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PII: S0305-4470(04)70895-1

3125

Icosahedral multi-component model sets

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Received 13 October 2003, in final form 13 January 2004 Published 18 February 2004 Online at stacks.iop.org/JPhysA/37/3125 (DOI: 10.1088/0305-4470/37/9/005)

Abstract

A quasi-periodic packing Q of interpenetrating copies of C, most of them only partially occupied, can be defined in terms of the strip projection method for any icosahedral cluster C. We show that in the case when the coordinates of the vectors of C belong to the quadratic field $\mathbb{Q}[\sqrt{5}]$ the dimension of the superspace can be reduced, namely Q can be re-defined as a multi-component model set by using a six-dimensional superspace.

PACS number: 61.44.Br

1. Introduction

An icosahedral quasi-crystal can be regarded as a quasi-periodic packing of copies of a welldefined icosahedral atomic cluster. Most of these interpenetrating copies are only partially occupied. From a mathematical point of view, an icosahedral cluster C can be defined as a finite union of orbits of a three-dimensional (3D) representation of the icosahedral group, and there exists an algorithm [3, 4] which leads from C directly to a pattern Q which can be regarded as a union of interpenetrating partially occupied translations of C. This algorithm, based on the strip projection method and group theory, represents an extended version of the model proposed by Katz and Duneau [12] and independently by Elser [8] for the icosahedral quasi-crystals.

The dimension of the superspace used in the definition of Q is rather large, and the main purpose of this paper is to present a way to reduce this dimension. It is based on the notion of *multi-component model set*, an extension of the notion of *model set*, proposed by Baake and Moody [2].

2. Quasi-periodic packings of icosahedral clusters

It is known that the icosahedral group $Y = 235 = \langle a, b | a^5 = b^2 = (ab)^3 = e \rangle$ has five irreducible non-equivalent representations, and its character table is

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(1)

	1e	12 <i>a</i>	15b	20ab	$12a^{2}$
Γ_1	1	1	1	1	1
Γ_2	3	τ	-1	0	au'
Γ_3	3	au'	-1	0	τ
Γ_4	4	-1	0	1	-1
Γ_5	5	0	1	-1	0

where $\tau = (1 + \sqrt{5})/2$ and $\tau' = (1 - \sqrt{5})/2$.

A realization of Γ_2 in the usual 3D Euclidean space $\mathbb{E}_3 = (\mathbb{R}^3, \langle, \rangle)$ is the representation $\{T_g : \mathbb{E}_3 \longrightarrow \mathbb{E}_3 \mid g \in Y\}$ generated by the rotations $T_a, T_b : \mathbb{E}_3 \longrightarrow \mathbb{E}_3$

$$T_a(\alpha, \beta, \gamma) = \left(\frac{\tau - 1}{2}\alpha - \frac{\tau}{2}\beta + \frac{1}{2}\gamma, \frac{\tau}{2}\alpha + \frac{1}{2}\beta + \frac{\tau - 1}{2}\gamma, -\frac{1}{2}\alpha + \frac{\tau - 1}{2}\beta + \frac{\tau}{2}\gamma\right)$$
$$T_b(\alpha, \beta, \gamma) = (-\alpha, -\beta, \gamma).$$
(2)

The entries of the matrices of T_a , T_b in the basis {(1, 0, 0), (0, 1, 0), (0, 0, 1)}

$$T_a = \frac{1}{2} \begin{pmatrix} \tau - 1 & -\tau & 1 \\ \tau & 1 & \tau - 1 \\ -1 & \tau - 1 & \tau \end{pmatrix} \qquad T_b = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
(3)

belong to the quadratic field $\mathbb{Q}[\sqrt{5}] = \mathbb{Q}[\tau]$. In the case of this representation, there are the trivial orbit $Y(0, 0, 0) = \{(0, 0, 0)\}$ of length 1, the orbits

$$Y(\alpha, \alpha\tau, 0) = \{T_g(\alpha, \alpha\tau, 0) \mid g \in Y\} \quad \text{where} \quad \alpha \in (0, \infty)$$
(4)

of length 12 (vertices of a regular icosahedron), the orbits

$$Y(\alpha, \alpha, \alpha) = \{T_g(\alpha, \alpha, \alpha) \mid g \in Y\} \quad \text{where} \quad \alpha \in (0, \infty)$$
(5)

of length 20 (vertices of a regular dodecahedron), the orbits

$$Y(\alpha, 0, 0) = \{T_g(\alpha, 0, 0) \mid g \in Y\} \qquad \text{where} \quad \alpha \in (0, \infty) \tag{6}$$

of length 30 (vertices of an icosaidodecahedron), and all the other orbits are of length 60.

Let C be a fixed icosahedral cluster containing only orbits of length 12, 20 and 30. It can be defined as

$$\mathcal{C} = \bigcup_{x \in S} Yx = \bigcup_{x \in S} \{T_g x \mid g \in Y\} = \{T_g x \mid g \in Y, x \in S\} = YS$$
(7)

where the set S contains a representative of each orbit. Since $\mathbb{Q}[\tau]$ is dense in \mathbb{R} , we can assume that

$$S \subset \{(\alpha, \alpha\tau, 0) \mid \alpha \in \mathbb{Q}[\tau], \alpha > 0\} \cup \{(\alpha, \alpha, \alpha) \mid \alpha \in \mathbb{Q}[\tau], \alpha > 0\}$$
$$\cup \{(\alpha, 0, 0) \mid \alpha \in \mathbb{Q}[\tau], \alpha > 0\}$$

without a significant loss of generality in the description of atomic clusters. Since the orbits of Y of length 12, 20 and 30 are symmetric with respect to the origin, the cluster C has the form

$$\mathcal{C} = \{e_1, e_2, \dots, e_k, -e_1, -e_2, \dots, -e_k\}$$
(8)

and for each vector $e_i = (e_{i1}, e_{i2}, e_{i3})$ the coordinates e_{i1}, e_{i2}, e_{i3} belong to $\mathbb{Q}[\tau]$.

Let $\varepsilon_1 = (1, 0, \dots, 0), \varepsilon_2 = (0, 1, 0, \dots, 0), \dots, \varepsilon_k = (0, \dots, 0, 1)$ be the canonical basis of \mathbb{E}_k . For each $g \in Y$, there exist the numbers $s_1^g, s_2^g, \dots, s_k^g \in \{-1, 1\}$ and a permutation of the set $\{1, 2, \dots, k\}$ denoted also by g such that,

$$T_g e_j = s_{g(j)}^g e_{g(j)}$$
 for all $j \in \{1, 2, \dots, k\}.$ (9)

Theorem 1 [3, 4]. The formula

$$g\varepsilon_j = s_{g(j)}^g \varepsilon_{g(j)} \tag{10}$$

defines the orthogonal representation

$$g(x_1, x_2, \dots, x_k) = \left(s_1^g x_{g^{-1}(1)}, s_2^g x_{g^{-1}(2)}, \dots, s_k^g x_{g^{-1}(k)}\right)$$
(11)

of Y in \mathbb{E}_k .

Theorem 2 [3, 4]. The subspace

$$E = \{ (\langle u, e_1 \rangle, \langle u, e_2 \rangle, \dots, \langle u, e_k \rangle) \mid u \in \mathbb{E}_3 \}$$
(12)

of \mathbb{E}_k is Y-invariant and the vectors

$$v_1 = \varrho(e_{11}, e_{21}, \dots, e_{k1}) \qquad v_2 = \varrho(e_{12}, e_{22}, \dots, e_{k2}) \qquad v_3 = \varrho(e_{13}, e_{23}, \dots, e_{k3})$$

where $\varrho = 1/\sqrt{(e_{11})^2 + (e_{21})^2 + \dots + (e_{k1})^2}$ form an orthonormal basis of *E*.

Theorem 3 [3, 4]. *The subduced representation of Y in E is equivalent to the representation of Y in* \mathbb{E}_3 , *and the isomorphism of representations*

$$\mathcal{I}: \mathbb{E}_3 \longrightarrow E \qquad \mathcal{I}u = (\varrho \langle u, e_1 \rangle, \varrho \langle u, e_2 \rangle, \dots, \varrho \langle u, e_k \rangle) \tag{13}$$

with the property $\mathcal{I}(\alpha, \beta, \gamma) = \alpha v_1 + \beta v_2 + \gamma v_3$ allows us to identify the 'physical' space \mathbb{E}_3 with the subspace E of \mathbb{E}_k .

Theorem 4 [3, 4]. *The matrix of the orthogonal projector* $\pi : \mathbb{E}_k \longrightarrow \mathbb{E}_k$ *corresponding to* E *in the basis* { $\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_k$ } *is*

$$\pi = \varrho^2 \begin{pmatrix} \langle e_1, e_1 \rangle & \langle e_1, e_2 \rangle & \cdots & \langle e_1, e_k \rangle \\ \langle e_2, e_1 \rangle & \langle e_2, e_2 \rangle & \cdots & \langle e_2, e_k \rangle \\ \vdots & \vdots & \vdots & \vdots \\ \langle e_k, e_1 \rangle & \langle e_k, e_2 \rangle & \cdots & \langle e_k, e_k \rangle \end{pmatrix}.$$
(14)

Let $\kappa = 1/\varrho$, $\mathbb{L} = \kappa \mathbb{Z}^k$, $\pi^{\perp} : \mathbb{E}_k \longrightarrow \mathbb{E}_k$, $\pi^{\perp} x = x - \pi x$ be the orthogonal projector corresponding to the subspace

$$E^{\perp} = \{ x \in \mathbb{E}_k \mid \langle x, y \rangle = 0 \text{ for all } y \in E \}$$
(15)

and let \mathbb{K} be a set obtained by shifting the hypercube

$$[0,\kappa]^k = \{(x_1, x_2, \dots, x_k) \mid 0 \leqslant x_i \leqslant \kappa\}$$

such that no point of $\pi^{\perp}(\mathbb{L})$ belongs to the boundary of $K = \pi^{\perp}(\mathbb{K})$.

Theorem 5 [3, 4]. *The* \mathbb{Z} *-module* $\mathbb{L} \subset \mathbb{E}_k$ *is Y-invariant,* $\pi(\kappa \varepsilon_i) = \mathcal{I}e_i$ *, that is* $\pi(\kappa \varepsilon_i) = e_i$ *if we take into consideration the identification* $\mathcal{I} : \mathbb{E}_3 \longrightarrow E$ *, and*

$$\pi(\mathbb{L}) = \mathbb{Z}e_1 + \mathbb{Z}e_2 + \dots + \mathbb{Z}e_k.$$
⁽¹⁶⁾

The pattern defined by using the strip projection method [12]

$$\mathcal{Q} = \{\pi x \mid x \in \mathbb{L}, \pi^{\perp} x \in K\}$$
(17)

can be regarded as a union of interpenetrating copies of C, most of them only partially occupied. For each point $\pi x \in Q$, the set of all the arithmetic neighbours of πx

$$\{\pi y \mid y \in \{x + \kappa \varepsilon_1, \dots, x + \kappa \varepsilon_k, x - \kappa \varepsilon_1, \dots, x - \kappa \varepsilon_k\}, \pi^{\perp} y \in K\}$$

is contained in the translated copy

$$\{\pi x + e_1, \dots, \pi x + e_k, \pi x - e_1, \dots, \pi x - e_k\} = \pi x + C$$

of the *G*-cluster *C*. The fully occupied clusters occurring in Q correspond to the points $x \in \mathbb{L}$ satisfying the condition [12]

$$\pi^{\perp}x \in K \cap \bigcap_{i=1}^{k} (\pi^{\perp}(\kappa\varepsilon_i) + K) \cap \bigcap_{i=1}^{k} (-\pi^{\perp}(\kappa\varepsilon_i) + K).$$
(18)

Generally, only a small part of the clusters occurring in Q can be fully occupied. A fragment of Q can be obtained by using, for example, the algorithm presented in [16]. The main difficulty is the rather large dimension *k* of the superspace \mathbb{E}_k used in the definition of Q.

3. Icosahedral multi-component model sets

We shall re-define the pattern Q as a multi-component model set by using a 6D subspace of \mathbb{E}_k . The automorphism

$$\varphi: \mathbb{Q}[\tau] \longrightarrow \mathbb{Q}[\tau] \tag{19}$$

of the quadratic field $\mathbb{Q}[\tau]$ that maps $\sqrt{5} \mapsto -\sqrt{5}$ has the property $\varphi(\tau) = \tau'$. The representation (2) is related through φ to the representation $\{T'_g : \mathbb{E}_3 \longrightarrow \mathbb{E}_3 \mid g \in Y\}$ belonging to Γ_3 generated by the rotations $T'_a, T'_b : \mathbb{E}_3 \longrightarrow \mathbb{E}_3$

$$T_{a}^{\prime}(\alpha,\beta,\gamma) = \left(\frac{\tau^{\prime}-1}{2}\alpha - \frac{\tau^{\prime}}{2}\beta + \frac{1}{2}\gamma, \frac{\tau^{\prime}}{2}\alpha + \frac{1}{2}\beta + \frac{\tau^{\prime}-1}{2}\gamma, -\frac{1}{2}\alpha + \frac{\tau^{\prime}-1}{2}\beta + \frac{\tau^{\prime}}{2}\gamma\right)$$

$$T_{b}^{\prime}(\alpha,\beta,\gamma) = (-\alpha,-\beta,\gamma).$$
(20)

If instead of the representation (2) and cluster C, we start from the representation (20) and the cluster

$$\mathcal{C}' = \{e'_1, e'_2, \dots, e'_k, -e'_1, -e'_2, \dots, -e'_k\}$$
(21)

where

$$e'_{i} = (e'_{i1}, e'_{i2}, e'_{i3}) = (\varphi(e_{i1}), \varphi(e_{i2}), \varphi(e_{i3}))$$
(22)

then we get the same representation of *Y* in \mathbb{E}_k and the *Y*-invariant subspace

$$E' = \{ (\langle u, e'_1 \rangle, \langle u, e'_2 \rangle, \dots, \langle u, e'_k \rangle) \mid u \in \mathbb{E}_3 \}.$$
(23)

The vectors

$$v'_1 = \varrho'(e'_{11}, e'_{21}, \dots, e'_{k1})$$
 $v'_2 = \varrho'(e'_{12}, e'_{22}, \dots, e'_{k2})$ $v'_3 = \varrho'(e'_{13}, e'_{23}, \dots, e'_{k3})$
where $\varrho' = 1/\sqrt{(e'_{11})^2 + (e'_{21})^2 + \dots + (e'_{k1})^2}$ form an orthonormal basis of E' , and the matrix of the orthogonal projector $\pi' : \mathbb{E}_k \longrightarrow \mathbb{E}_k$ corresponding to E' in the basis $\{\varepsilon_1, \varepsilon_2, \dots, \varepsilon_k\}$ is

$$\pi' = {\varrho'}^2 \begin{pmatrix} \langle e_1', e_1' \rangle & \langle e_1', e_2' \rangle & \cdots & \langle e_1', e_k' \rangle \\ \langle e_2', e_1' \rangle & \langle e_2', e_2' \rangle & \cdots & \langle e_2', e_k' \rangle \\ \cdots & \cdots & \cdots & \cdots \\ \langle e_k', e_1' \rangle & \langle e_k', e_2' \rangle & \cdots & \langle e_k', e_k' \rangle \end{pmatrix}.$$
(24)

Theorem 6. The projectors π and π' are orthogonal, that is

 $\pi\pi'=\pi'\pi=0$

and the projector $\pi + \pi'$ corresponding to the subspace $\mathcal{E} = E \oplus E'$ has rational entries.

Proof. Consider the linear mapping

$$A: \mathbb{E}_3 \longrightarrow \mathbb{E}_3: u \mapsto Au$$
 where $Au = \sum_{i=1}^n \langle u, e_i \rangle e'_i$.

Since A is a morphism of representations

$$A(T_g u) = \sum_{i=1}^k \langle T_g u, e_i \rangle e'_i = \sum_{i=1}^k \langle u, T_g^{-1} e_i \rangle e'_i$$
$$= T'_g \left(\sum_{i=1}^k \langle u, T_g^{-1} e_i \rangle T'_g^{-1} e'_i \right) = T'_g \left(\sum_{i=1}^k \langle u, e_i \rangle e'_i \right) = T_g(Au)$$

between the irreducible non-equivalent representations (2) and (20), from Schur's lemma it follows that A = 0, that is $\sum_{i=1}^{k} \langle u, e_i \rangle e'_i = 0$ for any $u \in \mathbb{E}_3$. Particularly, we have

$$\sum_{i=1}^{k} \langle e_j, e_i \rangle \langle e'_i, e'_i \rangle = \left\langle \sum_{i=1}^{k} \langle e_j, e_i \rangle e'_i, e'_i \right\rangle = 0$$

whence $\pi \pi' = 0$. In a similar way we can prove that $\pi' \pi = 0$. Since

$${\varrho'}^2 \langle e'_i, e'_j \rangle = \varphi(\varrho^2 \langle e_i, e_j \rangle)$$

we get $\varrho'^2 \langle e'_i, e'_j \rangle + \varrho^2 \langle e_i, e_j \rangle \in \mathbb{Q}$, that is the projector $\pi + \pi'$ has rational entries.

Theorem 7. The collection of spaces and mappings

$$\pi x \leftarrow x : E \quad \stackrel{\pi}{\longleftarrow} \quad \begin{array}{c} \mathcal{E} \quad \stackrel{\pi'}{\longrightarrow} \quad E' : x \rightarrow \pi' x \\ \cup \\ \mathcal{L} \end{array}$$

$$(25)$$

where $\mathcal{L} = (\pi + \pi')(\mathbb{L})$, is a cut and project scheme [2, 14].

Proof. Since, in view of theorems 5 and 6, we have

$$\pi'(\mathcal{L}) = \pi'(\pi + \pi')(\mathbb{L}) = \pi'(\mathbb{L}) = \sum_{i=1}^{k} \mathbb{Z}e'_i$$

the set $\pi'(\mathcal{L})$ is dense in E'. For each $x \in \mathcal{L}$ there is $\kappa y \in \mathbb{L}$ with $y \in \mathbb{Z}^k$ such that $x = (\pi + \pi')(\kappa y)$. If $\pi x = 0$ then $\pi(\pi + \pi')(\kappa y) = 0$, whence $\pi(\kappa y) = 0$. But, $\pi(\kappa y) = \kappa \pi y$, and hence we have $\pi y = 0$. Since $y \in \mathbb{Z}^k$, from $\pi y = 0$ we get $\pi' y = 0$, whence $x = (\pi + \pi')y = 0$. This means that π restricted to \mathcal{L} is injective.

Let $E'' = \mathcal{E}^{\perp} = \{x \in \mathbb{E}_k \mid \langle x, y \rangle = 0 \text{ for all } y \in \mathcal{E}\}$ and let $\pi'' : \mathbb{E}_k \longrightarrow \mathbb{E}_k, \pi'' x = x - \pi x - \pi' x$ be the corresponding orthogonal projector (see figure 1). The lattice $L = \mathbb{L} \cap \mathcal{E}$ is a sublattice of \mathcal{L} , and necessarily $[\mathcal{L} : L]$ is finite. Since π'' has rational entries the projection $\mathbb{L}'' = \pi''(\mathbb{L})$ of \mathbb{L} on E'' is a discrete countable set. Let $\mathcal{Z} = \{z_i \mid i \in \mathbb{Z}\}$ be a subset of \mathbb{L} such that $\mathbb{L}'' = \pi''(\mathcal{Z})$ and $\pi'' z_i \neq \pi'' z_j$ for $i \neq j$. The lattice \mathbb{L} is contained in the union of the cosets $\mathcal{E}_i = z_i + \mathcal{E} = \{z_i + x \mid x \in \mathcal{E}\}$

$$\mathbb{L} \subset \bigcup_{i \in \mathbb{Z}} \mathcal{E}_i.$$
⁽²⁶⁾

Since $\mathbb{L} \cap \mathcal{E}_i = z_i + L$ the set

$$= (\pi + \pi')(\mathbb{L} \cap \mathcal{E}_i) = (\pi + \pi')z_i + L$$
(27)

 $\mathcal{L}_i = (\pi + \pi')(\mathbb{L} \cap$ is a coset of *L* in \mathcal{L} for any $i \in \mathbb{Z}$.



Figure 1. The decompositions $\mathbb{E}_k = E \oplus E^{\perp} = E \oplus E' \oplus E'' = \mathcal{E} \oplus E''$.

Only for a finite number of cosets \mathcal{E}_i the intersection

$$K_i = K \cap \mathcal{E}_i = K \cap \pi^{\perp}(\mathcal{E}_i) = \pi^{\perp}(\mathbb{K} \cap \mathcal{E}_i) \subset \pi'' z_i + E'$$
(28)

is non-empty. By changing the indexation of the elements of \mathcal{Z} if necessary, we can assume that the subset of E'

$$\mathcal{K}_i = \pi'(K_i) = \pi'(\mathbb{K} \cap \mathcal{E}_i) \subset E' \tag{29}$$

has a non-empty interior only for $i \in \{1, ..., m\}$. The 'polyhedral' set \mathcal{K}_i satisfies the conditions:

- (a) $\mathcal{K}_i \subset E'$ is compact;
- (b) $\mathcal{K}_i = \overline{\operatorname{int}(\mathcal{K}_i)};$
- (c) The boundary of \mathcal{K}_i has the Lebesgue measure 0

for any $i \in \{1, ..., m\}$. This allows us to re-define Q in terms of the 6D superspace \mathcal{E} as a multi-component model set [2]

$$Q = \bigcup_{i=1}^{m} \{ \pi x \mid x \in \mathcal{L}_i, \pi' x \in \mathcal{K}_i \}.$$
(30)

It is known [6] that this is the minimal embedding for a 3D quasi-periodic point set with icosahedral symmetry. The main difficulty in this new approach is the determination of the 'atomic surfaces' \mathcal{K}_i .

4. Concluding remarks

There exist several models for the icosahedral quasi-crystals, and almost all of them are defined by using, directly or indirectly, a 6D superspace. We hope that the 6D version of our model presented in this paper will help crystallographers to compare our model with other models, and to use it. In the case of certain computer calculations based on our model the kD version seems to be more advantageous than the 6D one.

Elser and Henley [7] and Audier and Guyot [1] have obtained models for icosahedral quasi-crystals by decorating the Ammann rhombohedra occurring in a tiling of the 3D space defined by projection [8, 12]. In his quasi-unit cell picture, Steinhardt [15] has shown (following an idea of Gummelt [10]) that the atomic structure can be described entirely by using a single repeating cluster which overlaps (shares atoms with) neighbouring clusters. The model is determined by the overlap rules and the atom decoration of the unit cell. Some important models have been obtained by Yamamoto and Hiraga [17, 18], Katz and Gratias [13] and Gratias *et al* [9] by using the section method in a 6D superspace decorated with

several polyhedra (acceptance domains). Janot and de Boissieu [11] have shown that a model of a icosahedral quasi-crystal can be generated recursively by starting from a pseudo-Mackay cluster and using some inflation rules. In the case of all these models, one has to add or shift some points in order to fill the gaps between the clusters, and one has to eliminate some points from interpenetrating clusters if they become too close. These geometric corrections increase the number of local configurations and are difficult to explain energetically. In the case of all these models, only for a very small part of the points are the neighbouring points distributed on the vertices of the generating cluster.

Our mathematical model is different. The patterns Q have the remarkable mathematical properties of the patterns obtained by projection [12, 14]. They are exactly defined (no correction rules are necessary), and each point of the pattern (without exception) is the centre of a more or less occupied copy of C. The clusters corresponding to neighbouring points share several points. The arithmetic neighbours of a point are disposed at the same distance independently of the considered point, and in agreement with the orientation of the generating cluster (there is a strict short and long range order). For each atom there is the tendency to dispose its neighbours in the same configuration, namely to become the centre of the same cluster. The reduction of the dimension of the superspace has led us in a natural way to the use of several sublattices, each of them with a specific window.

Several extensions of the presented model are possible. In this paper we have tried to avoid any unnecessary complication and to present a both simple and relevant version. We have considered a particular window and clusters containing only orbits of length 12, 20 and 30 (the experimental data show that these are the clusters occurring in most cases).

If we start from $S = \{(1, \tau, 0)\}$ we re-obtain the well-known model proposed by Katz and Duneau, and independently by Elser. In this case k = 6 and m = 1, that is we obtain directly a model set defined in a 6D superspace. For each point $\pi x \in Q$ (without exception) the arithmetic neighbours of πx are distributed on the vertices of the icosahedron $\pi x + C$. The pattern Q is a union of interpenetrating copies of C (generally, partially occupied), has a uniform distribution of points and it is not necessary to eliminate/add new points. A similar situation occurs in all our models.

As concerns the reduction of the superspace dimension, the reader can find an worked example with m = 4 in [5]. It concern the 2D Penrose case, but the situation in the case of our icosahedral patterns is similar.

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