Symmetries and Spectral Properties of Aperiodic Structures

Überblick über die schriftliche Habilitationsleistung
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Contents

1 Overview

This text summarises the articles on which this application for habilitation is based, namely, references [1] to [15]. The remainder of this section gives a brief overview of all results. Section 2 contains the basic facts and definitions underlying these results. In Sections 3, 4, 5, each subsection summarises one, two, or three of the references [1] to [15] separately. These subsections are ordered into sections according to their relation. This text is organised in a way such that the reader may switch to any subsection after reading Sections 1 and 2.

The references belonging to this application for habilitation are cited by numbers. Further relevant references are cited by letters.

1.1 Mathematical theory of aperiodic order

The discovery of alloys with sharp diffraction images which show non-crystallographic symmetries (quasicrystals) by Shechtman et al [SBGC] initiated extensive studies of such nonperiodic, but highly ordered structures. In fact, the discovery of Shechtman et al was anticipated by theoretical models like the Penrose tilings [PEN] or the three dimensional examples by Kramer [KRA]. But it was the impact of the discovery of real world quasicrystals that fuelled the search for further examples in the realm between crystallographic structures and entirely chaotic structures, the mathematical description of their properties, the understanding of possible symmetries of quasiperiodic structures, and the need of a precise definition of order.

During the last two decades a lot of progress has been made, accumulating in a mathematical theory of aperiodic order. It turned out that many mathematical disciplines are relevant to this field. There are connections to discrete geometry, combinatorics, harmonic analysis (the work under consideration falls essentially under these three topics), dynamical systems, topology, number theory and statistical mechanics. One fundamental result here is that the diffraction spectrum of any regular model set (see [HOF], [SCHL], or Theorem 2.1 below) is a countable sum of Dirac deltas (it is 'pure point'). The proof uses methods from the theory of dynamical systems. As a consequence, one standard method to decide whether a given structure has pure point spectrum is to establish that it *is* a regular model set. Unfortunately, this yields only a sufficient condition for pure point spectrum in the general case, not a necessary condition.

1.2 Pure point spectrum

The articles [2, 4, 6, 15] are dedicated to the problem of determining the model set property for some given structure. In [4] we obtain a necessary and sufficient condition for a lattice substitution system to have pure point spectrum, where we built upon an earlier result [LMS]. Lattice substitution systems are the most intensively studied instances of nonperiodic point sets supported on a lattice in $\mathbb{R}^d$.

In [2, 6] Galois duals (or more general, star-duals) of model sets are studied. Galois duality was introduced by Thurston in 1989 [THU]. In [2] it was shown how to use Galois duality to prove the model set property (thus pure point spectrum) for certain model sets in $\mathbb{R}^2$. In [6] the concept of Galois duality was generalized to locally Abelian groups, using Moody's star map. This more general concept is thus called star-duality. It is shown in [6] how this concept yields rigorous proofs for the model set property, thus for pure point spectrum, of many 'nice' aperiodic structures. In particular it was applied to reprove the model set property of Penrose tilings and Ammann-Beenker tilings, by computing their star-duals.

1.3 Beyond pure point spectrum

Today, there are a lot of results on aperiodic structures with pure point spectrum, whereas the structures with mixed spectrum and/or continuous spectrum are poorly understood. There are very few non-pure point examples where any detailed result is known about their spectra. Even results for single examples seem hard to achieve here. Results in this direction are obtained in [1, 3, 5, 7, 9].

SCD tilings are prominent classes of aperiodic tilings in $\mathbb{R}^3$. In [1] it was shown, that the diffraction spectrum of incommensurate SCD tilings is singular continuous apart from a central line. This was only the second example so far where rigorous results about the nature of non pure point spectra of deterministic aperiodic structures could be established.

In [3, 5] we aimed for a similar result for the Conway-Radin pinwheel tiling. This tiling is the most prominent instance of deterministic structures in the plane, where the tiles occur in infinitely many orientations. Several partial results are obtained in [3], in particular on the frequency module of the tiling, and a radial version of the Poisson summation formula. However, since there is evidence of the presence of absolutely continuous parts in the spectrum, this case seems harder than the SCD tilings.

Many results on the pinwheel tiling were generalised to all primitive substitution tilings with tiles in infinitely many orientations in [7, 9]. This includes the equidistribution of the orientations of the tiles (*statistical circular symmetry*), a kind of repetitivity (with respect to an appropriate topology of the tiling spaces), and circular symmetry of the diffraction spectrum, and hence purely singular spectrum (apart from 0).

1.4 Symmetries and colour symmetries

In the articles mentioned above the study of the symmetry of the structure under consideration is essential. In particular, these structures show statistical circular symmetry, which implies the perfect circular symmetry of the autocorrelation and thus of the diffraction spectrum. The articles [10, 11, 12, 13, 14] contain further results on possible symmetries of aperiodic structures. In [13] the possible symmetries of a large class of aperiodic hyperbolic structures ('Böröczky tilings') are classified. The importance of these structures lies in their universality: Böröczky's construction is the only one known today which yields deterministic hyperbolic tilings in any dimension.

The study of colour symmetries of crystallographic structures in Euclidean space is a classical topic, see for instance [SCHB]. It was kind of surprising that very few results are published on colour symmetries of regular hyperbolic structures. This inspired the papers [11, 12]. They give an enumeration of perfect colourings of regular hyperbolic tilings [12] and concrete realizations of some of them [11].

The possible symmetries of plane quasiperiodic tilings are well understood, compare for instance [HRB]. These symmetries can be well described in rings of cyclotomic integers. Thus the papers [10, 14] deal with colour symmetries of cyclotomic integers, yielding results on the algebraic strucutre of colour groups of perfect colourings of those.

Finally, [8] answered an open question raised in [FR]: In a tiling of $\mathbb{R}^d$ by convex polytopes, is there a point $x \in \mathbb{R}^d$ which is vertex of exactly one of the polytopes? The answer is negative for all dimensions d, when the tiling is locally finite. (Otherwise, counterexamples are easily constructed, see [8], Figure 1.)

2 Preliminaries

In the following we state some preliminaries. The closed ball of radius r centred in $x \in \mathbb{R}^d$ is denoted by $B_r(x)$. A *lattice* in $\mathbb{R}^d$ is the $\mathbb{Z}$-span of d linearly independent vectors in $\mathbb{R}^d$. More general, in any topological group G, a lattice is a discrete cocompact subgroup of G. By $\mathbb{H}^d$ we denote d-dimensional hyperbolic space. The closure of A is denoted by $\mathrm{cl}(A)$.

Let Λ be a point set in $\mathbb{R}^d$. In order to rule out some pathological cases, we require Λ to be a Delone set.

Definition A set $\Lambda \subset \mathbb{R}^d$ is a *Delone set*, if there are $R > r > 0$, such that

1. For all $x \in \mathbb{R}^d$, $B_R(x)$ contains at least one element of Λ (Λ is *relatively dense*), and
2. For all $x \in \mathbb{R}^d$, $B_r(x)$ contains at most one element of Λ (Λ is *uniformly discrete*).

Sometimes Delone sets are also called separated nets or (r,R)-sets. Each lattice in $\mathbb{R}^d$ is a Delone set. A Delone set Λ (more generally, any set Λ in $\mathbb{R}^d$) is called *aperiodic*, if $\Lambda = \Lambda + t$ implies $t = 0$. Otherwise, Λ is called periodic. Moreover, Λ is called *crystallographic*, if the set of translations fixing Λ is a lattice in $\mathbb{R}^d$. In particular, any lattice is crystallographic. Two important properties to describe highly ordered, but aperiodic, Delone sets are given in the following definition.

Definition Let $\Lambda \subset \mathbb{R}^d$ be a Delone set. Λ has *finite local complexity*, if for any $r > 0$, there are only finitely many translation classes of $B_r(x) \cap \Lambda$.
Λ is called *repetitive*, if for any $B_r(x) \cap \Lambda$ the set

$$\{y \,|\, B_r(y) \cap \Lambda \text{ is a translate of } B_r(x) \cap \Lambda\}$$

is relatively dense in $\mathbb{R}^d$.

Loosely speaking, finite local complexity means that there are only finitely many different local constellations fitting into a ball of radius r. Repetitivity means that a copy of each local constellation in Λ occurs 'everywhere' in Λ.

Note that one may define repetitivity alternatively with respect to congruence, rather than to translations. Whenever we want to emphasise which one is considered, we will write 'repetitive with respect to translation (respectively congruence)'. A third notion is stated in [7], see also Subsection 4.3.

2.1 Diffraction measures

By regarding each element of a Delone set Λ as an atomic position, Λ can serve as a model of some physical solid. Thus we may be interested in the diffraction image of Λ. In a physical experiment, this would be the outcome of an X-ray experiment, where the X-ray is scattered by Λ (respectively a large, but finite portion of Λ). In mathematics, the appropriate analogue of the diffraction image is the Fourier transform of the autocorrelation measure of Λ (see below, or [Hof] for details). In order to turn Λ into a measure — on which we can perform a Fourier transform — we assign to Λ its *Dirac comb*: Let δ_x denote the normed Dirac measure in x: $\delta_x(M) = 1$ if $x \in M$, and 0 else. The Dirac comb of Λ is

$$\delta_\Lambda = \sum_{x \in \Lambda} \delta_x,$$

Since Λ is a Delone set, δ_Λ is a translation bounded (positive) measure. The *autocorrelation measure* γ_Λ of Λ is the volume averaged convolution of δ_Λ with itself:

$$\gamma = \gamma_\Lambda = \lim_{r\to\infty} \frac{1}{\operatorname{vol} B_r(0)} \sum_{x,y\in\Lambda\cap B_r(0)} \delta_{x-y},$$

where the limit is taken in the vague topology. In general, it is not clear whether this limit exists. But since δ_Λ is translation bounded, there exists at least one convergent subsequence. So we consider each convergent subsequence, separately whenever we speak of the limit in the sequel. Now, the *diffraction measure* of Λ is the Fourier transform $\widehat{\gamma}_\Lambda$ of γ_Λ. Whenever it is convenient, we may use the framework of tempered distributions (see for instance [RUD], [SCHW]) to compute the Fourier transform of γ_Λ or its properties.

By construction, the autocorrelation measure is positive definite. Since the Fourier transform of a positive definite measure in $\mathbb{R}^d$ is again a positive measure in $\mathbb{R}^d$ [RS], the diffraction measure $\widehat{\gamma} = \widehat{\gamma}_\Lambda$ decomposes by Lebesgue's decomposition theorem uniquely into three parts, with respect to Lebesgue measure in $\mathbb{R}^d$:

$$\widehat{\gamma} = \widehat{\gamma}_{pp} + \widehat{\gamma}_{sc} + \widehat{\gamma}_{ac}.$$

Here, $\widehat{\gamma}_{ac}$ denotes an absolutely continuous measure (a measure which can be described by a density function, by the Radon-Nikodym theorem). $\widehat{\gamma}_{pp}$ denotes a pure point measure, that is, a countable sum of (weighted) Dirac measures. $\widehat{\gamma}_{sc}$ denotes a singular continuous measure. That is, $\widehat{\gamma}_{sc}$ vanishes on single points, but its support has Lebesgue measure zero.

A fundamental question in the theory of aperiodic order is:

What kind of matter diffracts?

In our framework, this asks for a classification of Delone sets according to their diffraction measure. For instance, one would like to find a necessary and sufficient condition on a Delone set having pure point diffraction (that is, the diffraction measure is a pure point measure), or purely continuous diffraction (that is, the pure point part vanishes apart from the origin). Today, a general answer is out of reach. One of the deepest results in this direction is Theorem 2.1 below. Two particular problems derived from the question above motivated the work under consideration: How to apply Theorem 2.1 efficiently? (That is, how to prove pure point spectrum efficiently.) And can we find Delone sets — deterministic ones, say — where we can prove rigorous results on their spectrum, if it is not pure point?

2.2 Model sets

A model set in general is given as follows: Let G, H be two locally compact Abelian groups, and let L be a lattice in $G \times H$. Let $W \subset H$ have nonempty interior and compact closure in H. Furthermore, let π_1 and π_2 be projections from $G \times H$ to G respectively H, such that $\pi_1|_L$ is injective, and $\pi_2(L)$ is dense in W. The following diagram may illustrate the situation.

$$\begin{array}{ccccc} G & \xleftarrow{\pi_1} & G\times H & \xrightarrow{\pi_2} & H \\ \cup & & \cup & & \cup \\ \Lambda & & L & & W \end{array} \tag{1}$$

Let Λ contain all $\pi_1(x)$, where $x \in L$, such that $\pi_2(x)$ is contained in W:

$$\Lambda = \{\pi_1(x) \,|\, x \in L, \pi_2(x) \in W\}.$$

Then Λ is called a *model set*. If, in addition to the conditions above, the boundary of W has Haar measure zero, then Λ is a *regular model set*.

Regular model sets share many properties with lattices: They are Delone sets, they have finite local complexity, they are usually repetitive, but in general they are aperiodic. The relevance of regular model sets in connection with diffraction measures is based on the following result by Hof [HOF] for $G \times H = \mathbb{R}^d$, and Schlottmann [SCHL] for the general case.

Theorem 2.1 *All regular model sets have pure point diffraction measure.*

This result can be used to show pure point diffraction for some given Delone set Λ by establishing that Λ is a regular model set. Many Delone sets are immediately seen not to be model sets, for instance random point sets, or more generally: any Delone set without finite local complexity. A vast number of appropriate candidates (deterministic, with finite local complexity, repetitive) are given by substitution tilings.

2.3 Substitution tilings and iterated function systems

Informally, a tile substitution is given by a finite number of *prototiles* (compact sets) $T_1, \dots, T_m$, an inflation factor $\lambda > 1$, and a rule how to dissect each inflated tile λT_i into tiles congruent to the prototiles $T_1, \dots, T_m$. Illustrations are given in Figures 1 and 2. The process of inflating and subdividing is called a *tile substitution*. The tile substitution σ can be repeated, starting with a single tile T_i. In each step we obtain a finite collection of non-overlapping tiles, the *supertiles* $\sigma^k(T_i)$. Any pattern occurring in such a supertile is called *legal* (with respect to σ). Any tiling of $\mathbb{R}^d$ — or more general, of some metric space — which contains only legal patterns, is called *substitution tiling* (with substitution σ). For a more formal definition see [2] or [7]. Tile substitutions are a simple and powerful method to generate a lot of aperiodic tilings. For a wealth of examples, see [FRH]. By assigning to each prototile some control point, one can easily derive a Delone set from a substitution tiling by considering the set of all control points, compare Figure 2. It is also possible to formulate substitutions for Delone sets. But for historical and illustrative reasons, one usually sticks to substitution tilings.

A tile substitution σ is *primitive*, if for each prototile T_i there is $k \geq 1$ such that $\sigma^k(T_i)$ contains copies of all prototiles $T_1, \dots, T_m$. Commonly, a tile substitution is required to be primitive in order to rule out pathological cases.

A formal definition of a tile substitution can be given by a digit set matrix. Let $\mathcal{D} = (\mathcal{D}_{ij})_{1 \leq i,j \leq m}$, where each entry $\mathcal{D}_{ij}$ is a finite (possibly empty) set of translation vectors. Using $\mathcal{D}$, we can write the tile substitution σ as

$$\sigma(T_j) = \bigcup_{1 \leq i \leq m} \bigcup_{t \in \mathcal{D}_{ij}} \{T_i + t\} \quad (1 \leq j \leq m).$$

Since σ is known to be a tile substitution, it follows

$$\lambda T_j = \bigcup_{T \in \sigma(T_j)} T = \bigcup_{1 \leq i \leq m} \bigcup_{t \in \mathcal{D}_{ij}} T_i + t \quad (1 \leq j \leq m), \tag{2}$$

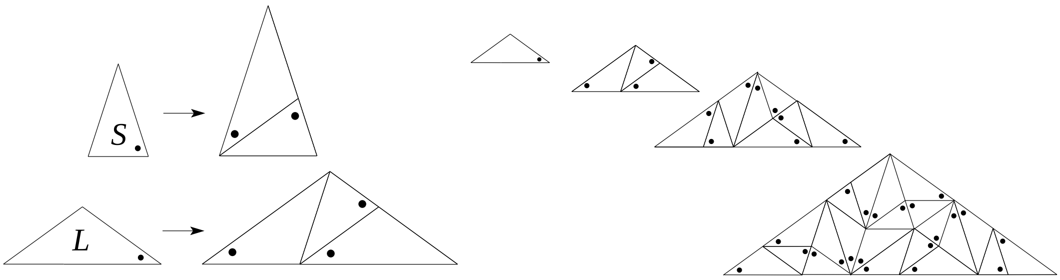

Figure 1: An example of a tile substitution with two prototiles S, L and inflation factor $\lambda = \frac{\sqrt{5}+1}{2}$ (left) and the first three iterations of the substitution on the prototile L (right). This substitution yields the famous Penrose tilings. The dots on the triangles indicate their orientation. They may also serve as control points in order to derive a Delone set from the tiling.

where the unions are non-overlapping. Since $\lambda > 1$, multiplication of the last equation by λ^{-1} yields a (multi-component) iterated function system. An *iterated function system* (IFS) with one component is an equation of the form

$$K = \bigcup_{1 \le i \le n} f_i(K),$$

where each f_i is a contraction. It is well known that each iterated function system possesses a unique nonempty compact solution [HUT]. This is also true for multi component IFS, see for instance [SI]. Thus the digit set matrix together with the substitution factor λ determines the prototiles uniquely.

It is a simple consequence of the Perron-Frobenius theorem that, for a primitive tile substitution, the digit set matrix determines the inflation factor uniquely. (To be precise: the leading eigenvalue of the matrix of the cardinalities in $\mathcal{D}$ is λ^d.) Thus the digit set matrix alone already determines the prototiles and the inflation factor. Let us list these facts in a comprehensive form.

- Each tile substitution σ can be defined by a digit set matrix $\mathcal{D}$.
- Such a digit set matrix defines an IFS, whose unique solutions are the prototiles of σ.
- If σ is primitive, $\mathcal{D}$ determines σ uniquely.

Note that sometimes substitutions are considered which do not fulfil (2). That is, the union of tiles in $\sigma(T_i)$ is not longer similar to T_i. We consider here *self-similar* substitutions only, that is, those which fulfil (2).

2.4 Symmetry

Let $(\mathbb{X}, d)$ be a metric space. An *isometry* is a map $f : \mathbb{X} \to \mathbb{X}$ where for all $x, y \in \mathbb{X}$: $d(x,y) = d(f(x), f(y))$. The symmetry group $S(X)$ of some set $X \subset \mathbb{X}$ is the group of all isometries f with $f(X) = X$.

By definition, an aperiodic tiling has no translational symmetry. But it may possess other symmetries. For instance, there are two Penrose tilings (out of uncountably many) showing fivefold dihedral symmetry [GSH]. Nevertheless, *all* Penrose tilings show statistical tenfold dihedral symmetry in the sense that each tile occurs in each of the ten possible orientations with the same frequency, roughly spoken. In the following, we have to assume that each tiling under consideration is well behaved in the sense that it looks locally alike everywhere. Formally, we require *uniform patch frequency* up to congruence, see [7], Section 6, Equation (4).

A precise definition of statistical symmetry needs some care and can be found in [9]. Two cases have to be distinguished: Either the tiles in a given tiling occur in finitely many orientations only, or in infinitely many orientations. In the first case, it makes sense to define the frequency $\mathrm{freq}(T_i, \alpha)$ of tiles of type T_i in orientation α (compare [9], equation (1)). The angles α where $\mathrm{freq}(T_i, \alpha)$ does not vanish allow the definition of statistical symmetry of the tiling under consideration.

It may sound surprising at a first glance that the second case — the tiles in the tiling occur in infinitely many orientations — actually occurs for deterministic tilings, say, for substitution tilings. References [5, 7, 9] contain a lot of examples where it occurs. In this case, all values $\mathrm{freq}(T_i, \alpha)$, defined as above, may vanish. Thus we define *statistical circular symmetry* by requiring that the orientations of the tiles in the tiling are equidistributed in $[0, 2\pi[$. For the full definition, see [9], or [7], Definition 3.2.

A further type of symmetry is colour symmetry. The study of colour symmetries of crystallographic patterns — like lattices — is a classical topic. For a thorough survey see [SCHB].

In brief words, a colour symmetry is the following: Let $\mathbb{X}$ be a metric space (in our case either $\mathbb{R}^d$ or $\mathbb{H}^d$) and X either a tiling or a point set in $\mathbb{X}$. To each element of X we assign an additional attribute, say, one of finitely many colours. Formally, this is described by a surjective map $c : X \to \{1, \ldots, k\}$. Let f be an isometry in $\mathbb{X}$ and π a permutation on k letters. The pair (f, π) is called a *colour symmetry* of X, if $c(f(x)) = \pi(c(x))$ for all $x \in X$. In plain words, f fixes the coloured object (X, c), up to a global permutation of colours. The set of all colour symmetries of (X, c) is called its *colour symmetry group* (or k-colour symmetry group, if the number of colours should be emphasised).

Applied to crystallographic Delone sets in $\mathbb{R}^d$, the concept of colour symmetry generalises the classification of crystallographic groups. For instance, it is a classical result that there are 17 distinct crystallographic groups in $\mathbb{R}^2$ (the 'wallpaper groups'). 'Distinct' means, that no two of them can be transformed into each other by an affine transformation. An analogue for colour groups is the result that there are 46 distinct crystallographic 2-colour symmetry groups in $\mathbb{R}^2$ and 23 distinct crystallographic 3-colour symmetry groups [GSH]. It is hard to judge who achieved these two results first, since there has been confusion about the meaning of 'distinct' for a long time, see [SCHB].

The work under consideration takes first steps beyond the framework described above, by studying colourings in the hyperbolic plane, and colourings of cyclotomic integers. Thereby it concentrates on the study of perfect colourings. A colouring is called *perfect*, if each symmetry of the uncoloured pattern X yields a colour symmetry.

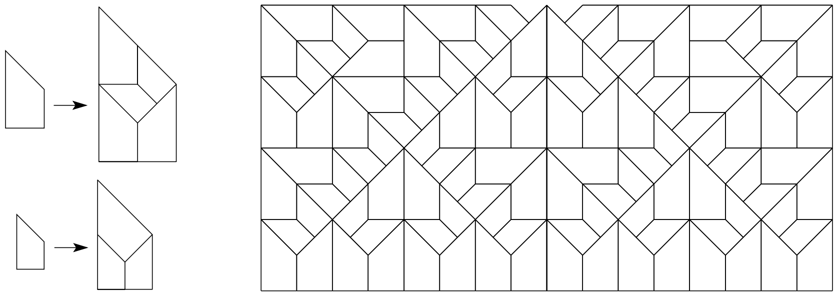

Figure 2: A tiling whose translation module is a lattice.

3 Pure point spectrum

3.1 Computing modular coincidences

Article [4]: An important class of aperiodic tilings, or aperiodic Delone sets, are lattice substitution systems (LSS). Historically, they arise from aperiodic substitution tilings whose translation module is a lattice. The translation module of a tiling $\mathcal{T}$ is the $\mathbb{Z}$-span of the difference set $\mathcal{D}_{\mathcal{T}}$ of $\mathcal{T}$:

$$\mathcal{D}_{\mathcal{T}} = \{x \,|\, \exists T, T' \in \mathcal{T} : T = T' + x\}.$$

Such a tiling is shown in Figure 2. It was first realized in [BMS] how to generate LSS as model sets by choosing H (compare (1)) as a ring of p-adic integers. In [LMS] this result has been generalised. In particular, it was shown that a lattice substitution system has pure point diffraction if *and only if* it is a regular model set. Moreover, an algorithm was derived which decides whether a given lattice substitution system consists of model sets. This algorithm used modular coincidences (see [LMS] or [4], Section 3). The drawback of this algorithm is the following: If the given LSS consists of model sets, it answers YES after finitely many steps, but the number of steps is a priori unknown. If the given LSS does not consist of model sets, the algorithm does not terminate.

In [4] we established the connection between modular coincidence and a generalisation of Dekking coincidence (see [DEK] or [4], Appendix A). Dekking coincidence can be applied to symbolic one-dimensional substitution sequences, and it is very simple to compute. By generalising Dekking coincidence to LSS in arbitrary dimension and establishing the equivalence with modular coincidence (Theorem 4.4), we were able to give an a priori upper bound on the number of steps of the algorithm discussed above (Theorem 4.5). Moreover, we obtained several simple conditions to decide whether a given LSS consists of model sets or not (Corollaries 4.6, 4.7, 4.9). By the results in [LMS], this answers also the question whether the given LSS has pure point diffraction or not. These conditions could be easily applied to most LSS in the literature. For instance, out methods enabled us to prove for the first time that the example in Figure 2 does not have pure point diffraction.

Article [4] was produced in close cooperation with Bernd Sing in Greifswald and Bielefeld. The main results were achieved together, and both authors contributed equally to the text.

3.2 Star-duality of model sets

Articles [2], [6], [15]: In his seminal paper [THU] Thurston noticed already in 1989 that a model set in $\mathbb{R}$ which possesses a substitution σ gives rise to an IFS in the internal space $H = \mathbb{R}^e$. The solution of this dual IFS is the window W. Moreover, this dual IFS defines a tile substitution in H. Thurston called this tile substitution the *Galois dual* of σ, since it could easily be expressed in terms of Galois conjugates of the data defining σ. This idea can be used to determine the model set property — and thus the pure point diffractivity — of a given substitution tiling. Note that for a given tiling, or the corresponding point set Λ, the construction of the lattice L and the internal space H (compare (1)) is standard, see [SI], or [6], Section 3, for a detailed discussion of the case of two prototiles. The IFS in H yields W. The problem is to show the following points:

- W has nonempty interior,
- the boundary of W has Haar measure zero, and
- Λ indeed consists of *all* projected points from $G \times W$ (maybe up to a zero set, this does not affect the pure point diffractivity).

Article [2] illustrates Thurston's Galois duality using certain one-dimensional tilings. Their Galois duals in $H = \mathbb{R}^2$ are obtained, and it is shown that these Galois dual tilings — respectively the set of their control points — are regular model sets, thus pure point diffractive. This is possible by the fact that the window of the Galois dual tilings lives in $G = \mathbb{R}$, and is just an interval. So the three points above can easily be checked. This idea can be employed further: whenever the solution of the dual IFS, that is, the window W, is a polytope, the three points are easily checked.

In [6], Galois duality is generalized to the case of non-Euclidean H. The key is the so called *star map*: In (1), the projection π_1 is invertible on $\pi_1(L)$. Thus we can define the map

$$\star : \pi_1(L) \to H, \quad x \mapsto x^\star = \pi_2 \pi_1^{-1}(x).$$

One benefit of the star map is that many facts can be stated in a simple manner. For instance, we obtain the identity $W = \mathrm{cl}(\Lambda^\star)$, where $\Lambda^\star = \{x^\star \,|\, x \in \Lambda\}$.

It turns out that — with the appropriate embedding of the lattice L, see the exemplary outline in [2], Equation (9) — the star map is the same as the Galois dual of Thurston, if $H = \mathbb{R}^e$. But using the star map generalises the notion of duality to arbitrary internal spaces H. With the help of the so defined star duality we can easily write down the IFS yielding the window in internal space H: If σ is given by a digit set matrix $\mathcal{D}$, the IFS in H is given just by $(\mathcal{D}^T)^\star$. This is outlined in [6], and applied to the two most famous substitution tilings: The Penrose tiling and the Ammann Beenker tiling. Since their windows are polytopes, the model set property of both examples is easily established. Note that this has been done before several times.

A new result is the following: As outlined in Subsection 2.3, the internal IFS, given by $(\mathcal{D}^T)^\star$, defines a dual substitution. In this way we obtain in [6] the dual substitution for the Penrose tiling (Theorem 3.1) — which has been done before with much more effort [BKSZ] — and the dual substitution for the Ammann Beenker tiling (Theorem 3.2), which apperas here for the first time.

In [6] the question is raised about self-dual substitutions with respect to star duality. A necessary condition and a sufficient condition are obtained for a substitution to be self-dual. A complete characterisation for one-dimensional substitutions with two prototiles is obtained in [15]. Theorem 6.3

lists four conditions which are equivalent for a substitution to be self-dual in this case. Furthermore, the equivalence of several notions of duality which occur in the literature is established in this special case (Theorem 5.7). In particular, a connection to automorphisms on the free group F_2 is established: an automorphism $\varphi \in \mathrm{Aut}(F_2)$ is conjugate to its inverse, up to permutation of letters, if and only if the corresponding substitution is a primitive substitution for a model set with connected window and $H = \mathbb{R}$ (Theorem 5.7 in connection with Theorem 1.1).

Both authors provided equally to article [15]. Sections 1, 2, 3 are provided by F., Section 4 is provided by V. Berthé, Sections 5 and 6 are provided by both authors.

4 Beyond pure point spectrum

4.1 SCD patterns have singular diffraction

Article [1]: Up today, for many Delone sets with pure point diffraction, the spectrum is known explicitly. In contrast, there are very few cases where anything is known about the continuous part in their diffraction. One exception is the diffraction of the Thue-Morse sequence, see [KAK], [BG2]. Its spectrum is singular continuous (plus some pure point part, depending on the scatter intensities), even though the closure of its support is the whole line.

Another Delone set where it was possible to prove results on the nature of the diffraction measure are SCD patterns. SCD pattern stands for the set of control points in an SCD tiling ('Schmitt-Conway-Danzer tiling'). SCD tilings are tilings in $\mathbb{R}^3$ by a single prototile. It is the only single prototile known so far which admits *only* aperiodic tilings. (There are several sets of two or more prototiles which allow only aperiodic tilings, in $\mathbb{R}^2$ or $\mathbb{R}^3$.) In particular, in any generic SCD tiling the tiles occur in infinitely many orientations.

In [1] we were able to show that the diffraction spectrum of SCD patterns do not have an absolutely continuous part (Theorem 2.1). In the generic case, the pure point part is contained on a single line ℓ, and the singular continuous part is supported on a set of concentric cylinders centred in ℓ (Theorem 2.5).

The proofs use explicit calculations within the framework of tempered distributions and utilise the fact that the autocorrelation measure of SCD patterns is invariant under arbitrary rotations about ℓ.

Both authors contributed equally to Article [1].

4.2 Pinwheel diffraction

Articles [3], [5]: After obtaining the results on the diffraction measure of SCD tilings, we turned to the most prominent instance of tilings with tiles in infinitely many orientations: the Conway-Radin pinwheel tiling of the plane [RAD]. It was known already that its autocorrelation measure is invariant under rotations about the origin (see [RAD], [MPS], or [3], Theorem 6) and consequently, the pure point part of its diffraction spectrum vanishes apart from the origin. As usual, we translated the pinwheel tiling into a point set Λ by assigning to each tile a control point (see for instance [3], Figure 5). In order to study the diffraction further, we determined the frequency module of the autocorrelation ([3], Claim 5) by determining the frequencies of the smallest constellation in the pinwheel tilings, namely, of its vertex stars. Frequency of a constellation C means the average number of congruent copies of C per unit area. The frequency module is the $\mathbb{Z}$-span of the frequencies of all 2-point constellations. The introduction of an alternative substitution rule for the pinwheel tiling (the kite-domino substitution, see [3], Figure 4) allowed for the determination of the frequency module.

Moreover, we obtained a radial analogue of Poisson's summation formula (Theorem 3). The motivation was to apply it to the autocorrelation of the pinwheel tiling. It turned out that it can be successfully applied to a simple model for powder diffraction. This is basically the union of copies of the integer lattice $\mathbb{Z}^2$, see [3], Proposition 5.

Regarding the diffraction of the pinwheel tiling, we were able to establish partial results only. However, our approach allowed for a numerical investigation of the diffraction with unmatched precision. Our results support the conjecture that the diffraction of the pinwheel tiling has a singular part, which is concentrated on concentric rings about the origin (similar to SCD patterns), but that it also has an absolutely continuous part, in contrast to SCD patterns.

Article [3] developed in strong cooperation of the first two authors. The first author provided more of the diffraction results, the second author provided more of the geometrical results. The third author provided the numerical results and most of the typesetting.

Article [5] gives a short report on the results of [3] with focus on physical implications. F.s contribution was mainly commentarial and in providing the results of [3].

4.3 Substitution tilings with statistical circular symmetry

Articles [7], [9]: The key in establishing singular spectrum for SCD patterns and pinwheel tilings was the circular symmetry of the autocorrelation. This circular symmetry in turn is the result of the statistical circular symmetry of SCD tilings and pinwheel tilings. In [7] it was shown that *all* primitive substitution tilings with tiles in infinitely many orientations are of statistical circular symmetry. Thus it is not possible for such tilings to have some 'preferred' orientations. Consequently, all of them have circular symmetric autocorrelation, and circular symmetric — hence purely continuous — diffraction spectrum.

Moreover, two infinite series of substitution tilings with statistical circular symmetry are given explicitly. This implies that circular statistical symmetry is not necessarily an exotic property for substitution tilings, but may be even a kind of generic case. Finally, it is shown that all such tilings possess a kind of repetitivity, namely, w-repetitivity ([7], Theorem 6.3). It is well known — and easy to see — that all primitive substitution tilings are repetitive with respect to congruence (compare Section 2). In contrast, no tiling of statistical circular symmetry is repetitive with respect to translations. However, there is a notion of repetitivity in between these two: A tiling, respectively its corresponding point set Λ, is *w-repetitive* (for wiggle-repetitive), if for any $r > 0, \varepsilon > 0$, for each $B_r(x) \cap \Lambda$ the set

$$\{y \,|\, B_r(y) \cap \Lambda \text{ is a translate of } B_r(x) \cap \Lambda, \text{ up to a rotation by } \alpha \leq \varepsilon\}$$

is uniformly dense. In plain words, there is $R > 0$ such that each ball of radius R contains a copy of $B_r(x) \cap \Lambda$, up to a rotation by less than ε. Theorem 6.3 in [7] establishes w-repetitivity for all primitive substitution tilings with statistical circular symmetry. The relevance of this result is that the dynamical system of the hull of a tiling (see [9], Section 4, and references there) is minimal if and only if the tiling is repetitive.

Article [9] gives an overview over most results of [7], provides the detailed proof how the circular symmetry of the diffraction measure follows from the statistical circular symmetry of the tiling

(Theorems 3.2, 3.3), and a result about equidistribution of orientations of tiles in tilings with finitely many orientations (Theorem 2.3). Cum grano salis, one may summarise these results as follows: in each primitive substitution tiling, each orientation accours with the same frequency. But compare the example in [9], Figure 1.

5 Symmetry groups and colour symmetry groups

5.1 Colour symmetries of cyclotomic integers

Articles [10], [14]: After the discovery of quasicrystals it seemed natural to ask for their colour symmetries, in analogy to colour symmetries of crystallographic structures. Many aperiodic structures in the plane with nontrivial symmetry (be it statistical or perfect) are based on cyclotomic integers $\mathcal{M}_n = \mathbb{Z}[e^{2\pi i/n}]$. For instance, the vertices of the famous Ammann-Beenker tilings of the plane form a subset of $\mathcal{M}_8$, compare [14], Figure 2. This leads to the study of colour symmetries of $\mathcal{M}_n$, which are — for $n = 5, n \geq 7$ — dense in the plane. A first step was the determination of the number of perfect colourings of cyclotomic integers with class number one [B], [BG1]. This topic is more combinatorial in nature. Based on their approach, we studied in [14] the algebraic properties of perfect colourings of $\mathcal{M}_n$ with class number one by identifying perfect colourings with ideals in $\mathcal{M}_n$. In particular, it was shown that all ideals in $\mathcal{M}_n$ yield chirally perfect colourings (Theorem 3.4), and that they are perfect depending on the factorisation of the generator q of the ideal. This breaks down beyond the (finitely many) class number one cases. Furthermore, we established results on the algebraic nature of the colour symmetry group H (Section 3) and of the colour preserving group K (Section 4). The algebraic structure of K was established for all but finitely many cases.

The second part of [10] is mainly based on the results in [14]. It discusses the cases $\mathcal{M}_5, \mathcal{M}_8$ and $\mathcal{M}_{12}$ in more detail. The first part of [10] studies point groups of lattices L which are suitable to generate model sets with symmetries which can be described in the framework of cyclotomic integers.

F. provided and wrote down essentially all results in [14], motivated by, and in discussion with, M.L.A.N. de las Peñas during her visit in Bielefeld. These results were presented in more detail in the second part of [10] for special cases, where F.s contribution was mainly to provide the more general results of [14].

5.2 Colour symmetries of regular hyperbolic tilings

Articles [11], [12]: As mentioned in Section 2, the study of colour symmetries in $\mathbb{R}^d$ has a long tradition. So it is kind of surprising that next to nothing is known about colour symmetries in $\mathbb{H}^d$. One of the first questions one may ask is: For which number k of colours does there exist a perfect colouring of a regular tiling in $\mathbb{H}^d$? Reference [12] answers this questions for small values of k, where small means approximately less than 30. This is achieved by identifying perfect colourings with left cosets in the symmetry group of the regular hyperbolic tiling by p-gons, where at each vertex q tiles intersect. This group is a Coxeter group

$$G_{p,q} = \langle a,b,c \,|\, a^2, b^2, c^2, (ab)^p, (bc)^q, (ac)^2 \rangle.$$

Now perfect colourings can be counted by counting subgroups of Coxeter groups, given by this finite presentation. Unfortunately, this is a problem which cannot be computed efficiently. This limits the number of colours to be considered to 30 to 50.

In a similar way, chirally perfect colourings can be counted. These are colourings which are perfect with respect to the direct symmetry group (the subgroup $\bar{G}_{p,q}$ of $G_{p,q}$ containing no reflections). This problem is even harder to compute, since the different subgroups of $\bar{G}_{p,q}$ has to be distinguished up to conjugacy in $G_{p,q}$. This limits the number of colours to be considered to less than 20 in some cases.

Article [11] gives some concrete realisations of colourings of regular hyperbolic tilings with 10 colours. In this article, the theoretical framework is due to F., where the concrete realisations were found by R. Lück.

5.3 Symmetries of aperiodic hyperbolic tilings

Article [13]: In 1974, K. Böröczky published a construction of tilings of $\mathbb{H}^2$ by a single prototile. This construction can be extended to any dimension, yielding tilings of $\mathbb{H}^d$. His aim was to show that there is no such natural notion of density in $\mathbb{H}^d$ as in Euclidean space $\mathbb{R}^d$. It was soon realized that his tilings are aperiodic, in the sense that their symmetry groups are not cocompact. (That is, they have no compact fundamental domain with respect to $\mathbb{H}^d$.)

In plain words, the construction goes as follows. Let us describe it for $\mathbb{H}^3$ first. (Compare also [13], Figure 2, for the case $\mathbb{H}^2$.) Consider a collection of concentric horospheres, where consecutive horospheres have equal distance. Each horosphere is conformal to the Euclidean plane $\mathbb{R}^2$. So consider a partition of each horosphere into the canonical tiling of $\mathbb{R}^2$ by unit squares. Erect on each square a prism, such that the top of the prism is made of four squares of the next layer. This yields a tiling of $\mathbb{H}^3$, where each tile carries four tiles on its top. Analogues are possible in any dimension.

The main result of [13] is the classification of all possible symmetry groups of Böröczky tilings in $\mathbb{H}^d$ (Theorem 6.1). It turns out that the symmetry group of a Böröczky tiling in $\mathbb{H}^{d+1}$ is either isomorphic to the symmetry group B_k of a k-dimensional cube ($k \le d$, possibly $k = 0$, thus trivial), or to the direct product $\mathbb{Z} \times B_k$. In particular, the symmetry group may be infinite, but never cocompact.

Analogues of this construction allow many further tilings of $\mathbb{H}^d$, for instance by embedding a plane Euclidean substitution tiling $\mathcal{T}$ on one horosphere, embedding the successors $\sigma(\mathcal{T}), \sigma^2(\mathcal{T}), \ldots$ in the horospheres above, and the predecessors $\sigma^{-1}(\mathcal{T}), \sigma^{-2}(\mathcal{T}), \ldots$ in the horospheres below. The results in [13] can be easily generalised to such tilings.

The article developed over five years in close cooperation of both authors, with some interruptions. Both authors contributed equally to it.

5.4 The lonely vertex problem

Article [8] falls slightly out of the scope of the work discussed above. It concerns a problem in classical convex geometry. Nevertheless, its motivation lies in local properties of tilings, and in establishing finite local complexity of certain substitution tilings.

The question is: In a locally finite tiling by convex polytopes in $\mathbb{R}^d$, is it possible that there is $x \in \mathbb{R}^d$ which is vertex of exactly one of the polytopes? (A tiling is locally finite, if each ball $B_r(x)$ intersects only finitely many tiles.) In other words, can there be a vertex of some polytope in the tiling which intersects no neighbouring polytope in a vertex? In [8] the answer is shown to be negative for all dimensions. A central result is Theorem 2.1. In plain words, it states that the indicator function of a convex spherical polytope without antipodal points (*A-type*) can not equal a finite linear combination of indicator functions of convex spherical polytopes which all contain antipodal points (*B-type*). From

Theorem 2.1 follows that the sphere cannot be partitioned into some B-type polytopes and exactly one A-type polytope (Theorem 2.4). Furthermore, this yields a negative answer to the question above (Theorem 2.5).

In addition, these results are used to show that each tile substitution, where the $\mathbb{Z}$-span of the vertices of the prototiles is a lattice, is of finite local complexity.

Both authors contributed equally to [8]. The problem itself was posed by F., the application to finite local complexity of tilings, too. However, the most fundamental result, Theorem 2.1, is due to A. Glazyrin.

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