LETTER TO THE EDITOR

Icosahedral multi-component model sets

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Abstract. A quasiperiodic 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 6-dimensional superspace.
1. Introduction

An icosahedral quasicrystal can be regarded as a quasiperiodic packing of copies of a well-defined icosahedral atomic cluster. Most of these interpenetrating copies are only partially occupied. From a mathematical point of view, an icosahedral cluster can be defined as a finite union of orbits of a 3-dimensional representation of the icosahedral group, and there exists an algorithm which leads from the cluster directly to a pattern which can be regarded as a union of interpenetrating partially occupied translations of the cluster. This algorithm, based on the strip projection method and group theory, represents an extended version of the model proposed by Katz & Duneau and independently by Elser for the icosahedral quasicrystals.

The dimension of the superspace used in the definition of the pattern 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. Quasiperiodic packings of icosahedral clusters

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

\[
\begin{array}{c|cccccc}
\Gamma & 1 & e & 12 & a & 15 & b & 20 & ab & 12 & a^2 \\
\hline
\Gamma_1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
\Gamma_2 & 3 & \tau & 1 & 0 & \tau' & 0 & 1 & 0 & 1 & 0 \\
\Gamma_3 & 3 & \tau' & 1 & 0 & \tau & 0 & 1 & 0 & 1 & 0 \\
\Gamma_4 & 4 & -1 & 0 & 1 & -1 & 0 & 1 & -1 & 0 & 1 \\
\Gamma_5 & 5 & 0 & 1 & -1 & 0 & 1 & -1 & 0 & 1 & 0 \\
\end{array}
\]

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

A realization of \( \Gamma_2 \) in the usual 3-dimensional Euclidean space \( E_3 = (\mathbb{R}^3, \langle, \rangle) \) is the representation \( \{ T_g : E_3 \to E_3 \mid g \in Y \} \) generated by the rotations \( T_a, T_b : E_3 \to E_3 \)

\[
\begin{align*}
T_a(\alpha, \beta, \gamma) &= \left( \frac{\tau-1}{2} \alpha - \frac{1}{2} \beta + \frac{1}{2} \gamma, \frac{\tau}{2} \alpha + \frac{1}{2} \beta - \frac{1}{2} \gamma, -\frac{1}{2} \alpha + \frac{1}{2} \beta + \frac{1}{2} \gamma \right) \\
T_b(\alpha, \beta, \gamma) &= (-\alpha, -\beta, \gamma).
\end{align*}
\]

In the case of this representation there are the trivial orbit \( Y(0,0,0) = \{(0,0,0)\} \) of length 1, the orbits

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

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

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

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

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

of length 30 (vertices of an icosidodecahedron), 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

$$C = \bigcup_{x \in S} Yx = \bigcup_{x \in S} \{T_gx \mid g \in Y\} = \{T_gx \mid g \in Y, \ x \in S\} = YS$$

(6)

where the set $S$ contains a representative of each orbit. The entries of the matrices of rotations $T_a$, $T_b$ in the basis $\{(1,0,0), (0,1,0), (0,0,1)\}$

$$T_a = \frac{1}{2} \begin{pmatrix} \tau - 1 & -\tau & 1 \\ \tau & 1 & \tau - 1 \\ -1 & \tau - 1 & \tau \end{pmatrix} \quad T_b = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

(7)

belong to the quadratic field $\mathbb{Q}[\sqrt{5}] = \mathbb{Q}[\tau]$. 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

$$C = \{ e_1, e_2, ..., e_k, -e_1, -e_2, ..., -e_k \}$$

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

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

(9)

**Theorem 1.** \[ \boxed{23} \] The formula

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

(10)

defines the orthogonal representation

$$g(x_1, x_2, ..., x_k) = (s_1^g x_{g^{-1}(1)}, s_2^g x_{g^{-1}(2)}, ..., s_k^g x_{g^{-1}(k)})$$

(11)

of $Y$ in $\mathbb{E}_k$.

**Theorem 2.** \[ \boxed{23} \] The subspace

$$E = \{ \langle u, e_1 \rangle, \langle u, e_2 \rangle, ..., \langle u, e_k \rangle \mid u \in \mathbb{E}_3 \}$$

(12)

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

$$v_1 = g(e_{11}, e_{21}, ..., e_{k1}) \quad v_2 = g(e_{12}, e_{22}, ..., e_{k2}) \quad v_3 = g(e_{13}, e_{23}, ..., e_{k3})$$

where $g = 1/\sqrt{(e_{11})^2 + (e_{22})^2 + ... + (e_{k1})^2}$ form an orthonormal basis of $E$.

**Theorem 3.** \[ \boxed{23} \] The subduced representation of $Y$ in $E$ is equivalent with the representation of $Y$ in $\mathbb{E}_3$, and the isomorphism of representations

$$\mathcal{I'} : \mathbb{E}_3 \longrightarrow E \quad \mathcal{I'} u = (g < u, e_1 >, g < u, e_2 >, ..., g < u, e_k >)$$

(13)
with the property $I(\alpha, \beta, \gamma) = \alpha v_1 + \beta v_2 + \gamma v_3$ allows us to identify the ‘physical’ space $E_3$ with the subspace $E$ of $E_k$.

**Theorem 4.** Let $I$ with the property $E$ and $E_k$ be regarded as a union of interpenetrating copies of $E$, corresponding to the subspace $E$. Theorem 4.

**Theorem 5.** The matrix of the orthogonal projector $\pi : E_k \rightarrow E_k$ corresponding to $E$ in the basis $\{\varepsilon_1, \varepsilon_2, ..., \varepsilon_k\}$ is

$$\pi = \varrho^2 \left( \begin{array}{cccc} \langle e_1, e_1 \rangle & \langle e_1, e_2 \rangle & \cdots & \langle e_1, e_k \rangle \\ \langle e_2, e_1 \rangle & \langle e_2, e_2 \rangle & \cdots & \langle e_2, e_k \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle e_k, e_1 \rangle & \langle e_k, e_2 \rangle & \cdots & \langle e_k, e_k \rangle \end{array} \right).$$

(14)

Let $\kappa = 1/\varrho$, $L = \kappa Z^k$, $K = [0, \kappa]^k = \{ (x_1, x_2, ..., x_k) | 0 \leq x_i \leq \kappa \}$, and let $K = \pi^*(K)$, where $\pi^* : E_k \rightarrow E_k$, $\pi^* x = x - \pi x$ is the orthogonal projector corresponding to the subspace

$$E^\perp = \{ x \in E_k \mid \langle x, y \rangle = 0 \text{ for all } y \in E \}.$$

(15)

**Theorem 5.** The $Z$-module $L \subset E_k$ is $Y$-invariant, $\pi(\kappa \varepsilon_i) = \lambda e_i$, that is, $\pi(\kappa \varepsilon_i) = e_i$ if we take into consideration the identification $I : E_3 \rightarrow E$, and

$$\pi(L) = \lambda e_1 + \lambda e_2 + ... + \lambda e_k.$$

(16)

The pattern defined by using the strip projection method 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 $\pi x$

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

is contained in the translated copy

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

of the $G$-cluster $C$. The fully occupied clusters occurring in $Q$ correspond to the points $x \in L$ satisfying the condition

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

(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 [8]. The main difficulty is the rather large dimension $k$ of the superspace $E_k$ 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 6-dimensional subspace of $E_k$. The automorphism

$$\varphi : Q[\tau] \rightarrow Q[\tau]$$

(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 $\varphi$ to the representation $\{ T_g : \mathbb{E}_3 \to \mathbb{E}_3 \mid g \in Y \}$ belonging to $\Gamma_3$ generated by the rotations $T_a', T_b' : \mathbb{E}_3 \to \mathbb{E}_3$

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

(20)

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

$$C' = \{ e_1', e_2', ..., e_k', -e_1', -e_2', ..., -e_k' \}$$

(21)

where

$$e_i' = (e_{i,1}, e_{i,2}, e_{i,3}) = (\varphi(e_{i,1}), \varphi(e_{i,2}), \varphi(e_{i,3}))$$

(22)

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

$$E' = \{ (\langle u, e_1' \rangle, \langle u, e_2' \rangle, ..., \langle u, e_k' \rangle) \mid u \in \mathbb{E}_3 \}.$$ (23)

The vectors

$$v_1' = g'(e_{1,1}', e_{2,1}', ..., e_{k,1}') \quad v_2' = g'(e_{1,2}', e_{2,2}', ..., e_{k,2}') \quad v_3' = g'(e_{1,3}', e_{2,3}', ..., e_{k,3}')$$

where $g' = 1/\sqrt{(e_{1,1})^2 + (e_{2,1})^2 + ... + (e_{k,1})^2}$, form an orthonormal basis of $E'$, and the matrix of the orthogonal projector $\pi' : \mathbb{E}_k \to \mathbb{E}_k$ corresponding to $E'$ in the basis \{ $e_1, e_2, ..., e_k$ \} is

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

**Theorem 6.** The projectors $\pi$ and $\pi'$ 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

$$A : \mathbb{E}_3 \to \mathbb{E}_3 : u \mapsto Au \quad \text{where} \quad Au = \sum_{i=1}^{k} \langle u, e_i \rangle e_i'.$$

Since $A$ is a morphism of representations

$$A(T_g u) = \sum_{i=1}^{k} \langle T_g u, e_i \rangle e_i' = \sum_{i=1}^{k} \langle u, T_g^{-1} e_i \rangle e_i'$$

$$= T_{g'} \left( \sum_{i=1}^{k} \langle u, T_g^{-1} e_i \rangle T_g' e_i' \right) = T_{g'} \left( \sum_{i=1}^{k} \langle u, e_i \rangle e_i' \right) = T_g(Au)$$
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

\[
\sum_{i=1}^{k} \langle e_j, e_i \rangle \langle e_i', e_i' \rangle = \langle \sum_{i=1}^{k} \langle e_j, e_i \rangle e_i', e_i' \rangle = 0
\]

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

\[
\varrho^2 \langle e_i', e_j' \rangle = \varphi \left( \varrho^2 \langle e_i, e_j \rangle \right)
\]

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

\[
\pi x \leftarrow x : E \xrightarrow{\pi} \mathcal{E} \xrightarrow{\pi'} E' : x \rightarrow \pi'x
\]

\(\mathcal{L}\)

where \(\mathcal{L} = (\pi + \pi')(\mathbb{L})\), is a cut and project scheme \([11, 7]\).

**Proof.** Since, in view of theorem 5, 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 \(\pi\) restricted to \(\mathcal{L}\) is injective.

Let \(E'' = \mathcal{E}^\perp = \{x \in \mathbb{E}_k \mid \langle x, y \rangle = 0\) for all \(y \in \mathcal{E}\}\) and let \(\pi'' : \mathbb{E}_k \rightarrow \mathbb{E}_k\), \(\pi'' x = x - \pi x - \pi' x\) be the corresponding orthogonal projector. The lattice \(L = \mathbb{L} \cap \mathcal{E}\) is a sublattice of \(\mathcal{L}\), and necessarily \([\mathcal{L} : L]\) is finite. Since \(\pi''\) 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 \(\mathcal{E}_i = z_i + \mathcal{E} = \{z_i + x \mid x \in \mathcal{E}\}\)

\[
\mathbb{L} \subset \bigcup_{i \in \mathbb{Z}} \mathcal{E}_i.
\]

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

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

is a coset of \(L\) in \(\mathcal{L}\) for any \(i \in \mathbb{Z}\).

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

\[
K_i = K \cap \mathcal{E}_i = \pi'(\mathbb{K} \cap \mathcal{E}_i) \subset \pi'' z_i + E'
\]

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

\[
\mathcal{K}_i = \pi'(K_i) = \pi'(\mathbb{K} \cap \mathcal{E}_i) \subset E'
\]
has a non-empty interior only for \( i \in \{1, \ldots, m\} \). The ‘polyhedral’ set \( \mathcal{K}_i \) satisfies the conditions:

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

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

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

It is known [4] that this is the minimal embedding for a 3-dimensional quasiperiodic point set with icosahedral symmetry. The main difficulty in this new approach is the determination of the ‘atomic surfaces’ \( \mathcal{K}_i \).

Acknowledgments

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