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QUASILATTICES IN $\mathbb{E}^3$ AND THEIR PROJECTION FROM LATTICES IN $\mathbb{E}^n$

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Abstract - Theoretical studies are reported on the structure of non-periodic quasilattices associated with the icosahedral group. The construction is based on dualization and projection of lattices and on induction and subduction of group representations.

I - INTRODUCTION

This report deals with theoretical studies /1−5/ of non-periodic space fillings and quasilattices obtained by projection of high-dimensional hypercubic lattices to $\mathbb{E}^3$. These studies are concentrated on groups and in particular on the icosahedral group $A(5)$. The work was stimulated by the paradigm of non-periodic 2-dimensional patterns given by Penrose /6/, by the algebraic theory of these patterns developed by de Bruijn /7/, and by the proposal of Mackay /8/ to use two rhombohedral cells in $\mathbb{E}^3$ as a basis for non-periodic 3-dimensional crystallography.

In abstract terms, traditional crystallography deals with the action of space groups on Euclidean space. The space groups have a non-trivial translation subgroup and hence give rise to periodic lattices. What then is the group theory and crystallography of non-periodic quasilattices in $\mathbb{E}^3$, and how does it relate to traditional crystallography?

These questions require full attention through the remarkable experimental discovery of solid matter phases of AlMn by Shechtman, Blech, Gratias and Cahn /9/. We cannot give here an account of the relevant contributions following this work, compare /10/, and return to a brief survey of theoretical work carried out in cooperation with Haase, Kramer, Lalvani and Mackay.

II - THE HYPERCUBIC LATTICE IN $\mathbb{E}^n$ AND ITS PROJECTION TO $\mathbb{E}^3$.

In the Euclidean space $\mathbb{E}^n$ consider an orthonormal basis $\mathbf{b}_1, \ldots, \mathbf{b}_n$ and its dual $\mathbf{b}_1^*, \ldots, \mathbf{b}_n^*$,

$$\mathbf{b}_i^* \cdot \mathbf{b}_j = \delta_{ij}, \quad i, j = 1, \ldots, n.$$ 

The hypercubic lattice $Y$ is the lattice invariant under the translation group $T$ whose elements are generated by the starred basis. Its cells are the fundamental domains or transversals on $\mathbb{E}^n$ under the action of $T$. By use of the basis $\mathbf{b}_1^*, \ldots, \mathbf{b}_n^*$, the points of a cell with index system $(k_1, \ldots, k_n)$, $k_j = \pm 1, \pm 3, \ldots$
may be characterized as
\[ \{ y | \frac{1}{2}(k_1-2) \leq y \cdot b_1 < \frac{1}{2}k_1, \ i = 1, \ldots, n \}. \]
Upon choosing a fixed shift vector \( \gamma \) and decomposing \( \gamma \) as \( \gamma = x + \gamma \),
we speak of a cell referred to the shift vector \( \gamma \) as
\[ \{ x | \frac{1}{2}(k_1-2) \leq (x + \gamma) \cdot b_1 < \frac{1}{2}k_1, \ i = 1, \ldots, n \}. \]
Consider for \( 1 \leq q < n \) an orthogonal decomposition of the space \( \mathbb{R}^n \),
\[ \mathbb{R}^n = \mathbb{R}^q + \mathbb{R}^{n-q}, \quad \mathbb{R}^q \perp \mathbb{R}^{n-q} \]
and of the vectors
\[ \gamma = x_1 + x_2, \quad x = x_1 + x_2. \]
The cell with given index system intersects with \( \mathbb{R}^q \) if there is a point \( x_1, \gamma = x_1 + \gamma \) such that
\[ \frac{1}{2}(k_1-2) \leq (x_1 + \gamma) \cdot b_1 < \frac{1}{2}k_1, \ i = 1, \ldots, n. \]
Introducing the projections
\[ b_{11}, \ldots, b_{n1} \]
of the basis vectors from \( \mathbb{R}^n \) to \( \mathbb{R}^q \) and the numbers \( y_i = (\gamma \cdot b_i) \), these equations determine in \( \mathbb{R}^q \) an \( n \)-grid \( Y_1 \) whose cells are formed by intersections of \( n \) hyperplanes orthogonal to the vectors just specified and shifted by the numbers \( y_i \),
\[ \frac{1}{2}(k_1-2) \leq x_i \cdot b_{1i} + y_i < \frac{1}{2}k_1, \ i = 1, \ldots, n. \]
A dual lattice or quasilattice \( Z_1 \) is formed in \( \mathbb{R}^q \) by associating to any hyperface with fixed index \( j \) of a cell of \( Y_1 \) a dual edge corresponding to the vector \( b_{j1} \). Upon decomposing the shift vector as
\[ \gamma = Y_1 + Y_2 \]
the part of this vector in \( \mathbb{R}^q \) amounts to an overall shift of the quasilattice whereas the complementary part determines the structure of the quasilattice.
This construction described in /2/ is modified in /11/. There we determine in the space \( \mathbb{R}^n \) the duals to the \( p \)-boundaries of a cell which intersects with the subspace \( \mathbb{R}^q \) and then construct the standard dual \((n-p)\)-boundaries in \( \mathbb{R}^n \) which form a quasilattice in \( \mathbb{R}^n \). This quasilattice \( Z \) is then projected to \( \mathbb{R}^q \). This modified approach uses standard crystallographic dualization in \( \mathbb{R}^n \) throughout.

III - GROUP ANALYSIS FOR THE PROJECTION
The lattice \( Y \) in \( \mathbb{R}^n \) has as its full space group the semidirect product group
\[ T \rtimes \Omega(n) \]
where \( \Omega(n) \) is the hyperoctahedral point group. This latter group contains all permutations of the symmetric group \( S(n) \) and all reflections
\[ b_i^* = \varepsilon_i b_i^*, \quad \varepsilon_i = \pm 1. \]
Given a subgroup \( H \subset \Omega(n) \), the representation of \( \Omega(n) \) in \( \mathbb{R}^n \) subduces irreducible representation spaces of \( H \) which may serve as candidates for \( \mathbb{R}^q \). The projection from \( \mathbb{R}^n \) to \( \mathbb{R}^q \) then commutes with the action of \( H \). This construction is applied in /2/ to various groups and leads
to periodic and non-periodic space fillings and (quasi-)lattices, compare Table 1.

Table 1 Examples for the projection $\mathbb{E}^n \rightarrow \mathbb{E}^q + \mathbb{E}^{n-q}$

<table>
<thead>
<tr>
<th>n</th>
<th>q</th>
<th>space group</th>
<th>point group</th>
<th>subgroup</th>
<th>$\mathbb{E}^q + \mathbb{E}^{n-q}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>2</td>
<td>$T(n)A\Omega(n)$</td>
<td>$\Omega(n)$</td>
<td>$S(n)$</td>
<td>$\mathbb{E}^2 + \mathbb{E}^1$</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>$T(4)A\Omega(4)$</td>
<td>$\Omega(4)$</td>
<td>$T_d S(4)$</td>
<td>$\mathbb{E}^3 + \mathbb{E}^1$</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>$T(5)A\Omega(5)$</td>
<td>$\Omega(5)$</td>
<td>$C(5)$</td>
<td>$\mathbb{E}^2 + \mathbb{E}^2 + \mathbb{E}^1$</td>
</tr>
<tr>
<td>6</td>
<td>3</td>
<td>$T(6)A\Omega(6)$</td>
<td>$\Omega(6)$</td>
<td>$A(5)$</td>
<td>$\mathbb{E}^3 + \mathbb{E}^3$</td>
</tr>
</tbody>
</table>

IV - GROUP AND SUBGROUP ANALYSIS FOR QUASILATTICES ASSOCIATED WITH THE ICOSAHEDRAL GROUP

Since the icosahedral group $A(5)$ is not compatible in $\mathbb{E}^3$ with translational symmetry, this group is an interesting candidate for the group $H$ considered in section III. In /12/ we investigate spaces $\mathbb{E}^n$ which arise in this way. The dihedral subgroups $D(m)$, $m = 5, 3, 2$ of $A(5)$ are employed to establish the chain of point groups $D(m) < A(5) < \Omega(60/(2m))$, $m = 5, 3, 2$.

Representation theory of these groups shows that the irrep $|31^2|$ of $A(5)$ contains the non-trivial 1-dimensional representations of the dihedral groups which we denote by $\hat{c}$. This representation of $D(m)$ induces an orthogonal representation of dimension $n = |A(5)|/|D(m)| = 60/(2m) = 6, 10, 15$.

By construction, this representation yields an embedding of $A(5)$ into $\Omega(60/(2m))$. Moreover the construction assures that the subduction from $\Omega(60/(2m))$ contains the 3-dimensional representation $|31^2|$ of $A(5)$. If the 3-dimensional subspace for this representation is chosen for the projection, one obtains three types of quasilattices associated with the icosahedral group. In /12/ we analyze all the composite and elementary cells for these quasilattices. For the cases $n = 6, 10$ and 15, the number of elementary rhombohedra is 2, 5 and 14 respectively.
Table 2 Subduction of irreducible representations from A(5) to D(m).

A(5):

| 5 | 32 | 31^2_+ | 31^2_- |

D(5):

| o | 0 | 0 | 1 | 1 |

| 1 | 0 | 1 | 1 | 0 |

| 2 | 0 | 1 | 1 | 0 |

D(3):

| o | 1 | 1 | 1 | 0 | 0 |

| 0 | 1 | 0 | 1 | 1 |

| 1 | 0 | 1 | 2 | 1 | 1 |

D(2):

| o | 1 | 1 | 2 | 0 | 0 |

| 0 | 1 | 1 | 1 | 1 |

| 1 | 0 | 1 | 1 | 1 |

| 1 | 0 | 1 | 1 | 1 |

V - THE QUASILATTICE ASSOCIATED WITH D(5) < A(5) < O(6)

This quasilattice is constructed in /2/ and analyzed in more detail in /3/. We briefly describe the main features. The hypercubic lattice is given in \( \mathbb{E}^6 \), and the embedding D(5) < A(5) < O(6) in terms of the analysis given in /12/ is obtained by inducing from D(5). In the reduction to A(5) one finds the two irreps

\[ |31^2_+|, |31^2_-| \]

in the notation of Table 2. These 3-dimensional representations yield two orthogonal subspaces

\( \mathbb{E}^3_1, \mathbb{E}^3_2 \)

of the initial space \( \mathbb{E}^6 \). The projection of the hypercubic lattice from \( \mathbb{E}^6 \) to \( \mathbb{E}^2 \) yields a hexagrid whose planes are parallel to six pairs of faces of the regular dodecahedron. The elementary dual cells are two rhombohedra discussed already by Kowalewski /13/ in relation to the rhombic triacontahedron found by Kepler /14/. Mackay /8/ introduced these cells as candidates for a quasilattice in \( \mathbb{E}^3 \).

The quasilattice contains composite cells in the form of three zonohedra with 12, 20, and 30 rhombus faces /3/. Another characteristic of the quasilattice is the existence of infinite 2-dimensional layers consisting of packed rhombohedral cells. Any cell in this layer has four edges vertical to a pair of faces of the regular dodecahedron.

Six sets of parallel systems of layers continue through the full quasilattice.

The quasilattice can be described as a set of

\[ \{6\} = 20 \]

interpenetrating periodic lattices. Each sublattice is based on 3 of the six vectors perpendicular to the faces of the dodecahedron. It contains the corresponding rhombus cells whose center is distorted from the average periodic position.

The shift vector \( Y \) is analyzed in /3/ with respect to the structure of the quasilattice. This analysis is carried out in the complementary space \( \mathbb{E}^3_1 \) and it is considerably extended in /11/. It is shown that the vector \( Y \), is confined to the interior of a Kepler zone, defined as the interior of a triacontahedron.
For any vertex in the quasilattice there is a corresponding vertex in the Kepler zone, and the vertices in this zone can be connected to form an infinite graph $K$. The continuation of this graph is completely determined by the diagnosis of this vertex in the Kepler zone, and so the graph contains all the information on the matching rules for the quasilattice. An example of a graph is given in Fig. 1.

Fig. 1. Part of a graph $K$ in the Kepler zone. The Kepler zone is the interior of a triacontahedron. This triacontahedron is shown here in a projection along a 2-fold axis. The open circles mark points which form the vertices of the graph $K$ and are connected by edge lines. The graph contains 32 vertices which are projections of vertices of the hypercube in $E^6$. The broken line indicates the continuation of the infinite graph $K$ to a new set of points. To this graph there corresponds a quasilattice with icosahedral point symmetry. It contains a central triacontahedron whose faces are covered by 30 rhombic dodecahedra.

The diffraction from the quasilattice has been studied in an approximation where there is one scattering center at each vertex. A simple long-range approximation is obtained from the description in terms of 20 sublattices $/3, 4, 5/*. The interference of contributions from different sublattices yields strong maxima of the intensity at positions determined by the Fibonacci numbers.

In the same approximation of one center per vertex, projections of the quasilattice have been computed along the 5-, 3-, and 2-fold axis. Results are shown in Figs. 2-4. These computed results show many features of experimental results obtained by Urban and collaborators $/15*/$. 
Fig. 2. Projections of points on vertex positions of the quasi-lattice into a plane along the 5-fold axis.

Fig. 3. Projection of points on vertex positions of the quasi-lattice into a plane along the 3-fold axis.
Projection of points on vertex positions of the quasi-lattice into a plane along the 2-fold axis.

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COMMENTS AFTER THE P. KRAMER TALK:

M.V. JARIC.-

Suggested "standard" orientations of the icosahedra in the physical, $\mathbb{R}_3$, and complementary, $\mathbb{R}_3^\perp$, spaces.
Remark:

Since several recent papers on icosahedral quasicrystals all use different orientations of the reference icosahedra in the two three-dimensional complements of the six-dimensional hyperspace, and since transformations of the relevant tensorial quantities from one coordinate system to another might be quite complicated, I suggest that we standardise the orientation of these icosahedra in a similar way that the orientation of a cube is typically taken to have coordinate axes as the four-fold axes. I recommend that we use the fact that the tetrahedral group is a subgroup of the icosahedral group and that the two inequivalent three dimensional representations of the icosahedral group both subduce the same three dimensional vector representation of the tetrahedral group. A simple standard orientation of a tetrahedron is the one in which its two-fold axes coincide with the coordinate axes. The two icosahedra are then oriented so that they contain the tetrahedron in the way shown in the enclosed figure. In this way, we can, for example, construct relevant icosahedral tensors by building from the tetrahedral tensors which are particularly simple in the given orientation.