DISCRETE TOMOGRAPHY OF F-TYPE ICOSAHEDRAL MODEL SETS

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Abstract. We address the problem of uniquely reconstructing F-type icosahedral quasicrystals from few images produced by quantitative high resolution transmission electron microscopy and explain recent results in the discrete tomography of these sets.

1. Introduction

Motivated by the request of materials science for the unique reconstruction of quasicrystalline structures from a small number of images produced by quantitative high resolution transmission electron microscopy (HRTEM), the discrete tomography (DT) of F-type icosahedral model sets is concerned with the inverse problem of uniquely reconstructing finite patches of these aperiodic point sets from their (discrete parallel) X-rays in several directions. As for the discrete analogue of parallel X-rays in computerized tomography (CT), the X-ray of a finite subset of Euclidean 3-space in a certain direction assigns to each line parallel to this direction the number of points of the set on this line. In fact, for some crystals the technique QUANTITEM (QUantitative ANALysis of The Information from Transmission Electron Microscopy) can approximately measure the number of atoms lying on lines parallel to directions that guarantee HRTEM images of high resolution, i.e., yield dense lines in the crystal; cf. [15, 17]. Therefore, the classical setting of DT deals with the corresponding inverse problem for (periodic) lattices; cf. [12, 9, 10, 11]. Since F-type icosahedral model sets are commonly regarded as good mathematical models for many icosahedral quasicrystals [8] and since it is reasonable to expect that future developments in technology will extend the technique QUANTITEM to classes of quasicrystals, we feel that it is about time to explain recent results in the DT of these sets in a manner that is easily accessible for practitioners. In particular, special emphasis is put on illustrating the problems that arise in the DT of aperiodic model sets. For detailed proofs and related results, we refer the interested reader to [4, 5, 13, 14].

2. F-type icosahedral model sets

We denote the golden ratio by $\tau$, i.e., $\tau = (1 + \sqrt{5})/2$. Note that $\tau$ is a root of $X^2 - X - 1 \in \mathbb{Z}[X]$, whence it is an algebraic integer of degree 2 over $\mathbb{Q}$. The unique non-trivial Galois automorphism of the real quadratic number field $\mathbb{Q}(\tau) = \mathbb{Q}(\sqrt{5}) = \mathbb{Q} \oplus \mathbb{Q}\tau$, determined by $\sqrt{5} \mapsto -\sqrt{5}$, will be denoted by $'$, hence $\tau' = 1 - \tau$. Throughout this text, elements of Euclidean 3-space will be written as row vectors. The standard face-centred icosahedral module of quasicrystallography is given by

$$\mathcal{M}_F := \mathbb{Z}[\tau](2, 0, 0) \oplus \mathbb{Z}[\tau](\tau + 1, \tau, 1) \oplus \mathbb{Z}[\tau](0, 0, 2),$$

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where $\mathbb{Z}[\tau] = \mathbb{Z} \oplus \mathbb{Z} \tau$ is the ring of integers in $\mathbb{Q}(\tau)$; cf. [2, 7]. Clearly, $\mathcal{M}_F$ is a free $\mathbb{Z}[\tau]$-module of rank 3 that spans all of $\mathbb{R}^3$. In particular, it is a free $\mathbb{Z}$-module of rank 6. Moreover, $\mathcal{M}_F$ has full icosahedral symmetry, i.e., it is invariant under the action of the rotation group $Y$ of the regular icosahedron centred at the origin $0 \in \mathbb{R}^3$ with orientation such that each coordinate axis passes through the mid-point of an edge, thus coinciding with 2-fold axes of the icosahedron. Due to the connection with the icosian ring, we prefer to use the scaled version $L := \frac{1}{2} \mathcal{M}_F \subset \mathbb{Q}(\tau)^3$ instead of $\mathcal{M}_F$ itself; cf. [7] and references therein.

**Definition 2.1.** Let the map $^* : L \rightarrow \mathbb{R}^3$ be defined by applying the Galois conjugation $'$ coordinatewise. Given a subset $W \subset \mathbb{R}^3$ with $\emptyset \neq W^\circ \subset W \subset \overline{W^\circ}$ and $\overline{W^\circ}$ compact, and any $t \in \mathbb{R}^3$, we obtain an $F$-type icosahedral model set $\Lambda(t, W)$ by setting

$$\Lambda(t, W) := t + \{ \alpha \in L \mid \alpha^* \in W \}$$

The map $^* : L \rightarrow \mathbb{R}^3$ is the so-called star map of $\Lambda(t, W)$ and $W$ is referred to as the window of $\Lambda(t, W)$. The model set $\Lambda(t, W)$ is called generic if it satisfies $\partial W \cap L^* = \emptyset$. Moreover, it is called regular if the boundary $\partial W$ has Lebesgue measure 0 in $\mathbb{R}^3$. For a window $W \subset \mathbb{R}^3$, we denote by $\mathcal{I}_g^F(W)$ the set of generic $F$-type icosahedral model sets with a window of the form $s + W$, where $s \in \mathbb{R}^3$.

We refer the reader to [14] for the corresponding cut and project scheme and to [16, 6] for related general settings and background. $F$-type icosahedral model sets $\Lambda$ are aperiodic Delone subsets of 3-space. Moreover, if $\Lambda$ is regular, then $\Lambda$ is pure point diffractive. If $\Lambda$ is both generic and regular, and, if a suitable translate of its window has the full icosahedral
symmetry of $L^*$, then $\Lambda$ has full icosahedral symmetry in the sense of symmetries of LI-classes, meaning that a discrete structure has a certain symmetry if the original and the transformed structure are locally indistinguishable; cf. [3, 14] and references therein for details.

**Example 2.2.** For a generic regular F-type icosahedral model set with full icosahedral symmetry, consider $\Lambda := \Lambda(0, s + W)$, where $s := 10^{-3}(1, 1, 1)$ and $W$ is the regular icosahedron centred at the origin $0 \in \mathbb{R}^3$ with orientation such that $(\tau', 0, 1)$ and $(-\tau', 0, 1)$ belong to its vertices; see Figure 1 for an illustration.

3. Complexity

The fundamental notion in DT is the following.

**Definition 3.1.** Let $F$ be a finite subset of $\mathbb{R}^3$, let $u \in S^2$ be a direction, and let $\mathcal{L}_u$ be the set of lines in direction $u$ in $\mathbb{R}^3$. The (discrete parallel) X-ray of $F$ in direction $u$ is the function $X_u F : \mathcal{L}_u \to \mathbb{N}_0 := \mathbb{N} \cup \{0\}$, defined by

$$X_u F(\ell) := \text{card}(F \cap \ell) = \sum_{x \in \ell} 1_F(x).$$

Moreover, the support $(X_u F)^{-1}(\mathbb{N})$ of $X_u F$, i.e., the (finite) set of lines in $\mathcal{L}_u$ which pass through at least one point of $F$, is denoted by $\text{supp}(X_u F)$. Further, we denote by $\mathcal{L}^L_u$ the subset of $\mathcal{L}_u$ consisting of all lines in $\mathcal{L}_u$ which pass through at least one point of $L$.

Let $U \subset S^2$ be a finite set of pairwise non-parallel directions and let $F$ be a finite subset of $\mathbb{R}^3$. Clearly, $F$ is contained in its grid with respect to the X-rays in the directions of $U$ given by

$$G^F_U := \bigcap_{u \in U} \left( \bigcup_{\ell \in \text{supp}(X_u F)} \ell \right).$$
Figure 3. The grid $G$ that is generated by the slice $S$ from Figure 2 with respect to two $L^{(\tau,0,1)}$-directions with slopes 0 and $\tan(2\pi/5)$, respectively.

In fact, if there are more directions in $U$ than elements in $F$, one even has $F = G^F_U$; cf. [14, Proposition 5.3]. Since after about 3 to 5 images taken by HR TEM, typical (quasi)crystalline probes may be damaged or even destroyed by the radiation energy, this result is meaningless in practice. Consequently, one has to deal with grids that are much bigger than their generating finite sets; see Figure 3 for an illustration in the plane. In fact, for a finite subset $F$ of a fixed F-type icosahedral model set, its grid can contain points of a different translate of $L$ than $F$ itself; see [4, Figure 5] for illustrations of this phenomenon in the case of planar sets. As mentioned in the introduction, only directions that yield dense lines in a fixed F-type icosahedral model set $\Lambda$ are reasonable in view of applications in practice. Therefore, we may restrict ourselves to $\Lambda$-directions, i.e., directions parallel to non-zero interpoint vectors of $\Lambda$. It turns out that the set of $\Lambda$-directions is exactly the set of $L$-directions (defined analogously) for any F-type icosahedral model set $\Lambda$; cf. [14, Proposition 3.20].

Definition 3.2 (Reconstruction Problem). Let $W \subset \mathbb{R}^3$ be a window and let $u_1, \ldots, u_m \in S^2$ be $m \geq 2$ pairwise non-parallel $L$-directions. The corresponding reconstruction problem is defined as follows.

Reconstruction.
Given functions $p_{u_j} : \mathcal{L}_{u_j} \rightarrow \mathbb{N}_0$, $j \in \{1, \ldots, m\}$, whose supports are finite and satisfy $\text{supp}(p_{u_j}) \subset \mathcal{L}_{u_j}^L$, decide whether there exists a finite subset $F$ of an element of $\mathcal{I}^F_g(W)$ that satisfies $X_{u_j}F = p_{u_j}$, $j \in \{1, \ldots, m\}$, and, if so, construct one such $F$.

In the case of planar lattices and two lattice directions, the above reconstruction problem clearly is intimately related with the problem of reconstructing 0-1-matrices from their row and column sums. Though, for aperiodic model sets the problem is much more involved due to the complication with the window. Below, an $L$-direction will be called an $L^{(\tau,0,1)}$-direction if it lies in the hyperplane orthogonal to $(\tau,0,1)$, the latter representing a 5-fold axis of the icosahedral symmetry of $L$. Observing first that generic F-type icosahedral model sets can be sliced orthogonal to $(\tau,0,1)$ into (planar) cyclotomic model sets that are based on the
The image $G^\star$ of the grid $G$ from Figure 3 under the star map together with $S^\star$ and the corresponding decagonal window already shown in Figure 2. Note that the star map naturally extends to $\mathbb{Q}(\tau)^3$ which contains the grid $G$. Although the star map may change the directions and the relative position of parallel lines, the marginal sums are being preserved. In fact, $G^\star$ is the grid generated by $S^\star$ with respect to the directions that have slopes 0 and $\tan(2\pi/10)$, respectively. The reconstruction task is to find a subset of $G^\star$ that lies in a translate of $L^\star$, fits the marginal sums and lies in a suitable translate of the interior of the window.

Theorem 3.3. [14, Theorem 4.3] When restricted to two $L^{(\tau,0,1)}$-directions and polyhedral windows, the problem RECONSTRUCTION can be solved in polynomial time in the real RAM-model of computation.

Remark 3.4. For a detailed analysis of the complexities of the reconstruction problem in the case of B-type icosahedral model sets, we refer the reader to [13, Chapter 3]. Note that even in the case of planar lattices and the Turing machine as the model of computation the corresponding reconstruction problem is NP-hard for three or more lattice directions (defined analogous to $\Lambda$-directions); cf. [10]. Therefore, it seems to be rather obvious that one cannot expect a generalization of Theorem 3.3 to the case of three or more $L$-directions.

4. Uniqueness

In general, the above reconstruction problem can possess rather different solutions. Therefore, one is led to the investigation of the uniqueness problem of finding a small number of suitably prescribed $L$-directions that eliminate these non-uniqueness phenomena.

Definition 4.1. Let $\mathcal{E}$ be a collection of finite subsets of $\mathbb{R}^3$ and let $U \subset \mathbb{S}^2$ be a finite set of directions. We say that $\mathcal{E}$ is determined by the $X$-rays in the directions of $U$ if different elements of $\mathcal{E}$ cannot have the same $X$-rays in the directions of $U$.

Below, a finite subset $C$ of a Delone set $\Lambda \subset \mathbb{R}^3$ is called a convex subset of $\Lambda$ if it satisfies the equation $C = \text{conv}(C) \cap \Lambda$; cf. [9] for the lattice case. The set of all convex subsets of
Λ will be denoted by $\mathcal{C}(\Lambda)$. Using the slicing of F-type icosahedral model sets into certain cyclotomic model sets again, one obtains the following fundamental result.

**Theorem 4.2.** [14, Theorem 5.12]

(a) There is a set $U \subset S^2$ of four pairwise non-parallel $L^{(\tau,0,1)}$-directions such that, for all generic F-type icosahedral model sets $\Lambda$, the set $\mathcal{C}(\Lambda)$ is determined by the X-rays in the directions of $U$.

(b) For all generic F-type icosahedral model sets $\Lambda$ and all sets $U \subset S^2$ of three or less pairwise non-parallel $L^{(\tau,0,1)}$-directions, the set $\mathcal{C}(\Lambda)$ is not determined by the X-rays in the directions of $U$.

In fact, for a generic F-type icosahedral model set $\Lambda$, the set $\mathcal{C}(\Lambda)$ is determined by the X-rays in the directions of any set $U$ of four pairwise non-parallel $L^{(\tau,0,1)}$-directions with the property that there is no $U$-polygon in $\Lambda$; cf. [13]. Here, for a set $U$ of $L^{(\tau,0,1)}$-directions, a $U$-polygon in $\Lambda$ is a planar non-degenerate convex polygon $P$ with all its vertices in $\Lambda$ such that any line in $\mathbb{R}^3$ that is parallel to a direction of $U$ and passes through a vertex of $P$ also meets another vertex of $P$. It turns out that one can choose four pairwise non-parallel $L^{(\tau,0,1)}$-directions which provide uniqueness and yield dense lines in F-type icosahedral model sets; cf. [14, Example 5.13 and Remark 5.14] for examples and details. Moreover, there are even four pairwise non-parallel $L^{(\tau,0,1)}$-directions which provide uniqueness, yield dense lines in F-type icosahedral model and have the property that, in an approximative sense, for any fixed window $W \subset \mathbb{R}^3$ whose boundary $\partial W$ has Lebesgue measure 0 in $\mathbb{R}^3$, the set $\bigcup_{\Lambda \in \mathcal{I}_F} \mathcal{C}(\Lambda)$ is determined by the corresponding X-rays; cf. [14] for details. This setting, which we already used in the definition of the reconstruction problem, is highly relevant in practice of quantitative HR TEM because it reflects the fact that, due to the icosahedral symmetry of genuine F-type icosahedral quasicrystals, the determination of the rotational orientation of a quasicrystalline probe in an electron microscope can rather easily be achieved in the diffraction mode. Though, in general, the X-ray images taken in the high-resolution mode do not allow us to locate the examined sets. Therefore, as already explained in [4, 14], in order to prove practically relevant and rigorous results, one has to deal with the whole local indistinguishability class of a regular, generic F-type icosahedral model set $\Lambda$, rather than dealing with a single fixed one.

5. **Outlook**

Although the presented results answer some of the basic problems of DT of F-type icosahedral model sets, there is still a lot to do to create a tool that is as satisfactory for the application in materials science as is CT in its medical or other applications. Foremost, this is due to the fact that there is always some noise involved when physical measurements are taken, whereas the results in this text can only be applied when exact data is given. Therefore, it is necessary to study stability and instability results in DT of F-type icosahedral model sets in the future [1].

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References

[1] Alpers, A.; Gritzmann, P.: On stability, error correction, and noise compensation in discrete tomography. SIAM J. Discrete Math. 20 (2006) 227–239.

[2] Baake, M.: Solution of the coincidence problem in dimensions $d \leq 4$. In: R. V. Moody (Ed.): The Mathematics of Long-Range Aperiodic Order. NATO-ASI Series C 489. Kluwer, Dordrecht (1997), pp. 9–44.; revised version arXiv:math/0605222v1 [math.MG]

[3] Baake, M.: A guide to mathematical quasicrystals. In: Suck, J.-B.; Schreiber, M.; Häussler, P. (Eds.): Quasicrystals. An Introduction to Structure, Physical Properties, and Applications. Springer, Berlin (2002), pp. 17–48. arXiv:math-ph/9901014v1

[4] Baake, M.; Gritzmann, P.; Huck, C.; Langfeld, B.; Lord, K.: Discrete tomography of planar model sets. Acta Cryst. A62 (2006) 419–433; arXiv:math/0609393v1 [math.MG]

[5] Baake, M.; Huck, C.: Discrete tomography of Penrose model sets. Philos. Mag. 87 (2007) 2839–2846; arXiv:math-ph/0610056v1

[6] Baake, M.; Moody, R. V. (Eds.): Directions in Mathematical Quasicrystals. CRM Monograph Series, vol. 13, AMS, Providence, RI (2000).

[7] Baake, M.; Pleasants, P. A. B.; Rehmann, U.: Coincidence site modules in 3-space. Discr. Comput. Geom. 38 (2006) 111–138; arXiv:math/0609793v1 [math.MG]

[8] de Boissieu, M.; Guyot, P.; Audier, M.: Quasicrystals: quasicrystalline order, atomic structure and phase transitions. In: Hippert, F.; Gratias, D. (Eds.): Lectures on Quasicrystals. EDP Sciences, Les Ulis (1994), pp. 1–152.

[9] Gardner, R. J.; Gritzmann, P.: Discrete tomography: determination of finite sets by X-rays. Trans. Amer. Math. Soc. 349 (1997) 2271–2295.

[10] Gardner, R. J., Gritzmann, P., Prangenberg, D.: On the computational complexity of reconstructing lattice sets from their X-rays. Discrete Math. 202 (1999) 45–71.

[11] Gritzmann, P.: On the reconstruction of finite lattice sets from their X-rays. In: E. Ahronovitz; C. Fiorio (Eds.): Lecture Notes on Computer Science, pp. 19–32. Springer, London (1997).

[12] Herman, G. T.; Kuba, A. (Eds.): Discrete Tomography: Foundations, Algorithms, and Applications. Birkhäuser, Boston (1999).

[13] Huck, C.: Discrete Tomography of Delone Sets with Long-Range Order. PhD Thesis (Universität Bielefeld), Logos Verlag, Berlin (2007).

[14] Huck, C.: Discrete tomography of icosahedral model sets. Submitted. arXiv:0706.3005v2 [math.MG]

[15] Kisielowski, C.; Schwander, P.; Baumann, F. H.; Seibt, M.; Kim, Y.; Ourmazd, A.: An approach to quantitative high-resolution transmission electron microscopy of crystalline materials. Ultramicroscopy 58 (1995) 131–155.

[16] Moody, R. V.: Model sets: a survey. In: Axel, F.; Dénoyer, F.; Gazeau, J.-P. (Eds.): From Quasicrystals to More Complex Systems. EDP Sciences, Les Ulis, and Springer, Berlin (2000), pp. 145–166. arXiv:math/0002020v1 [math.MG]

[17] Schwander, P.; Kisielowski, C.; Seibt, M.; Baumann, F. H.; Kim, Y.; Ourmazd, A.: Mapping projected potential, interfacial roughness, and composition in general crystalline solids by quantitative transmission electron microscopy. Phys. Rev. Lett. 71 (1993) 4150–4153.

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