THE DIFFRACTION PATTERN OF SELFSIMILAR TILINGS

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Abstract.

The discrete part of the diffraction pattern of self-similar tilings, called the Bragg spectrum, is determined. Necessary and sufficient conditions for a wave vector q to be in the Bragg spectrum are derived. It is found that the Bragg spectrum can be non-trivial only if the scaling factor ϑ of the tiling is a PV-number. In this case, the Bragg spectrum is entirely determined by the scaling factor ϑ and the *translation module* of the tiling. Three types of Bragg spectra can be distinguished, belonging to *quasiperiodic*, *limit-periodic* and *limit-quasiperiodic* structures, respectively.

1. Introduction

The selfsimilarity properties of quasicrystals have triggered considerable interest in selfsimilar tilings, which are used as simple models to describe the structure of quasicrystals. Most of the tilings used for this purpose can be obtained as a cut through a higher-dimensional periodic structure, and are thus quasiperiodic by construction. This implies, in particular, that their Fourier transform contains Bragg peaks on a module of finite rank. However, there are also many interesting self-similar tilings which are defined only in terms of an iterated substitution procedure. In each step of this substitution, the finite tiling obtained so far is scaled by a linear factor ϑ, and then each scaled tile is replaced by a specific cluster of tiles of the original size. In this way, starting from a single tile or any other admissible seed, the whole space can be eventually be covered.

The question then arises whether such substitution tilings also show Bragg diffraction, and if so, what the support of their Bragg spectrum is. More precisely, one would like to know whether the Bragg spectrum of a substitution tiling is that of a quasiperiodic structure, such as a quasicrystal, or whether it is that of a more general almost periodic structure. Some early attempts to answer these questions have been made by Bombieri and Taylor (1986, 1987) in the case of one-dimensional substitution tilings. Bombieri and Taylor observed that the algebraic properties of the largest eigenvalue ϑ of the substitution matrix plays an important role for the existence of a non-trivial Bragg spectrum. More precisely, for a non-trivial Bragg spectrum it is necessary that ϑ is a so-called PISOT-VIJAYARAGHAVAN-number (PV-number).

The analysis of Bombieri and Taylor had later been generalized to two and more dimensions (Godrèche and Luck, 1989; Godrèche, 1989; Godrèche and Luck, 1990), but only a few particular cases were treated in detail. In (Godrèche and Luck, 1989), several substitutions for tilings with Robinson triangles were studied, among them substitutions yielding Penrose tilings, as well as partially random substitutions. In (Godrèche, 1989) and (Godrèche and Luck, 1990), substitutions generating so called *limit-periodic* tilings were analyzed, thereby leaving the realm of quasiperiodic tilings. The discussion of all these examples appears somewhat ad hoc and specific to the particular case that was treated. From these examples, and in analogy to the one-dimensional case, it was concluded that a non-trivial Bragg spectrum exists if and only if the largest eigenvalue of the substitution matrix is a PV-number. It remained unclear, however, what precisely determined the *support* of the Bragg spectrum, and which properties of the substitution were really essential for the Bragg spectrum. To determine the (complete) support of the Bragg spectrum, a precise anaysis of the relative placement of tiles in the tiling is necessary, without which one risks to find only a subset of the Bragg spectrum, as was the case in (Godrèche and Luck, 1989).

It is evident that by studying only particular examples, it is difficult to determine the properties which are really essential for the problem. We therefore propose here a more systematic approach. We shall consider a whole class of general substitution tilings. For this class of substitution tilings we shall systematically work out the necessary and sufficient conditions for a wave vector q to be in the Bragg spectrum. It will turn out that two properties of the substitution completely determine the Bragg spectrum: the linear scaling factor ϑ, and the *translation module* T of the tiling. For a non-trivial Bragg spectrum, the scaling factor ϑ must be a

PV-number. Although this is equivalent to the largest eigenvalue of the substitution matrix being a PV-number, it is conceptually much more natural to formulate this requirement as a property of the scaling factor. If ϑ is a PV-number, the Bragg spectrum then is determined by ϑ and the translation module T, and we shall give a complete and constructive description of the Bragg spectrum.

We should remark that in this paper we are interested only in the Bragg spectrum of the tiling, that is, in the *discrete* part of its diffraction pattern. Our methods can not exclude the existence of a continuous component in the diffraction pattern, and they do not provide any information on that continuous part. However, the diffraction pattern of a tiling is closely related to the spectrum of a tiling dynamical system associated with the tiling (Dworkin, 1993; Hof, 1995b). It can be shown that if this dynamical spectrum is purely discrete, then the diffraction pattern is purely discrete, too. Since there are criteria for the pure discreteness of the dynamical spectrum (Solomyak, 1995), these criteria can be used to establish also the pure discreteness of the diffraction pattern. This has been done for several of the examples we shall present.

Our paper is organized as follows. In Section 2, a detailed description of the class of substitutions covered by this paper is given. In particular, we shall confine ourselves to substitutions which scale all tiles by a common, uniform factor ϑ. We further require that the substitution generates only tilings within a single local isomorphism class, which implies that the substitution must be primitive. The structure of the tilings generated by such substitutions is then analyzed in some detail. In particular, we shall discuss the translation module, which will play an important role for the Bragg spectrum.

In Section 3 we first give a more precise definition of what we mean by Bragg spectrum. We then propose to use a simplified criterion for the determination of this Bragg spectrum, the justification of which is given in Appendix A. Using this criterion, necessary and sufficient conditions for a wave vector q being in the Bragg spectrum are then derived (Theorem 2). The characterization of the Bragg spectrum obtained in Theorem 2 is still rather implicit, however.

Using the Theorem of Pisot and Vijayaraghavan (Theorem 3), we shall then make the characterization of the Bragg spectrum much more explicit in Section 4. Theorem 4 will give a completely constructive description of the Bragg spectrum of a substitution tiling. Tilings with Bragg spectra of three different types can be distinguished, which we classify as *quasiperiodic*, *limit-periodic*, and *limit-quasiperiodic*, respectively.

In Section 5 we briefly discuss the appropriate concept of point symmetry for non-periodic tilings, before we illustrate our general theory with numerous examples in Section 6. Subsection 6.1 is devoted to one-dimensional examples, whereas two- and three-dimensional examples are presented in Subsection 6.2. We finally conclude in Section 7.

2. Selfsimilar Tilings

We first have to recall a few basic facts about selfsimilar tilings. Many of these are well-known, see e.g. (Lunnon and Pleasents, 1987; Geerse and Hof, 1991; de Bruijn, 1990). Consider a set of m prototiles $t_i \subset \mathbb{R}^d$, and suppose a substitution process $\mathcal{S}$ acting on copies of these prototiles is given, which replaces each tile t_i by a (1^{st} order) supertile $t_i^{(1)}$ of the same shape, but larger by a linear factor ϑ. Each of these supertiles $t_i^{(1)}$ is composed in a specific way of tiles t_j from the original set of prototiles. Moreover, each prototile t_i is supposed to carry a "diffraction density", which is given by some finite measure $\mu_i^{(0)}$ on t_i. Prototiles which differ either by geometric shape, orientation in space, diffraction density, or behaviour under substitution, are considered to be distinct. Since supertiles are composed of tiles t_j, the substitution process can be iterated. Starting with a single tile as a seed, by repeated substitutions and translations (de Bruijn, 1990) one can generate tilings covering larger and larger parts of $\mathbb{R}^d$, and eventually all of $\mathbb{R}^d$. Unless the tilings generated in this way are periodic, there are uncountably many different ones covering the entire space (de Bruijn, 1990; Danzer and Dolbilin, 1995). Each of these tilings is selfsimilar, and can be partitioned into a hierarchy of supertiles $t_i^{(n)} = \mathcal{S}(t_i^{(n-1)})$ of all orders, where we have set $t_i^{(0)} = t_i$. In the following we shall assume in addition that for any $r > 0$ the tilings generated by the substitution contain, up to translations, only finitely many different local patches of diameter up to r. We say then that the tiling has *finite number of local patterns* (Solomyak, 1995). Substitutions with a constant scaling factor ϑ, as described above, are often called *inflations*.

Definition: *Two tilings $\mathcal{T}_1$ and $\mathcal{T}_2$ are called locally isomorphic if every finite part of $\mathcal{T}_1$ occurs also in $\mathcal{T}_2$, and vice versa.*

Local isomorphism is an equivalence relation between tilings. In the following, we shall consider only substitutions which generate tilings within a single *local isomorphism class* (LI class) . Let S be the matrix whose entries S_{ij} denote the number of copies of t_j contained in $t_i^{(1)}$. This matrix S, whose entries are non-negative, is called the *substitution matrix.*

Definition: *A matrix S with non-negative entries is called* reducible *if there exists a permutation matrix T such that $T^{-1}ST$ is non-trivially block-diagonal,* irreducible *otherwise. Furthermore, S is called* primitive *if there exists a finite power S^n of S, all of whose entries are strictly positive.*

In order that the substitution $\mathcal{S}$ generates only tilings within a single local isomorphism class, the substitution matrix S must be irreducible, for otherwise the substitution would generate tilings containing only a subset of the tiles, and this subset would depend on the seed. By the same reasoning we conclude that any finite power of S must be irreducible as well. It can be shown (Gantmacher, 1959; Seneta, 1973), however, that if S is irreducible, but not primitive, there exists a finite power S^n of S which is reducible. Therefore, we can restrict ourselves to substitutions with a primitive substitution matrix, which we simply call *primitive substitutions*, and we shall assume that the substitution matrix S has strictly positive entries, which can always be achieved by passing to a suitable power of the substitution.

All tilings generated by a primitive substitution are in the same local isomorphism class (LI class), called the LI class of the substitution (Lunnon and Pleasents, 1987), but there may exist tilings in this LI class which can not directly be reached as the limit of a sequence of substitutions (Lunnon and Pleasents, 1987). Some such substitution sequences may have limiting tilings which cover only a cone in $\mathbb{R}^d$, and it may be possible that by combining several such cones a tiling in the same LI class is obtained which cannot be reached otherwise. However, there can only be finitely many such exceptional tilings in the LI class (Lunnon and Pleasents, 1987), and the LI class is already fully determined by the regular substitution tilings. Exceptional tilings cannot be distinguished from regular ones by any local means.

Definition: *A set $X \subset \mathbb{R}^d$ is called* relatively dense *if there exists $R < \infty$ such that any ball $B(R) \subset \mathbb{R}^d$ of radius R has non-zero intersection with X.*

Definition: *A tiling $\mathcal{T}$ of $\mathbb{R}^d$ is called* repetitive*, if for every finite part $\mathcal{F} \subset \mathcal{T}$ the set of all (translational) copies of $\mathcal{F}$ in $\mathcal{T}$ is relatively dense.*

Since the substitution fixes the LI class of the tilings it generates, every finite part of a tiling in the LI class must be contained in some supertile $t_i^{(n)}$ of some finite order n. This immediately implies that a primitive substitution tiling is repetitive. Since every supertile $t_i^{(1)}$ contains at least one copy of all the t_j, the set of all t_i is certainly relatively dense for every i, and due to the selfsimilarity the same must hold for supertiles of any order. We also note that the repetitivity implies that every finite part which occurs in a tiling occurs with a positive density.

Theorem 1. *(Perron) A primitive matrix S has a real positive eigenvalue λ, which is a simple root of the characteristic polynomial of S, and which is strictly larger in magnitude than any other eigenvalue of S. The right and left eigenvectors associated with λ have strictly positive entries.*

A proof of Theorem 1 can be found in (Gantmacher, 1959; Seneta, 1973). Since with each iteration of the substitution the volume of the tiling scales with a factor ϑ^d, the leading eigenvalue of S must be ϑ^d. The components of the left eigenvector of S associated with ϑ^d are proportional to the relative volumes of the tiles, whereas those of the right eigenvector can be interpreted as the relative frequencies of the different tiles in the infinite tiling. Due to the uniqueness of the largest eigenvalue, tiles, as well as supertiles, have a well defined density. The same holds actually true for any finite part contained in the tiling.

We now write the substitution in a more explicit form. For that purpose, we have to fix a reference point on each prototile. If a copy of tile t_i is placed in space in such a way that its reference point is at the origin of $\mathbb{R}^d$, we denote its diffraction density by $\mu_i^{(0)}$, where $\mu_i^{(0)}$ is some bounded measure. A translated copy of t_i whose reference point is at $x \in \mathbb{R}^d$ then carries the translated diffraction density $\mathsf{T}(x)\cdot\mu_i^{(0)}$, where $\mathsf{T}(x)$ is the translation operator defined by $(\mathsf{T}(x)\cdot\mu)(f) = \mu(f_x)$, with $f_x(y) = f(y-x)$. The reference points on the supertiles $t_i^{(n)}$ are induced by those of their predecessors $t_i^{(n-1)}$: they are just scaled, together with the tile. With such a choice of reference points, the diffraction densities $\mu_i^{(n+1)}$ carried by the $(n+1)^{th}$ order supertiles $t_i^{(n+1)}$ can be expressed by the diffraction densities of the previous generation:

$$\mu_i^{(n+1)} = \sum_{j=1}^{m} \sum_{\ell=1}^{S_{ij}} \mathsf{T}(\vartheta^n d_{ij\ell}) \cdot \mu_j^{(n)}, \tag{1}$$

where m is the number of prototiles. The translation vectors $d_{ij\ell}$ denote the relative positions of the reference points of the first order supertile $t_i^{(1)}$ and its constituent tiles; $d_{ij\ell}$ points from the reference point on $t_i^{(1)}$ to the reference point of the ℓ^{th} copy of t_j contained in $t_i^{(1)}$ (there are S_{ij} such copies of t_j in $t_i^{(1)}$). In the n^{th} iteration, all translation vectors $d_{ij\ell}$ have to be scaled by a factor ϑ^n, which follows directly from our choice of reference points on the supertiles of all orders.

Consider now a finite patch $\mathcal{P}$ contained in the tiling, fix a reference point on $\mathcal{P}$, and denote by X the set of reference points of all (translated) copies of $\mathcal{P}$ in the tiling. The $\mathbb{Z}$-span of the set $\{z \in \mathbb{R}^d | z = x-y, x \in X, y \in X\}$ is called the *translation module* of the patch $\mathcal{P}$, and is denoted by $T(\mathcal{P})$. Clearly, $T(\mathcal{P})$ is a free $\mathbb{Z}$-module of finite rank. If a patch $\mathcal{P}_1$ is a subset of another patch $\mathcal{P}_2$, its translation module $T(\mathcal{P}_1)$ contains the translation module $T(\mathcal{P}_2)$ as a submodule. Of particular importance are the translation modules of tiles and supertiles. For these we use the notation $T_i^{(n)} = T(t_i^{(n)})$.

The $\mathbb{Z}$-span of the union $\bigcup_i T_i^{(n)}$ is denoted by $T^{(n)}$, where i runs over all tile types. $T^{(n)}$ is called the translation module of order n of the tiling. For $T^{(0)}$ we simply write T, and call it the *translation module of the tiling*. Since the tile $t_i^{(n)}$ is contained in $t_i^{(n+1)}$, we have $T_i^{(n+1)} \subseteq T_i^{(n)}$, and due to the selfsimilarity of the tiling we have $\vartheta T_i^{(n)} \subseteq T_i^{(n+1)}$, so that $\vartheta T_i^{(n)} \subseteq \vartheta T_i^{(n)}$, and consequently $\vartheta T^{(n)} \subseteq \vartheta T^{(n)}$. In other words, multiplication by ϑ maps a translation module $T^{(n)}$ into itself. With respect to a basis of the module, the action of ϑ on the module is described by an integral matrix M. Two cases have to be distinguished. If $|\det(M)| = 1$, we have $T^{(n)} = \vartheta T^{(n)}$, and therefore the translation modules of all orders are equal. In fact, since any finite patch $\mathcal{P}$ is contained in some supertile $t_j^{(n)}$, even in one of any given type j, all translation modules $T(\mathcal{P})$ must be equal, whatever the patch $\mathcal{P}$ is. On the other hand, if $|\det(M)| > 1$, multiplication by ϑ maps a translation module into submodule, so that $T^{(n+1)}$ may be a true submodule of $T^{(n)}$, of index up to $|\det(M)|$ in $T^{(n)}$. This is actually what happens, unless there is some further symmetry present in the substitution. For instance, we might consider a substitution which generates a periodic tiling, in which case the translation module of any patch can not be smaller than the translation lattice of the tiling. To prevent such cases, it is often required that any tiling $\mathcal{T}$ has a unique predecessor $\mathcal{T}'$ such that $\mathcal{S}\mathcal{T}' = \mathcal{T}$. Such tilings are said to have the *unique composition property* (Solomyak, 1995), which ensures the non-periodicity of the tiling. Larger patches then have in general truly smaller translation modules, and the intersection of the translation modules of all possible finite patches, which is called the limit translation module (Baake et al., 1991), consists just of the zero element. Since all our arguments go through without the unique composition property, we shall not impose it here, however.

It is important that the translation module can be determined with a finite amount of work. Since every tile occurs at least once in every supertile, the translation module of a tile is generated by distances between copies of this tile, which are either within the same supertile, or within neighboring supertiles. Since the tiling has finitely many local patterns, there are only finitely many such distance vectors to be considered.

Since in the case $|\det(M)| = 1$ all translation modules $T(\mathcal{P})$ are identical, the limit translation module $\cap_{\mathcal{P}} T(\mathcal{P})$ then necessarily is non-trivial. This is the case whenever ϑ is a unit in the ring $\mathbb{Z}[\vartheta]$. We emphasize that so far we have not made any assumptions on the number-theoretic nature of ϑ, other than ϑ being algebraic. This results holds, in particular, also for non-PV-numbers ϑ. For some particular examples, this had been shown already by Klitzing (Klitzing, 1995a), but the result actually is completely general.

After this excursion into translation modules we return to formula (1) and consider the free $\mathbb{Z}$-module $\mathcal{D}$ generated by the translation vectors $\vartheta^n d_{ij\ell}$ occurring in (1). Clearly, $\mathcal{D}$ contains the translation module T as a submodule, and therefore contains any translation module $T(\mathcal{P})$. However, $\mathcal{D}$ depends on the choice of reference points on the tiles, and we have an interest in choosing them such that the module $\mathcal{D}$ becomes as small as possible. For this purpose, we choose as reference points certain fixed points of the substitution. We start with the first tile type, and consider an affine map f which maps the first order supertile $t_1^{(1)}$ onto one of its constituent tiles $t_1^{(0)}$ (there is at least one). Since f is a contraction, it has unique fixed point, which we choose as the reference point for the tile $t_1^{(0)} = f(t_1^{(1)})$. The reference points on the n^{th} order supertiles are then determined by scaling the tile $t_1^{(0)}$ with its reference point to the size of the supertile.

For the other tile types $j > 1$, we choose a reference point on the first order supertile $t_j^{(1)}$, namely the reference point of one of the tiles $t_1^{(0)}$ contained in $t_j^{(1)}$. The reference points on $t_j^{(0)}$ and on higher order supertiles are then again determined be scaling.

With these choices we have achieved that the differences between reference points of supertiles of order $n \geq 1$ are always contained in the translation module T_1, and consequently in T. Hence, the differences between reference points of any tiles are contained in $\vartheta^{-1}T$. This immediately implies the following lemma:

Lemma 1. *The reference points on the tiles can be chosen in such a way that the $\mathbb{Z}$-span of the vectors $\vartheta^n d_{ij\ell}$, $n \geq 0$, is contained in $\vartheta^{-1}T$.*

We finally remark that the special reference points chosen above are very similar to the *control points* used by other authors (Kenyon, 1994; Solomyak, 1995), although for the tile types $j > 1$ they are not exactly the same.

3. Fourier Transform and the Diffraction Pattern

The recursion relation (1) for the diffraction densities $\mu_i^{(n+1)}$ can readily be transformed into one for their Fourier transforms:

$$\widehat{\mu}_i^{(n+1)}(q) = \sum_{j=1}^{m} \left(\sum_{\ell=1}^{S_{ij}} e(-q \cdot \vartheta^n d_{ij\ell}) \right) \cdot \widehat{\mu}_j^{(n)}(q), \tag{2}$$

where we have set $e(x) = \exp(2\pi i x)$. Equation (2) can be written as a matrix equation:

$$\widehat{\mu}^{(n+1)}(q) = F_n(q)\widehat{\mu}^{(n)}(q), \tag{3}$$

with $F_n(q)$ an $m\times m$ complex matrix. As it will turn out, a wave vector q will be in the discrete part of the diffraction pattern of the density $\mu^{(\infty)}$ if and only if the Fourier amplitude vector $\widehat{\mu}^{(n)}(q)$ has a component which grows asymptotically as fast as the volume of the system, which is proportional to ϑ^{dn}. In this paper, we shall only be interested in the discrete part of the diffraction pattern, which is called the *Bragg spectrum*.

Before we proceed, however, we have to give a more precise definition of the diffraction pattern. For more details, we refer to (Hof 1995b, 1995a, 1992. For any measure μ we define the measure $\widetilde{\mu}$ by $\widetilde{\mu}(f) = \mu(\widetilde{f})$, where the function $\overline{f}$ is given by $\widetilde{f}(x) = \overline{f}(-x)$. By μ_Λ we denote the diffraction density on the tiling constrained to some bounded, measurable set Λ, of volume $|\Lambda|$. In a diffraction experiment carried out on such a finite system, one measures the *structure factor*, given by

$$\widehat{\gamma}_\Lambda(q) = \frac{1}{|\Lambda|}|\widehat{\mu}_\Lambda(q)|^2, \tag{4}$$

which is nothing but the Fourier transform of the measure

$$\gamma_\Lambda = \frac{1}{|\Lambda|}\mu_\Lambda * \widetilde{\mu}_\Lambda, \tag{5}$$

where $*$ denotes convolution of measures. Division by $|\Lambda|$ in (4) and (5) is necessary because otherwise neither of them has a well-defined infinite volume limit. The infinite volume limit of γ_Λ, however, exists and is unique under physically fairly mild conditions on the diffraction density μ. We shall henceforth assume that γ_Λ has a unique infinite volume limit γ, which we call the *correlation measure*. Crystallographers call this correlation measure the *Patterson function*, although in our context it is a measure, not a function. The correlation measure is a distribution of positive type (Gel'fand and Vilenkin, 1964), which implies that its Fourier transform is a positive measure. Therefore, the structure factor (4) converges to a well-defined positive measure $\widehat{\gamma}$, which we call the *diffraction pattern*. In particular, $\widehat{\gamma}$ has a well-defined discrete or pure point component, $\widehat{\gamma}_{pp}$, which we call the *Bragg spectrum*.

If the Fourier transform $\widehat{\mu}$ of μ itself is a measure, and thus has a well-defined discrete component $\widehat{\mu}_{pp}$, one can show (Hof, 1995b, 1995a, 1992) that

$$\widehat{\gamma}_{pp}(\{q\}) = |\widehat{\mu}_{pp}(\{q\})|^2 \quad \forall q \in \mathbb{R}^d. \tag{6}$$

Unfortunately, in many interesting cases $\widehat{\mu}$ is not a measure, and even if it is, this is very difficult to prove. However, one can show (Hof 1995b, 1992, 1995a) that if the infinite volume limit

$$g(q) := \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} \widehat{\mu}_\Lambda(q) \tag{7}$$

exists and is unique, then

$$|g(q)|^2 = \widehat{\gamma}_{pp}(\{q\}) \quad \forall q \in \mathbb{R}^d. \tag{8}$$

By a unique infinite volume limit we mean, in particular, that it exists uniformly in the position of the finite box Λ. If this requirement is not satisfied, the set of wave vectors q for which $\overline{\lim}_{|\Lambda|\to\infty}(1/|\Lambda|)|\widehat{\mu}_\Lambda| > 0$ (which is called the *Fourier-Bohr spectrum* of μ) is, in general, only a subset of the Bragg spectrum. Such an example is given in (Allouche and Mendès France, 1995).

For the diffraction densities μ carried by our primitive substitution tilings one can show (Appendix A) that the infinite volume limit (7) indeed exists and is unique. We can therefore identify elements of the Bragg spectrum ("Bragg peaks") as those wave vectors for which

$$\lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} |\widehat{\mu}_\Lambda(q)| > 0. \tag{9}$$

Using the criterion (9) for the Bragg spectrum will considerably simplify our task. Since the volume of the n^{th} substitution of any seed is a constant times ϑ^{nd}, we set $F_n^\circ(q) = F_n(q)/\vartheta^d$, and similarly $S_\circ = S/\vartheta^d$. For a generic diffraction density on the tiles, the wave vector q then is in the Bragg spectrum if and only if the sequence of matrix products

$$P_n^\circ(q) = F_n^\circ(q) \cdots F_0^\circ(q) \tag{10}$$

does not converge to zero. We write "generic diffraction density" because otherwise the initial amplitude vector might be in the kernel of one of the P_n°, or in the kernel of the limit of (10). Unless stated otherwise, we shall assume in the following that the diffraction density is generic in this sense, in which case we can simply talk about the *Bragg spectrum of the tiling*, instead of the Bragg spectrum of a particular diffraction density on the tiling.

We note that the matrices $F_n(q)$, and therefore also the matrices $P_n^\circ(q)$, depend on the choice of the reference points on the tiles. In particular, if we move the reference point on tile t_i by a vector x_i, the matrices $F_n(q)$ transform according to

$$\widetilde{F}_n(q) = D_{n+1}^{-1}(q) F_n(q) D_n(q), \tag{11}$$

where $D_n(q)$ is the diagonal matrix with entries $e(-\vartheta^n q \cdot x_i)$. The product $P_n^\circ(q)$ then becomes

$$\widetilde{P}_n^\circ(q) = D_{n+1}^{-1}(q) P_n^\circ(q) D_0(q), \tag{12}$$

which shows that the property of q being in the Bragg spectrum does not depend on the choice of the reference points on the tiles.

Before we continue, we have to introduce some notation. If $x \in \mathbb{R}^d$ is a vector, we denote by $\|x\|$ its L^∞-norm. This norm on vectors induces a norm on matrices, also denoted by $\|\cdot\|$. Although used only in Chapter 4, we remark already now that if $x \in \mathbb{R}$ is a number, $\|x\|$ has a different meaning: $\|x\|$ then denotes the (positive) distance of x to the nearest integer. Since the L^∞-norm occurs only in the present Chapter, there should be no confusion on the meaning of $\|x\|$. Finally, we recall that $S_\circ = S/\vartheta^d$ is primitive, with leading eigenvalue 1. Let r and ℓ be the right and left eigenvectors of $S_\circ$ corresponding to this eigenvalue, written as a column matrix and a row matrix, respectively. We then set

$$S_\circ^\infty = \frac{r \cdot \ell}{\ell \cdot r}, \tag{13}$$

which is the projector on the eigenspace of the largest eigenvalue of $S_\circ$.

Lemma 2. *The primitive matrix $S_\circ = S/\vartheta^d$ satisfies $\lim_{n\to\infty} S_\circ^n = S_\circ^\infty$.*

Proof. There exists $A \in GL_n(\mathbb{C})$ such that $J = AS_\circ A^{-1}$ is in Jordan form. J is block-diagonal, with a 1×1 block $J_1 = 1$, and further blocks of the form $J_k = \lambda_k \cdot I + N_k$, where the $\lambda_k < 1$ are the other eigenvalues of $S_\circ$, I is the identity, and the matrices N_k are nilpotent. If d_k is the dimension of J_k, we have $\|J_k^n\| \le C_k |\lambda_k|^{n-d_k}$, with C_k some constant, so that J_k^n asymptotically vanishes for $k > 1$. Therefore, we have $\lim_{n\to\infty} S_\circ^n = A^{-1}PA$, with P the one-dimensional orthogonal projector on the eigenspace of J with eigenvalue 1. □

Theorem 2. *Consider a primitive substitution tiling with scaling factor ϑ, and let T be its translation module. For any fixed wave vector q, we have the following:*

i) If there exists $x \in T$ such that $e(\vartheta^n q \cdot x) \not\to 1$, then the sequence $P_n^\circ(q)$ converges to zero.

ii) If $e(\vartheta^n q \cdot x) \to 1$ $\forall x \in T$, we can chose reference points on the tiles such that $F_n^\circ(q)$ converges to $S_\circ$, with $\|F_n^\circ(q) - S_\circ\| < b\rho^n$ for some $\rho < 1$. Moreover, the sequence $P_n^\circ(q)$ then converges, and the limit $P_\infty^\circ = \lim_{n\to\infty} P_n^\circ$ satisfies $S_\circ^\infty P_\infty^\circ = P_\infty^\circ$. Furthermore, there exists $k \in \mathbb{N}$ such that $\lim_{n\to\infty} F_n^\circ(q) \cdots F_k^\circ(q) \neq 0$.

Proof. Consider the matrix element

$$(F_n(q))_{ij} = \sum_\ell e(\vartheta^n q \cdot d_{ij\ell}) = e(\vartheta^n q \cdot d_{ij1}) \sum_\ell e(\vartheta^n q \cdot x_{ij\ell}),$$

where $x_{ij\ell} = d_{ij\ell} - d_{ij1}$. The $x_{ij\ell}$ are a generating set of the translation module T. If there exists $x \in T$ such that $e(\vartheta^n q \cdot x) \not\to 1$, the same must hold for one of the $x_{ij\ell}$, which implies that $\underline{\lim}_{\, n\to\infty} |(F_n^\circ(q))_{ij}| < (S_\circ)_{ij}$ for some pair ij. In particular, there exists $\epsilon > 0$ such that for all members in a subsequence $F_{n_m}^\circ$ we have $|(F_{n_m}^\circ)_{ij}| \leq (1-\epsilon)(S_\circ)_{ij}$. Since, in addition, $|(F_n^\circ)_{k\ell}| \leq (S_\circ)_{k\ell}\ \forall n, k, \ell$, for those $F_{n_m}^\circ$ we have

$$\begin{aligned} |(F_{n_m+1}^\circ F_{n_m}^\circ F_{n_m-1}^\circ)_{k\ell}| &\leq (S_\circ^3)_{k\ell} - \epsilon (S_\circ)_{ki}(S_\circ)_{ij}(S_\circ)_{j\ell} \\ &\leq (S_\circ^3)_{k\ell}(1-\alpha\epsilon), \end{aligned}$$

where

$$\alpha = \frac{(\min\limits_{ij}\ (S_\circ)_{ij})^3}{\max\limits_{ij}\ (S_\circ^3)_{ij}} > 0$$

(recall that $(S_\circ)_{k\ell} > 0\ \forall k, \ell$). Together with the uniform boundedness of the $S_\circ^k$ (see the proof of Lemma 2) this proves the convergence to zero.

Conversely, if $e(\vartheta^n q \cdot x) \to 1\ \forall x \in T$, by Lemma 1 we can choose reference points on the tiles such that $e(\vartheta^n q \cdot d_{ij\ell}) \to 1\ \forall d_{ij\ell}$, which implies $F_n^\circ(q) \to S_\circ$. Exponential convergence $\|F_n^\circ(q) - S_\circ\| < b\rho^n$ follows from $|1 - e(x)| = 2|\sin(\pi x)| \leq 2\pi \|x\|$ and Theorem 3 (see next section).

Concerning the convergence of P_n° we first note that the matrices P_n° are uniformly bounded. We therefore have for all $n > N$

$$\begin{aligned} \|P_n^\circ - {S_\circ}^{n-N} P_N^\circ\| &= \|\sum_{\ell=N+1}^{n} {S_\circ}^{n-\ell}(F_\ell^\circ(q) - S_\circ) P_{\ell-1}^\circ(q)\| \\ &\leq \sum_{\ell=N+1}^{n} \|{S_\circ}^{n-\ell}\| \cdot \|F_\ell^\circ(q) - S_\circ\| \cdot \|P_{\ell-1}^\circ(q)\| \\ &\leq C \sum_{\ell=N+1}^{n} \rho^\ell \leq C'\ \rho^{n+1} \end{aligned} \tag{14}$$

This then implies that for all $n \geq N \geq m$

$$\begin{aligned} \|P_n^\circ(q) - P_N^\circ(q)\| \leq{}& \|P_n^\circ(q) - {S_\circ}^{n-m} P_m^\circ(q)\| \\ &+ \|P_N^\circ(q) - {S_\circ}^{N-m} P_m^\circ(q)\| \\ &+ \|{S_\circ}^{n-m} - {S_\circ}^{N-m}\| \cdot \|P_m^\circ(q)\|, \end{aligned}$$

which by Lemma 2 proves that $P_n^\circ(q)$ is a Cauchy sequence. $S_\circ^\infty P_\infty^\circ = P_\infty^\circ$ follows from (14) (choose $n = 2N$).

Next we write $B_n = F_n^\circ - S_\circ$, with $\|B_n\| \le b\rho^n$, and expand the product $F_{k+m}^\circ \cdots F_k^\circ = (S_\circ + B_{k+m}) \cdots (S_\circ + B_k)$. Each term in this expansion contains ℓ factors B_i, all having different indices, and at most $\ell + 1$ factors which are powers of $S_\circ$, where $0 \le \ell \le m+1$. From the proof of Lemma 2 it follows that the set of all powers of $S_\circ$ is uniformly bounded, $\|S_\circ^n\| \le C$ for all $n \ge 0$. We therefore have the estimate

$$\begin{aligned} \|F_{k+m}^\circ \cdots F_k^\circ\| &\ge \|S_\circ^{m+1}\| - \sum_{\ell=1}^{m} \frac{1}{\ell!} \left(\sum_{n=k}^{k+m} \|B_n\| \right)^\ell C^{\ell+1} \\ &\ge 1 - C \sum_{i=1}^{m} \frac{1}{\ell!} \left(\frac{bC\rho^k}{1-\rho} \right)^\ell \\ &\ge 1 - C \left(\exp\left(\frac{bC\rho^k}{1-\rho} \right) - 1 \right), \end{aligned} \tag{15}$$

where we have used that $\|S_\circ^n\| \ge 1$ for all $n \ge 0$. Clearly, there exists an integer $k > 0$ such that the lower bound (15) is positive, from which the last assertion of Theorem 2 follows. □

Theorem 2 gives necessary and sufficient conditions that a wave vector q belongs to the Bragg spectrum, at least if the tiling is decorated with a generic diffraction density. For a non-generic decoration, the initial Fourier amplitude vector might be in the kernel of $S_\circ^\infty$, so that the Bragg peak would be extinct. But even for a generic decoration, we cannot completely exclude that a Bragg peak is extinct. However, if this is the case the amplitude vector must be in the kernel of $S_\circ^\infty$ already after a *finite* number of iterations (which may depend on q).

Apart from such additional extinctions, which by Theorem 2 are under control, the Bragg spectrum therefore can be identified with the set of those wave vectors q for which $e(\vartheta^n q \cdot x) \to 1$ for all x in the translation module T. This latter set clearly forms a $\mathbb{Z}$-module, and shall be called the *Fourier module* of the tiling, henceforth denoted by $\mathcal{F}$. In any case, the Bragg spectrum always is contained in the Fourier module, and in typical cases, where there are no extinctions, the two are identical.

4. The Fourier Module of a Substitution Tiling

The characterization of the Bragg spectrum in terms of the Fourier module, as it was obtained in the previous section, is still rather implicit. In this section, we shall give a more explicit and constructive description of the Fourier module.

We first have to recall a few basic facts on algebraic numbers. More details can be found in any standard textbook, see, e.g., (Borevich and Shafarevich, 1966). A polynomial $p(x) = a_r x^r + a_{r-1}x^{r-1} + \cdots + a_0$ with integer coefficients is called $\mathbb{Z}$-*irreducible*, if its coefficients are coprime, the leading coefficient a_r is positive, and $p(x)$ cannot be factorized into integral polynomials of lower degree. A number α is called *algebraic of degree* r if there exists a $\mathbb{Z}$-irreducible polynomial $p_\alpha(x) = a_r x^r + a_{r-1}x^{r-1} + \cdots + a_0$ of degree r, which has α as one of its roots. This polynomial $p_\alpha(x)$ is uniquely determined by α. The roots of $p_\alpha(x)$, denoted by $\alpha_1 = \alpha, \alpha_2, \ldots, \alpha_r$, are said to be (algebraic) conjugates of each other. If the leading coefficient $a_r = 1$, α is called an *algebraic integer*. Particular algebraic integers are those of degree 1, namely the rational (ordinary) integers. If $|a_0| = |\prod_i \alpha_i| = 1$, we say that α is a *unit*, meaning that it is a unit in the ring $\mathbb{Z}[\alpha]$.

The field $\mathbb{Q}(\alpha)$ is the algebraic closure of the union of the field of rational numbers, $\mathbb{Q}$, and the algebraic number α. $\mathbb{Q}(\alpha)$ can be regarded as a vector space over $\mathbb{Q}$, of dimension r. Multiplication by $\beta \in \mathbb{Q}(\alpha)$ induces a linear mapping $\xi \to \beta\xi$ on this vector space. If B is the matrix of this mapping with respect to a basis in $\mathbb{Q}(\alpha)$, we define the *trace* $Tr(\beta)$ (Borevich and Shafarevich, 1966) as the trace of the matrix B. In particular, if β is an algebraic integer, its trace is a rational integer. Moreover, if $\beta_1 = \beta$ and $\beta_2, \ldots, \beta_r$ are the conjugates of β, we have $Tr(\beta) = \sum_{i=1}^r \beta_r$. If $\omega_1, \ldots, \omega_r$ is a basis of $\mathbb{Q}(\alpha)$, one can show (Borevich and Shafarevich, 1966) that the matrix $g_{ij} = Tr(\omega_i\omega_j)$ is positive definite. The trace therefore provides us with a natural, positive definite scalar product $\beta \cdot \gamma = Tr(\beta\gamma)$ in the vector space $\mathbb{Q}(\alpha)$. In particular, for every basis $\omega_1, \ldots, \omega_r$ of $\mathbb{Q}(\alpha)$ there is a unique dual basis $\omega_1^*, \ldots, \omega_r^*$, defined by $Tr(\omega_i\omega_j^*) = \delta_{ij}$.

Definition: *An algebraic integer $\vartheta > 1$ of degree r is called a* Pisot-Vijayaraghavan*-number, a* Pisot*-number, or simply a* PV*-number, if all its other conjugates $\vartheta_2, \ldots, \vartheta_r$ satisfy $|\vartheta_i| < 1$.*

From now on, $\forall x \in \mathbb{R}$ we denote by $\|x\|$ the positive distance of x to the nearest integer.

Theorem 3. *(Pisot, Vijayaraghavan) Suppose that $\vartheta > 1$ is a real algebraic integer of degree r, and that $\lambda \in \mathbb{R}$. Then the following statements are equivalent:*

i) $\|\lambda\vartheta^n\| \to 0$ *as* $n \to \infty$.
ii) There exist constants $\rho < 1$ and b such that $\|\lambda\vartheta^n\| < b\rho^n \ \forall n \in \mathbb{N}$.
iii) ϑ *is a* PV*-number, and* $\lambda = \vartheta^{-k}\mu$ *for some integer* $k \geq 0$ *and some number* $\mu \in \mathbb{Q}(\vartheta)$ *such that* $Tr(\vartheta^j\mu) \in \mathbb{Z}$, $(0 \leq j \leq r-1)$.

A proof of Theorem 3, which will be our main tool in the analysis of the Fourier module of a substitution tiling, can be found in (Cassels, 1957).

We now recall that multiplication by ϑ maps the translation module T into itself. With respect to a basis of T, this linear mapping is described by a matrix M with integral entries. Clearly, ϑ is an eigenvalue of M, and therefore must be an algebraic integer. Since $|1 - e(x)| = 2|\sin(\pi x)|$ has the same set of zeros as $\|x\|$, $e(\vartheta^n q \cdot x) \to 1$ is equivalent to $\|\vartheta^n q \cdot x\| \to 0$, so that Theorem 3 implies that the Fourier module of a substitution tiling can be non-trivial only if ϑ is a PV-number. Therefore, from now on we shall assume that ϑ is a PV-number.

Since a primitive substitution tiling is repetitive, the $\mathbb{R}$-span of the translation module is $\mathbb{R}^d$, and so the eigenvalue ϑ of M must have multiplicity at least d, from which it follows that the characteristic polynomial of M contains a factor $(p(x))^d$, where $p(x)$ is the minimal irreducible polynomial of ϑ. Therefore, the translation module T has rank at least rd. On the other hand, by methods similar to those used in (Kenyon, 1994) one can show that there always exists a basis $b_1, \dots, b_d$ of $\mathbb{R}^d$ such that the translation module T is contained in $b_1\mathbb{Q}(\vartheta) \oplus \cdots \oplus b_d\mathbb{Q}(\vartheta)$, from which it immediately follows (Borevich and Shafarevich, 1966) that T cannot have rank bigger than rd. One basically shows that for a primitive substitution tiling the linear mapping M on T extends continuously to a linear mapping on $\mathbb{R}^d$ (where T is dense), which implies the desired result. Therefore, from now on we can assume that the translation module T has minimal rank rd.

From the action of M on T it is clear that with $p(\vartheta) = 0$ we also have $p(M) = 0$. By Cayley-Hamilton we can then bring M to block-diagonal form, where the characteristic polynomial of each block is $p(x)$. Since the roots of $p(x)$ are all simple roots, each of these blocks is diagonalizable over $\mathbb{C}$, so that also M is diagonalizable over $\mathbb{C}$. If the case $r = 1$, when ϑ is a rational integer, the rank of T is d, so that T is a lattice, and $M = \vartheta \cdot I$. On the other hand, if $r > 1$ we can regard M as a linear mapping on a space $\mathbb{R}^n$, where $n = rd$ is the rank of T. We shall use coordinates in $\mathbb{R}^n$ in which M is diagonal. These coordinates may be complex, but this does not pose any problem. $\mathbb{R}^n$ can be split into a direct sum $\mathbb{R}^n = \mathbb{R}^d \oplus \mathbb{R}^{n-d}$, such that M leaves both $\mathbb{R}^d$ and $\mathbb{R}^{n-d}$ separately invariant. If π and π' denote the orthogonal projectors on $\mathbb{R}^d$ and $\mathbb{R}^{n-d}$, respectively, then M commutes with both π and π'. On $\mathbb{R}^d$, M acts as $\vartheta \cdot I$, whereas on $\mathbb{R}^{n-d}$ it acts as a contraction. The latter follows from the fact that all eigenvalues $\lambda_i \neq \vartheta$ of M are conjugates of ϑ, and ϑ is a PV-number. We note that T can be regarded as being embedded in the linear subspace $\mathbb{R}^d$ of $\mathbb{R}^n$.

For each translation module T of minimal rank $n = rd$, we shall now define a *dual module* T^*. In the case $r = 1$, where T is a lattice, the dual module T^* is simply the dual lattice of T, defined by $T^* = \{y \in \mathbb{R}^d | y \cdot x \in \mathbb{Z} \ \forall x \in T\}$. If $b_1, \dots, b_d$ is a basis of T, the dual basis $b_1^*, \dots, b_d^*$, defined by $b_i \cdot b_j^* = \delta_{ij}$, is a basis of T^*. In the case $r > 1$ there exists a lattice

$L \subset \mathbb{R}^n$ such that $\pi L = T$, where π is again the projector on $\mathbb{R}^d$ which commutes with M. If L^* is the dual lattice of L, we set for the dual module $T^* = \pi L^*$. It is important here that, although there is no unique lattice L which projects on T, the definition of T^* does not depend on the choice of L. Any lattice L with $\pi L = T$ shall be called a *lift* of T, and gives rise to the same dual module T^*. The construction of the dual module T^* is reminiscent of the cut and project method for the construction of quasicrystals and their Fourier transform.

We are now ready to give a second, much more explicit characterization of the Fourier module $\mathcal{F}$ of a selfsimilar tiling. The following Theorem states that these two characterizations are equivalent.

Theorem 4. *Let T be the translation module of a primitive substitution tiling with scaling factor ϑ. Then the following statements are equivalent:*

i) $e(\vartheta^n q \cdot x) \to 1 \ \forall x \in T$.

ii) $q = \vartheta^{-m} k$, *where $m \geq 0$ is an integer, and k is in the dual module T^*.*

Proof. We first show that ii) implies i). Consider first the case $r = 1$. Since ϑ then is an integer, by the definition of the dual lattice we have $e(\vartheta^n q \cdot x) = e(\vartheta^{n-m} k \cdot x) = 1$ for all $n \geq m$, $x \in T$. In the case $r > 1$, let L be a (fixed) lift of T, and L^* the dual lattice of L. For each $x \in T$, let X denote its unique lift to L, satisfying $\pi X = x$. In a similar way, for $k \in T^*$, let K denote its lift to L^*. Since $MT \subset T$, for $x \in T$ and $k \in T^*$ we then have

$$1 = e(K \cdot M^n X) = e(K \cdot \pi M^n X) \cdot e(K \cdot \pi' M^n X). \tag{16}$$

Since π commutes with M, and $\pi M = \vartheta \pi$, the first factor in (16) simply reads $e(\vartheta^n k \cdot x)$, and since π' commutes with M, and $\pi' M$ is a contraction, the second factor in (16) converges to 1 as $n \to \infty$. Therefore, if $q \in T^*$, we have $e(\vartheta^n q \cdot x) \to 1$ for all $x \in T$. Evidently, the same holds true if $q = \vartheta^{-m} k$, with $k \in T^*$.

Next, we show that i) implies ii). We first consider the case where T is a one-dimensional module $\mathbb{Z}[\vartheta]$, which is of rank r and has a basis $1, \vartheta, \ldots, \vartheta^{r-1}$. We note that $\vartheta^k \to (\vartheta^k, \vartheta_2^k, \ldots, \vartheta_r^k)$ defines a lift of $\mathbb{Z}[\vartheta]$ to a lattice $L \subset \mathbb{R}^r$. In this representation M is diagonal, $M = \operatorname{diag}(\vartheta, \vartheta_2, \ldots, \vartheta_r)$. Since $1, \vartheta, \ldots, \vartheta^{r-1}$ is also a basis of $\mathbb{Q}(\vartheta)$, this lift can be extended to $\mathbb{Q}(\vartheta)$. The embedding of the lift of $\mathbb{Q}(\vartheta)$ in $\mathbb{R}^r$ is chosen in such a way that the scalar product on the lift of $\mathbb{Q}(\vartheta)$ which is induced by the standard scalar product on $\mathbb{R}^r$ is identical to the scalar product defined by the trace on $\mathbb{Q}(\vartheta)$. From Theorem 3 we know that $\|\vartheta^n \lambda\| \to 0$ if and only if $\lambda = \vartheta^{-m} \mu$, with $Tr(\vartheta^j \mu) \in \mathbb{Z}$, $(0 \leq j \leq r-1)$. Since $1, \vartheta, \ldots, \vartheta^{r-1}$ is a basis of $\mathbb{Z}[\vartheta]$ this simply means that μ is in the dual module of $\mathbb{Z}[\vartheta]$.

We now proceed to the next level of generality. If $d > 1$, we consider the case where $T = a_1 \mathbb{Z}[\vartheta] \oplus \ldots \oplus a_d \mathbb{Z}[\vartheta]$. The vectors a_i need not be orthogonal, but they should be linearly independent over $\mathbb{R}$. The vectors a_i are then a basis of $\mathbb{R}^d$, and so let a_i^* be the dual basis. We now decompose $x \in T$ as $x = \sum x_i a_i$, and any wave vector q as $q = \sum q_i a_i^*$. Then we have $e(\vartheta^n q \cdot x) = \prod_i e(\vartheta^n q_i x_i)$, which implies that q is in the Fourier module of T if and only if, for all i, q_i is in the dual module of $\mathbb{Z}[\vartheta]$. On the other hand, a lift of T can be obtained by taking the direct sum of the lifts of the submodules $a_i\mathbb{Z}[\vartheta]$, which shows that $T^* = a_1^*\mathbb{Z}[\vartheta] \oplus \ldots \oplus a_d^*\mathbb{Z}[\vartheta]$ is nothing but the dual module of T. This proves Theorem 4 also in this case.

In the most general case, T contains at least a submodule T' of the form $T' = a_1\mathbb{Z}[\vartheta] \oplus \ldots \oplus a_d\mathbb{Z}[\vartheta]$. Since T and T' have the same rank, T/T' is finite. With respect to a basis b_i of T and a basis c_i of T', there exists an integral matrix A such that $T' = AT$, where $|\det(A)|$ is equal to $|T/T'|$. Any $y \in T$ can therefore be written as $y = A^{-1}x$, with $x \in T'$. Since $T \subset T'$, the Fourier module of a structure with translation module T will be contained in the Fourier module of a structure with translation module T'. Therefore, we can assume that a wave vector q in the Fourier module of T is of the form $\vartheta^{-m}k$, with $k \in T'^*$. If we express k with respect to the dual basis c_i^* of T'^*, we have $e(\vartheta^{n-m}k \cdot y) \to 1$ for all $y \in T$ if and only if $e(\vartheta^{n-m}k \cdot A^{-1}x) = e(\vartheta^{n-m}(A^T)^{-1}k \cdot x) \to 1$ for all $x \in T'$, where A^T is the transpose of A. This implies $(A^T)^{-1}k \in T'^*$, or $k \in A^T T'^*$. On the other hand, if L is a lift of T', then $A^{-1}L$ clearly is a lift of T, and therefore $A^T T'^*$ is the dual module of T. □

It is implicit in Theorem 4 that there are three essentially different types of Fourier modules which can occur. Since ϑ is an algebraic integer, ϑ can either be a rational integer, or an irrational algebraic integer. In the latter case, we have to distinguish between ϑ being a unit, or not a unit. Note that if $\vartheta > 1$ is a rational integer, it can never be a unit.

In the rest of this section, we shall describe these three situations in general terms. These descriptions are intended to provide an intuitive understanding of the situation, and are therefore not always completely rigorous. Also, by calling a structure limit-periodic, quasiperiodic, or limit-quasiperiodic, which all are special types of *almost-periodic* structures, we do not imply here that their diffraction spectrum is purely discrete, as one would usually do.

The Limit-Periodic Case. If ϑ is a rational integer, T must be a lattice, and the Fourier module $\mathcal{F}$ is given by

$$\mathcal{F} = \bigcup_{k \geq 0} \vartheta^{-k} T^*, \tag{17}$$

where T^* is the dual lattice of T. This is the Fourier module of a *limit-periodic* structure. The name "limit-periodic" can be understood as follows.

If we retain only a finite union in (17),

$$\mathcal{F}_n = \bigcup_{0 \le k \le n} \vartheta^{-k} T^* = \vartheta^{-n} T^*, \tag{18}$$

we obtain the Fourier module of a periodic structure, whose lattice of translation symmetries is $\vartheta^n T$. By increasing n step by step, this lattice of translation symmetries is broken to a sublattice, and again to a sublattice, and so on. In the limit, an aperiodic structure is obtained, which is the limit of a sequence of periodic structures, whose translation lattices form a sequence of successive sublattices. We note that the module (17) is not finitely generated, for ϑ^{-1} maps any finite rank submodule of $\mathcal{F}$ into a module which is strictly bigger.

The Quasiperiodic Case. If ϑ is irrational, and moreover is a unit in the ring $\mathbb{Z}[\vartheta]$, we have $\det(M) = \vartheta\vartheta_2 \cdots \vartheta_r = \pm 1$, so that $\vartheta T = MT = T$, and consequently $\vartheta^{-1} T^* = (M^T)^{-1} T^* = T^*$. Therefore, the Fourier module $\mathcal{F}$ is simply given by

$$\mathcal{F} = T^*. \tag{19}$$

This Fourier module is finitely generated, and structures with a finitely generated Fourier module are called *quasiperiodic*. Quasiperiodic structures can be understood as the intersection of some periodic structure in a space $\mathbb{R}^n$, where n is the rank of T, with a d-dimensional hyperplane $\mathbb{R}^d \subset \mathbb{R}^n$, which is incommensurate with the lattice of the periodic structure. The lattice of this periodic structure is nothing but a lift of the translation module T. We finally remark that, although quasiperiodic structures can be obtained as the limit of a sequence of periodic approximant structures (Janssen, 1991), the translation lattices of these approximant structures do not form a sequence of successive sublattices. For this reason, quasiperiodic structures are *not* limit-periodic.

The Limit-Quasiperiodic Case. This case is, in a certain sense, a combination of the previous two cases. Now, ϑ is irrational, and it is *not* a unit in $\mathbb{Z}[\vartheta]$. Hence, $|\det(M)| > 1$, and $\vartheta^{-k} T^* = (M^T)^{-k} T^*$ is a true submodule of $\vartheta^{-(k+1)} T^*$. The Fourier module therefore is

$$\mathcal{F} = \bigcup_{k \ge 0} \vartheta^{-k} T^*, \tag{20}$$

where this time T^* is the Fourier module of a quasiperiodic structure. If we consider, in analogy to the limit-periodic case, a finite union

$$\mathcal{F}_n = \bigcup_{0 \le k \le n} \vartheta^{-k} T^* = \vartheta^{-n} T^*, \tag{21}$$

we obtain the Fourier module of a quasiperiodic structure with translation module $\vartheta^n T$. A structure with Fourier module (20) can therefore be obtained as the limit of a sequence of quasiperiodic structures, whose translation modules form a sequence of successive submodules. It is therefore natural to call such structures *limit-quasiperiodic*, in analogy to the limit-periodic case. The term "limit-quasiperiodic" had first been introduced in (Gähler, 1991). As in the limit-periodic case, the Fourier module of a limit-quasiperiodic structure is not finitely generated. A limit-quasiperiodic structures can be understood as a planar section through a simpler structure in a higherdimensional space $\mathbb{R}^n$, which is, unlike in the quasiperiodic case, not periodic, but rather limit-periodic.

5. Substitution Tilings With A Non-Trivial Point Symmetry

So far we haven't said anything about point symmetry. In fact, the existence of a non-trivial Bragg spectrum relies exclusively on the existence of certain translational symmetries, and is completely independent of the presence of point symmetry elements. However, at least in more than one dimension, the most appealing examples of self-similar tilings are certainly those which are highly symmetric, so that it is worthwhile to say a few words about point symmetry. For a discussion of point symmetry and related topics we refer also to (Baake and Schlottmann, 1995).

We shall say that a tiling admits a point symmetry element $g \in O(d)$, if g maps the tiling into another tiling in the *same local isomorphism class* (LI class). Since an LI class consists of tilings which are locally indistinguishable from each other, this means that the rotated (or reflected) tiling can not be distinguished from the original one by any local means. For non-periodic structures, this concept of point symmetry seems to be a very appropriate one. It identifies the point group of a tiling with that of its LI class. An element $g \in O(d)$ is in the point group of the tiling if it leaves its LI class invariant, not pointwise, but as a set. Since in the case of a periodic tiling the LI class consists of a single element, this definition of point symmetry reduces to the usual one in the periodic case.

We emphasize that an LI class with point group $G \subset O(d)$ does not necessarily contain any particular tiling wich is globally G-symmetric. Rather, the converse is true: the existence of a globally G'-symmetric tiling in a LI-class implies that the point group G of the LI-class contains G' as a subgroup. For instance, the point group of the Penrose tiling is D_{10}, which contains, in particular, 10-fold rotations, although there is no single Penrose tiling with more than 5-fold rotational symmetry, and most Penrose tilings have no symmetry at all.

We also emphasize that the point group G of a tiling has nothing to do with the presence or absence of local patches which are G-symmetric, a misconception which, unfortunately, is very popular. A completely unsymmetric tiling may contain highly symmetric local patches, and a highly symmetric tiling may contain only completely unsymmetric local patches.

Let us now return to self-similar tilings, generated by substitutions. Since the LI class of a substitution tiling is generated by its substitution, the resulting LI class will be G-symmetric if and only if the substitution is G-symmetric, i.e., if it commutes with G. This means that for every tile there must be a whole G-orbit of tiles, including the diffraction densities carried by these tiles, and all tiles in a given G-orbit must have the same behaviour under substitution. If $g \in G$ is a point group element, e.g., a rotation, and $g(\mu_i^{(n)})$ are the rotated diffraction densities on the rotated tiles $g(t_i^{(n)})$, these rotated diffraction densities must behave under the substitution as

$$g(\mu_i^{(n+1)}) = \sum_{j=1}^{m} \sum_{\ell=1}^{S_{ij}} \mathsf{T}\left(g(\vartheta^n d_{ij\ell})\right) \cdot g(\mu_j^{(n)}). \tag{22}$$

The presence of the point symmetry G in the substitution has two consequences. The first one is that the translation module of the substitution tiling will be G-symmetric, and the same holds true for the Fourier module. The second consequence is that the substitution matrix commutes with the point group G, where the latter acts as a permutation of the tiles. This implies that the left and right ϑ^d-eigenvectors of S, whose components are strictly positive, must be constant on G-orbits. For this reason, not only the Fourier module, but also the intensities of the Bragg peaks will be G-symmetric.

6. Some Illustrative Examples

6.1. ONE-DIMENSIONAL EXAMPLES

There is a vast literature on one-dimensional substitutional sequences. We just mention (Queffelec, 1987; Luck et al., 1993; Allouche and Mendès France, 1995), where further references can be found. The one-dimensional case is somewhat particular in that one first considers, in general, an abstract substitution acting on words in a finite alphabet. Having generated an infinite word, one then replaces in a second step the letters in the infinite word by intervals of different lengths, producing a one-dimensional *self-similar tiling*. Another possibility is to replace the letters by numbers, producing a *self-similar sequence of numbers*. This second possibility is equivalent to a tiling with differently decorated unit-length intervals, where the decoration is a function of the letters.

In either case, one has to check whether such a tiling fits into the general framework developed in this paper. We have always assumed that under substitution all tiles scale with the same factor ϑ, and this condition must be carefully verified, because in one dimension there are no geometric constraints for the choice of the interval lengths. Given a substitution matrix S, the admissible relative tile lengths are already completely fixed. These tile lengths must be proportional to the components of the ϑ left eigenvector of S. Therefore, the Fibonacci tiling, consisting of intervals of length $\tau \equiv (1+\sqrt{5})/2$ and 1, does fit into our framework, whereas the Fibonacci *sequence*, considered as an abstract 01-sequence, does not. For two-letter substitutions, the case of arbitrary tile lengths has been studied in detail in (Kolář et al., 1993).

If we fix the scaling factor ϑ and the number of different tiles, there may still be several different substitutions with this scaling factor, with different ratios of the tile sizes. Such examples can be found in (Lück, 1993) for the scaling factors $1+\sqrt{2}$ and $2+\sqrt{3}$, which are important for quasiperiodic tilings with eight- and twelve-fold symmetry, respectively.

As explained above, if ϑ is irrational, a self-similar sequence of numbers will never fit into our framework. If ϑ is an integer, however, and if, moreover, each letter is substituted by a word of the same length, a substitution sequence of numbers is covered by our general theory. Substitution sequences with these special properties are so-called *automatic sequences* (Allouche and Mendès France, 1995), and include the Thue-Morse sequence, the Rudin-Shapiro sequence, the period-doubling sequence, the paper-folding sequence, and many others (Allouche and Mendès France, 1995).

For substitutions with an integer scaling factor one would expect a limit-periodic Fourier module. However, some of these automatic sequences are ill-behaved in the sense that extinctions occur. As an example, we consider the Thue-Morse sequence, whose substitution acts as $a \to ab$, $b \to ba$. If the infinite word is replaced by a sequence of numbers on $\mathbb{Z}$, by Theorem 2 the Fourier module can only contain elements of the form $q = 2^{-n}m$, where n is a non-negative integer, and m an integer, which is odd if $n \geq 1$ (note that $\vartheta = 2$). For such a q, the matrix $F_k(q)$ then reads

$$F_k(q) = \begin{pmatrix} 1 & e(2^{k-n}m) \\ e(2^{k-n}m) & 1 \end{pmatrix}. \tag{23}$$

In particular, since $e(1/2) = -1$, we have for $q = 2^{-n}m$ (m odd)

$$F_n(q)F_{n-1}(q) = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = 0, \tag{24}$$

so that in the case $n \geq 1$ the intensity exactly vanishes after a finite number of iterations. Therefore, for a generic choice of the numbers a and b, the Thue-Morse sequence has a Fourier module $\mathcal{F} = \mathbb{Z}$. On all other points of the limit-periodic Fourier module, the intensities are extinct. The situation is, in fact, even worse: in the literature, the favourite choice for a and b is $a = 1$ and $b = -1$, in which case the initial Fourier amplitude vector is in the kernel of S. Therefore, with this non-generic decoration *all* Bragg peaks are extinct.

Since the Bragg spectrum of the Thue-Morse sequence is at most a module of rank one, but the Thue-Morse sequence is non-periodic, it is clear that the Thue-Morse sequence must also have a continuous component in its diffraction pattern. This continuous component happens to be singular continuous (Peyrière, 1975).

As far as the Bragg spectrum is concerned, the Rudin-Shapiro sequence is very similar to the Thue-Morse sequence. Also in this case, extinctions occur after a finite number of iterations, and the surviving Bragg peaks are removed by a non-generic decoration that is usually considered in the literature (Allouche and Mendès France, 1995; Queffelec, 1987).

Such pathological behaviour, as for the Thue-Morse and the Rudin-Shapiro sequence, seems to be limited to dimension one and integer scaling factor ϑ. No other examples are currently known. The paper-folding sequence, on the other hand, shows the full limit-periodic Fourier module (Allouche and Mendès France, 1995), as one would have expected.

6.2. EXAMPLES IN DIMENSIONS TWO AND THREE

The simplest example of a limit-periodic tiling in more than one dimension is certainly the two-dimensional chair tiling (Godrèche and Luck, 1990). It consists of one tile (the "chair"), which occurs in four different orientations. The chair tiling has a scaling factor $\vartheta = 2$ and D_4 symmetry, in the sense of Section 5. The second power of the substitution of a chair, which is the first one in which all chair orientations show up, is shown in Fig. 1, together with a larger piece of a chair tiling. The translation module of the chairs of one orientation is indicated with dots. It is a rectangular lattice. Chairs which are rotated by $\pm 90°$ have a correspondingly rotated translation module, so that the total translation module is a square lattice (recall that in the case of a non-unit substitution, the translation modules of different patches, and in particular of different tiles, need not be identical).

Very similar to the chair tiling is the sphinx tiling (Godrèche, 1989), which is also limit-periodic. This tiling consists of right and left sphinxes, both of which occur in six orientations. The scaling factor ϑ is again 2, and the tiling has D_6 symmetry. The translation module of a single sphinx tile

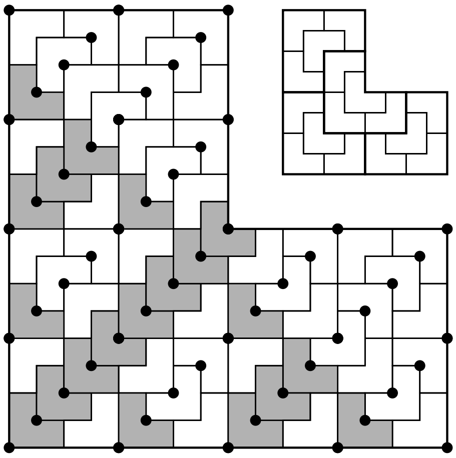

Figure 1. Second substitution of a chair (top right), and a larger piece of a chair tiling. All chairs of one given orientation are shaded, and the translation module of these chairs is indicated by dots.

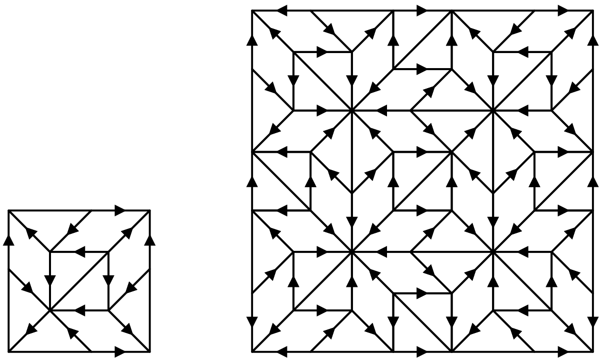

Figure 2. First and second substitution of a square in the octagonal Ammann tiling. All squares are divided into two triangles, and the square and rhombus edges are decorated with arrows, in order to make the substitution of all tiles unique.

is a rectangular lattice (with lattice constants 1 and $\sqrt{3}$), and the union of the translation modules of all tiles is a hexagonal lattice. We note that with the methods of (Solomyak, 1995) one can show that both the chair and the sphinx tiling have a purely discrete diffraction pattern.

The quasiperiodic case is probably the one with the richest choice of examples. The simplest one is certainly the octagonal Ammann-Beenker Tiling (Ammann et al., 1992; Beenker, 1982), which is usually described in terms of squares and 45° rhombi. However, in order to ensure that every tile can be substituted by a set of *entire* tiles, we shall divide here the

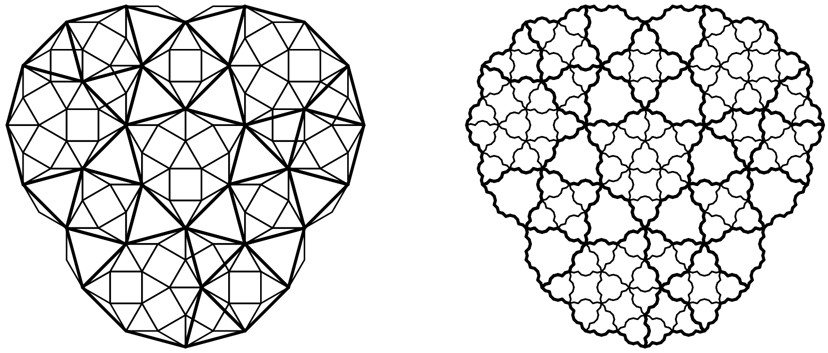

Figure 3. Substitution of a patch of the shield tiling, with polygonal tiles (left) and with fractalized tiles (right).

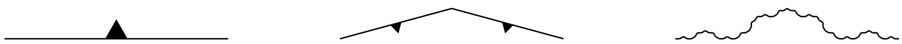

Figure 4. A straight bond (left) is replaced by a buckled bond (middle). The black triangle indicates the direction into which the next buckling will occur. If this buckling procedure is iterated, one arrives in the limit at the fractal bond shown on the right.

square along one of its diagonals into two triangles. In Fig. 2, the first and the second substitution of a square, or, more precisely, a patch consisting of two triangles, is shown. From Fig. 2, the substitutions of all kinds of tiles can easily be read off. Since the substitutions of the triangles are asymmetric, we have to decorate all tiles with arrows on the edges, in order to make the substitution unique. One easily convinces oneself that the translation module of the octagonal Ammann tiling is the module generated by the tile edges.

There are many other well-known tilings for which it is necessary to divide some or all tiles into several smaller ones, if we want to generate them by a substitution which replaces tiles by entire tiles. However, there are also examples for which it is not enough to divide the tiles into finitely many such pieces. One such example is the dodecagonal Socolar tiling (Socolar, 1989; Klitzing, 1995b), another one the dodecagonal shield tiling (Niizeki and Mitani, 1987; Gähler, 1988b). For these, it proves necessary to introduce fractalized tiles. Here, we shall have a closer look at the shield tiling, for which there exists a substitution which does not only scale the tiling by a certain factor, but also rotates it by 15° (Niizeki and Mitani, 1987). Since the shield tiling is only 12-fold symmetric, in the strict sense this substitution does not map a tiling into one of the same LI class. All even powers of this substitution, however, leave the LI class invariant, and if we identify tilings which are rotated by 15° with respect to each other,

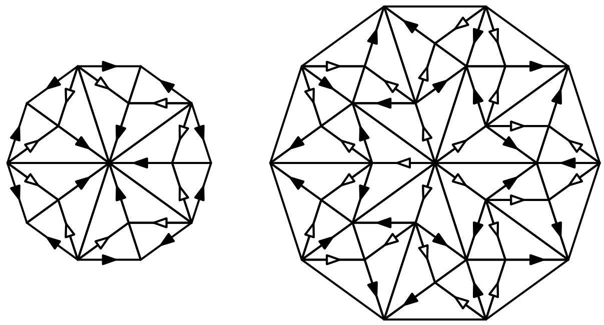

Figure 5. A patch of the Penrose tiling (left), together with its substitution (right). Rhombs are divided into two triangles each, and rhomb edges are decorated with two kinds of arrows, on order to make the substitution of a tile unique.

the same holds true also for odd powers. If we want to generate the shield tiling by this substitution by replacing each tile by a set of entire tiles, we must replace the polygonal tiles by tiles with fractal boundaries, which are adapted to the substitution. In Fig. 3, the substitution of a patch of the shield tiling is shown, both with polygonal tiles and with fractal tiles. In the version with polygonal tiles one can see that in each substitution step the bonds want to buckle to one side, depending on their environment. If this buckling is iterated, as explained in Fig. 4, we obtain in the limit a fractal bond, which is invariant under substitution. In terms of tiles with these fractalized edges, the substitution then has the required properties, as is evident from Fig. 3. We note that Fig. 3 does not completely specify the substitution. For a complete specification, the tiles would have to carry markings (Gähler, 1993) which break their symmetry.

The best known quasiperiodic example is certainly the Penrose tiling (Penrose 1974, 1979; de Bruijn, 1981). Here, we consider its rhombic variant. As for the Ammann-Beenker tiling, to make the substitution unique the edges of the rhombi have to be decorated with arrows, and each of the rhombi has to be divided into two Robinson triangles (de Bruijn, 1990), in order that tiles are substituted by entire tiles. The substitution of a patch of the Penrose tiling is shown in Fig. 5. A new feature of the Penrose tiling is that its translation module T is not the module generated by the rhombus edges, which we denote by T'. Rather, its translation module is smaller, and has only index 5 in T'. We have to recall here (de Bruijn, 1981) that the vertices of the Penrose tiling fall into four different classes, or rather five classes, one of which is empty. If $e_1, \ldots, e_4$ is a basis of rhombus edge vectors generating T', we can write any vertex in a unique way as $\sum_i n_i e_i$, where the n_i are integers. The class of a vertex then is determined by the value $\sum_i n_i \pmod 5$. Since a vertex patch, including its orientation, uniquely determines the class of a vertex (de Bruijn, 1981), the translation module clearly cannot be bigger than the module generated by the differences between vertices of the *same* class, which is of index 5 in T'. One easily convinces oneself that this module indeed is the translation module. Using mistakenly T' as the translation module of the Penrose tiling would only lead to a submodule of the true Fourier module of the Penrose tiling.

In order to find the complete Bragg spectrum of the Penrose tiling, it is therefore important to correctly determine its translation module. Would one choose reference points on the tiles such that their differences generate T' instead of T (which is easily achieved by taking a random choice of vertices as reference points), and would one then require that the matrices $F_n(q)$ converge to S, this would lead to the (wrong) conclusion that the Fourier module of the Penrose tiling is the dual module of T', which is only a submodule of index 5 of the true Fourier module of the Penrose tiling. The examples in (Godrèche and Luck, 1989), which are based on the Penrose Tiling, suffer precisely from this problem: only a submodule of the true Fourier module has been determined in (Godrèche and Luck, 1989).

A similar problem arises with the icosahedral Danzer tiling (Danzer, 1989), which is the only 3D example which we shall mention here. Also in the Danzer tiling, the vertices fall into three different classes which are not translationally equivalent, so that some care is needed in the determination of the translation module.

As a last quasiperiodic example, we mention a square-triangle tiling introduced by Stampfli (Stampfli, 1986), whose substitution is depicted in Fig. 6. Here again, squares and triangles have to be divided into smaller tiles (only partially indicated in Fig. 6). Squares have to be cut into two rectangular half-squares, and triangles into six right-angled triangles. The scaling factor for this example is $2 + \sqrt{3}$. We remark that edges may have two kinds of environments, depending on their directions. If we divide the 12-fold star of all possible edge directions into two 6-fold stars, the type of an edge is of one or the other kind, depending on the 6-fold star into which the edge direction falls. Accordingly, there are two kinds of triangles, which have either all edges of one kind, or all edges of the other kind. On the other hand, there is only one kind of square, which is two-fold symmetric, since it contains edges of both kinds. Clearly, this subdivision into two inequivalent sets of edges prevents tilings generated by this substitution from being 12-fold symmetric. The substitution from Fig. 6 has only 6-fold symmetry, even though one easily convinces oneself that the translation module of this square-triangle tiling is 12-fold symmetric. We therefore have here an example where the *positions* of the Bragg peaks, governed by the translation module, are 12-fold symmetric, whereas the *intensities* of the Bragg peaks,

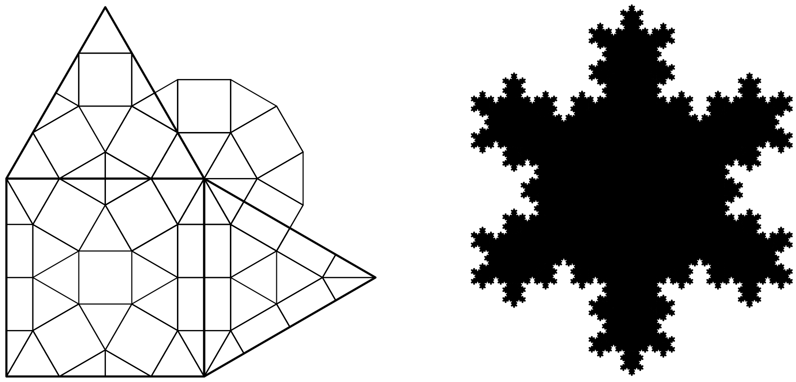

Figure 6. On the left, the substitution of a dodecagonal square-triangle tiling is shown. There are two kinds of edges, depending on their direction, and therefore two kinds of triangles (see text). The vertices of the first order supertiles are all decorated with the same dodecagonal patch. The set of these dodecagonal patches, whose interior is only hexagonally symmetric, determines the complete tiling. On the right, the atomic surface for the vertices of the tiling is shown. It has a fractal boundary and is six-fold symmetric.

which are governed by the symmetry of the substitution matrix S, are only 6-fold symmetric.

The set of vertices of this square-triangle tiling can be obtained as a plane cut through a 4-dimensional periodic structure, which consists of a lattice in which each node is decorated by an “atomic surface”. This atomic surface, first determined in (Gähler, 1988a), is shown in Fig. 6. An interesting feature of this tiling is that its atomic surface has a fractal boundary. Moreover, the atomic surface clearly is six-fold symmetric, which corroborates our symmetry analysis above. Other selfsimilar tilings with fractal atomic surfaces have been given in (Luck et al., 1993; Godrèche et al., 1993; Zobetz, 1992).

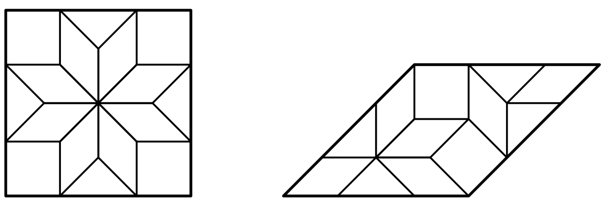

Figure 7. Substitution of a square and a rhombus, leading to a limit-quasiperidic structure.

Limit-quasiperiodic examples occur much less frequently in the literature. As the only example of more than one dimension that we are aware of we mention the one given in (Watanabe et al., 1987), which has a scaling factor $2+\sqrt{2}$ and is eightfold symmetric. The substitution of its tiles, a square and a 45° rhombus, is shown in Fig. 7. Again, the square has to be divided into two half-squares. Since the substitution of the rhomb is asymmetric, Fig. 7 does not completely specify the substitution. Markings would be needed to break the symmetry of the rhombi. Since *any* sufficient symmetry breaking of the rhombi (both mirror symmetries must be broken) will lead to a limit-quasiperiodic structure, we shall not choose a specific symmetry breaking.

7. Discussion and Conclusions

In this paper, a detailed study of the Bragg spectrum of self-similar tilings generated by primitive substitutions has been presented. Necessary and sufficient conditions for a wave vector q to be in the Bragg spectrum have been worked out. In has been shown that, apart from possible extinctions, which we neglect in this discussion, the Bragg spectrum is entirely determined by the linear scaling factor ϑ and the translation module T of the tiling. In particular, a necessary condition for the existence of a non-trivial Bragg spectrum is that ϑ is a PV-number. It appears very natural that ϑ and T have a decisive influence on the Bragg spectrum. For a wave vector q to be in the Bragg spectrum, the waves scattered from identical patches throughout the whole tiling must interfere constructively. The relative placement of identical patches is therefore of vital importance. It is determined by the translation module T on the one hand, and by the scaling factor ϑ on the other hand, which governs the fluctuations in the distribution of identical patches.

If ϑ is a PV-number, the support of the Bragg spectrum is determined by further properties of ϑ, and by the translation module T. Depending on ϑ, three different types of Bragg spectra can be distinguished. If ϑ is a unit in the ring $\mathbb{Z}[\vartheta]$, which is possible only if ϑ is irrational, the tiling is *quasiperiodic*, and its Bragg spectrum is given by the dual T^* of the translation module. If ϑ is not a unit, the Bragg spectrum is not finitely generated. It is then given by the infinite union $\bigcup_{k\geq 0}\vartheta^{-k}T^*$, where T^* is again the dual module of T. Depending on whether ϑ is a rational integer, or an irrational algebraic integer, two subcases can be distinguished in the non-unit case. If ϑ is a rational integer, the tiling is *limit-periodic*, and the dual module T^* is a lattice. If ϑ is an irrational algebraic integer, the tiling is *limit-quasiperiodic*, and the dual module T^* is a general finite rank module. A limit-quasiperiodic structure can be seen as a planar cut through a higher-dimensional limit-periodic structure.

Given its important role in the previous literature, it may be somewhat surprising that the properties of the substitution matrix S play only a minor role in our analysis. Basically, we have only assumed that S is primitive, in order to make sure that only tilings within a single LI class are generated by the substitution. All other properties of S turned out to be irrelevant for the Bragg spectrum. Of course, the largest eigenvalue ϑ^d of S must be a PV-number, but this is only a simple consequence of ϑ being a PV-number. Apart from that, the substitution matrix S is not important. In particular, its other eigenvalues do not play any role, and it does not matter whether any of these other eigenvalues has a modulus larger than one. This has already been remarked for the sphinx tiling (Godrèche, 1989), and as a further example where the second largest eigenvalue is larger than one we may cite the Danzer tiling (Danzer, 1989).

Acknowledgements

During the early stages of this work, FG has benefitted from discussions with Claude Godrèche and Jean-Marc Luck, and RK has benefitted from discussions with Peter Pleasants. These discussions are gratefully acknowledged.

A. Existence of the Infinite Volume Limit

In this appendix we shall justify our criterion (9) on q being in the Bragg spectrum. For this we have to show that the infinite volume limit (7) exists and is unique.

For any bounded set Λ and $\rho > 0$ we define $\partial_\rho\Lambda$ to be the set of those $x \in \mathbb{R}^d$ whose distance to the boundary of Λ, $\partial\Lambda$, is less than ρ. A sequence of bounded sets Λ_n is called a *van Hove sequence* (Hof, 1992) if $\lim_{n\to\infty} |\Lambda_n|^{-1}|\partial_\rho\Lambda_n| = 0$ for any $\rho > 0$ (here again, $|\Lambda|$ denotes the volume of Λ). We say that the infinite volume limit $\lim_{|\Lambda|\to\infty} |\Lambda|^{-1}\widehat{\mu}_\Lambda(q)$ exists *in the sense of van Hove* if it exists and is unique for any van Hove sequence Λ_n.

In the following, we shall show that if μ is the diffraction density of a primitive substitution tiling, the infinite volume limit $\lim_{|\Lambda|\to\infty} |\Lambda|^{-1}\widehat{\mu}_\Lambda(q)$ exists in the sense of van Hove for all $q \in \mathbb{R}^d$. We first introduce some notation. If t is any tile or supertile in the tiling, we denote by μ_t the diffraction density constrained to that particular tile, and by $\widehat{\mu}_t(q)$ its Fourier transform at wave vector q. If the tiles t_1 and t_2 are translated copies of each other, we write $t_1 \sim t_2$. We then have $\widehat{\mu}_{t_1}(q) = e(q \cdot d)\widehat{\mu}_{t_2}(q)$, where $d = d(t_1, t_2)$ is the distance vector between t_1 and t_2. For each tile type i and every substitution generation n we fix a reference copy $t_i^{(n)}$, and we denote by m_{in} its volume. According to a theorem by Geerse and Hof (1991), the infinite volume limit $\lim_{|\Lambda|\to\infty} |\Lambda|^{-1}\widehat{\mu}_\Lambda(q)$ then exists in the sense of van Hove if and only if

$$\lim_{n\to\infty} \max_i \sup_{t\sim t_i^{(n)}} \frac{1}{m_{in}} |\widehat{\mu}_t(q) - \widehat{\mu}_{t_i^{(n)}}(q)| = 0. \tag{25}$$

Since

$$\frac{1}{m_{in}} |\widehat{\mu}_t(q) - \widehat{\mu}_{t_i^{(j)}}(q)| = |1 - e(q \cdot d(t, t_i^{(n)}))| \frac{|\widehat{\mu}_{t_i^{(n)}}(q)|}{m_{in}}, \tag{26}$$

we have to show that for all i at least one of the two factors on the right hand side of (26) converges to zero as $n \to \infty$. There are two cases to be considered. If there exists an x in the translation module T such that $e(x \cdot q) \not\to 1$, then by Theorem 2 we have $m_{in}^{-1} |\widehat{\mu}_{t_i^{(n)}}(q)| \to 0 \;\forall q$. On the other hand, if $e(x \cdot q) \to 1 \;\forall x \in T$, we use the fact that any pair of supertiles is contained in a single supertile of some order N. This then implies that the distance vector $d(t, t_i^{(n)})$ can be written as

$$d(t, t_i^{(n)}) = \sum_{k=n}^{N-1} \vartheta^k d_k,$$

where each d_k is the difference of two of the translation vectors $d_{ij\ell}$ occurring in the substitution. By Theorem 3 we therefore have the estimate

$$|1 - e(q \cdot d(t, t_i^{(n)}))| \leq 2\pi \| q \cdot d(t, t_i^{(n)}) \| \leq \sum_{k=n}^{N-1} 2\pi \| \vartheta^k q \cdot d_k \| \leq \sum_{k=n}^{N-1} b_k \rho^k$$

for some $\rho < 1$. The constants b_k depend on $q \cdot d_k$, but since the number of different translation vectors $d_{ij\ell}$ is finite (and independent of N), we can replace the constants b_k by their maximum, b, so that we arrive at

$$\sup_{t\sim t_i^{(n)}} |1 - e(q \cdot d(t, t_i^{(n)}))| \leq \sum_{k=n}^{N-1} b\rho^k \leq \frac{b}{1-\rho} \rho^n,$$

which proves that (25) is satisfied also in this case.

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