0.1 Combinatorial problems of (quasi-)crystallography

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0.1.1 Introduction

The discovery of non-periodic solids has motivated the construction of numerous examples of aperiodic tiling models, and led to the systematic theory of cut and project or model sets, as they are now called, see [1–3] for details and further references. Most combinatorial questions of crystallography, such as sublattice or shelling structures, have a natural analogue for aperiodic systems (we will explain the technical terms in more detail later on). However, the traditional methods of crystallography do not apply. Fortunately, the most important systems possess a high degree of symmetry, which manifests itself in an intimate relation to algebraic number theory [4]. This relationship has been exploited successfully to tackle combinatorial questions for quasicrystals [5–9].

Interestingly, this approach also simplifies the treatment of crystals. A fairly common feature is the use of Dirichlet series generating functions, which emerges from the observation that many counting functions, when properly normalised, can be expressed in terms of multiplicative arithmetic functions, see [10] for background material. This leads to a systematic and unified approach which will be summarised in this article. Besides explicit results, the generating functions also allow a precise calculation of asymptotic properties.

There are various other combinatorial problems, such as the determination of coordination sequences and coronae, the orbit structure under inflation, or general complexity considerations. The results are usually encapsulated in terms of generating functions, compare [11] for background material. In this expository article, we will concentrate on problems that are connected with Dirichlet series generating functions, and only summarize other developments.

To be able to explain the concepts in a simple fashion, we shall mainly use two examples, namely the triangular lattice, written as $\varGamma = \mathbb{Z}[\xi_3]$ with $\xi_3 = \exp(2\pi\mathrm{i}/3) = (-1+\mathrm{i}\sqrt{3})/2$, the set (ring) of Eisenstein integers, and the vertex set of the twelvefold symmetric shield tiling, see Fig. 1. We concentrate on explicit results for these examples, and refer to original sources for a more general exposition and for details on the asymptotic behaviour.

0.1.2 Counting general sublattices

Let us first consider the triangular lattice $\varGamma = \mathbb{Z}[\xi_3]$, or, in fact, any planar lattice, i.e., the integer span of two vectors in the plane that are linearly independent over $\mathbb{R}$. Our first question is for the number $\ell_2(m)$ of *sublattices* $\varGamma'$ of given index $m = [\varGamma : \varGamma']$. This is a multiplicative

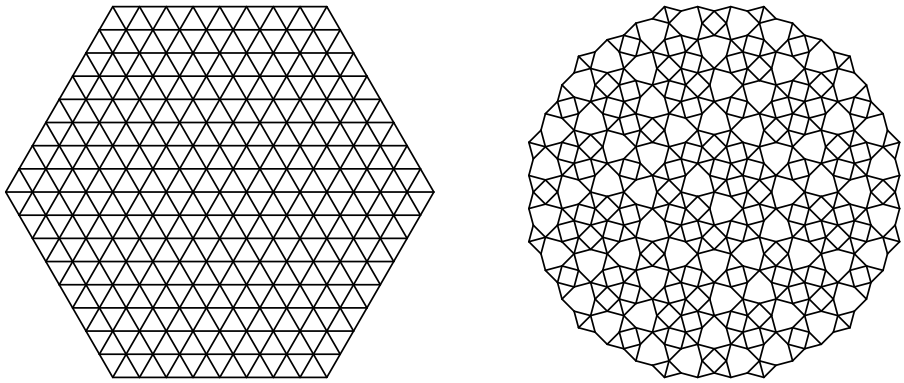

Figure 1: Finite patches of the triangular lattice and the twelvefold shield tiling.

function, i.e., $\ell_2(mn) = \ell_2(m)\,\ell_2(n)$ for m, n coprime. Due to multiplicativity, it is best encoded in a Dirichlet series generating function, where one obtains [5, Eq. (3.9)]

$$\begin{aligned} F_2(s) &= \sum_{m=1}^{\infty} \frac{\ell_2(m)}{m^s} = \zeta(s)\,\zeta(s-1) = \prod_p \frac{1}{1-p^{-s}}\,\frac{1}{1-p^{1-s}} \qquad (1)\\ &= 1 + \tfrac{3}{2^s} + \tfrac{4}{3^s} + \tfrac{7}{4^s} + \tfrac{6}{5^s} + \tfrac{12}{6^s} + \tfrac{8}{7^s} + \tfrac{15}{8^s} + \tfrac{13}{9^s} + \tfrac{18}{10^s} + \tfrac{12}{11^s} + \tfrac{28}{12^s} + \ldots \end{aligned}$$

Here, $\zeta(s) = \sum_{m=1}^{\infty} m^{-s}$ is Riemann's zeta function, p in the product runs over all rational primes, by which, following the usual convention, we mean the primes of $\mathbb{Z}$. Furthermore, $\ell_2(m) = \sum_{d|m} d$ is the ordinary divisor function, compare [10] for details.

The corresponding question is well defined also for $L = \mathbb{Z}[\xi_{12}]$, $\xi_{12} = \exp(2\pi\mathrm{i}/12)$, when considered as a (free) $\mathbb{Z}$-module of rank 4. The number of full rank submodules of index m, $\ell_4(m)$, is again multiplicative and has the generating function [5, App. A]

$$\begin{aligned} F_4(s) &= \sum_{m=1}^{\infty} \frac{\ell_4(m)}{m^s} = \zeta(s)\,\zeta(s-1)\,\zeta(s-2)\,\zeta(s-3) \qquad (2)\\ &= 1 + \tfrac{15}{2^s} + \tfrac{40}{3^s} + \tfrac{155}{4^s} + \tfrac{156}{5^s} + \tfrac{600}{6^s} + \tfrac{400}{7^s} + \tfrac{1395}{8^s} + \tfrac{1210}{9^s} + \tfrac{2340}{10^s} + \tfrac{1464}{11^s} + \ldots \end{aligned}$$

where $\ell_4(m) = \sum_{d_1\cdot\ldots\cdot d_4=m} d_1^0\, d_2^1\, d_3^2\, d_4^3$ with the sum running over positive d_i only. The answer is the same for all $\mathbb{Z}$-modules of rank 4. They include the cyclotomic rings $\mathbb{Z}[\xi_n]$ with $n \in \{5, 8, 12\}$, which are important for quasicrystals [12]. Note that we follow the mathematical convention to restrict to $n \not\equiv 2\ (4)$ because $\mathbb{Z}[\xi_n] = \mathbb{Z}[\xi_{2n}]$ for n odd.

Clearly, this combinatorial question is purely algebraic, and the method also applies to counting finite index subgroups of finitely generated free Abelian groups, see [5, App. A] for details. The generating function for counting index m subgroups of $\mathbb{Z}^n$ reads

$$F_n(s) = \sum_{m=1}^{\infty} \frac{\ell_n(m)}{m^s} = \zeta(s)\,\zeta(s-1)\cdot\ldots\cdot\zeta(s-n+1) \qquad (3)$$

and gives the formula $\ell_n(m) = \sum_{d_1\cdot\ldots\cdot d_n=m} d_1^0\, d_2^1 \cdot\ldots\cdot d_n^{n-1}$.

0.1.3 Counting similarity sublattices

Let us turn to (geo)metric properties and ask for the number $a_6(m)$ of *triangular* sublattices of Γ of a given index m, which coincides with the number of ideals of $\mathbb{Z}[\xi_3]$ of norm m because $\mathbb{Z}[\xi_3]$ is a principal ideal domain [13]. The answer is given by the Dedekind zeta function of the cyclotomic (also, quadratic) field $\mathbb{Q}(\xi_3) = \mathbb{Q}(\sqrt{-3})$, i.e., one obtains [14, Eq. (9)]

$$\begin{aligned} \zeta_{\mathbb{Q}(\xi_3)}(s) &= \sum_{m=1}^{\infty} \frac{a_6(m)}{m^s} = \frac{1}{1-3^{-s}} \prod_{p\equiv 1\,(3)} \frac{1}{(1-p^{-s})^2} \prod_{p\equiv 2\,(3)} \frac{1}{1-p^{-2s}} \qquad (4)\\ &= 1+\tfrac{1}{3^s}+\tfrac{1}{4^s}+\tfrac{2}{7^s}+\tfrac{1}{9^s}+\tfrac{1}{12^s}+\tfrac{2}{13^s}+\tfrac{1}{16^s}+\tfrac{2}{19^s}+\tfrac{2}{21^s}+\tfrac{1}{25^s}+\ldots \end{aligned}$$

where, e.g., $p \equiv 1(3)$ means that the corresponding product runs over all rational primes congruent to 1 modulo 3.

The corresponding question for the module $\mathbb{Z}[\xi_{12}]$ is answered by the Dedekind zeta function [15] of the cyclotomic field $\mathbb{Q}(\xi_{12})$, which reads [14, Eq. (13)]

$$\begin{aligned} \zeta_{\mathbb{Q}(\xi_{12})}(s) &= \sum_{m=1}^{\infty} \frac{a_{12}(m)}{m^s} \qquad (5)\\ &= \frac{1}{1-4^{-s}} \frac{1}{1-9^{-s}} \prod_{p\equiv 1\,(12)} \frac{1}{(1-p^{-s})^4} \prod_{p\equiv -1 \text{ or } \pm 5\,(12)} \frac{1}{(1-p^{-2s})^2}\\ &= 1+\tfrac{1}{4^s}+\tfrac{1}{9^s}+\tfrac{4}{13^s}+\tfrac{1}{16^s}+\tfrac{2}{25^s}+\tfrac{1}{36^s}+\tfrac{4}{37^s}+\tfrac{2}{49^s}+\tfrac{4}{52^s}+\tfrac{4}{61^s}+\ldots \end{aligned}$$

These two generating functions also have an interpretation in terms of planar colourings [14, 16, 17]: $a_6(m)$ is (up to permutation) the number of colourings of the triangular lattice Γ where one colour occupies a similarity (hence triangular) sublattice of Γ of index m and the remaining colours occupy its cosets. The function $a_{12}(m)$ then counts the colourings of $\mathbb{Z}[\xi_{12}]$ via similarity submodules of index m, all of which are principal ideals of $\mathbb{Z}[\xi_{12}]$ as the latter is a principal ideal domain, see [6, 15] for details. For a discussion of the corresponding colour groups, see [16].

This approach can be extended to all cyclotomic fields with class number one (the corresponding rings of integers are then principal ideal domains), see [14, 15, 18], and references given there, for details.

0.1.4 Counting coincidence sublattices

Another geometric problem, with interesting applications to grain boundaries and twinning phenomena in crystals and quasicrystals, is the classification of sublattices of Γ that can be seen as the intersection of Γ with a rotated copy of itself. These are the *coincidence sublattices*, see [5] for details, and the corresponding coincidence index is called Σ-factor in materials science. Once more, the generating function (for the number of coincidence sublattices of index m) is best written as a Dirichlet series, where, using $\Gamma = \mathbb{Z}[\xi_3]$, one finds

$$\begin{aligned} \Phi_{\mathbb{Z}[\xi_3]}(s) &= \prod_{p\equiv 1\,(3)} \frac{1+p^{-s}}{1-p^{-s}} = \frac{1}{1+3^{-s}} \frac{\zeta_{\mathbb{Q}(\xi_3)}(s)}{\zeta(2s)} \qquad (6)\\ &= 1+\tfrac{2}{7^s}+\tfrac{2}{13^s}+\tfrac{2}{19^s}+\tfrac{2}{31^s}+\tfrac{2}{37^s}+\tfrac{2}{43^s}+\tfrac{2}{49^s}+\tfrac{2}{61^s}+\tfrac{2}{67^s}+\tfrac{2}{73^s}+\ldots \end{aligned}$$

which is derived in [8, Sec. IV.A].

Behind this combinatorial problem is a group structure. It turns out that the set of rotations R such that $\varGamma \cap R\varGamma$ is a coincidence sublattice of $\varGamma$ forms a group, called $\mathrm{SOC}(\varGamma)$, which is isomorphic to $C_6 \otimes \mathbb{Z}^{(\aleph_0)}$, see [19] for details, in particular on the structure of this Abelian group. Also, the possible coincidence indices $[\varGamma : (\varGamma \cap R\varGamma)] =: \varSigma(R)$ (excluding 0 and ∞) form a monoid (a semigroup with unit), generated by the (rational) primes $p \equiv 1 \ (3)$.

The formulation with cyclotomic integers admits an extension of the previous results to $\mathbb{Z}[\xi_{12}]$, where the generating function for the number of coincidence submodules of $\mathbb{Z}[\xi_{12}]$ of index m is [8, Sec. IV.F]

$$\begin{aligned} \Phi_{\mathbb{Z}[\xi_{12}]}(s) &= \prod_{p\equiv 1\,(12)} \left(\frac{1+p^{-s}}{1-p^{-s}}\right)^2 \prod_{p\equiv \pm 5\,(12)} \frac{1+p^{-2s}}{1-p^{-2s}} = \frac{\zeta_{\mathbb{Q}(\xi_{12})}(s)}{\zeta_{\mathbb{Q}(\sqrt{3})}(2s)} \\ &= 1 + \tfrac{4}{13^s} + \tfrac{2}{25^s} + \tfrac{4}{37^s} + \tfrac{2}{49^s} + \tfrac{4}{61^s} + \tfrac{4}{73^s} + \tfrac{4}{97^s} + \tfrac{4}{109^s} + \tfrac{4}{157^s} + \ldots \end{aligned} \tag{7}$$

Here, $\zeta_{\mathbb{Q}(\sqrt{3})}(s)$ is the Dedekind zeta function of the quadratic field $\mathbb{Q}(\sqrt{3})$, i.e.,

$$\zeta_{\mathbb{Q}(\sqrt{3})}(s) = \frac{1}{1-2^{-s}} \frac{1}{1-3^{-s}} \prod_{p\equiv \pm 1\,(12)} \frac{1}{(1-p^{-s})^2} \prod_{p\equiv \pm 5\,(12)} \frac{1}{1-p^{-2s}} \,. \tag{8}$$

There is one subtlety in the application of this result to a *discrete* point set such as the vertex set of the shield tiling. A small acceptance correction factor is needed, which can be calculated explicitly, except for situations where the window has fractal boundary, as in [20]. Further details, together with a general discussion of the case of n-fold symmetry, can be found in [8].

0.1.5 Central shelling

Let us discuss the shelling problem, first in its version for the *central* shelling. Here, one asks for the number of points of $\varGamma = \mathbb{Z}[\xi_3]$ on circles of radius r around the origin. The result is usually given in terms of lattice theta functions, see [21, Ch. 4] for an extensive exposition. However, in our situation, it can also be encapsulated in a Dirichlet series. To this end, one considers only radii $r > 0$ and divides the corresponding shelling number, $c(r^2)$, by 6, which is the trivial symmetry factor. If a shell is non-empty, we have $r^2 = x\,\overline{x}$ with $x \in \varGamma$, and $r^2 = m$ is a (rational) integer. What then remains is the multiplicative function $a_6(m)$ whose generating function was given above, in a different context, in Eq. (5). Further details and references are given in [22].

In the case of $\mathbb{Z}[\xi_{12}]$, the central shelling function c depends on $r^2 \in \mathbb{Z}[\xi_{12} + \overline{\xi}_{12}] = \mathbb{Z}[\sqrt{3}\,]$, and one needs the primes of $\mathbb{Z}[\sqrt{3}\,]$ (see [13] for details) to derive a formula for $c(r^2)$, compare [18]. Let us write $\tilde{p}$ for a prime in $\mathbb{Z}[\sqrt{3}\,]$, and let $t(\tilde{p})$ be the highest power t such that $\tilde{p}^{\,t}$ divides r^2, written as $\tilde{p}^{\,t} \| r^2$. Then, whenever $t(\tilde{p})$ is odd for a $\tilde{p}$ that is also a prime in $\mathbb{Z}[\xi_{12}]$ (i.e., an inert prime), one has $c(r^2) = 0$. Otherwise, one finds the formula

$$c(r^2) = 12 \prod_{\substack{\tilde{p}\,|\,r^2 \\ \tilde{p}\ \text{splits}}} \big(t(\tilde{p}) + 1\big) \tag{9}$$

$\mathbb{Z}$	$\mathbb{Z}[\sqrt{3}]$	$\mathbb{Z}[\xi_{12}]$
2	$2 = (2-\sqrt{3})\cdot(1+\sqrt{3})^2$	$1+\sqrt{3}$ prime
3	$3 = (\sqrt{3})^2$	$\sqrt{3}$ prime
$p \equiv 1\ (12)$	$p = \tilde{p}\,\tilde{p}'$	$\tilde{p} = P\,\overline{P},\ \tilde{p}' = P'\,\overline{P'}$
$p \equiv -1\ (12)$	$p = \tilde{p}\,\tilde{p}'$	$\tilde{p}, \tilde{p}'$ prime
$p \equiv \pm 5\ (12)$	p prime	$p = P\,\overline{P}$

Table 1: Splitting structure of primes for $\mathbb{Z}[\xi_{12}]$. Here, $'$ is a Galois automorphism of $\mathbb{Q}(\xi_{12})$ which acts as $\sqrt{3} \mapsto -\sqrt{3}$ in $\mathbb{Q}(\sqrt{3})$, and $\overline{\ }$ denotes complex conjugation. Note that $2-\sqrt{3} = (2+\sqrt{3})^{-1}$ is a unit in $\mathbb{Z}[\sqrt{3}]$.

where the product runs only over a representative set of those primes $\tilde{p}$ of $\mathbb{Z}[\sqrt{3}]$ that split in the extension to $\mathbb{Z}[\xi_{12}]$. In this example, they are precisely the primes that originate from rational primes $p \equiv 1\ (12)$ and $p \equiv \pm 5\ (12)$.

Fortunately, the function $c(r^2)$ need not be calculated for all possible values of r^2. Since the units of $\mathbb{Z}[\sqrt{3}]$ are of the form $\pm(2+\sqrt{3})^{\ell}$ with $\ell \in \mathbb{Z}$, all positive units are actually totally positive, i.e., also their algebraic conjugate in $\mathbb{Q}(\sqrt{3})$ is positive. The fundamental unit is $2+\sqrt{3} = (1+\xi_{12})(1+\overline{\xi}_{12})$, hence all positive units are of the form $u = x\,\overline{x}$ with $x \in \mathbb{Z}[\xi_{12}]$, and this implies that $c(r^2)$ only depends on the (principal) ideal of $\mathbb{Z}[\sqrt{3}]$ that is generated by r^2, compare the proof of theorem 1 in [7]. So, whenever $s^2 = ur^2$ with u a positive unit, we have $c(s^2) = c(r^2)$. Also, one can see that $c\big(r^2\big) = c\big((r^2)'\big)$, where $'$ denotes algebraic conjugation in $\mathbb{Q}(\sqrt{3})$, defined by the Galois automorphism $\sqrt{3} \mapsto -\sqrt{3}$, compare Table 1.

Can the result be given in an even simpler way? Suppose, for a moment, that the function $c(r^2)$ would only depend on the *norm* of r^2, i.e., on $m = r^2\,(r^2)'$, where m is a rational integer. This would mean that $c(r^2) = 12 f(m)$ with $f(m)$ a multiplicative arithmetic function, whose Dirichlet series turns out to be

$$
\begin{aligned}
C_{12}(s) &= \sum_{m=1}^{\infty} \frac{f(m)}{m^s} \qquad (10)\\
&= \frac{1}{1-4^{-s}}\,\frac{1}{1-9^{-s}} \prod_{p\equiv 1\,(12)} \frac{1}{\left(1-p^{-s}\right)^2}\\
&\quad \times \prod_{p\equiv -1\,(12)} \frac{1}{1-p^{-2s}} \prod_{p\equiv \pm 5\,(12)} \frac{1}{\left(1-p^{-2s}\right)^2}\\
&= 1 + \tfrac{1}{4^s} + \tfrac{1}{9^s} + \tfrac{2}{13^s} + \tfrac{1}{16^s} + \tfrac{2}{25^s} + \tfrac{1}{36^s} + \tfrac{2}{37^s} + \tfrac{2}{49^s} + \tfrac{2}{52^s} + \tfrac{2}{61^s} + \ldots
\end{aligned}
$$

As can be seen from the exact shelling formula (9), this cannot provide the general answer. However, it is correct for many cases, and is then by far the simplest way to calculate $c(r^2)$.

The first non-trivial value of m where this fails is $m = 169 = 13^2$. Observing that $13 = (4+\sqrt{3})(4-\sqrt{3}) = \tilde{p}\tilde{p}'$ in $\mathbb{Z}[\sqrt{3}]$, the possible values of r^2 with norm m are $\tilde{p}^2$, $\tilde{p}\tilde{p}'$ and $(\tilde{p}')^2$, with shelling numbers 36, 48 and 36, respectively. Since $f(169) = 3$, we get a

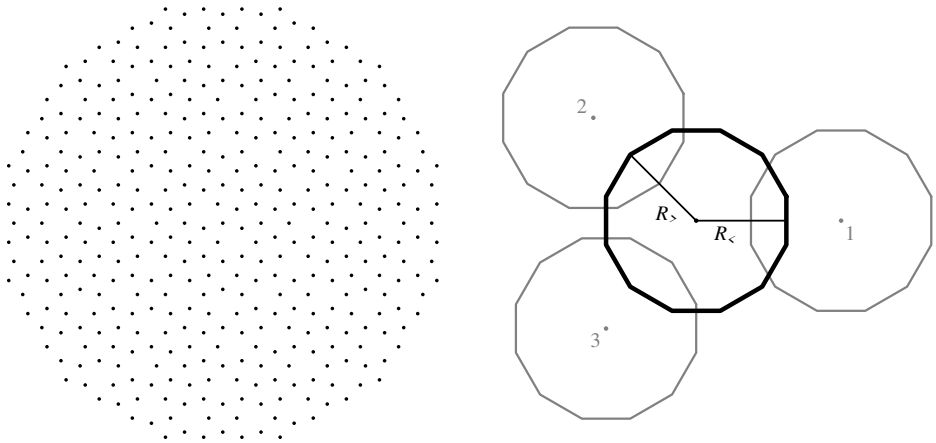

Figure 2: Vertex set of the shield tiling and its dodecagonal window (black). Also shown are three shifted copies of the window (grey), see text for details, as needed for Table 2.

wrong answer for the middle case this way. This is an example with a prime $p \equiv 1 \ (12)$. The contributions to non-empty shells from the other rational primes are properly counted by the Dirichlet series (10) because they either correspond to a unique prime in $\mathbb{Z}[\sqrt{3}]$ or to primes which do not split in the step from $\mathbb{Z}[\sqrt{3}]$ to $\mathbb{Z}[\xi_{12}]$, see Table 1.

So, let us assume that r is the radius of a non-empty shell, i.e., $t(\tilde{p})$ is even for all inert primes $\tilde{p}$ of $\mathbb{Z}[\sqrt{3}]$. Then, $12f(m)$ with $m = r^2\,(r^2)'$ gives the correct shelling number if, whenever m is divisible by a rational prime $p \equiv 1 \ (12)$, r^2 is divisible by either $\tilde{p}$ or $\tilde{p}'$, compare Table 1, but never by both. Beyond this situation, one has to use formula (9).

Eq. (9), together with the partial simplification of Eq. (10), gives the result for the central shelling of the full module. When passing to a model set [1], which is a discrete subset of the full module, an obvious selection takes place for the possible radii. Furthermore, a correction factor may become necessary which depends on the window chosen, see [18] for details. A systematic approach to a complete generating function would employ summatory functions of arithmetic characters [15], which is postponed to future work.

0.1.6 Averaged shelling

In this last application, we are interested in the *average* number of points on shells of radius r, where the average is taken over all points of our point set as possible centres. In the lattice situation, the averaged and central shelling numbers coincide, but this is not so for model sets [1, 22]. To be specific, we explain this for the vertex set of the shield tiling. As for model sets in general, all averages needed are well defined and unique.

Let us first describe the vertex set of the shield tiling [23] in algebraic terms. We use $L = \mathbb{Z}[\xi_{12}]$ as above, together with the Galois automorphism $\star$ of $\mathbb{Q}(\xi_{12})$ given by $\xi_{12} \mapsto (\xi_{12})^5$.

r^2	representative	orbit length	norm	shift type	$a(r^2)$
$2-\sqrt{3}$	$1-\xi$	12	1	2	$8-2\sqrt{3}$
$4-2\sqrt{3}$	$\xi+\overline{\xi}-1$	12	4	1	2
$6-3\sqrt{3}$	$1-\xi+\xi^2-\xi^3$	12	9	2	$4-2\sqrt{3}$
1	1	12	1	1	8
$5-2\sqrt{3}$	$2-\xi$	24	13	3	$10-4\sqrt{3}$
2	$1+\xi^3$	12	4	2	$48-24\sqrt{3}$
$4-\sqrt{3}$	$\xi+\xi^2-2$	24	13	3	6
$8-3\sqrt{3}$	$3\xi-\xi^3-1$	24	37	3	$-76+44\sqrt{3}$
3	$\xi+\overline{\xi}$	12	9	1	$-4+\frac{16}{3}\sqrt{3}$
$7-2\sqrt{3}$	$2-2\xi-\xi^2$	24	37	3	$20-\frac{32}{3}\sqrt{3}$
$2+\sqrt{3}$	$1+\xi$	12	1	2	$48-22\sqrt{3}$
4	2	12	16	1	$2+\frac{4}{3}\sqrt{3}$

Table 2: Averaged shelling numbers $a(r^2)$ for the shield tiling of edge length $2\sin(\pi/12) = \sqrt{2-\sqrt{3}}$, for all possible distances $0 < r \leq 2$. Representative elements (with $\xi = \xi_{12}$) and orbit lengths refer to the point symmetry group D_{12} of the tiling. The norm of r^2 is $m = r^2\,(r^2)'$, and the shift types are explained in Fig. 2.

This is the star map of the standard model set construction [1], which gives

$$\varLambda \;=\; \{x \in L \mid x^\star \in W\} \tag{11}$$

where the window W is a relatively compact set with non-empty interior. For the shield tiling, we choose W as a regular dodecagon of edge length 1, hence of inradius $R_< = (2+\sqrt{3})/2$ and circumradius $R_> = \sqrt{2+\sqrt{3}}$, see Fig. 2 for the correct orientation.

If the window is centred at 0, the model set is singular, while generic examples are obtained by shifting the window, i.e., $\varLambda^u \;=\; \{x \in L \mid x^\star \in W+u\}$, for almost all $u \in \mathbb{R}^2$. The shortest distance between points in a generic $\varLambda^u$ is $(\sqrt{3}-1)/\sqrt{2}$. Joining such points by edges results in a shield tiling; different generic choices of u result in locally indistinguishable shield tilings.

Table 2 lists all distances $0 < r \leq 2$ between points of $\varLambda$ which occur with positive frequency, together with a representing point in L. The corresponding orbit length is given w.r.t. the point symmetry group D_{12}. Here, it coincides with the value of the central shelling number $c(r^2) = 12\,f(m)$, as calculated by means of Eq. (9) or Eq. (10). For larger values of r^2, $c(r^2)$ can comprise several D_{12}-orbits, but only complete ones because the window is twelvefold and reflection symmetric. For the averaged shelling, we need to calculate the relative overlap area of the window W and a shifted copy (the so-called covariogram of W), where the shift is the star image of the representing vector [18]. For our examples, all three relative orientations indicated in Fig. 2 emerge, with squared midpoint distance $(r^2)'$ in $\mathbb{Q}(\sqrt{3}\,)$. The resulting averaged shelling number (last column) is always an element of $\mathbb{Q}(\sqrt{3}\,)$. More precisely, all averaged shelling numbers are in $\frac{1}{3}\mathbb{Z}[\sqrt{3}\,]$. This follows from the fact that the frequency mod-

ule of the vertex set of the shield tiling is $\frac{1}{36}\mathbb{Z}[\sqrt{3}]$. The frequency module is the $\mathbb{Z}$-span of the frequencies of all possible finite patches and can be determined from the topological invariants of the shield tiling [24].

For the overlap scenarios 1 and 2 of Fig. 2, where the shifts are along the two principal reflection axes of the dodecagon, the covariogram has a relatively simple form. We find

$$h_1(s) \;=\; \begin{cases} 1-\frac{1}{3}s, & 0\le s<1 \\ \frac{15+2\sqrt{3}}{18}-\frac{2\sqrt{3}}{9}s+\frac{2\sqrt{3}-3}{18}s^2, & 1\le s<2R_<-1 \\ \frac{5+2\sqrt{3}}{6}-\frac{2}{3}s+\frac{2\sqrt{3}-3}{6}s^2, & 2R_<-1\le s<2R_< \\ 0, & 2R_<\le s \end{cases} \tag{12}$$

and

$$h_2(s) \;=\; \begin{cases} 1-\frac{\sqrt{2}(\sqrt{3}-1)}{3}s+\frac{7-4\sqrt{3}}{6}s^2, & 0\le s<R_> \\ \frac{5+\sqrt{3}}{6}-\frac{\sqrt{2}}{3}s+\frac{2-\sqrt{3}}{6}s^2, & R_>\le s<R_>+\sqrt{2} \\ \frac{4+2\sqrt{3}}{3}-\frac{\sqrt{2}(1+\sqrt{3})}{3}s+\frac{1}{6}s^2, & R_>+\sqrt{2}\le t<2R_> \\ 0, & 2R_>\le s \end{cases} \tag{13}$$

These functions have to be multiplied by the orbit length to give the averaged shelling number, resp. the corresponding contribution to it.

In Table 2, the four examples of type 3, where the shift is not along a symmetry direction, were calculated separately (and exactly). We do not give the more involved general formula for the covariogram of the regular dodecagon, but mention that

$$h(s) \;=\; \frac{2}{\pi}\arccos\Bigl(\frac{s}{2R}\Bigr)-\frac{s}{\pi R}\sqrt{1-\Bigl(\frac{s}{2R}\Bigr)^2}\,, \tag{14}$$

with $R=\sqrt{3/\pi}\,R_>$, is a very good approximation. It is obtained by replacing the dodecagon W with a disk of equal area, hence of radius R. This function is also known as Euclid's hat, see [25, p. 100] and references given there for details.

The averaged shelling in one dimension is rather simple and can be given in closed form [22], though no appropriate approach via generating function has been formulated so far. In two dimensions, the example of the Ammann-Beenker rhombus tiling with eightfold symmetry is treated in [18, 22], while examples with tenfold symmetry are shown in [22] (rhombic Penrose tiling) and [26] (Tübingen triangle tiling). So, with the example shown here, the standard symmetries in the plane are covered. Again, the understanding in terms of generating functions is missing, and in three or more dimensions, the averaged shelling has not been looked at thoroughly so far.

0.1.7 Other combinatorial questions

Another combinatorial problem, which can be seen as a variant of the shelling problem, is the determination of the coordination structure [21, 27, 28]. This needs a graph structure in

addition to the point set, and is usually formulated for tilings. Once again, one can ask for the number of points in the nth coordination shell (or corona), or for the analogous averaged quantity. The latter is more suitable for non-periodic (face to face) tilings. If they are constructed by a primitive inflation rule, or by the standard cut and project method (e.g., in its dualization version [29]), we know that all averages exist and the problem is well posed.

Let us first consider the situation of a lattice. If we denote the number of points at graph distance n by s_n, one uses the ordinary power series generating function $S(x) = \sum_{n=0}^{\infty} s_n\, x^n$. For the class of root lattices and root graphs, these generating functions are rather simple and can be given in closed form, see [27, 30]. For aperiodic tilings, one faces the same difficulties as for the averaged shelling discussed above. The rhombic Penrose tiling and its octagonal sibling, the Ammann-Beenker tiling, are discussed in [28]. Once again, the averaged coordination numbers seem to be "nice" numbers. This is due to the structure of the corresponding frequency modules, and can be quantified [24].

Closely related is the more general question for the patch counting function, which is a direct measure of the local complexity of the structure. For example, it is well known that Sturmian sequences possess $n + 1$ different words of length n. This is the smallest complexity possible for any non-periodic structure in one dimension. To what extent this can be generalized to higher dimensions is still unsettled, see [31] for details. In order to come to a natural analogue to the statement about the Sturmian sequences, one could make use of the knowledge obtained from the shelling function discussed above. It provides the possible shell radii and hence the sizes of the patches to be considered.

The method of iterated inflation is, besides the projection method, the most frequently used approach to generate aperiodic tilings with long-range order. Under some mild conditions, the resulting structure is linearly repetitive, see [32] for details on this concept. Inflation also acts naturally on the set of all tilings that are locally indistinguishable (LI) to the fixed point constructed, i.e., on the entire LI class. In view of the high degree of (local) repetitivity, one is also interested in the orbit structure of the LI class under the inflation I. Let a_n denote the number of fixed points of I^n, $n \geq 1$, and define

$$\zeta_{\mathrm{LI}}(z) \;=\; \exp\left(\sum_{m=1}^{\infty} \frac{a_m}{m}\, z^m\right) \tag{15}$$

so that $\frac{z\zeta'_{\mathrm{LI}}(z)}{\zeta_{\mathrm{LI}}(z)} = \sum_{m=1}^{\infty} a_m\, z^m$ is the usual power series generating function of the sequence $\{a_m \mid m \geq 1\}$. The object $\zeta_{\mathrm{LI}}(z)$ is called a dynamical zeta function, see [33] and references given therein for background material.

This function can be calculated systematically, as explained in [34]. The cycle structure of inflation can also be extracted, e.g., by means of the Euler product expansion

$$\frac{1}{\zeta_{\mathrm{LI}}(z)} \;=\; \prod_{n=1}^{\infty} (1 - z^n)^{c_n} \tag{16}$$

where c_n is the number of n-cycles under inflation. Clearly, $a_n = \sum_{m|n} m\, c_m$, and an inversion is possible employing the Möbius function, compare [10].

If the tiling admits a construction by the projection method, it also admits a universal torus parametrization [35, 36]. The latter will be one-to-one on generic members of the LI class, but

	Fibonacci	Penrose
LI class	$\dfrac{1-z}{1-z-z^2}$	$\dfrac{(1-z-z^2)^2(1+z)}{(1-3z+z^2)(1+z-z^2)^3(1-z)}$
torus	$\dfrac{1-z^2}{1-z-z^2}$	$\dfrac{(1-z-z^2)^2(1+z-z^2)^2}{(1-3z+z^2)(1-z)^2(1+z)^4}$

Table 3: Dynamical zeta functions for the inflation action on the Fibonacci chain and the rhombic Penrose tiling, both on the full LI classes and on their torus parametrizations.

multiple-to-one on singular members. Consequently, since inflation is compatible with this reduction step, there is another dynamical zeta function, this time for the orbit structure on the torus. Both types of zeta functions are known to be rational. Two examples are summarized in Table 3, further examples can be found in [34, 35, 37].

0.1.8 Open problems

The above examples demonstrate that a systematic and unified approach to combinatorial problems of (quasi)crystallography is possible, at least in the planar case. The situation is more involved in dimensions $d \geq 3$, where satisfactory results so far exist only for the most symmetric cases, i.e., those with (hyper)cubic or (hyper)icosahedral symmetry [5–7, 9, 38]. Still, even some of these cases leave room for improvement and simplification, e.g., along the lines mentioned around Eq. (10).

On the other hand, model sets with high symmetry are closely related to lattices in higher dimensions, where many of these questions are still open, compare [21]. One may expect some progress at least for the class of root lattices, hence also for quasicrystals derived from them [39]. Further progress is also needed in the investigation of colour symmetry groups, see [16] for a summary of the present state of affairs.

A big mystery is the meaning of the averaged shelling function. For the standard tilings with all magic properties (inflation rule, perfect matching rules, pure point diffraction etc.), the averaged shelling numbers always seem to be "nice" (being algebraic integers or rationals with bounded denominator), while this is not the case for model sets with generic windows. This phenomenon points towards another function defined by these numbers, with various analytic and topological consequences, but we do not know how to substantiate this at present.

Acknowledgment

It is a pleasure to thank Robert V. Moody, Peter A. B. Pleasants and Alfred Weiss for cooperation and helpful discussions. We are grateful to Franz Gähler and Tilmann Gneiting for providing relevant material and information. This work was supported by Deutsche Forschungsgemeinschaft (Ba 1070/7). Finally, we express our gratitude to the Erwin Schrödinger International Institute for Mathematical Physics in Vienna for support during a stay in autumn 2002, where this manuscript was completed.

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