

Discrete tomography of icosahedral model sets

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The discrete tomography of mathematical quasicrystals with icosahedral symmetry is investigated, placing emphasis on reconstruction and uniqueness problems. The work is motivated by the requirement in materials science for the unique reconstruction of the structures of icosahedral quasicrystals from a small number of images produced by quantitative high-resolution transmission electron microscopy.

1. Introduction

Discrete tomography (DT) is concerned with the inverse problem of retrieving information about some finite object from (generally noisy) information about its slices; see the book by Herman & Kuba (1999). A typical example is the *reconstruction* of a finite point set in Euclidean 3-space from its line sums in a small number of coplanar directions [see Fishburn *et al.* (1997), Gardner & Gritzmann (1999) and Gardner *et al.* (1999)]. More precisely, a (discrete parallel) X-ray of a finite subset of \mathbb{R}^3 in direction u is the corresponding line sum function, *i.e.* it gives the number of points of the set on each line in \mathbb{R}^3 parallel to u . This concept should not be confused with X-rays in diffraction theory, which provide rather different information on the underlying structure that is based on statistical pair correlations [see Cowley (1995), Fewster (2003) and Guinier (1994)]. The interest in the DT of *aperiodic model sets* is mainly motivated by the requirement in materials science for the unique reconstruction of quasicrystals from their images under quantitative high-resolution transmission electron microscopy (HRTEM) in a small number of high-density directions, *i.e.* directions that yield densely occupied lines in the quasicrystalline structure. For a gentle introduction to the DT of aperiodic model sets including an extended bibliography, we refer the reader to Baake, Gritzmann, Huck *et al.* (2006).

In the present paper, we consider icosahedral model sets in 3-space, which are commonly regarded as good mathematical models for many icosahedral quasicrystals in nature like the aluminium alloys AlMn and AlCuFe; see de Boissieu *et al.* (1994) for further examples. It will be crucial for our approach that generic icosahedral model sets can be sliced into certain planar cyclotomic model sets (Proposition 3.11), whose DT we have studied earlier [see Baake, Gritzmann, Huck *et al.* (2006) and Huck (2007*a,b*)].

Using the above slicing and the results from Baake, Gritzmann, Huck *et al.* (2006), it was shown in Huck (2007*b*) that the algorithmic problem of reconstructing finite subsets of generic icosahedral model sets Λ with polyhedral windows given X-rays in two nonparallel Λ -directions that are parallel to the slices can be solved in polynomial time in the real random access machine (RAM) model of computation (Theorem 4.3). Here, a Λ -direction is parallel to a nonzero interpoint vector of Λ . Since this reconstruction problem can possess rather different solutions, we also study the *uniqueness problem* of finding a small number of suitably prescribed Λ -directions that eliminate these non-uniqueness phenomena [see Gardner & Gritzmann (1997, 1999), Fishburn *et al.* (1991) and Fishburn & Shepp (1999)]. More precisely, a subset \mathcal{E} of the set of all finite subsets of a fixed icosahedral model set Λ is said to be determined by the X-rays in a finite set U of directions if different sets in \mathcal{E} cannot have the same X-rays in the directions of U . Since any fixed finite number of X-rays in Λ -directions is insufficient to determine the entire class of finite subsets of a fixed icosahedral model set Λ by Proposition 5.1, it is necessary to impose some restriction in order to obtain positive uniqueness results. For our main uniqueness result, we consider the natural class of convex subsets of a fixed icosahedral model set Λ . They are bounded sets $C \subset \Lambda$ whose convex hulls contain no new points of Λ . Here, by using the above slicing and the results from Huck (2007*a,b*), it is shown that there are four pairwise nonparallel Λ -directions that are parallel to the slices such that the set of convex subsets of any icosahedral model set Λ are determined by their X-rays in these directions (Theorem 5.8). In fact, it turns out that one can even choose four Λ -directions which provide uniqueness and yield dense lines in icosahedral model sets, the latter making this result look promising in view of real applications (Example 5.9 and Remark 5.10). Finally, we demonstrate that, in an approximate sense, the last result extends to the far more general and relevant situation, where one deals with a whole family of generic icosahedral model sets at the same

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time, rather than dealing with a single fixed icosahedral model set.

2. Preliminaries and notation

We denote the norm in Euclidean d -space \mathbb{R}^d by $\|\cdot\|$. The unit sphere in \mathbb{R}^d is denoted by \mathbb{S}^{d-1} , i.e. $\mathbb{S}^{d-1} = \{x \in \mathbb{R}^d \mid \|x\| = 1\}$. Moreover, the elements of \mathbb{S}^{d-1} are also called *directions*. For $r > 0$ and $x \in \mathbb{R}^d$, $B_r(x)$ is the open ball of radius r about x . Recall that a homothety $h : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is given by $x \mapsto \lambda x + t$, where $\lambda \in \mathbb{R}$ is positive and $t \in \mathbb{R}^d$. For a subset $S \subset \mathbb{R}^d$, $k \in \mathbb{N}$ and $R > 0$, we denote by $\text{card}(S)$, $\mathcal{F}(S)$, $\mathcal{F}_{\leq k}(S)$, $\text{int}(S)$, $\text{cl}(S)$, $\text{bd}(S)$, $\text{conv}(S)$ and $\mathbb{1}_S$ the cardinality, the set of finite subsets, the set of finite subsets of S having cardinality less than or equal to k , the interior, the closure, the boundary, the convex hull and the characteristic function of S , respectively. The *centroid* of an element $F \in \mathcal{F}(\mathbb{R}^d)$ is defined as $(\sum_{x \in F} x) / \text{card}(F)$. A direction $u \in \mathbb{S}^{d-1}$ is called an *S-direction* if it is parallel to a nonzero element of the difference set $S - S$ of S . Throughout this text, elements of \mathbb{R}^d will be written as row vectors. For a nonzero element v of \mathbb{R}^d , we denote by v^\perp the hyperplane in \mathbb{R}^d orthogonal to v .

Definition 2.1. Let $d \in \mathbb{N}$ and let $F \in \mathcal{F}(\mathbb{R}^d)$. Furthermore, let $u \in \mathbb{S}^{d-1}$ be a direction and let \mathcal{L}_u^d be the set of lines in direction u in \mathbb{R}^d . Then, the (*discrete parallel*) *X-ray of F in direction u* is the function $X_u F : \mathcal{L}_u^d \rightarrow \mathbb{N}_0 := \mathbb{N} \cup \{0\}$, defined by

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

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

Lemma 2.2. [Lemmas 5.1 and 5.4 of Gardner & Gritzmann (1997).] Let $d \in \mathbb{N}$ and let $u \in \mathbb{S}^{d-1}$ be a direction. For all $F, \tilde{F} \in \mathcal{F}(\mathbb{R}^d)$, one has:

- (a) $X_u F = X_u \tilde{F}$ implies $\text{card}(F) = \text{card}(\tilde{F})$;
- (b) If $X_u F = X_u \tilde{F}$, the centroids of F and \tilde{F} lie on the same line parallel to u .

Definition 2.3. Let $d \geq 2$, let $U \subset \mathbb{S}^{d-1}$ be a finite set of pairwise nonparallel directions, and let $F \in \mathcal{F}(\mathbb{R}^d)$. We define the *grid of F with respect to the X-rays in the directions of U* as

$$G_U^F := \bigcap_{u \in U} \left(\bigcup_{\ell \in \text{supp}(X_u F)} \ell \right).$$

We refer the reader to Fig. 5 of Baake, Gritzmann, Huck *et al.* (2006) and Figs. 3 and 4 of Huck (2008) for illustrations of grids of planar finite sets with respect to two X-rays in nonparallel directions. The following property follows immediately from the definition of grids.

Lemma 2.4. Let $d \geq 2$. If $U \subset \mathbb{S}^{d-1}$ is a finite set of pairwise nonparallel directions, then for all $F, \tilde{F} \in \mathcal{F}(\mathbb{R}^d)$, one has

$$(X_u F = X_u \tilde{F} \ \forall u \in U) \implies F, \tilde{F} \subset G_U^F = G_U^{\tilde{F}}.$$

Definition 2.5. Let $d \geq 2$, let $\mathcal{E} \subset \mathcal{F}(\mathbb{R}^d)$, and let $m \in \mathbb{N}$. Further, let $U \subset \mathbb{S}^{d-1}$ be a finite set of directions. We say that \mathcal{E} is *determined by the X-rays in the directions of U* if, for all $F, \tilde{F} \in \mathcal{E}$, one has

$$(X_u F = X_u \tilde{F} \ \forall u \in U) \implies F = \tilde{F}.$$

Definition 2.6. Let $d \in \mathbb{N}$ and let $S \subset \mathbb{R}^d$. A bounded subset C of S is called a *convex subset of S* if it satisfies the equation $C = \text{conv}(C) \cap S$. Moreover, the set of all convex subsets of S is denoted by $\mathcal{C}(S)$.

3. Icosahedral versus cyclotomic model sets

We shall always denote the golden ratio by τ , i.e. $\tau = [1 + (5)^{1/2}]/2$. Moreover, by \cdot' we will denote the unique nontrivial Galois automorphism of the real quadratic number field $\mathbb{Q}(\tau) = \mathbb{Q}(5^{1/2}) = \mathbb{Q} \oplus \mathbb{Q}\tau$ (determined by $5^{1/2} \mapsto -5^{1/2}$), whence $\tau' = -1/\tau = 1 - \tau$. Note that τ is an algebraic integer of degree 2 over \mathbb{Q} (a root of $X^2 - X - 1 \in \mathbb{Z}[X]$). Moreover, $\mathbb{Z}[\tau] = \mathbb{Z} \oplus \mathbb{Z}\tau$ is the ring of integers in $\mathbb{Q}(\tau)$; cf. Hardy & Wright (1979).

Consider the following scaled (by $\frac{1}{2}$) versions of the standard body-centred and face-centred icosahedral modules \mathcal{M}_B and \mathcal{M}_F of quasicrystallography, defined as

$$L_B := \mathbb{Z}[\tau](0, 1, 0) \oplus \mathbb{Z}[\tau]_{\frac{1}{2}}(-1, -\tau', \tau) \oplus \mathbb{Z}[\tau]_{\frac{1}{2}}(1, 1, 1)$$

and

$$L_F := \mathbb{Z}[\tau](0, 1, 0) \oplus \mathbb{Z}[\tau]_{\frac{1}{2}}(-1, -\tau', \tau) \oplus \mathbb{Z}[\tau](1, 0, 0),$$

respectively; cf. Baake (1997) and Baake, Pleasants & Rehmman (2006), and references therein. The icosahedral modules are well known objects to crystallographers, as they appear in the indexing of Bragg peaks in icosahedral structures. For the connection with the icosian ring, see Chen *et al.* (1998), Moody (2000) and Moody & Patera (1993). Obviously, both L_B and its subgroup L_F (of index 4) are free $\mathbb{Z}[\tau]$ -modules of rank 3, and are hence free \mathbb{Z} -modules of rank 6. Moreover, both modules have icosahedral symmetry, i.e. they are invariant under the action of the group Y_h of 120 symmetries of the regular icosahedron centred at the origin $0 \in \mathbb{R}^3$ with orientation such that each coordinate axis passes through the midpoint of an edge, thus coinciding with twofold axes of the icosahedron. By definition, model sets arise from so-called cut and project schemes [see Baake & Moody (2000) and Moody (2000) for general background material, and Baake (2002) for a gentle introduction]. In the case of Euclidean internal spaces, these are commutative diagrams of the

following form, where π and π_{int} denote the canonical projections; cf. Moody (2000).

$$\begin{array}{ccccc} \mathbb{R}^d & \xleftarrow{\pi} & \mathbb{R}^d \times \mathbb{R}^m & \xrightarrow{\pi_{\text{int}}} & \mathbb{R}^m \\ \cup & & \cup_{\text{lattice}} & & \cup_{\text{dense}} \\ L & \xleftrightarrow{1-1} & \tilde{L} & \longrightarrow & L^* \end{array} \quad (1)$$

Here, \tilde{L} is a lattice in $\mathbb{R}^d \times \mathbb{R}^m$. Further, we assume that the restriction $\pi|_{\tilde{L}}$ is injective and that the image $\pi_{\text{int}}(\tilde{L})$ is a dense subset of \mathbb{R}^m . Letting $L := \pi(\tilde{L})$, the bijectivity of the (co-)restriction $\pi|_{\tilde{L}}$ allows us to define a map $\cdot^*: L \rightarrow \mathbb{R}^m$ by $\alpha^* := \pi_{\text{int}}((\pi|_{\tilde{L}})^{-1}(\alpha))$. Then, one has $L^* = \pi_{\text{int}}(\tilde{L})$ and, further, $\tilde{L} = \{(l, l^*) \mid l \in L\}$.

Definition 3.1. Given a subset $W \subset \mathbb{R}^m$ with $\emptyset \neq \text{int}(W) \subset W \subset \text{cl}(\text{int}(W))$ and $\text{cl}(\text{int}(W))$ compact, a so-called *window*, and any $t \in \mathbb{R}^d$, we obtain a *model set*

$$\Lambda(t, W) := t + \Lambda(W)$$

relative to the above cut and project scheme [equation (1)] by setting

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

Moreover, \mathbb{R}^d (respectively \mathbb{R}^m) is called the *physical* (respectively *internal*) space. The map $\cdot^*: L \rightarrow \mathbb{R}^m$, as defined above, is called the *star map* of $\Lambda(t, W)$, W is referred to as the *window* of $\Lambda(t, W)$ and L is called the *underlying \mathbb{Z} -module* of $\Lambda(t, W)$. The model set $\Lambda(t, W)$ is called *generic* if it satisfies $\text{bd}(W) \cap L^* = \emptyset$. Moreover, it is called *regular* if the boundary $\text{bd}(W)$ has Lebesgue measure 0 in \mathbb{R}^m .

We refer the reader to Moody (2000) for details and general properties of model sets, and to Baake & Moody (2000) for general background. In the following, we assume that the reader is acquainted with the basic terminology of model sets as presented in Moody (2000). Clearly, every translate of a window is again a window. From now on, L will always denote one of the icosahedral modules above.

Definition 3.2. *Icosahedral model sets* $\Lambda_{\text{ico}}^L(t, W)$ with underlying \mathbb{Z} -module L arise from the cut and project scheme [equation (1)] by choosing the star map $\cdot^*: L \rightarrow \mathbb{R}^3$ to be the \mathbb{Q} -linear monomorphism of Abelian groups that is given by applying the Galois conjugation \cdot' coordinatewise. We further denote by \mathcal{I}_g^L the set of generic icosahedral model sets with underlying \mathbb{Z} -module L . Additionally, for a window $W \subset \mathbb{R}^3$, we set

$$\mathcal{I}_g^L(W) := \{\Lambda_{\text{ico}}^L(t, s + W) \mid t, s \in \mathbb{R}^3\} \cap \mathcal{I}_g^L.$$

We refer the reader to Moody (2000) and Pleasants (2000) for details and related general settings. Both in the B-type and the F-type case, we shall denote by \cdot^{-*} the inverse of the co-restriction of the corresponding star map $\cdot^*: L \rightarrow L^*$ to its image. The images of both maps $\tilde{\cdot}: L \rightarrow \mathbb{R}^3 \times \mathbb{R}^3$, defined by $\alpha \mapsto (\alpha, \alpha^*)$, are indeed lattices in $\mathbb{R}^3 \times \mathbb{R}^3$. In fact, the terminology originates from the fact that these images have a natural interpretation as a body-centred lattice in 6-space (a

weight lattice of type D_6^*) in the B-type case and as a face-centred lattice in 6-space (a root lattice of type D_6) in the F-type case; see Chen *et al.* (1998) and Conway & Sloane (1999) for background. Finally, one can easily verify that, in any case, the image L^* is a dense subset of \mathbb{R}^3 .

Remark 3.3. Let Λ be an icosahedral model set with underlying \mathbb{Z} -module L and window W . Then Λ is an aperiodic Meyer set. In particular, it is an aperiodic Delone set of finite local complexity. Moreover, if Λ is regular, then Λ is pure point diffractive, *i.e.* the Fourier transform of the auto-correlation density that arises by placing a delta peak (point mass) on each point of Λ looks purely point-like; cf. Schlottmann (2000). If Λ is both generic and regular, and if a suitable translate of the window W has the full icosahedral symmetry of L^* , then Λ also has this 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 (LI) (*i.e.* up to translation, every finite patch in Λ also appears in any of the other elements of its LI-class and *vice versa*); see Baake (2002) for details. Typical examples are balls and suitably oriented versions of the icosahedron, the dodecahedron, the rhombic triacontahedron (the latter also known as Kepler’s body) and its dual, the icosidodecahedron.

Example 3.4. A generic regular B-type icosahedral model set with full icosahedral symmetry Y_h is given by $\Lambda_{\text{ico}}^L := \Lambda_{\text{ico}}^L(0, s + W)$, where L is the body-centred icosahedral module from above, $s := 10^{-3}(1, 1, 1)$ and W is the regular icosahedron centred at the origin with orientation such that $(\tau', 0, 1)$ and $(-\tau', 0, 1)$ belong to its set of vertices; see Fig. 1 for an illustration.

From now on, we always let $\zeta_5 := e^{2\pi i/5}$, as a specific choice of a primitive fifth root of unity in \mathbb{C} . Occasionally, we identify \mathbb{C} with \mathbb{R}^2 . It is well known that the fifth cyclotomic field $\mathbb{Q}(\zeta_5)$ is an algebraic number field of degree 4 over \mathbb{Q} . Moreover, the field extension $\mathbb{Q}(\zeta_5)/\mathbb{Q}$ is a Galois extension with Abelian Galois group $G(\mathbb{Q}(\zeta_5)/\mathbb{Q}) \simeq (\mathbb{Z}/5\mathbb{Z})^\times$, where $a \pmod{5}$ corresponds to the automorphism given by $\zeta_5 \mapsto \zeta_5^a$; cf. Theorem 2.5 of Washington (1997). Note that, restricted to the quadratic field $\mathbb{Q}(\tau)$, both the Galois automorphism of $\mathbb{Q}(\zeta_5)/\mathbb{Q}$ that is given by $\zeta_5 \mapsto \zeta_5^3$ and its complex conjugate automorphism (*i.e.* the automorphism given by $\zeta_5 \mapsto \zeta_5^2$) induce the unique nontrivial Galois automorphism \cdot' of $\mathbb{Q}(\tau)/\mathbb{Q}$ (determined by $\tau \mapsto 1 - \tau$). Further, $\mathcal{O}_5 := \mathbb{Z}[\zeta_5]$ is the ring of integers in $\mathbb{Q}(\zeta_5)$; cf. Theorem 2.6 of Washington (1997). The ring \mathcal{O}_5 also is a $\mathbb{Z}[\tau]$ -module of rank two, *i.e.* one has $\mathcal{O}_5 = \mathbb{Z}[\tau] \oplus \mathbb{Z}[\tau]\zeta_5$; cf. Lemma 1(a) of Baake, Gritzmam, Huck *et al.* (2006). Since ζ_5^3 is another primitive fifth root of unity in \mathbb{C} , one also has $\mathcal{O}_5 = \mathbb{Z}[\tau] \oplus \mathbb{Z}[\tau]\zeta_5^3$. Note that both nontrivial Galois automorphisms of $\mathbb{Q}(\zeta_5)/\mathbb{Q}$ mentioned above map \mathcal{O}_5 into itself.

Definition 3.5. *Cyclotomic model sets* $\Lambda_{\text{cyc}}^5(t, W)$ with underlying \mathbb{Z} -module \mathcal{O}_5 arise from the cut and project scheme [equation (1)] by choosing the star map $\cdot^*: \mathcal{O}_5 \rightarrow \mathbb{R}^2$ to be

either the nontrivial Galois automorphism of $\mathbb{Q}(\zeta_5)/\mathbb{Q}$, defined by $\zeta_5 \mapsto \zeta_5^3$, or its complex conjugate automorphism.

We refer the reader to Baake, Gritzmam, Huck *et al.* (2006) for a proof that this definition leads indeed to a cut and project scheme.

Example 3.6. For illustrations of cyclotomic model sets with underlying \mathbb{Z} -module \mathcal{O}_5 , see Fig. 2(a) and Fig. 3; cf. Proposition 3.11 and Example 3.12 below.

We shall now demonstrate that icosahedral model sets Λ can be sliced into cyclotomic model sets with underlying

\mathbb{Z} -module \mathcal{O}_5 , where the slices are intersections of Λ with translates of the hyperplane $H := (\tau, 0, 1)^\perp$ and are thus orthogonal to a fivefold axis of the icosahedral symmetry of L . We further set $H' := (\tau', 0, 1)^\perp$. The following result is immediate.

Lemma 3.7. The following equations hold:

- (a) $L \cap H = \mathbb{Z}[\tau](0, 1, 0) \oplus \mathbb{Z}[\tau]^{\frac{1}{2}}(-1, -\tau', \tau)$;
- (b) $(L \cap H)^* = L^* \cap H'$.

Definition 3.8. We denote by Φ the \mathbb{R} -linear isomorphism $\Phi: H \rightarrow \mathbb{C}$, determined by $(0, 1, 0) \mapsto 1$ and $\frac{1}{2}(-1, -\tau', \tau) \mapsto \zeta_5$. Further, Φ^* will denote the \mathbb{R} -linear isomorphism $\Phi^*: H' \rightarrow \mathbb{C}$, determined by $(0, 1, 0) \mapsto 1$ and $\frac{1}{2}(-1, -\tau, \tau') \mapsto \zeta_5^3$.

Lemma 3.9. The maps Φ and Φ^* are isometries of Euclidean vector spaces, where H, H' and \mathbb{C} are regarded as two-dimensional Euclidean vector spaces in the canonical way. Moreover, identifying \mathbb{C} with the xy plane in \mathbb{R}^3 , Φ and Φ^* extend uniquely to direct rigid motions of \mathbb{R}^3 , i.e. elements of the group $SO(3, \mathbb{R})$.

Proof. The first assertion follows from the following identities:

$$\begin{aligned} \|r(0, 1, 0) + s\frac{1}{2}(-1, -\tau', \tau)\| &= |r + s\zeta_5| = (r^2 + s^2 - rs\tau')^{1/2}, \\ \|r(0, 1, 0) + s\frac{1}{2}(-1, -\tau, \tau')\| &= |r + s\zeta_5^3| = (r^2 + s^2 - rs\tau)^{1/2}. \end{aligned}$$

The additional statement is immediate.

Lemma 3.10. Via restriction, the maps Φ and Φ^* induce isomorphisms of rank-two $\mathbb{Z}[\tau]$ -modules:

$$L \cap H \xrightarrow{\Phi} \mathcal{O}_5 \xleftarrow{\Phi^*} L^* \cap H'.$$

Proof. This follows from the definition of Φ and Φ^* together with Lemma 3.7.

Proposition 3.11. Let Λ be a generic icosahedral model set with underlying \mathbb{Z} -module L , say $\Lambda = \Lambda_{\text{ico}}^L(t, W)$. Then, for every $\lambda \in \Lambda$, one has the identity

$$\Phi((\Lambda \cap (\lambda + H)) - \lambda) = \{z \in \mathcal{O}_5 \mid z^{*5} \in W_\lambda\},$$

where *5 is the Galois automorphism of $\mathbb{Q}(\zeta_5)/\mathbb{Q}$, defined by $\zeta_5 \mapsto \zeta_5^3$, and

$$W_\lambda := \Phi^*((W \cap ((\lambda - t)^* + H')) - (\lambda - t)^*).$$

Thus, the sets of the form

$$\Phi((\Lambda \cap (\lambda + H)) - \lambda),$$

where $\lambda \in \Lambda$, are cyclotomic model sets with underlying \mathbb{Z} -module \mathcal{O}_5 .

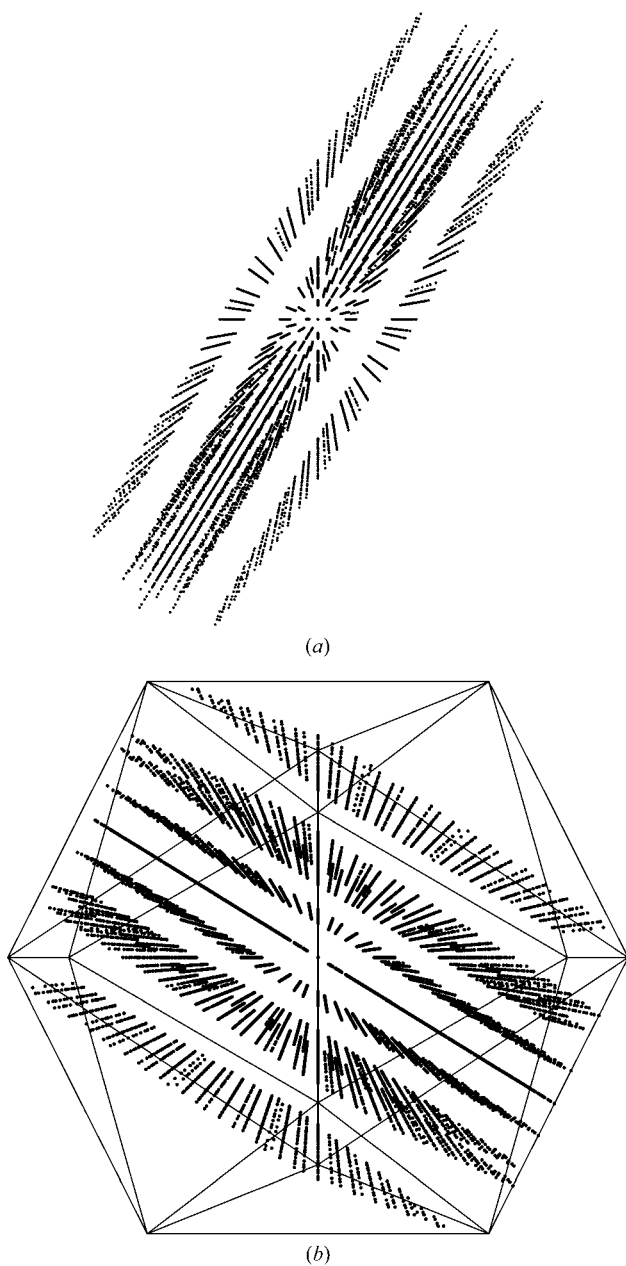


Figure 1
(a) A few slices of a patch of the icosahedral model set Λ_{ico}^L and (b) their * -images inside the icosahedral window in the internal space, both seen from the positive x axis.

Proof. First, consider $\Phi(\mu)$, where $\mu \in (\Lambda \cap (\lambda + H)) - \lambda$. It follows that $\mu \in L \cap H$ and $(\mu + (\lambda - t))^* = \mu^* + (\lambda - t)^* \in W$. Using Lemmas 3.7 and 3.10, one can now verify that

$$\Phi(\mu)^{*s} = \Phi^*(\mu^*) \in W_\lambda.$$

Conversely, suppose that $z \in \mathcal{O}_5$ satisfies $z^{*s} \in W_\lambda$. Since $z^{*s} \in \mathcal{O}_5$, Lemmas 3.9 and 3.10 show that there is a unique $\mu \in L^* \cap H'$ with $z^{*s} = \Phi^*(\mu)$ and $\mu + (\lambda - t)^* \in W$. One can now verify that $\mu^{-*} \in (\Lambda \cap (\lambda + H)) - \lambda$ and $\Phi(\mu^{-*}) = z$. This proves the claimed identity. The assertion follows.

Example 3.12. For an illustration of the content of Proposition 3.11 in the case of the icosahedral model set Λ_{ico}^L from Example 3.4, see Figs. 2 and 3.

We shall now establish a relation between icosahedral model sets and their underlying \mathbb{Z} -modules. We denote by m_τ the $\mathbb{Z}[\tau]$ -module endomorphism of $\mathbb{Q}(\tau)^3$, given by multiplication by τ , i.e. $\alpha \mapsto \tau\alpha$. Furthermore, we denote by m_τ^* the $\mathbb{Z}[\tau]$ -module endomorphism of $(\mathbb{Q}(\tau)^3)^*$, given by $\alpha^* \mapsto (\tau\alpha)^*$.

Lemma 3.13. The map m_τ^* is contractive with contraction constant $1/\tau \in (0, 1)$, i.e. the equality $\|m_\tau^*(\alpha^*)\| = (1/\tau) \|\alpha^*\|$ holds for all $\alpha \in \mathbb{Q}(\tau)^3$.

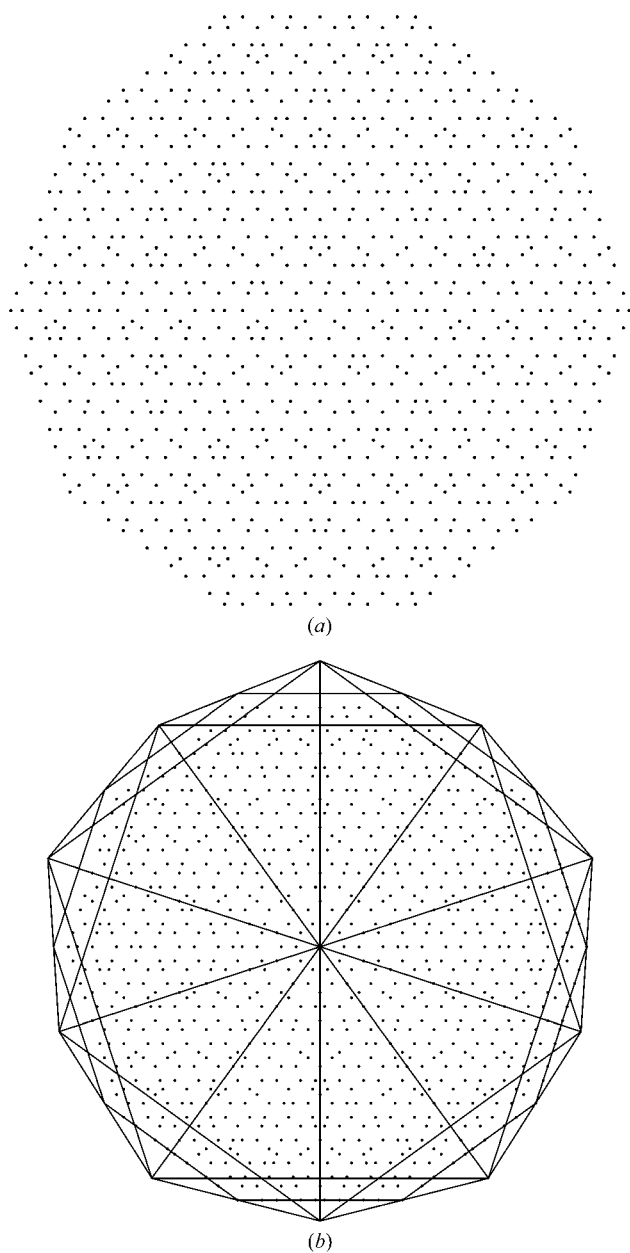


Figure 2
(a) The central slice of the patch of Λ_{ico}^L from Fig. 1 and (b) its *s -image inside the (marked) decagon $(s + W) \cap H'$. Views (a) and (b) are seen from perpendicular viewpoints.

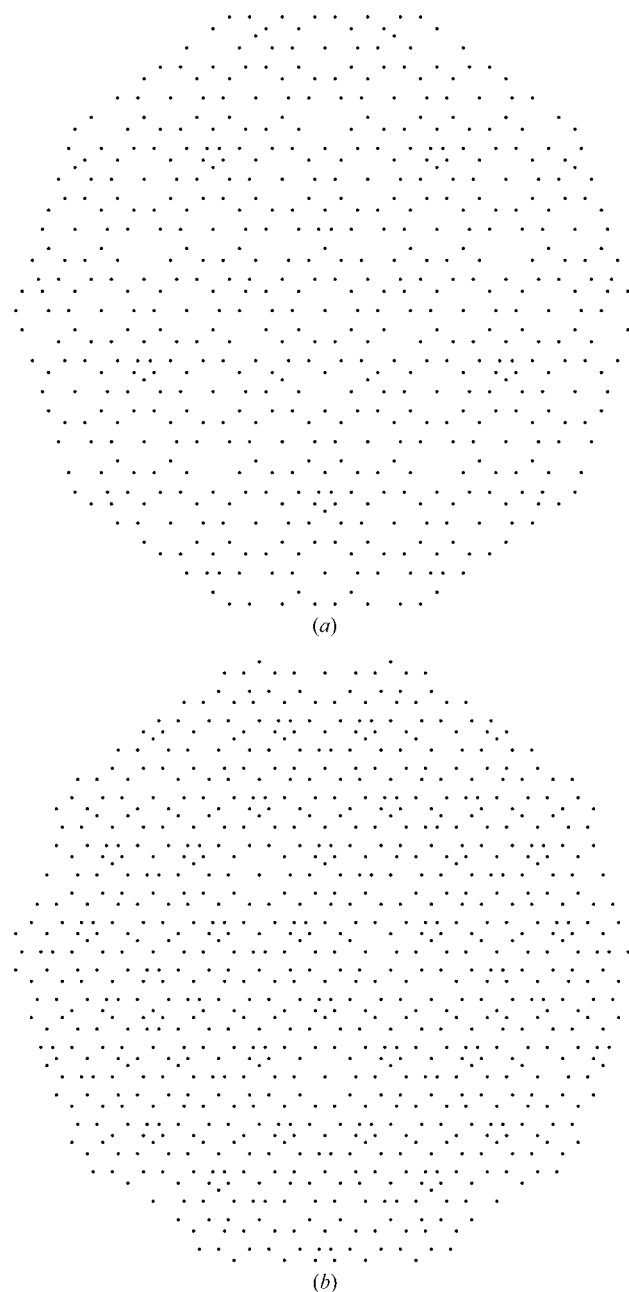


Figure 3
Another two slices of the patch of Λ_{ico}^L from Fig. 1. Views (a) and (b) are seen from perpendicular viewpoints.

Proof. For $\alpha \in \mathbb{Q}(\tau)^3$, observe that $\|m_\tau^*(\alpha^*)\| = \|(\tau\alpha)^*\| = \|\tau'\alpha^*\| = (1/\tau) \|\alpha^*\|$.

Lemma 3.14. Let Λ be an icosahedral model set with underlying \mathbb{Z} -module L , say $\Lambda = \Lambda_{\text{ico}}^L(t, W)$. Then, for any $F \in \mathcal{F}(L)$, there is a homothety $h: \mathbb{R}^3 \rightarrow \mathbb{R}^3$ such that $h(F) \subset \Lambda$.

Proof. From $\text{int}(W) \neq \emptyset$ and the denseness of L^* in \mathbb{R}^3 , one gets the existence of a suitable $\alpha_0 \in L$ with $\alpha_0^* \in \text{int}(W)$. Consider the open neighbourhood $V := \text{int}(W) - \alpha_0^*$ of 0 in \mathbb{R}^3 . Since the map m_τ^* is contractive by Lemma 3.13 (in the sense which was made precise in that lemma), the existence of a suitable $k \in \mathbb{N}$ is implied such that $(m_\tau^*)^k(F^*) \subset V$. Hence, one has $\{(\tau^k\alpha + \alpha_0)^* \mid \alpha \in F\} \subset \text{int}(W) \subset W$ and, further, $h(F) \subset \Lambda$, where $h: \mathbb{R}^3 \rightarrow \mathbb{R}^3$ is the homothety given by $x \mapsto \tau^k x + (\alpha_0 + t)$.

As an easy application of Lemma 3.14, one obtains the following result on the set of Λ -directions for icosahedral model sets Λ , which we shall use without further discussion.

Proposition 3.15. Let Λ be an icosahedral model set with underlying \mathbb{Z} -module L . Then, the set of Λ -directions is precisely the set of L -directions.

Proof. Since one has $\Lambda - \Lambda \subset L$, every Λ -direction is an L -direction. For the converse, let $u \in \mathbb{S}^2$ be an L -direction, say parallel to $\alpha \in L \setminus \{0\}$. By Lemma 3.14, there is a homothety $h: \mathbb{R}^3 \rightarrow \mathbb{R}^3$ such that $h(\{0, \alpha\}) \subset \Lambda$. It follows that $h(\alpha) - h(0) \in (\Lambda - \Lambda) \setminus \{0\}$. Since $h(\alpha) - h(0)$ is parallel to α , the assertion follows.

By similar arguments to those above, one can show the following relative of the last result.

Proposition 3.16. Let Λ be a cyclotomic model set with underlying \mathbb{Z} -module \mathcal{O}_5 . Then, the set of Λ -directions is precisely the set of \mathcal{O}_5 -directions.

4. Complexity

In the practice of quantitative HRTEM, the determination of the rotational orientation of a quasicrystalline probe in an electron microscope can rather easily be achieved in the diffraction mode. This is due to the icosahedral symmetry of genuine icosahedral quasicrystals. However, the X-ray images taken in the high-resolution mode do not allow us to locate the examined sets. Therefore, as already pointed out in Baake, Gritzmans, Huck *et al.* (2006), in order to prove practically relevant and rigorous results, one has to deal with the *non-anchored case* of the whole LI class $\text{LI}(\Lambda)$ of a regular, generic icosahedral model set Λ , rather than dealing with the *anchored case* of a single fixed icosahedral model set Λ ; recall Remark 3.3 for the equivalence relation given by local indistinguishability and see also Gritzmans & Langfeld (2008).

Remark 4.1. The LI class of a lattice M in \mathbb{R}^3 simply consists of all translates of M in \mathbb{R}^3 . In particular, $\text{LI}(M)$ simply consists of

one translation class. The entire LI class $\text{LI}(\Lambda_{\text{ico}}^L(t, W))$ of a regular, generic icosahedral model set $\Lambda_{\text{ico}}^L(t, W)$ can be shown to consist of all generic icosahedral model sets of the form $\Lambda_{\text{ico}}^L(t, s + W)$ and all patterns obtained as limits of sequences of generic icosahedral model sets of the form $\Lambda_{\text{ico}}^L(t, s + W)$ in the local topology (LT). Here, two patterns are ε -close if, after a translation by a distance of at most ε , they agree on a ball of radius $1/\varepsilon$ around the origin; see Baake (2002) and Schlottmann (2000). Each such limit is then a subset of some $\Lambda_{\text{ico}}^L(t, s + W)$, but s might not be in a generic position. Note that the LI class $\text{LI}(\Lambda)$ of an icosahedral model set Λ contains uncountably many (more precisely, 2^{\aleph_0}) translation classes; cf. Baake (2002) and references therein.

In view of the complication described above, we must make sure that we deal with finite subsets of generic icosahedral model sets of the form $\Lambda_{\text{ico}}^L(t, s + W)$, *i.e.* subsets whose \cdot^* -image lies in the interior of the window. This restriction to the generic case is the proper analogue of the restriction to perfect lattices and their translates in the crystallographic case. Analogous to the lattice case (Gardner & Gritzmans, 1999; Gardner *et al.*, 1999) and the case of cyclotomic model sets (Baake, Gritzmans, Huck *et al.*, 2006), the main algorithmic problems of the DT of icosahedral model sets are as follows.

Definition 4.2. (Consistency, Reconstruction and Uniqueness problems). Let $W \subset \mathbb{R}^3$ be a window, and let $u_1, \dots, u_m \in \mathbb{S}^2$ be $m \geq 2$ pairwise nonparallel L -directions. The corresponding consistency, reconstruction and uniqueness problems are defined as follows.

CONSISTENCY. Given functions $p_{u_j}: \mathcal{L}_{u_j}^3 \rightarrow \mathbb{N}_0$, $j \in \{1, \dots, m\}$, whose supports are finite and satisfy $\text{supp}(p_{u_j}) \subset \mathcal{L}_{u_j}^L$, decide whether there is a finite set F which is contained in an element of $\mathcal{I}_g^L(W)$ and satisfies $X_{u_j}F = p_{u_j}$, $j \in \{1, \dots, m\}$.

RECONSTRUCTION. Given functions $p_{u_j}: \mathcal{L}_{u_j}^3 \rightarrow \mathbb{N}_0$, $j \in \{1, \dots, m\}$, 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 $\mathcal{I}_g^L(W)$ that satisfies $X_{u_j}F = p_{u_j}$, $j \in \{1, \dots, m\}$, and, if so, construct one such F .

UNIQUENESS. Given a finite subset F of an element of $\mathcal{I}_g^L(W)$, decide whether there is a different finite set \tilde{F} that is also a subset of an element of $\mathcal{I}_g^L(W)$ and satisfies $X_{u_j}F = X_{u_j}\tilde{F}$, $j \in \{1, \dots, m\}$.

One has the following tractability result, which was proved for the case of B-type icosahedral model sets by combining the results from the last section with those presented in Baake, Gritzmans, Huck *et al.* (2006); cf. Theorem 3.33 of Huck (2007b) for the details. The proof for the F-type case is similar. For the sake of brevity, we prefer to omit the straightforward details here. Below, L -directions that lie in H will be called L^H -directions.

Theorem 4.3. When restricted to two L^H -directions and polyhedral windows, the problems CONSISTENCY, RECON-

STRUCTION and UNIQUENESS as defined above can be solved in polynomial time in the real RAM model of computation.

For a detailed analysis of the complexities of the above algorithmic problems in the B-type case, we refer the reader to ch. 3 of Huck (2007b). Note that even in the anchored planar lattice case \mathbb{Z}^2 (and the Turing machine as the model of computation) the corresponding problems CONSISTENCY, RECONSTRUCTION and UNIQUENESS are NP-hard for three or more \mathbb{Z}^2 -directions (Gardner & Gritzmann, 1999; Gardner *et al.*, 1999). Therefore, it seems to be rather obvious that one cannot expect a generalization of Theorem 4.3 to three or more L^H -directions.

5. Uniqueness

We start off with some uniqueness results which only deal with the anchored case of determining finite subsets of a fixed icosahedral model set Λ by X-rays in L -directions. The following negative result follows from Proposition 3.1 of Huck (2009).

Proposition 5.1. Let Λ be an icosahedral model set with underlying \mathbb{Z} -module L and let $U \subset \mathbb{S}^2$ be an arbitrary but fixed finite set of pairwise nonparallel L -directions. Then $\mathcal{F}(\Lambda)$ is not determined by the X-rays in the directions of U .

The first positive result follows immediately from Fact 3.3 of Huck (2009).

Proposition 5.2. Let Λ be an icosahedral model set with underlying \mathbb{Z} -module L . Further, let $U \subset \mathbb{S}^2$ be any set of $k + 1$ pairwise nonparallel L -directions, where $k \in \mathbb{N}_0$. Then, $\mathcal{F}_{\leq k}(\Lambda)$ is determined by the X-rays in the directions of U . Moreover, for all $F \in \mathcal{F}_{\leq k}(\Lambda)$, one has $G_U^F = F$.

Since icosahedral model sets have finite local complexity, the following result is a direct consequence of Proposition 3.5 of Huck (2009); cf. Remark 3.3.

Proposition 5.3. Let Λ be an icosahedral model set with underlying \mathbb{Z} -module L and let $r > 0$. Then there is a set U of two nonparallel L -directions such that the set of subsets of patches of radius r of Λ are determined by the X-rays in the directions of U . Moreover, there is a set U of three pairwise nonparallel L -directions such that, for all subsets F of patches of radius r of Λ , one has $G_U^F = F$.

Note that, although looking promising at first sight, neither of the last two results can comply with the restriction to few high-density directions mentioned earlier. The following result follows immediately from Theorem 2.54 of Huck (2007b); see also Theorem 15 of Huck (2007a).

Theorem 5.4. The following assertions hold:

(a) There is a set $U \subset \mathbb{S}^1$ of four pairwise nonparallel \mathcal{O}_5 -directions such that, for all cyclotomic model sets Λ with underlying \mathbb{Z} -module \mathcal{O}_5 , the set $\mathcal{C}(\Lambda)$ is determined by the X-rays in the directions of U .

(b) For all cyclotomic model sets Λ with underlying \mathbb{Z} -module \mathcal{O}_5 and all sets $U \subset \mathbb{S}^1$ of three or fewer pairwise nonparallel \mathcal{O}_5 -directions, the set $\mathcal{C}(\Lambda)$ is not determined by the X-rays in the directions of U .

In fact, for a cyclotomic model set Λ with underlying \mathbb{Z} -module \mathcal{O}_5 , the set $\mathcal{C}(\Lambda)$ is determined by the X-rays in the directions of any set U of four pairwise nonparallel \mathcal{O}_5 -directions having the property that there is no U -polygon in Λ ; cf. Lemma 1.83 and Theorem 2.29 of Huck (2007b) or Theorem 14 of Huck (2007a). Here, a U -polygon in Λ is a nondegenerate convex polygon P with all its vertices in Λ such that any line in \mathbb{R}^2 that is parallel to a direction of U and passes through a vertex of P also meets another vertex of P .

Example 5.5. The convex subsets of cyclotomic model sets with underlying \mathbb{Z} -module \mathcal{O}_5 are determined by the X-rays in the set U_5 of \mathcal{O}_5 -directions parallel to the elements of the set $\{(1 + \tau) + \zeta_5, (\tau - 1) + \zeta_5, -\tau + \zeta_5, 2\tau - \zeta_5\}$; cf. Theorem 2.56 and Example 2.57 of Huck (2007b) [see also Theorem 16 and Example 3 of Huck (2007a)].

Before we can present the first uniqueness result of this text that can comply with the restriction to few high-density directions, we need to observe the following property.

Lemma 5.6. Let $U \subset \mathbb{S}^2$ be a finite set of L^H -directions, and let $F, \tilde{F} \in \mathcal{F}(t + H)$, where $t \in \mathbb{R}^3$. If F and \tilde{F} have the same X-rays in the directions of U , then $\Phi(F - t)$ and $\Phi(\tilde{F} - t)$ have the same X-rays in the directions of $\Phi(U) \subset \mathbb{S}^1$.

Remark 5.7. By Lemmas 3.9 and 3.10, the set of L^H -directions maps under Φ bijectively onto the set of \mathcal{O}_5 -directions. Note also that, for a convex subset C of an icosahedral model set Λ and an element $\lambda \in \Lambda$, the intersection $C \cap (\lambda + H)$ is a convex subset of the slice $\Lambda \cap (\lambda + H)$ of Λ . Hence, $\Phi((C \cap (\lambda + H)) - \lambda)$ is a convex subset of $\Phi((\Lambda \cap (\lambda + H)) - \lambda)$.

By applying Theorem 5.4 to the various images $\Phi((\Lambda \cap (\lambda + H)) - \lambda)$, where Λ is an icosahedral model set and $\lambda \in \Lambda$, the proof of the following result now follows from Proposition 3.11, Lemma 5.6 and Remark 5.7.

Theorem 5.8. The following assertions hold:

(a) There is a set $U \subset \mathbb{S}^2$ of four pairwise nonparallel L^H -directions such that, for all generic icosahedral model sets Λ with underlying \mathbb{Z} -module L , the set $\mathcal{C}(\Lambda)$ is determined by the X-rays in the directions of U .

(b) For all generic icosahedral model sets Λ with underlying \mathbb{Z} -module L and all sets $U \subset \mathbb{S}^2$ of three or fewer pairwise nonparallel L^H -directions, the set $\mathcal{C}(\Lambda)$ is not determined by the X-rays in the directions of U .

An analysis of the proof of Theorem 5.8 shows that the result extends to the set of subsets C of generic icosahedral model sets Λ that are only H -convex, the latter meaning that, for all $\lambda \in \Lambda$, the sets $C \cap (\lambda + H)$ are convex subsets of the slices $\Lambda \cap (\lambda + H)$.

Example 5.9. By virtue of Example 5.5, we see that the convex subsets of generic icosahedral model sets Λ with underlying \mathbb{Z} -module L are determined by the X-rays in the L^H -directions of the set $U_{\text{ico}} := \Phi^{-1}(U_5)$.

Remark 5.10. By the results of Pleasants (2003), the directions that are determined by U_{ico} are likely to yield dense lines in icosahedral model sets. It follows that, in the practice of quantitative HRTEM, the resolution coming from these directions is likely to be rather high.

Finally, we wish to demonstrate that, in an approximate sense, part (a) of Theorem 5.8 even holds in the non-anchored case for regular generic icosahedral model sets. Before this, we need a consequence of Weyl's theory of uniform distribution; cf. Weyl (1916). This analytical property of regular icosahedral model sets was analysed in general by Schlottmann (1998, 2000) and Moody (2002). We need the following variant which relates the centroids of images of certain finite subsets of a regular icosahedral model set Λ under the star map to the centroid of its window.

Lemma 5.11. Let Λ be a regular icosahedral model set of the form $\Lambda = \Lambda_{\text{ico}}^L(0, W)$. Then, for all $a \in \mathbb{R}^3$, one has the identity

$$\lim_{r \rightarrow \infty} \frac{1}{\text{card}(\Lambda \cap B_r(a))} \sum_{\alpha \in \Lambda \cap B_r(a)} \alpha^* = \frac{1}{\text{vol}(W)} \int_W y \, d\lambda(y),$$

where λ denotes the Lebesgue measure on \mathbb{R}^3 .

Proof. This is a consequence of the uniform distribution of the points of Λ^* in the window, which gives the integral by Weyl's lemma. The proof of the uniform distribution property for model sets can be found in Schlottmann (1998) and Moody (2000, 2002).

We are now able to demonstrate that, in an approximate (and weak) sense to be clarified below, for any fixed window $W \subset \mathbb{R}^3$ whose boundary $\text{bd}(W)$ has Lebesgue measure 0 in \mathbb{R}^3 , the set $\cup_{\Lambda \in \mathcal{I}_g^L(W)} \mathcal{C}(\Lambda)$ is determined by the X-rays in the L^H -directions of U_{ico} defined in Example 5.9. Let

$$F, \tilde{F} \in \bigcup_{\Lambda \in \mathcal{I}_g^L(W)} \mathcal{C}(\Lambda),$$

say $F \in \mathcal{C}(\Lambda_{\text{ico}}^L(t, s + W))$ and $\tilde{F} \in \mathcal{C}(\Lambda_{\text{ico}}^L(\tilde{t}, \tilde{s} + W))$, where $t, \tilde{t}, s, \tilde{s} \in \mathbb{R}^3$, and suppose that F and \tilde{F} have the same X-rays in the directions of U_{ico} . If $F = \emptyset$, then, by Lemma 2.2(a), one also gets $\tilde{F} = \emptyset$. One may thus assume, without loss of generality, that F and \tilde{F} are non-empty. Hence, there is an element $\lambda \in F$ such that $F \cap (\lambda + H)$ and $\tilde{F} \cap (\lambda + H)$ are non-empty finite sets with the same X-rays in the directions of U_{ico} . Then, by Lemma 5.6, the non-empty finite subset $\Phi((F \cap (\lambda + H)) - \lambda)$ of \mathcal{O}_5 (cf. Lemma 3.10) and the non-empty finite subset $\Phi((\tilde{F} \cap (\lambda + H)) - \lambda)$ of \mathbb{C} have the same X-rays in the \mathcal{O}_5 -directions of $\Phi(U_{\text{ico}}) = U_5$. Using Lemma 2.4 in conjunction with Theorem 1.130 of Huck (2007b) [see also Theorem 12 of Huck (2007a)], one obtains

$$\begin{aligned} & \Phi((F \cap (\lambda + H)) - \lambda), \Phi((\tilde{F} \cap (\lambda + H)) - \lambda) \\ & \subset G_{U_5}^{\Phi((F \cap (\lambda + H)) - \lambda)} \subset \mathcal{O}_5. \end{aligned}$$

Thus, one gets

$$F \cap (\lambda + H), \tilde{F} \cap (\lambda + H) \subset t + L. \tag{2}$$

Since $\tilde{F} \cap (\lambda + H) \subset \tilde{t} + L$, equation (2) implies that $t + L$ meets $\tilde{t} + L$, the latter being equivalent to the identity $t + L = \tilde{t} + L$. Note also that the identity $t + L = \tilde{t} + L$ is equivalent to the relation $\tilde{t} - t \in L$. Trivially, one has

$$F - t \in \mathcal{C}(\Lambda_{\text{ico}}^L(0, s + W)).$$

One further obtains that

$$\tilde{F} - t \in \mathcal{C}(\Lambda_{\text{ico}}^L(\tilde{t} - t, \tilde{s} + W)) = \mathcal{C}(\Lambda_{\text{ico}}^L(0, (\tilde{s} + (\tilde{t} - t)^*) + W)).$$

Clearly, $F - t$ and $\tilde{F} - t$ again have the same X-rays in the directions of U_{ico} . Hence, by Lemma 2.2(b), $F - t$ and $\tilde{F} - t$ have the same centroid. Since the star map \cdot^* is \mathbb{Q} -linear, it follows that the finite subsets $(F - t)^*$ and $(\tilde{F} - t)^*$ of \mathbb{R}^3 also have the same centroid. Now, if one has

$$F - t = B_r(a) \cap \Lambda_{\text{ico}}^L(0, s + W)$$

and

$$\tilde{F} - t = B_{\tilde{r}}(\tilde{a}) \cap \Lambda_{\text{ico}}^L(0, (\tilde{s} + (\tilde{t} - t)^*) + W)$$

for suitable $a, \tilde{a} \in \mathbb{R}^3$ and large $r, \tilde{r} > 0$ (which is rather natural in practice), then Lemma 5.11 allows us to write

$$\begin{aligned} [1/\text{vol}(W)] \int_{s+W} y \, d\lambda(y) & \approx [1/\text{card}(F - t)] \sum_{x \in F - t} x^* \\ & = [1/\text{card}(\tilde{F} - t)] \sum_{x \in \tilde{F} - t} x^* \\ & \approx [1/\text{vol}(W)] \int_{(\tilde{s} + (\tilde{t} - t)^*) + W} y \, d\lambda(y). \end{aligned}$$

Consequently,

$$s + \int_W y \, d\lambda(y) \approx (\tilde{s} + (\tilde{t} - t)^*) + \int_W y \, d\lambda(y),$$

and hence $s \approx \tilde{s} + (\tilde{t} - t)^*$. The latter means that, approximately, both $F - t$ and $\tilde{F} - t$ are elements of the set $\mathcal{C}(\Lambda_{\text{ico}}^L(0, s + W))$. Now, it follows in this approximate sense from Example 5.9 that $F - t \approx \tilde{F} - t$, and, finally, $F \approx \tilde{F}$.

6. Outlook

For a more extensive account of both uniqueness and computational complexity results in the DT of Delone sets with long-range order, we refer the reader to Huck (2007b). This reference also contains results on the interactive concept of successive determination of finite sets by X-rays and further extensions of settings and results that are beyond our scope here; see also Huck (2007a). Although the results of this text and of Huck (2007b) give satisfying answers to the basic problems of the DT of icosahedral model sets, they represent only a very first step towards a tool that is as satisfactory for application in materials science as is computerized tomography in its medical or other applications. It would be interesting to have experimental tests in order to see how well

the above results work in practice. In fact, the group of K. Saitoh (Nagoya, Japan) is working on a practical realization. Since there is always some noise involved when physical measurements are taken, the latter also requires the ability to work with imprecise data. For this, it is necessary to study stability and instability in the DT of icosahedral model sets in the future; cf. Alpers & Gritzmann (2006).

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