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LETTER TO THE EDITOR

Penrose-type patterns obtained by projection from a 12-dimensional lattice

Nicolae Cotfas

Faculty of Physics, University of Bucharest, PO Box 76-54, Postal Office 76, Bucharest, Romania

E-mail: ncotfas@yahoo.com

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Abstract

We define a class of icosahedral patterns similar to the three-dimensional Penrose pattern by using the strip projection method in a 12-dimensional space.

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The three-dimensional (3D) Penrose tiling, which is a space filling with two rhombohedra discovered by Ammann, plays a fundamental role in quasicrystal physics. It is usually defined [1, 3] by using the strip projection method in a 6D space, but its first theoretic construction was done by Kramer *et al* [5] in terms of a 12D space. We shall use the term *Penrose pattern* to designate the set of all the vertices of this remarkable tiling.

It is well known that the calculated diffraction pattern of the Penrose pattern is similar to the observed patterns of certain quasicrystals as concerns the position of the Bragg peaks. The agreement is not good enough if we take into consideration the intensities of the peaks. On the other hand, the Penrose pattern cannot be used directly as a model since the frequency of occurrence of some fully occupied icosahedral clusters is high in real quasicrystals and very low or absent in the Penrose pattern.

The location of peaks depends essentially on the decomposition of the superspace we use. The decomposition of the 6D superspace used in the definition of the Penrose pattern is a good starting point in the description of the icosahedral quasicrystals. Some of the most important models [2, 4, 7] existing in quasicrystal physics are defined in terms of the section method by using this decomposition and some rather complicated atomic surfaces. Our aim is to look for an alternative mathematical approach.

The patterns we present in this letter seem to show that it is possible to change the intensities of the Bragg peaks keeping almost the same location, and to increase the frequency of occurrence of some fully occupied icosahedral clusters by changing the superspace we use.

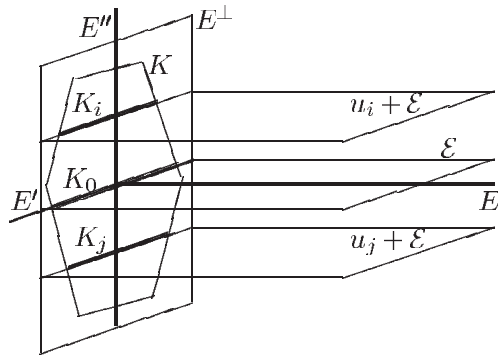


Figure 1. The decomposition $\mathbb{E}_{12} = E \oplus E' \oplus E''$.

The Penrose pattern is usually obtained [1, 3] in terms of the Euclidean 6D space \mathbb{E}_6 by using the orthogonal projectors $p, p' : \mathbb{E}_6 \rightarrow \mathbb{E}_6$ defined in the canonical basis $\varepsilon_1 = (1, 0, \dots, 0), \dots, \varepsilon_6 = (0, \dots, 0, 1)$ by the matrices

$$p = \frac{1}{2\sqrt{5}} \begin{pmatrix} \sqrt{5} & 1 & -1 & -1 & 1 & 1 \\ 1 & \sqrt{5} & 1 & -1 & -1 & 1 \\ -1 & 1 & \sqrt{5} & 1 & -1 & 1 \\ -1 & -1 & 1 & \sqrt{5} & 1 & 1 \\ 1 & -1 & -1 & 1 & \sqrt{5} & 1 \\ 1 & 1 & 1 & 1 & 1 & \sqrt{5} \end{pmatrix} \quad p' = I_6 - p \quad (1)$$

where I_6 is the 6×6 unit matrix. These projectors allow us to decompose \mathbb{E}_6 into a sum of orthogonal subspaces $\mathbb{E}_6 = \mathbb{E}_6^\parallel \oplus \mathbb{E}_6^\perp$, where $\mathbb{E}_6^\parallel = p(\mathbb{E}_6)$ and $\mathbb{E}_6^\perp = p'(\mathbb{E}_6)$. For any $\xi \in \mathbb{Z}^6$, the points of the set $p(\{\xi + \varepsilon_1, \xi - \varepsilon_1, \dots, \xi + \varepsilon_6, \xi - \varepsilon_6\})$ are the vertices of a regular icosahedron of centre $p\xi$. The Penrose pattern is the set

$$\mathcal{Q} = \{p\xi \mid \xi \in \mathbb{Z}^6, p'\xi \in p'(\gamma_6)\} \quad (2)$$

where $\gamma_6 = \{(\xi_1, \xi_2, \dots, \xi_6) \mid 0 < \xi_i < 1\}$.

Let $\lambda \in \{1, 2, 3, \dots\}$, $\kappa = \sqrt{1 + \lambda^2}$, and let $\mathcal{L} = \kappa\mathbb{Z}^{12}$. The matrices

$$\pi = \kappa^{-2} \begin{pmatrix} p & \lambda p \\ \lambda p & \lambda^2 p \end{pmatrix} \quad \pi' = \kappa^{-2} \begin{pmatrix} p' & \lambda p' \\ \lambda p' & \lambda^2 p' \end{pmatrix} \quad \pi'' = I_{12} - \pi - \pi' \quad (3)$$

define three orthogonal projectors $\pi, \pi', \pi'' : \mathbb{E}_{12} \rightarrow \mathbb{E}_{12}$ which allow us to decompose \mathbb{E}_{12} into the sum $\mathbb{E}_{12} = E \oplus E' \oplus E''$ of the orthogonal subspaces $E = \pi(\mathbb{E}_{12})$, $E' = \pi'(\mathbb{E}_{12})$ and $E'' = \pi''(\mathbb{E}_{12})$ with $\dim E = \dim E' = 3$ and $\dim E'' = 6$ (see figure 1).

Using the projectors π and $\pi^\perp = \pi' + \pi''$ we define the pattern

$$\mathcal{Q}_\lambda = \{\pi x \mid x \in \mathcal{L}, \pi^\perp x \in K\} \quad (4)$$

where $K = \pi^\perp(\gamma_{12})$ is the projection on $E^\perp = E' \oplus E''$ of the hypercube $\gamma_{12} = \{(x_1, x_2, \dots, x_{12}) \mid 0 < x_i < \kappa\}$. A fragment of \mathcal{Q}_λ can be obtained by using, for example, the general algorithm presented in [6] and a powerful enough computer.

Let $\Xi = \pi + \pi'$, $\mathcal{E} = E \oplus E' = \Xi(\mathbb{E}_{12})$, $\Lambda = \Xi(\mathcal{L})$, and let $\mathcal{L}'' = \pi''(\mathcal{L})$. Since λ is an integer and

$$\Xi = \kappa^{-2} \begin{pmatrix} I_6 & \lambda I_6 \\ \lambda I_6 & \lambda^2 I_6 \end{pmatrix} \quad \pi'' = \kappa^{-2} \begin{pmatrix} \lambda^2 I_6 & -\lambda I_6 \\ -\lambda I_6 & I_6 \end{pmatrix} \quad (5)$$

\mathcal{L}'' is a discrete subset of E'' , and Λ is a discrete subset of \mathcal{E} . There exists a countable set $\mathcal{U} = \{u_0, u_1, u_2, \dots\} \subset \mathcal{L}$ such that $\pi''(\mathcal{U}) = \mathcal{L}''$, $u_0 = (0, 0, \dots, 0)$, and $\pi''u_i \neq \pi''u_j$ for

$i \neq j$. The lattice \mathcal{L} is contained in the countable union of affine subspaces $\bigcup_{i=0}^{\infty} (u_i + \mathcal{E})$. Denoting $L = \mathcal{L} \cap \mathcal{E}$, we obtain $\mathcal{L} \cap (u_i + \mathcal{E}) = u_i + L$.

Since $\pi^\perp \mathcal{E} = E'$ we have $\pi^\perp (u_i + \mathcal{E}) = \pi'' u_i + E' = E^\perp \cap (u_i + \mathcal{E})$, and hence $\pi^\perp (\mathcal{L}) \subset \bigcup_{i=1}^{\infty} (\pi'' u_i + E')$. Only a finite number of the 3D subspaces $\pi'' u_i + E'$ intersect the bounded set K . By changing the indexation of the elements of \mathcal{U} if necessary, we can assume that $K \cap (\pi'' u_i + E') \neq \emptyset$ only for $i \in \{0, 1, \dots, k\}$. Denoting $K_i = K \cap (u_i + \mathcal{E}) = K \cap (\pi'' u_i + E')$ we obtain a definition of \mathcal{Q}_λ in terms of the 6D space \mathcal{E} , namely

$$\mathcal{Q}_\lambda = \bigcup_{i=0}^k \{\pi x \mid x \in \Xi u_i + L, \pi' x \in \pi'(K_i)\}. \quad (6)$$

By direct computation one can verify that, generally, the faces of K are not parallel to E'' , and hence, generally, the sets $\pi'(K_i)$ are distinct. This means that in order to define \mathcal{Q}_λ in terms of the 6D space \mathcal{E} , we have to distinguish some sublattices of Λ , and to use for each of them a specific window. This new definition of \mathcal{Q}_λ allows us to compare \mathcal{Q}_λ with the Penrose pattern, but, since the shapes of K_i seem to be very complicated, it is simpler to use the definition (4) than (6).

If we identify \mathbb{E}_{12} with $\{(\xi, \eta) \mid \xi, \eta \in \mathbb{E}_6\}$ then the vectors of the canonical basis of \mathcal{L} can be written as $e_1 = (\kappa \varepsilon_1, 0), \dots, e_6 = (\kappa \varepsilon_6, 0), e_7 = (0, \kappa \varepsilon_1), \dots, e_{12} = (0, \kappa \varepsilon_6)$. For any $x \in \mathcal{L}$ the points of the set $\pi(\{x + e_1, x - e_1, \dots, x + e_{12}, x - e_{12}\})$ are the vertices of two regular icosahedra of centre πx with the ratio of the radii λ .

The vectors w_1, w_2, \dots, w_6 , where

$$w_i = \Xi(\kappa \varepsilon_i, 0) = \kappa^{-1}(\varepsilon_i, \lambda \varepsilon_i) \quad (7)$$

form an orthonormal basis of the space \mathcal{E} , and since $\Xi(0, \kappa \varepsilon_i) = \lambda w_i$ we have $\Lambda = \sum_{i=1}^6 \mathbb{Z} w_i$, that is, Λ is the hypercubic lattice generated by $\{w_1, w_2, \dots, w_6\}$.

The matrix of the restriction $\pi_{1_\varepsilon} : \mathcal{E} \rightarrow \mathcal{E}$ of π to \mathcal{E} in the basis $\{w_1, w_2, \dots, w_6\}$ coincides with the matrix of $p : \mathbb{E}_6 \rightarrow \mathbb{E}_6$ in the basis $\{\varepsilon_1, \varepsilon_2, \dots, \varepsilon_6\}$ (see (1)). Indeed, denoting by p_{ij} the entries of the matrix p we have

$$\pi w_j = \kappa^{-1}(p \varepsilon_j, \lambda p \varepsilon_j) = \sum_{i=1}^6 p_{ij} \kappa^{-1}(\varepsilon_i, \lambda \varepsilon_i) = \sum_{i=1}^6 p_{ij} w_i. \quad (8)$$

This means that the decomposition $\mathcal{E} = E \oplus E'$ is identical with the decomposition $\mathbb{E}_6 = \mathbb{E}_6^\parallel \oplus \mathbb{E}_6^\perp$, and hence the pattern

$$\mathcal{Q}' = \{\pi x \mid x \in \Lambda, \pi' x \in K'\} \quad (9)$$

where $K' = \pi'(\{\alpha_1 w_1 + \alpha_2 w_2 + \dots + \alpha_6 w_6 \mid 0 < \alpha_i < 1\})$, is identical with the Penrose pattern.

The definition (6) shows that \mathcal{Q}_λ can be defined in terms of a 6D space by using the same decomposition as in the Penrose case. Therefore \mathcal{Q}_λ seems to have almost the same location of peaks in the calculated diffraction pattern as the Penrose pattern, but with different intensities. We think that the frequency of occurrence of the fully occupied icosahedra may be much higher in \mathcal{Q}_λ than in the Penrose pattern.

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