Quasicrystalline Combinatorics

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Abstract. Several combinatorial problems of (quasi)crystallography are reviewed with special emphasis on a unified approach, valid for both crystals and quasicrystals. In particular, we consider planar sublattices, similarity sublattices, coincidence sublattices and their module counterparts. The corresponding counting functions are encapsulated in Dirichlet series generating functions, with worked out results for the square lattice and the Tübingen triangle tiling. Finally, we discuss a novel approach to central and averaged shelling for these examples, also involving Dirichlet series.

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 model sets, see [13, 4, 17] for details and further references. Most combinatorial questions of crystallography, such as sublattice or shelling structures, have a natural analogue for aperiodic systems. However, the traditional methods of crystallography often 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 [15]. This relationship has been exploited successfully to tackle combinatorial questions for quasicrystals [2, 7, 14, 16, 19].

Interestingly, this approach also simplifies the treatment of crystals. One common feature is the use of Dirichlet series generating functions, which emerges from the observation that the counting functions, when properly normalised, can be expressed in terms of multiplicative arithmetic functions, see [1] 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.

We shall use the square lattice, written as $\mathbb{Z}^2 = \mathbb{Z}[i]$, the set (ring) of Gaussian integers, and the vertex set of the Tübingen triangle tiling (TTT) for explaining and illustrating our concepts, see figure 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.

2. Counting general sublattices

Let us consider $\mathbb{Z}[i]$. Our first question is for the number of *sublattices* of given index m, called $\ell_2(m)$. This is a multiplicative function, i.e. $\ell_2(mn) = \ell_2(m)\,\ell_2(n)$ for m, n coprime.

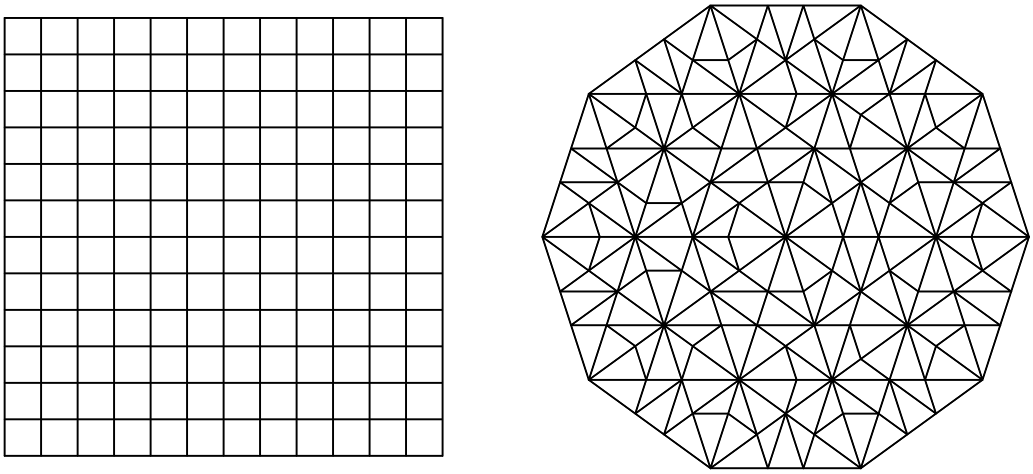

Figure 1. Finite patches of square lattice and Tübingen triangle tiling.

This suggests a Dirichlet series generating function, and one obtains [2, Eq. (3.9)]

$$F_2(s) = \sum_{m=1}^{\infty} \frac{\ell_2(m)}{m^s} \; = \; \zeta(s)\,\zeta(s-1) \; = \; \prod_p \frac{1}{1-p^{-s}}\,\frac{1}{1-p^{1-s}} \qquad (1)$$
$$= 1 + \tfrac{3}{2^s} + \tfrac{4}{3^s} + \tfrac{7}{4^s} + \tfrac{6}{5^s} + \tfrac{12}{6^s} + \tfrac{8}{7^s} + \tfrac{15}{8^s} + \tfrac{13}{9^s} + \tfrac{18}{10^s} + \tfrac{12}{11^s} + \tfrac{28}{12^s} + \tfrac{14}{13^s} + \ldots$$

where $\zeta(s) = \sum_{m=1}^{\infty} m^{-s}$ is Riemann's zeta function, p in the product runs over all (rational) primes, and $\ell_2(m) = \sum_{d|m} d$ is the ordinary divisor function, compare [1] for details.

The corresponding question is well defined also for $L = \mathbb{Z}[\xi]$, $\xi = \exp(2\pi i/5)$, 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 [2, App. A]

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

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.

Clearly, this combinatorial question is purely algebraic, and the method also applies to counting finite index subgroups of free Abelian groups, see [2, 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 $\ell_n(m) = \sum_{d_1 \cdot \ldots \cdot d_n = m} d_1^0\, d_2^1 \cdot \ldots \cdot d_n^{n-1}$.

3. Counting similarity sublattices

Let us turn to (geo)metric properties and ask for the number $a_4(m)$ of *square* sublattices of $\mathbb{Z}^2$ of a given index m, which coincides with the number of ideals of $\mathbb{Z}[i]$ of norm m. The answer is given by the Dedekind zeta function of the quadratic (or cyclotomic) field $\mathbb{Q}(i)$, i.e., one obtains [3, Eq. (7)]

$$\zeta_{\mathbb{Q}(i)}(s) = \sum_{m=1}^{\infty} \frac{a_4(m)}{m^s} = \frac{1}{1-2^{-s}} \prod_{p\equiv 1\,(4)} \frac{1}{(1-p^{-s})^2} \prod_{p\equiv 3\,(4)} \frac{1}{1-p^{-2s}} \tag{4}$$
$$= 1 + \tfrac{1}{2^s} + \tfrac{1}{4^s} + \tfrac{2}{5^s} + \tfrac{1}{8^s} + \tfrac{1}{9^s} + \tfrac{2}{10^s} + \tfrac{2}{13^s} + \tfrac{1}{16^s} + \tfrac{2}{17^s} + \tfrac{1}{18^s} + \tfrac{2}{20^s} + \dots$$

The corresponding question for the module $\mathbb{Z}[\xi]$ is answered by the Dedekind zeta function [18] of the cyclotomic field $\mathbb{Q}(\xi)$ which reads [3, Eq. (10)]

$$\zeta_{\mathbb{Q}(\xi)}(s) = \sum_{m=1}^{\infty} \frac{a_{10}(m)}{m^s} \tag{5}$$
$$= \frac{1}{1-5^{-s}} \prod_{p\equiv 1\,(5)} \frac{1}{(1-p^{-s})^4} \prod_{p\equiv -1\,(5)} \frac{1}{(1-p^{-2s})^2} \prod_{p\equiv \pm 2\,(5)} \frac{1}{1-p^{-4s}}$$
$$= 1 + \tfrac{1}{5^s} + \tfrac{4}{11^s} + \tfrac{1}{16^s} + \tfrac{1}{25^s} + \tfrac{4}{31^s} + \tfrac{4}{41^s} + \tfrac{4}{55^s} + \tfrac{4}{61^s} + \tfrac{4}{71^s} + \tfrac{1}{80^s} + \dots$$

These two generating functions also have an interpretation in terms of colourings: $a_4(m)$ is (up to permutation) the number of colourings of the square lattice where one colour occupies a sublattice of $\mathbb{Z}^2$ of index m and the remaining colours occupy its cosets. The function $a_{10}(m)$, in turn, counts the colourings of $\mathbb{Z}[\xi]$ via submodules of index m, all of which are similarity submodules because $\mathbb{Z}[\xi]$, as $\mathbb{Z}[i]$, is a principal ideal domain, see [18, 7] for details. For a discussion of the corresponding colour groups, see [12].

This approach can be extended to all cyclotomic fields with class number one (the corresponding rings of integers are then principal ideal domains), see [18, 3, 5], and references given there, for details.

4. Counting coincidence sublattices

Another geometric problem, with interesting applications to grain boundaries and twinning phenomena in (quasi)crystals, is the classification of sublattices of $\mathbb{Z}^2$ that can be seen as an intersection of $\mathbb{Z}^2$ with a rotated copy of itself. These are the *coincidence sublattices*, see [2] 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 (again using $\mathbb{Z}^2 = \mathbb{Z}[i]$) one finds [16]

$$\Phi_{\mathbb{Z}[i]}(s) = \prod_{p\equiv 1\,(4)} \frac{1+p^{-s}}{1-p^{-s}} = \frac{1}{1+2^{-s}} \frac{\zeta_{\mathbb{Q}(i)}(s)}{\zeta(2s)} \tag{6}$$
$$= 1 + \tfrac{2}{5^s} + \tfrac{2}{13^s} + \tfrac{2}{17^s} + \tfrac{2}{25^s} + \tfrac{2}{29^s} + \tfrac{2}{37^s} + \tfrac{2}{41^s} + \tfrac{2}{53^s} + \tfrac{2}{61^s} + \tfrac{4}{65^s} + \dots$$

which is derived in [2, Prop. 3.1].

Behind this combinatorial problem is a group structure. It turns out that the set of rotations R such that $\mathbb{Z}^2 \cap R\mathbb{Z}^2$ is a coincidence sublattice of $\mathbb{Z}^2$ forms a group, called $\mathrm{SOC}(\mathbb{Z}^2)$, which equals $\mathrm{SO}(2,\mathbb{Q})$, see [2, Thm. 3.3] for details. Also, the possible coincidence indices $[\mathbb{Z}^2 : (\mathbb{Z}^2 \cap R\mathbb{Z}^2)] =: \Sigma(R)$ (excluding 0 and ∞) form a monoid (a semigroup with unit), generated by the (rational) primes $p \equiv 1\ (4)$.

The formulation with cyclotomic integers admits the corresponding result for $\mathbb{Z}[\xi]$, and the generating function for the number of coincidence submodules of index m is [16]

$$\Phi_{\mathbb{Z}[\xi]}(s) = \prod_{p\equiv 1\,(5)} \left(\frac{1+p^{-s}}{1-p^{-s}}\right)^2 = \frac{1}{1+5^{-s}} \frac{\zeta_{\mathbb{Q}(\xi)}(s)}{\zeta_{\mathbb{Q}(\tau)}(2s)} \tag{7}$$
$$= 1 + \tfrac{4}{11^s} + \tfrac{4}{31^s} + \tfrac{4}{41^s} + \tfrac{4}{61^s} + \tfrac{4}{71^s} + \tfrac{4}{101^s} + \tfrac{8}{121^s} + \tfrac{4}{131^s} + \tfrac{4}{151^s} + \dots$$

where $\tau = (1+\sqrt{5})/2$ is the golden ratio and $\zeta_{\mathbb{Q}(\tau)}(s)$ is the Dedekind zeta function of the quadratic field $\mathbb{Q}(\tau)$, i.e.

$$\zeta_{\mathbb{Q}(\tau)}(s) \;=\; \frac{1}{1-5^{-s}} \prod_{p\equiv\pm1\,(5)} \frac{1}{(1-p^{-s})^2} \prod_{p\equiv\pm2\,(5)} \frac{1}{1-p^{-2s}}\,. \tag{8}$$

There is one subtlety in the application to the *discrete* point set of the TTT — a small acceptance correction factor is needed, which can be calculated explicitly from the cut and project scheme. This, together with a general discussion of the n-fold symmetry case, can be found in [16].

5. Central shelling

Let us come to the shelling problem, first in its version for the *central* shelling. Here, one asks for the number of points of $\mathbb{Z}[i]$ on circles of radius r around the origin. The result is usually given in terms of lattice theta functions, see [9, Ch. 4] for an extensive exposition, but, 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 4, which is the trivial symmetry factor. What remains, since $r^2 = m$ is an integer, is the multiplicative function $a_4(m)$ whose generating function was given above in equation (5). Further details and references are given in [6].

In the case of $\mathbb{Z}[\xi]$, the central shelling function c depends on $r^2 \in \mathbb{Z}[\xi+\bar{\xi}] = \mathbb{Z}[\tau]$, and one needs the primes of $\mathbb{Z}[\tau]$ (see [10, Appendix B] for details) to derive a formula for $c(r^2)$, compare [5]. Let us write $\tilde{p}$ for a prime in $\mathbb{Z}[\tau]$, and let $t(\tilde{p})$ be the highest power t such that $\tilde{p}^t | r^2$. Then, whenever $t(\tilde{p})$ is odd for a $\tilde{p}$ that is also a prime in $\mathbb{Z}[\xi]$ (i.e., an inert prime), one has $c(r^2) = 0$. Otherwise, one finds the formula

$$c(r^2) \;=\; 10 \prod_{\substack{\tilde{p}|r^2 \\ \tilde{p}\text{ splits}}} \big(t(\tilde{p})+1\big) \tag{9}$$

where the product runs only over those primes $\tilde{p}$ of $\mathbb{Z}[\tau]$ which split in the extension to $\mathbb{Z}[\xi]$. Here, they are precisely the primes that originate from rational primes $p \equiv 1$ (5).

Can the result be given in a simpler way? Suppose, for a moment, that the function $c(r^2)$ would only depend on the *norm* of r^2, i.e., on $m = r^2\,\sigma(r^2)$, where σ is the Galois automorphism of $\mathbb{Q}(\tau)$ defined by $\sqrt{5} \mapsto -\sqrt{5}$. Consequently, m is a rational integer. This would mean that $c(r^2) = 10f(m)$ with $f(m)$ a multiplicative arithmetic function, whose Dirichlet series turns out to be

$$\begin{aligned} C_{10}(s) &= \sum_{m=1}^{\infty} \frac{f(m)}{m^s} \\ &= \frac{1}{1-5^{-s}} \prod_{p\equiv1\,(5)} \frac{1}{(1-p^{-s})^2} \prod_{p\equiv-1\,(5)} \frac{1}{1-p^{-2s}} \prod_{p\equiv\pm2\,(5)} \frac{1}{1-p^{-4s}} \\ &= 1 + \tfrac{1}{5^s} + \tfrac{2}{11^s} + \tfrac{1}{16^s} + \tfrac{1}{25^s} + \tfrac{2}{31^s} + \tfrac{2}{41^s} + \tfrac{2}{55^s} + \tfrac{2}{61^s} + \tfrac{2}{71^s} + \tfrac{1}{80^s} + \tfrac{1}{81^s} + \ldots \end{aligned} \tag{10}$$

As can be seen from the exact shelling formula (9), this cannot be true in general. However, it gives the correct answer for many cases, and is then by far the simplest way to calculate $c(r^2)$. To be more precise, consider $m = r^2\,\sigma(r^2)$. Whenever m is not divisible by the square of *any* rational prime $p \equiv 1$ (5), we have $c(r^2) = 10f(m)$, where $f(m)$ is then 0, 1 or a power of 2.

The first value of m where this fails is $m = 121 = 11^2$. Since $11 = (3+\tau)(4-\tau) = \tilde{p}\tilde{p}'$ in $\mathbb{Z}[\tau]$, where we write $\tilde{p}'$ for $\sigma(\tilde{p})$, the possible values of r^2 with norm m are $\tilde{p}^2$, $\tilde{p}\tilde{p}'$ and $(\tilde{p}')^2$,

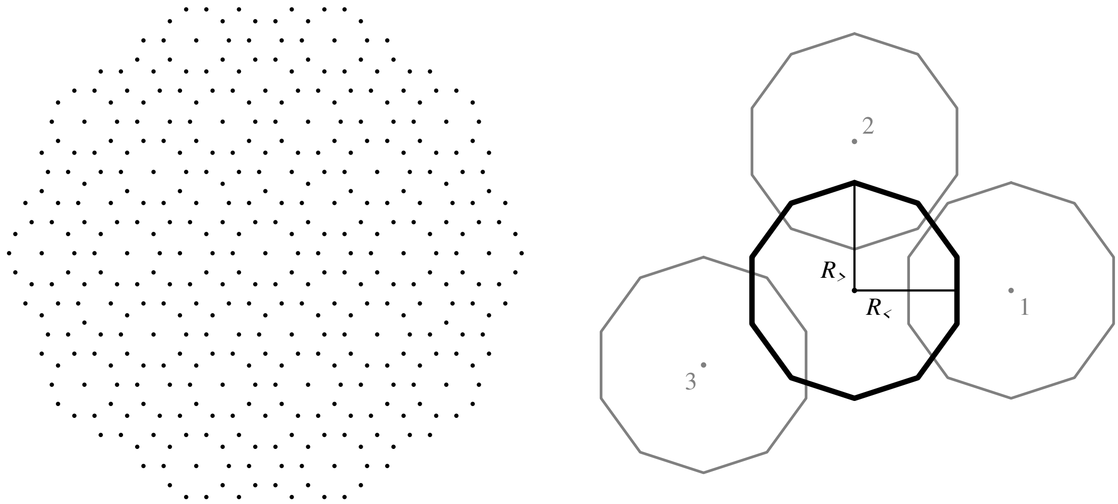

Figure 2. A TTT vertex set and its decagonal window (black). Also shown are three shifted copies of the window (grey), see text for details.

with shelling numbers 30, 40 and 30, respectively. Since $f(121) = 3$, we would get a wrong answer for the middle case. Nevertheless, $10f(m)$ still gives the correct shelling number if, whenever m is divisible by a rational prime $p \equiv 1\ (5)$ (whence $p = \tilde{p}\tilde{p}'$ is a complex splitting prime, and $\tilde{p}$ splits in the extension to $\mathbb{Z}[\xi]$), r^2 is divisible by either $\tilde{p}$ or $\tilde{p}'$, but never by both. Beyond this situation, one has to use formula (9).

Equation (9), together with the partial simplification of equation (10), gives the result for the central shelling of the full module. When passing to a model set [13], 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 [5] for details.

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 [6, 13]. Note that the averages needed do exist for model sets, so that the question posed is well defined. To be specific, we explain the averaged shelling for the vertex set of the TTT.

Let us first describe the TTT vertex set in algebraic terms. We use $L = \mathbb{Z}[\xi]$ as above, with $\xi = \exp(2\pi i/5)$, together with the Galois automorphism $\star$ of $\mathbb{Q}(\xi)$ given by $\xi \mapsto \xi^2$. This is the star map of the standard cut and project or model set construction [13], which gives

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

where the window W is a relatively compact set with nonempty interior. For the TTT, we choose W as a regular decagon of edge length $\tau/\sqrt{\tau+2}$, hence of inradius $R_< = \tau^2/2$ and circumradius $R_> = \tau^2/\sqrt{\tau+2}$, see figure 2 for the correct orientation.

This construction gives a triangle tiling with long (short) edges of lengths 1 $(1/\tau)$. If the window is centred at 0, the model set is singular, while generic examples are obtained by shifting the window, i.e. $\Lambda^u \;=\; \{x \in L \mid x^\star \in W + u\}$, for almost all $u \in \mathbb{R}^2$.

Table 1. Averaged shelling numbers for TTT for all possible distances $0 < r \leq 2$.

r^2	representative	orbit length	$t^2 = \sigma(r^2)$	shift type	shelling number
$2-\tau$	$\xi+\bar{\xi}$	10	$1+\tau$	1	$6-2\tau$
1	1	10	1	1	$28-14\tau$
$3-\tau$	$\xi^2-\bar{\xi}^2$	10	$2+\tau$	2	$-50+32\tau$
$4-\tau$	$1-\xi-\bar{\xi}^2$	20	$3+\tau$	3	$112-68\tau$
$1+\tau$	$\xi^2+\bar{\xi}^2$	10	$2-\tau$	1	$20-8\tau$
$2+\tau$	$\xi-\bar{\xi}$	10	$3-\tau$	2	$-44+30\tau$
4	2	10	4	1	$-18+12\tau$

Table 1 lists all distances $0 < r \leq 2$ between points of Λ, together with a representing point in L. The corresponding orbit length is given w.r.t. the point symmetry group D_{10}. Here, it coincides with the value of the central shelling number $c(r^2) = 10f(m)$, as calculated by means of equation (10). For larger values of r^2, $c(r^2)$ can comprise several D_{10}-orbits, but only complete ones because the window is tenfold and reflection symmetric. For the averaged shelling, we need to calculate the relative overlap area of the window W with a shifted copy (the so-called covariogram of W), where the shift is the star image of the representing vector [5]. For our examples, only the three relative orientations indicated in figure 2 emerge, with midpoint distance t, where t^2 is the algebraic conjugate of r^2 in $\mathbb{Q}(\tau)$. The resulting averaged shelling number (last column) is an element of $\mathbb{Z}[\tau]$ in all cases shown here. This is probably true in general, though we can only prove that they always lie in $\mathbb{Q}(\tau)$ at present.

For the overlap scenarios 1 and 2 of figure 2, where the shifts are along the two principal reflection axes of the decagon, the covariogram has a relatively simple form. Measuring the distance between the decagons in units of the circumradius, with $q = t/R_{>}$, we find

$$h_1(q) \;=\; \begin{cases} \frac{1}{5}[5-2\tau\frac{q}{\eta}+(\frac{q}{2\eta})^2], & 0 \leq q < \frac{2\eta}{\tau} \\ \frac{1}{5}[2-\frac{q}{\eta}+\tau^3(1-\frac{q}{2\eta})^2], & \frac{2\eta}{\tau} \leq q < 2\eta \\ 0, & 2\eta \leq q \end{cases} \tag{12}$$

where $\eta = \sqrt{2+\tau}/2$, and

$$h_2(q) \;=\; \begin{cases} \frac{1}{5}(5-2\tau q), & 0 \leq q < \frac{1}{\tau} \\ \frac{1}{5}(2\tau^2-4q+\frac{q^2}{\tau}), & \frac{1}{\tau} \leq q < \tau \\ \frac{\tau^2}{5}(2-q)^2, & \tau \leq q < 2 \\ 0, & 2 \leq q\,. \end{cases} \tag{13}$$

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

The averaged shelling number for the example of type 3 given in table 1 was calculated separately (and exactly). We do not give the general formula for the covariogram of the regular decagon, but mention that

$$h(q) \;=\; \frac{2}{\pi}\arccos\left(\frac{q}{2\rho}\right) - \frac{q}{\pi\rho}\sqrt{1-\left(\frac{q}{2\rho}\right)^2}, \tag{14}$$

with $\rho = \sqrt{\frac{5}{2\pi\tau}\sqrt{2+\tau}} \approx 0.9672$, is a very good approximation. It is obtained by replacing the decagon W with a disk of equal area, hence of radius $\rho R_{>}$. This function is also known as Euclid's hat, see [11, p. 100] and references given there for details.

7. 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 [2, 7, 8, 14, 19]. Still, even some of these cases leave room for improvement and simplification, e.g., along the lines mentioned around equation (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 [9]. One may expect some progress at least for the class of root lattices, hence also for quasicrystals derived from them. Further progress is also needed in the investigation of colour symmetry groups, see [12] for a summary of the present state of affairs.

Perhaps the biggest 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" ($\mathbb{Z}[\tau]$ numbers in the TTT example), while this is not the case for model sets with generic windows. This phenomenon points towards another function defined by these numbers that admits similarly nice analytic and topological interpretations, but we do not know how to substantiate this at present.

Acknowledgment

It is a pleasure to thank Robert V. Moody and Alfred Weiss for helpful discussions and suggestions. This work was partially supported by the German Research Council (DFG).

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