymbol{k})}.$$

2 An Experimental Mathematics Approach

This section presents some results that were obtained in a non-rigorous way using the method of guessing [8]. That is, for finding a linear differential equation

$$c_m(x) f^{(m)}(x) + \cdots + c_1(x) f'(x) + c_0(x) f(x) = 0$$

for a certain function $f(x)$, one computes the first terms of the Taylor expansion of $f(x)$ and then makes an ansatz with undetermined polynomial coefficients $c_j(x)$. If the resulting linear system is overdetermined (i.e., if sufficiently many Taylor coefficients were used) but still admits a nontrivial solution, then the detected ODE is very likely to be correct. Another strategy to gain confidence in the result, is to test it with further Taylor coefficients, that were not used in the computation. However, this method can never produce a rigorous proof of the result and there always remains a (very small) probability that the guess is wrong. For this reason, any result obtained in this fashion (e.g., the ODEs presented in [2, 3]) is termed a *conjecture*.

2.1 Starting from the Integral Representation

In this section we briefly recapitulate some previous work done by Broadhurst and Guttmann, who used the integral representation (3) of the LGF as a starting point.

Guttmann computed a differential equation for the LGF of the four-dimensional fcc lattice [2] (see also Theorem 1): for this purpose, the four-fold integral was rewritten as a double integral whose integrand was expanded as a power series. Term-by-term integration yielded a truncated Taylor expansion of the LGF which allowed him to apply the method of guessing.

Recently, Broadhurst had obtained an ODE for the LGF of the five-dimensional fcc lattice [3] (see also Theorem 3), a result that required several days of PARI calculations. Broadhurst's strategy consisted in expanding the integrand in (3) as a geometric series $\sum_{n=0}^{\infty} \lambda(\boldsymbol{k})^n z^n$ and in expanding $\lambda(\boldsymbol{k})^n$ using the multinomial theorem (which gives a $(m-1)$-fold sum if m is the number of summands in $\lambda(\boldsymbol{k})$). The inner terms can now be integrated using Wallis' formula

$$\int_0^{\pi} \cos(x)^{2n}\,\mathrm{d}x = \frac{\pi}{4^n}\binom{2n}{n}.$$

The structure function of the 5D fcc lattice consists of 10 summands. Thus the computation of the n-th Taylor coefficient of $P(\mathbf{0};z)$ requires the evaluation of a 9-fold sum, or in other words, has complexity $O(n^9)$.

2.2 Counting the walks

A different way to crank out as many Taylor coefficients of the LGF as necessary is to explicitly count all possible excursions with a certain number of steps. Let $a_n(\boldsymbol{x})$ be the number of walks from $\mathbf{0}$ to $\boldsymbol{x}$ with n steps and let c denote the coordination number of the lattice, then the lattice Green's function $P(\mathbf{0};z) = \sum_{n=0}^{\infty} a_n(\mathbf{0})(z/c)^n$, as we have already remarked earlier. The values of the $(d+1)$-dimensional sequence (d again denotes the dimensionality of the lattice) can be computed with the recurrence (6). To obtain the first n Taylor coefficients hence requires one to fill the $(d+1)$-dimensional array $\big(a_m(\boldsymbol{x})\big)_{0\leqslant m,x_1,\ldots,x_d<n}$ with values (by symmetry it suffices to consider the first octant only, which again by symmetry can be restricted to the wedge $x_1 \geqslant x_2 \geqslant \ldots \geqslant x_d$). Still, this has complexity $O(n^{d+1})$. Further optimizations consist in cutting off the regions where the sequence can be predicted

to be zero (e.g. when $x_j > n$ for some j), and to truncate the x_j-coordinates at $n/2$ (since we are interested in excursions, points too far from the origin $\mathbf{0}$ are not relevant). Although the complexity is better than before, computing the full array of values can be quite an effort. Again, in the example of the 5D fcc lattice, about 115 Taylor coefficients are necessary to recover the recurrence for $a_n(\mathbf{0})$ (which then gives rise to the differential equation of $P(\mathbf{0}; z)$), and hence the full array contains about $115 \cdot 58^5/5! \approx 6.3 \cdot 10^8$ values! Fortunately we can do better.

2.3 Multi-Step guessing

How can the recurrence for $a_n(\mathbf{0})$ be computed without calculating all the values of the multivariate sequence $a_n(\boldsymbol{x})$ in the box $[0, n]^{d+1}$ (or some slightly optimized version of it)? In the previous section, we first computed lots of data, then threw away most of it, and did a single guessing step. But the guessing can be done in several steps which we call *multi-step guessing*. The method is illustrated on the 5D fcc example. As before, we start with the recurrence (6) to crank out a moderate number of values for the six-dimensional sequence $a_n(x_1, \ldots, x_5)$, namely in the box $[0, 15]^6$, which takes about 30 seconds only. From this array, we pick the values of $a_n(x_1, x_2, x_3, 0, 0)$ which constitute a four-dimensional sequence that we denote with $b_n(x_1, x_2, x_3)$. The data is now used to guess recurrences for this new function b. One of these recurrences is

$$\begin{aligned}
&(n+1)b_n(x_1, x_2+3, x_3+1) - (n+1)b_n(x_1, x_2+1, x_3+3) + \\
&(n+1)b_n(x_1+1, x_2, x_3+3) - (n+1)b_n(x_1+1, x_2+3, x_3) + \\
&(n+1)b_n(x_1+1, x_2+3, x_3+4) - (n+1)b_n(x_1+1, x_2+4, x_3+3) - \\
&(n+1)b_n(x_1+3, x_2, x_3+1) + (n+1)b_n(x_1+3, x_2+1, x_3) - \\
&(n+1)b_n(x_1+3, x_2+1, x_3+4) + (n+1)b_n(x_1+3, x_2+4, x_3+1) + \\
&(n+1)b_n(x_1+4, x_2+1, x_3+3) - (n+1)b_n(x_1+4, x_2+3, x_3+1) + \\
&(x_2+2)b_{n+1}(x_1+1, x_2+2, x_3+3) - (x_3+2)b_{n+1}(x_1+1, x_2+3, x_3+2) - \\
&(x_1+2)b_{n+1}(x_1+2, x_2+1, x_3+3) + (x_1+2)b_{n+1}(x_1+2, x_2+3, x_3+1) + \\
&(x_3+2)b_{n+1}(x_1+3, x_2+1, x_3+2) - (x_2+2)b_{n+1}(x_1+3, x_2+2, x_3+1) = 0
\end{aligned}$$

which has the disadvantage that it does not allow us to compute the values $b_n(0, 0, 0)$ since the leading coefficient vanishes; unfortunately this phenomenon occurs frequently in this context. An additional recurrence that does not suffer from this handicap is much larger and therefore not reproduced here. Anyway, guessing these recurrences can be done in less than a minute.

Now these recurrences can be used to compute more values for the sequence $b_n(x_1, x_2, x_3)$ (in 30 seconds one can now go up to $n = 30$) which in turn are used to guess recurrences for $b_n(x_1, x_2, 0)$. These latter recurrences allow to compute $a_n(\mathbf{0}) = b_n(0, 0, 0)$ for $0 \leqslant n \leqslant 115$ in about 2.5 minutes. Voilà! The whole computation takes less than 5 minutes on a modest laptop. Of course it is a matter of trial and error to determine how many coordinates are set to 0 in each step (in the above example, we did 2 in the first step, 1 in the second, and again 2 in the third step).

3 A Computer Algebra Approach

Again, we want to emphasize that the results presented in the previous section are certainly nice, but lack mathematical rigor. To achieve ultimate confidence in their correctness we have to apply a different method. One possible such method is called *creative telescoping*, a short introduction of which is given in the following section. After that we are able to state our results in the form of theorems.

3.1 Creative Telescoping

This method has been popularized by Zeilberger in his seminal paper [9]. Since then it has been applied to innumerable identities involving hypergeometric summations, multisums, integrals of special functions, and various other kinds of problems. The basic idea is very simple and we illustrate it on the example of a definite integral $F(z) = \int_a^b f(x,z)\,\mathrm{d}x$. The main step in the algorithm consists in finding a partial differential equation for $f(x,z)$ that can be written in the form

$$\big(A(z, D_z) + D_x B(x, z, D_x, D_z)\big)(f(x,z)) = 0 \tag{8}$$

where the *telescoper* $A \in \mathbb{C}(z)\langle D_z\rangle$ and the *delta part* $B \in \mathbb{C}(x,z)\langle D_x, D_z\rangle$ are differential operators, with the previously introduced notation of D_x being the partial derivative w.r.t. x. By $\mathbb{C}(z)\langle D_z\rangle$ we denote the non-commutative Ore algebra that can be viewed as a polynomial ring in the "variable" D_z with rational function coefficients in $\mathbb{C}(z)$. The result of the algorithm is a (possibly) inhomogeneous linear ODE for the integral $F(z)$ that is obtained by integrating Equation (8):

$$A\big(F(z)\big) + \Big[B\big(f(x,z)\big)\Big]_{x=a}^{x=b} = 0.$$

In applications one frequently encounters the situation that the second part vanishes, yielding a homogeneous ODE. This is because many integrals that occur in practice, have *natural boundaries*. With our study of LGFs, we are in a similar situation: in Section 1.4 it was shown that the telescoper of (7) automatically annihilates the LGF. Nevertheless, in some of the present cases we did do the additional (but superfluous) check that the differential equation is indeed homogeneous by plugging in the boundaries of the integral, and got confirmation.

If this method is applied to a one-dimensional integral with hyperexponential integrand (i.e., its logarithmic derivative is a rational function), then it is called the Almkvist-Zeilberger algorithm. Its summation counterpart is the celebrated Zeilberger algorithm for hypergeometric summation. For our purposes we have to generalize the input class for the integrand to the so-called ∂-finite holonomic functions: a function $f(x_1,\dots,x_d)$ is called ∂-finite if for each x_i there exists a linear ODE for f with respect to x_i. If in addition f is holonomic (the definition of this notion is somewhat technical and is omitted here) then the existence of creative telescoping operators like (7) or (8) is guaranteed.

The first algorithm to compute (8) for general ∂-finite functions (our examples fall into this class, too) was proposed in [10]. It can deal with single integrations only and thus has to be applied iteratively for multiple integrals. Its main drawback is its complexity that makes it impossible to apply it to the problems discussed in this paper. In [11] we have developed a different approach to compute (8) which is much better suited for large examples involving multidimensional integrals. In addition, it can directly deal with multiple integrals by computing operators of the form (7), but in the present context it turned out to be more efficient to do the integrations step by step. Both algorithms are implemented in our Mathematica package `HolonomicFunctions` [12], and a detailed introduction into the topic is given in [13]. The following example demonstrates how this method is applied to the previously discussed two-dimensional lattice.

Example 3. Looking at the integrand of Equation (5) one realizes that it is not ∂-finite since no linear ODE with respect to k_1 can be found (and analogously for k_2). But by means of the simple substitutions $\cos k_1 \to x_1$ and $\cos k_2 \to x_2$ we can overcome this trouble: the integral now reads

$$P(z) = \frac{1}{\pi^2} \int_{-1}^{1} \int_{-1}^{1} \frac{\mathrm{d}x_1\, \mathrm{d}x_2}{(1 - z x_1 x_2)\sqrt{1-x_1^2}\sqrt{1-x_2^2}}. \tag{9}$$

Let $f(x_1, x_2, z)$ denote the above integrand; it is easily verified that it is a ∂-finite function. The three ODEs w.r.t. x_1, x_2, and z are given by the operators

$$\begin{aligned} G_1 &= (x_1x_2z - 1)D_z + x_1x_2, \\ G_2 &= (x_2^2 - 1)(x_1x_2z - 1)D_{x_2} + (2x_1x_2^2z - x_1z - x_2), \\ G_3 &= (x_1^2 - 1)(x_1x_2z - 1)D_{x_1} + (2x_1^2x_2z - x_1 - x_2z), \end{aligned}$$

so that $G_i\big(f(x_1, x_2, z)\big) = 0$ for $i = 1, 2, 3$. In this example, it is an easy exercise to check that the creative telescoping operator

$$z(z^2-1)D_z^2 + (3z^2-1)D_z + z \;+\; D_{x_1}\frac{x_2 - x_1^2x_2}{x_1x_2z - 1} \;+\; D_{x_2}\frac{x_2z - x_2^3z}{x_1x_2z - 1} \tag{10}$$

annihilates the integrand f. Indeed, it can be written as a linear combination

$$\left(\frac{z(z^2-1)}{x_1x_2z-1}D_z + \frac{x_1x_2z(z^2+1) - 3z^2 + 1}{(x_1x_2z-1)^2}\right)G_1 - \frac{x_2}{(x_1x_2z-1)^2}(zG_2 + G_3)$$

of the previously computed operators. It follows that the double integral (9) satisfies the ODE

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

whose solution is the elliptic integral $\mathbf{K}(z^2)$.

Alternatively, the two integrations can be performed in two steps (the strategy that will be applied to the higher-dimensional fcc lattices). In the first step (integration w.r.t. x_1) the following two creative telescoping operators are found:

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

They certify that the integral $\int_{-1}^{1} f(x_1, x_2, z)\,\mathrm{d}x_1$ is annihilated by $(x_2^2z^2-1)D_z+x_2^2z$ and $(x_2^2-1)(x_2^2z^2-1)D_{x_2}+x_2(2x_2^2z^2-z^2-1)$. Next the operator

$$z(z^2-1)D_z^2+(3z^2-1)D_z+z\;-\;D_{x_2}\frac{x_2z(x_2^2-1)}{(x_2^2z^2-1)}$$

which is a linear combination of the previous ones, again reveals the same ODE for the double integral. □

3.2 Results

Using the above methodology and software, we have computed differential equations for the LGFs of the fcc lattices in four, five, and six dimensions, and rigorously proved their correctness. Additionally, this allows the computation of the return probabilities in the respective lattices up to very high precision.

Theorem 1. *The lattice Green's function of the four-dimensional face-centered cubic lattice*

$$P(z)=\frac{1}{\pi^4}\int_0^\pi\int_0^\pi\int_0^\pi\int_0^\pi\frac{\mathrm{d}k_1\,\mathrm{d}k_2\,\mathrm{d}k_3\,\mathrm{d}k_4}{1-\frac{z}{6}\big(\cos k_1\cos k_2+\cos k_1\cos k_3+\cdots+\cos k_3\cos k_4\big)}$$

satisfies the differential equation

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

Proof. Here we give only an outline of the proof. The calculations in extenso are provided as a Mathematica notebook in the electronic supplementary material [14] (to be downloaded from http://www.koutschan.de/data/fcc/).

The substitutions $\cos k_j \to x_j$ transform the integrand of the four-fold integral to

$$f(x_1,\ldots,x_4,z)=\frac{1}{\big(1-\frac{z}{6}(x_1x_2+x_1x_3+\cdots+x_3x_4)\big)\cdot\prod_{j=1}^4\sqrt{1-x_j^2}}.\tag{11}$$

This expression is ∂-finite and thus a Gröbner basis of the zero-dimensional annihilating left ideal can be computed (`ann0` in the notebook). Next, operators $A_j(x_2,x_3,x_4,z,D_{x_2},D_{x_3},D_{x_4},D_z)$ and $B_j(x_1,x_2,x_3,x_4,z,D_{x_1},D_{x_2},D_{x_3},D_{x_4},D_z)$ for $1\leqslant j\leqslant 4$ are computed, such that $A_j+D_{x_1}B_j$ is an element in the left ideal generated by `ann0`. This fact can be easily tested by reducing it with the Gröbner basis: the remainder being 0 answers the membership question in an affirmative way. In the notebook, the A_j's are collected in the variable `ann0`, and the B_j's in the variable `delta1`. We conclude that A_1, A_2, A_3, and A_4 generate an annihilating left ideal for the integral $\int_0^\pi f(x_1,x_2,x_3,x_4,z)\,\mathrm{d}x_1$. In a similar fashion, the integrations with respect to x_2, x_3, and x_4 are performed, yielding a single ODE in z that annihilates $P(z)$. □

Note that this theorem confirms the conjectured result given in [2]. Guttmann also observed that the differential equation given in Theorem 1 has *maximal unipotent monodromy* (MUM), i.e., its indicial equation is of the form λ^n and hence has only 0 as a root, and additionally satisfies the *Calabi-Yau condition.* Many LGFs of other lattices fall into this class, too, and therefore this fact may not seem too surprising.

In order to receive the return probability in the four-dimensional fcc lattice, holonomic closure properties are applied to compute a differential equation for

$$\frac{P(z)}{1-z} = \sum_{n=0}^{\infty} \left(\sum_{k=0}^{n} p_k(\mathbf{0}) \right) z^n,$$

which in turn gives a recurrence for $f(n) = \sum_{k=0}^{n} p_k(\mathbf{0})$:

$$\begin{aligned}
&(n+2)(n+3)^2(n+4)(35n^2+420n+1252)f(n)+\\
&(n+3)(n+4)(595n^4+11375n^3+79874n^2+244384n+276024)f(n+1)+\\
&3(n+4)(1015n^5+24780n^4+240253n^3+1156976n^2+\\
&\quad 2769392n+2638272)f(n+2)+\\
&(3325n^6+107100n^5+1427695n^4+10080600n^3+39767416n^2+\\
&\quad 83134488n+71984160)f(n+3)-\\
&4(2065n^6+62580n^5+788848n^4+5295615n^3+19973086n^2+\\
&\quad 40139838n+33590844)f(n+4)-\\
&12(735n^6+25200n^5+359282n^4+2725632n^3+11601091n^2+\\
&\quad 26259960n+24690708)f(n+5)+\\
&288(35n^2+350n+867)(n+6)^4 f(n+6)=0.
\end{aligned}$$

The initial values

$$f(0)=1, \quad f(1)=1, \quad f(2)=\frac{25}{24}, \quad f(3)=\frac{19}{18}, \quad f(4)=\frac{1637}{1536}, \quad f(5)=\frac{549}{512}$$

are easily (of course, not by hand!) computed by counting the number of excursions of length up to 5. For the return probability

$$R = 1 - \left(\lim_{n\to\infty} f(n) \right)^{-1}$$

we need to evaluate the limit of the sequence $f(n)$. This can be done very accurately when knowing the asymptotics of the sequence. We apply the method described in [15], which has been implemented in Mathematica [16], and obtain the following basis of asymptotic solutions:

$$\begin{aligned}
s_1(n) &= \frac{1}{n^2}\left(-\frac{1}{2}\right)^n \left(1 - \frac{5}{6n} + \frac{67}{24n^2} + \frac{1459}{144n^3} + O\Big(\frac{1}{n^4}\Big)\right),\\
s_2(n) &= \frac{1}{n^2}\left(-\frac{1}{3}\right)^n \left(1 - \frac{5}{2n} + \frac{51}{8n^2} - \frac{143}{8n^3} + O\Big(\frac{1}{n^4}\Big)\right),\\
s_3(n) &= \frac{1}{n^2}\left(-\frac{1}{6}\right)^n \left(1 - \frac{45}{14n} + \frac{4633}{392n^2} - \frac{112407}{5488n^3} + O\Big(\frac{1}{n^4}\Big)\right),\\
s_4(n) &= \frac{1}{n^2}\left(-\frac{1}{8}\right)^n \left(1 - \frac{52}{9n} + \frac{812}{27n^2} - \frac{45820}{243n^3} + O\Big(\frac{1}{n^4}\Big)\right),
\end{aligned}$$

$$
\begin{aligned}
s_5(n) &= \frac{1}{n}\left(1 - \frac{1}{n} + \frac{7}{9n^2} - \frac{7}{18n^3} + O\Big(\frac{1}{n^4}\Big)\right), \\
s_6(n) &= 1.
\end{aligned}
$$

Obviously, the first four solutions do not significantly contribute as they tend to 0 very rapidly. Thus by taking into account $s_5(n)$ and $s_6(n)$ only, and computing the asymptotic expansion to a higher order (e.g., 30), allows us to obtain (at least) 100 correct digits of the limit.

Corollary 2. *The LGF of the four-dimensional fcc lattice, evaluated at $z = 1$ is*

$$P(1) \approx 1.10584379792120476018299547088585107443954623663875285836499,$$

and therefore the return probability is

$$R \approx 0.0957131541725628967353167649012101857007088196380173576877 4.$$

Note: Corollaries 2 and 4 have been confirmed independently by employing the certified numerics implemented in the Maple package `NumGfun` [17].

Theorem 3. *The lattice Green's function of the five-dimensional fcc lattice*

$$P(z) = \frac{1}{\pi^5}\int_0^\pi \cdots \int_0^\pi \frac{\mathrm{d}k_1\,\mathrm{d}k_2\,\mathrm{d}k_3\,\mathrm{d}k_4\,\mathrm{d}k_5}{1 - \frac{z}{10}\big(\cos k_1 \cos k_2 + \cos k_1 \cos k_3 + \cdots + \cos k_4 \cos k_5\big)}$$

satisfies the differential equation

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

Proof. The proof is very analogous to that of Theorem 1 and is given in detail in the supplementary material [14]. □

Again, we are happy to report that our proof confirms the conjectured ODE of [3]. Remarkably enough, the indicial equation of the differential equation presented in Theorem 3 is $\lambda^5(\lambda-1)$ and hence the ODE lacks MUM. For the same reason it is not a Calabi-Yau differential equation.

Corollary 4. *The LGF of the five-dimensional fcc lattice, evaluated at $z = 1$ is*

$$P(1) \approx 1.048852351354914851629563763699992759454025504652066403138 45,$$

and therefore the return probability is

$$R \approx 0.046576957463848024193374420594803291076402397746321129305 32.$$

Theorem 5. *The lattice Green's function of the six-dimensional face-centered cubic lattice*

$$P(z) = \frac{1}{\pi^6}\int_0^\pi \cdots \int_0^\pi \frac{\mathrm{d}k_1\,\mathrm{d}k_2\,\mathrm{d}k_3\,\mathrm{d}k_4\,\mathrm{d}k_5\,\mathrm{d}k_6}{1-\frac{z}{15}\big(\cos k_1\cos k_2+\cos k_1\cos k_3+\cdots+\cos k_5\cos k_6\big)}$$

satisfies a differential equation of order 8 and with polynomials coefficients of degree 43. Its leading coefficient is

$$z^6(z-3)(z-1)(z+4)(z+5)(z+9)(z+15)^2(z+24)(2z+3)(2z+15)$$
$$\times(4z+15)(7z+60)q(z)$$

where $q(z)$ stands for a certain irreducible polynomial of degree 25, and its indicial equation is $\lambda^6(\lambda-1)^2$. The full equation is too long to be printed here, but can be found in [14].

Proof. The proof is very analogous to that of Theorem 1 and is given in detail in the supplementary material [14]. □

As in the five-dimensional fcc lattice, the differential equation of Theorem 5 lacks MUM and therefore is not Calabi-Yau.

Corollary 6. *The LGF of the six-dimensional fcc lattice, evaluated at $z = 1$ is*

$$P(1) \approx 1.027749100627498839859363679273968502092439909001148724251 72,$$

and therefore the return probability is

$$R \approx 0.026999878287956124269364175426196380216122626762395014138 43.$$

We want to conclude this section with an overview of our results concerning the return probabilities, which reveals an interesting dependence on the dimension of the lattice:

Dimension	Return Probability
2	1
3	0.256318236504649
4	0.095713154172563
5	0.046576957463848
6	0.026999878287956

4 Outlook

While the calculations for Theorem 1 and Theorem 3 are performed in a few minutes respectively hours, it was a major effort of several days to compute the certificates that prove Theorem 5; they are several hundred MegaBytes in size. With the methods described in this paper and with the current hardware, it is completely out of the question to attack the fcc lattice in seven dimensions. An interesting question is whether the pattern that showed up in dimensions four to six continues. This would suggest a differential equation of order 10 with indicial equation $\lambda^7(\lambda-1)^3$. But who knows?

For the three corollaries we computed the approximations for the return probabilities with more than one hundred valid digits. But we have no clue what their exact values are. Banderier evaluated these numbers up to several thousand digits [18], but also he was unable to identify the closed forms. So we leave these questions open, as a challenge for future research.

Acknowledgments

Anthony Guttmann aroused my interest in computing LGFs during his talk at the 65th Séminaire Lotharingien de Combinatoire in Strobl, Austria. I would like to thank him for his encouragement and advice. I am grateful to my colleague Manuel Kauers for interesting discussions and for pointing me to the trick of multi-step guessing. This research was carried out while the author was employed at the Research Institute for Symbolic Computation (RISC), Linz, Austria. The author was supported by the Austrian Science Fund (FWF): P20162-N18.

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