Quasicrystallography from $B_n$ lattices

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Abstract. We present a group theoretical analysis of the hypercubic lattice described by the affine Coxeter-Weyl group $W_\infty (B_n)$. An $h$-fold symmetric quasicrystal structure follows from the hypercubic lattice whose point group is described by the Coxeter-Weyl group $W_\infty (B_n)$ with the Coxeter number $h=2n$. Higher dimensional cubic lattices are explicitly constructed for $n=4,5,6$ by identifying their rank-3 Coxeter subgroups and maximal dihedral subgroups. Decomposition of their Voronoi cells under the respective rank-3 subgroups $W(A_1)$, $W(H_2)\times W(A_1)$ and $W(H_3)$ lead to the rhombic dodecahedron, rhombic icosahedron and rhombic triacontahedron respectively. Projection of the lattice $B_4$ describes a quasicrystal structure with 8-fold symmetry. The $B_5$ lattice leads to quasicrystals with both 5-fold and 10-fold symmetries. The lattice $B_6$ projects on a 12-fold symmetric quasicrystal as well as a 3D icosahedral quasicrystal depending on the choice of subspace of projections. The projected sets of lattice points are compatible with the available experimental data.

1. Introduction
The first discovery of the icosahedral quasicrystal by D. Shechtman [1] attracted a lot of interest on the quasicrystallography. The 3D quasicrystals can be described by the Coxeter group $W(H_3)$ representing the icosahedral symmetry of order 120. The 2D quasicrystals exhibit 5-fold, 8-fold, 10-fold, 12-fold, and 18-fold symmetries [2, 3, 4, 5, 6]. Lubin and his collaborators [7] reported recently that a quasicrystallographic structure with 36-fold symmetry is possible. It seems there is no limitation on the order of the planar point symmetry of the quasicrystallography which can be described by the dihedral groups. This reminds us the classification of the Coxeter-Weyl groups with different Coxeter numbers $h$ [8, 9, 10, 11]. Every Coxeter-Weyl group has a dihedral subgroup $D_h$ of order $2h$. We illustrate relations between the affine Coxeter groups $W_\infty (B_n)$ and the $h$-fold symmetric quasicrystallography obtained from higher dimensional cubic lattices by orthogonal projections. A general projection technique of the higher dimensional cubic lattice has been proposed by Duneau and Katz [12] but without any discussion on the group theoretical aspects of the lattices.

The five-fold symmetric 2D quasicrystals as well as quasicrystals with icosahedral symmetry have been studied in the references [13, 14, 15, 16]. More elaborate discussions on the quasicrystal structures can be found in the set theoretic approach initiated by Yves Meyer [17,18] and later developed as Model Set by Robert V. Moody [19,20].

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The Lie group applications derived from the root systems of the Coxeter-Weyl groups are well known by the high energy physicists. The standard model of the High Energy Physics described by the Lie group $SU(3)\times SU(2)\times U(1)$ [21, 22, 23] is based on the Coxeter-Weyl group $W(A_1)\times W(A_1)$. The Grand Unified theories, $SU(5)\approx E_6$ [24], $SO(10)\approx E_7$ [25] and the exceptional group $E_6$ [26] depend on the respective Coxeter-Weyl groups $W(A_1)$, $W(D_4)$, and $W(E_6)$. One may assume that some of the Coxeter-Weyl groups may play an important role in the study of $h$-fold symmetric quasicrystallography. The argument goes as follows.

Every Coxeter group with a Coxeter number $h$ has a maximal dihedral subgroup $D_h$ of order $2h$ which acts in the Coxeter plane. In two recent papers [27, 28] it was proposed that a quasicrystallographic structure with $h$-fold symmetry can be determined by projections of the higher dimensional lattices onto the Coxeter planes. The Coxeter groups are characterized by their Coxeter exponents [8, 11]. This paper will study the general structure of the root lattice of the affine Coxeter group $W_\infty(B_n)$ which is the simple cubic lattice in $nD$ Euclidean space with the point symmetry determined by the Coxeter-Weyl group $W(B_n)$ of order $2^n n!$. The projections of the 5D cubic lattice onto a plane and the 6D cubic lattice into a 3D subspace have been studied earlier without using Coxeter group techniques [12, 29]. Projections of some 4D root lattices have been also studied earlier [30, 31, 32].

The paper is organized as follows. Section 2 deals with the general structure of the Coxeter-Weyl group $W(B_n)$ by identifying its maximal subgroups which could be useful for the projections of the hypercubic lattices. In Section 3 we study the rank-3 subgroups of the Coxeter-Weyl groups $W(B_3)$, $W(B_4)$, and $W(B_5)$ and projections of some of their polytopes into 3D Euclidean spaces. The projection of the Voronoi cell of the lattice $W(B_n)$ plays a crucial role in the description of the quasicrystallographic structures in 3D and 2D. Section 4 is devoted to the projection techniques of the lattices onto the Coxeter planes and the projection of the 6D cubic lattice into 3D subspace with icosahedral symmetry. Our predictions are confronted with experimental data in Section 5 and some conclusive remarks are added.

2. The Coxeter-Weyl group $W(B_n)$ and its Maximal Subgroups

The Coxeter-Weyl groups are well known [8, 9, 10, 11]. The classification includes an infinite series of crystallographic groups $A_n$, $B_n$, $C_n$, $D_n$, and a finite number of crystallographic exceptional groups $G_2$, $F_4$, $E_6$, $E_7$, $E_8$. Moreover, there are an infinite number of noncrystallographic dihedral Coxeter groups $I_\infty(h)$ ($h\geq 5$, $h\neq 6$) including two rank-3 and rank-4 noncrystallographic Coxeter groups $W(H_3)$ and $W(H_4)$ respectively. In this section we study the Coxeter-Weyl group $W(B_n)$ of rank $n$. It is represented by the Coxeter-Dynkin diagram shown in figure 1.

![Coxeter-Dynkin diagram](image)

**Figure 1.** Coxeter-Dynkin diagram of the Coxeter-Weyl group $W(B_n)$.

From left to right the nodes represent the long simple roots $\alpha_i$ ($i = 1, 2, \ldots, n - 1$) with norm $\sqrt{2}$ and the last simple root $\alpha_n$ is the short root with norm 1. Angle between any two adjacent simple roots with norm $\sqrt{2}$ is $120^\circ$ and the angle between the last two simple roots is $135^\circ$. Any two disconnected roots
are orthogonal to each other. The nodes also denote the reflection generators \( r_i \) whose action on an arbitrary vector \( \Lambda \) in the \( n \)-dimensional Euclidean space is given by

\[
    r_i \Lambda = \Lambda - \frac{2(\Lambda, \alpha_i)}{(\alpha_i, \alpha_i)} \alpha_i .
\]

The dual space of the root space is represented by the weight vectors \( \omega_i \) defined by

\[
    (\omega_i, \frac{2\alpha_i}{(\alpha_i, \alpha_i)}) = \delta_j .
\]

The Cartan matrix of the root space (Gram matrix) and the metric tensor in the dual space are defined respectively by the matrix elements

\[
    A_{ij} = \frac{2(\alpha_i, \alpha_j)}{(\alpha_j, \alpha_j)}, \quad G_{ij} = (\omega_i, \omega_j) = (A^{-1})_{ij} \frac{(\alpha_i, \alpha_j)}{2} .
\]

Let \( l_i (i=1,2,\ldots,n) \) denote the set of orthonormal vectors \( (l_i, l_j) = \delta_j \) in \( n \)-dimensional Euclidean space. The simple roots of \( \Lambda \) can be written as

\[
    \alpha_1 = l_1 - l_2, \alpha_2 = l_2 - l_3, \ldots, \alpha_{n-1} = l_{n-1} - l_n, \alpha_n = l_n .
\]

The root system consists of \( 2n \) short roots \( \pm l_i \) and \( 2(n-1) \) long roots \( \pm l_i \pm l_j (i \neq j) \). Reflection generators \( r_i \) act on the unit vectors as follows

\[
    r_i : l_1 \leftrightarrow l_2, r_2 : l_2 \leftrightarrow l_3, \ldots, r_{n-1} : l_{n-1} \leftrightarrow l_n, r_n : l_n \rightarrow -l_n .
\]

It is implicit that the reflection generators leave the other unit vectors (not shown) invariant. The weight vectors can be determined from \( \omega_i = (A^{-1})_{ij} \alpha_j \) as

\[
    \omega_1 = l_1, \omega_2 = l_1 + l_2, \ldots, \omega_{n-1} = l_1 + l_2 + \cdots + l_{n-1}, \omega_n = \frac{1}{2}(l_1 + l_2 + \cdots + l_n) .
\]

The highest weight vector \([33]\) in the weight space can be defined as

\[
    \Lambda = a_1 \omega_1 + a_2 \omega_2 + \cdots + a_n \omega_n \equiv (a_1, a_2, \ldots, a_n) \text{ with integer coefficients } a_i \geq 0 .
\]

An orbit of \( \Lambda \) under the group \( \Lambda \) will be denoted by \( \Lambda \) \( (B_n) \Lambda \equiv (a_1 a_2 \ldots a_n)_{B_n} \). With this notation, e.g., the orbits \((100\ldots0)_{B_n} = \pm l_1 \) and \((010\ldots0)_{B_n} = \pm l_1 \pm l_2 \) \((i \neq j)\) represent the sets of short roots and long roots respectively. The orbit \((00\ldots01)_{B_n} = \frac{1}{2}(\pm l_1 \pm l_2 \pm \cdots \pm l_n) \) represents the vertices of a cube in \( n \)-dimensional Euclidean space. We point out that the group \( \Lambda \) represents also the group obtained from the Coxeter-Dynkin diagram \( C_n \) where the short and long roots are represented by the roots \( \alpha_1 = l_1 - l_2, \alpha_2 = l_2 - l_3, \ldots, \alpha_{n-1} = l_{n-1} - l_n, \alpha_n = 2l_n \). Certain maximal subgroups of \( \Lambda \) can be useful in the study of quasicrystals. One of the maximal subgroup of the group \( \Lambda \) is the Coxeter-Weyl group \( \Lambda \) \( (D_n) \) with the Coxeter-Dynkin diagram given in figure 2. It consists of only long roots of norm \( \sqrt{2} \).

![Figure 2. Coxeter-Dynkin diagram of \( \Lambda \) \( (D_n) \)](image)

Denote by \( r_i' \) the reflection generators of \( \Lambda \) \( (D_n) \) and the simple roots by

\[
    \alpha_1', \alpha_2', \ldots, \alpha_{n-1}', \alpha_n' .
\]
The Coxeter-Dynkin diagram of $\Gamma$ with $(8)$ and the Coxeter element $a$. Define the generators decompose in such a way that the corresponding represents a rotation of order $2$. This is the dihedral group $D_4$ and $S_3$ of order 6. The automorphism group is then the group $Z_2$ generated by $\gamma$. There is one exception to this general result: the automorphism group of $D_4$ is larger than $W(B_n)$ since its Dynkin diagram symmetry is isomorphic to the symmetric group $S_3$ of order 6. The automorphism group is then the group $Aut(D_4) \approx W(D_4):Z_2 \approx W(D_n)$ where the group $Z_2$ is generated by $\gamma$. We note that the orbit $(00\ldots01)_{B_n}$ is the union of two orbits of $W(D_n)$.

The normal number $1$ is larger than $2$. One can choose a convenient set of orthogonal unit vectors obtained from the eigenvectors of the Cartan matrix $27, 28, 36$.

The root lattice is the simple cubic lattice which is invariant under the affine Coxeter group $W(B_n)$ that can be generated by adding a generator $r_0$ to the set of generators of the group $W(B_n)$.

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The generator $r_0$ represents a reflection with respect to the hyperplane bisecting the highest long root $\alpha_i = \omega_0 = l_1 + l_2$. Its action on an arbitrary vector is a translation.

A general vector of the root lattice then will be given by $v = \alpha_1 + \alpha_2 + \cdots + \alpha_n$. This indicates that a general vector of the lattice is the linear combinations of the unit vectors $l_i$ with integer coefficients. The primitive cell of the lattice can be chosen as the cube with the vertices $\alpha'_1 = l_1 - l_2, \alpha'_2 = l_2 - l_3, \ldots, \alpha'_{n-1} = l_{n-1} - l_n, \alpha'_n = l_{n-1} + l_n. \quad (6)$

The first $n-1$ simple roots are identical to the simple roots of the group $W(B_n)$. The generators of $W(D_n)$ transform the unit vectors as in (4) but the last generator differs in its action

$$r'_1 : l_1 \leftrightarrow l_2, r'_2 : l_2 \leftrightarrow l_3, \ldots, r'_{n-1} : l_{n-1} \leftrightarrow l_n, r'_n : l_{n-1} \leftrightarrow -l_n. \quad (7)$$

Then one can identify $r'_i = r_i$ for $(i = 1, 2, \ldots, n-1)$ and $r'_n = r_0$. The Coxeter-Dynkin diagram of $W(D_n)$ has a diagram symmetry $\gamma : \alpha'_{n-1} \leftrightarrow \alpha'_n$ which transforms $\gamma : l_n \rightarrow -l_n$ leaving the other unit vectors invariant and can be identified with $r_n$. It follows that the automorphism group of $D_4$ is $\text{Aut}(D_4) \approx W(D_4):Z_2 \approx W(D_n)$ where the group $Z_2$ is generated by $\gamma$. There is one exception to this general result: the automorphism group of $D_4$ is larger than $W(B_n)$ since its Dynkin diagram symmetry is isomorphic to the symmetric group $S_3$ of order 6. The automorphism group is then the group $Aut(D_4) \approx W(D_4):Z_2 \approx W(B_n)$. This is known as the triality of the $D_4$ symmetry. We note that the orbit $(00\ldots01)_{B_n}$ is the union of two orbits of $W(D_n)$.

The root lattice is the simple cubic lattice which is invariant under the affine Coxeter group $W(B_n)$ that can be generated by adding a generator $r_0$ to the set of generators of the group $W(B_n)$. The generator $r_0$ represents a reflection with respect to the hyperplane bisecting the highest long root $\alpha_i = \omega_0 = l_1 + l_2$. Its action on an arbitrary vector is a translation.
There are $2^n$ such cubes sharing the origin as a vertex. The Voronoi cells around the lattice points are congruent polytopes tiling the $n$-dimensional Euclidean space. The Voronoi cells of lattices are important in the theory of coding [37]. Denote by $V(0)$ the Voronoi cell around the origin. The vertices of the Voronoi polytope $V(0)$ can be determined as the intersection of the hyperplanes surrounding the origin. They are the hyperplanes determined as the orbits of the fundamental weights \( \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \) \( \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \) \( \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \) \( \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \) \( \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \, \, \mathbf{2} \, \, \mathbf{1} \).

The Voronoi polytope $V(0)$ is then a cube around the origin with the vertices \( (00\ldots01) \) \( (00\ldots01) \) \( (00\ldots01) \) \( (00\ldots01) \) \( (00\ldots01) \).

We emphasize here that the lattices generated by the affine Coxeter-Weyl group $W_u(C_n)$ are identical to the root and weight lattices of the Coxeter-Weyl group $W_u(D_n)$ [37]. The group $\text{Aut}(D_n) \approx W(C_n)$ should be taken into account when the point symmetry of the two lattices is of concern. Therefore in an $n$-dimensional Euclidean space with $n > 3$ one can construct five different lattices with affine Coxeter-Weyl groups, two for $W_u(A_n)$, two for $W_u(D_n)$, and the other is the simple cubic lattice described by $W_u(B_n)$. When $n$ coincides with the rank of the exceptional groups the number of lattice will be more than 5. The projection of the lattice onto the principal planes is nothing other than determination of the components of lattice vectors in the principal planes defined by the pairs of unit vectors \( (\hat{x}_1, \hat{x}_n), (\hat{x}_2, \hat{x}_{n-1}), \ldots \). Here the plane determined by the vectors \( (\hat{x}_1, \hat{x}_n) \) is known as the Coxeter plane. Note that for odd $n$ one of the unit vectors is unpaired that represents the direction orthogonal to all principal planes. The representations of the generators $R_1$ and $R_2$ of the dihedral subgroup can be put into block-diagonal matrices with $2 \times 2$ and/or $1 \times 1$ matrix entries. The component of the simple cubic lattice vector in the basis of $\hat{x}_i$ is given by

$$p_i = \frac{1}{\sqrt{h_{\hat{x}_i}}}(\sum_{j=1}^{n-1} a_j X_j + 2a_n), \ a_n \in \mathbb{Z}.$$  

This introduction on the hypercubic lattice will be useful in the following chapters where we study the 8-fold, 5-fold, 10-fold, and 12-fold symmetric quasicrystal structures induced by the projections of the lattices $B_4, B_5, \text{ and } B_6$.

**3. The Coxeter-Weyl groups $W(B_4), W(B_5), W(B_6)$ and projections of their polytopes into 3D subspaces**

The Voronoi cells of the root lattices of the Coxeter-Weyl groups $W(B_4), W(B_5), \text{ and } W(B_6)$ are projected on the rhombic dodecahedron, rhombic icosahedron, and rhombic triacontahedron respectively. A similar work, not in the context of the affine Coxeter groups, has been studied earlier by [40].

**3.1 The Coxeter-Weyl group $W(B_4)$ and projection of its fundamental polytopes into a 3D subspace with octahedral symmetry**

The vertices of the fundamental polytopes of the group $W(B_4)$ are given by
The first one represents the short roots of $W(B_4)$ which constitutes a 4D octahedron with 8 vertices whose facets (3-faces) are tetrahedra. The second polytope consists of 24 long roots as vertices and is known as the 24-cell with octahedral facets. Its full symmetry is the Coxeter-Weyl group $W(F_4)$ which embeds $W(B_4)$ as a subgroup with index 3. The third polytope with 32 vertices has two types of facets: tetrahedra and truncated octahedra. The last one is the 4D cube with 16 vertices consisting of the cubic facets.

The subspace we are interested in here is a 3D Euclidean space with the octahedral symmetry represented by the Coxeter-Weyl group $W(B_3)$ of order 48. Let us recall the isomorphism $W(B_3)$ $\cong Aut(D_4)$ $\cong Aut(A_4)$ = $W(A_3) : \mathbb{Z}_2$. Here one can choose the tetrahedral symmetry as the Coxeter-Weyl group $W(D_3)$ $\cong W(A_3)$ = $\langle r_1, r_2, r_3 \rangle$. The Dynkin diagram symmetry $\mathbb{Z}_2$ generated by $\gamma$ which permutes the unit vectors as $(l_1 \leftrightarrow l_2)$ and $l_3 \leftrightarrow l_4$ extends the group to the octahedral symmetry. It is clear that the vector $\frac{1}{2}(l_1 + l_2 + l_3 + l_4)$ is invariant under the octahedral subgroup. It is convenient to introduce a new set of orthonormal vectors defined by

$$
t_0 = \frac{1}{2}(l_1 + l_2 + l_3 + l_4), \quad t_1 = \frac{1}{2}(l_1 - l_2 + l_3 - l_4),$$

$$
t_2 = \frac{1}{2}(-l_1 + l_2 + l_3 - l_4), \quad t_3 = \frac{1}{2}(l_1 + l_2 - l_3 - l_4).$$

(15)

When the vectors in (14) are expressed in terms of the vectors $t_0, t_1, t_2,$ and $t_3$, it will be simpler to identify the 3D vertices of the 4D polytopes. The 4D octahedron projects onto a cube in 3D with the vertices $\frac{1}{2}(\pm t_1 \pm t_2 \pm t_3)$. The 24-cell projected into the 3D space represents two octahedra as well as one cuboctahedron. The polytope with 32 vertices is projected into one cube and two truncated tetrahedra.

The polytope $(0001)_{B_4}$ is more interesting since it constitutes the Voronoi cell of the 4D cubic lattice. When expressed in terms of the unit vectors $t_0, t_1, t_2,$ and $t_3$ and the component of an arbitrary vector along $t_0$ is deleted they will decompose under the octahedral group as two orbits, one with the vertices $(\pm t_1, \pm t_2, \pm t_3)$ representing the vertices of an octahedron and the other with vertices $\frac{1}{2}(\pm t_1 \pm t_2 \pm t_3)$ representing a cube. Union of these two orbits represents a rhombic dodecahedron with 14 vertices as shown in figure 3.
3.2 Projection of fundamental polytopes of the group $W(B_5)$ into 3D subspace with $W(H_2) \times C_2 \approx D_{10}$ symmetry

One of the fundamental orbits of the group $W(B_5)$ is the polytope $(10000)_{B_5} = \pm l_i (i = 1, 2, ..., 5)$ which represents an octahedron in 5D Euclidean space whose facets are 5-cells (4-simplexes). Its projection into a 3D space represents a pentagonal antiprism. To understand this better we have to define a new set of orthonormal vectors $\hat{\mathbf{x}}_i (i = 1, 2, ..., 5)$. The first four unit vectors $\hat{\mathbf{x}}_i (i = 1, 2, ..., 4)$ is obtained by using the eigenvectors of the Cartan matrix of $W(A_4)$ and the fifth vector is chosen to be orthogonal to the rest [36]

$$
\hat{\mathbf{x}}_1 = \frac{1}{\sqrt{2(2 + \sigma)}} (\alpha_1 + \tau \alpha_2 + \tau \alpha_3 + \alpha_4),
$$
$$
\hat{\mathbf{x}}_2 = \frac{1}{(2 + \sigma)\sqrt{2}} (\alpha_1 - \sigma \alpha_2 + \sigma \alpha_3 - \alpha_4),
$$
$$
\hat{\mathbf{x}}_3 = \frac{1}{\sqrt{2(2 + \tau)}} (\alpha_1 + \sigma \alpha_2 + \sigma \alpha_3 + \alpha_4),
$$
$$
\hat{\mathbf{x}}_4 = \frac{1}{(2 + \tau)\sqrt{2}} (\alpha_1 - \tau \alpha_2 + \tau \alpha_3 - \alpha_4),
$$
$$
\hat{\mathbf{x}}_5 = \frac{1}{\sqrt{5}} (\alpha_1 + 2\alpha_2 + 3\alpha_3 + 4\alpha_4 + 5\alpha_5).
$$

(16)

The unit vectors $l_i$ can be expressed as a linear combination $l_i = \sum_{j=1}^{5} b_{ij} \hat{\mathbf{x}}_j$ where the matrix $B$ is given by

$$
B = \frac{1}{\sqrt{|10|}} \begin{pmatrix}
  a & \tau & b & -\sigma & \sqrt{2} \\
  b & \sigma & -a & -\tau & \sqrt{2} \\
  0 & -2 & 0 & 2 & \sqrt{2} \\
 -b & \sigma & a & -\tau & \sqrt{2} \\
 -a & \tau & -b & -\sigma & \sqrt{2}
\end{pmatrix},
$$

(17)

$$
a = \sqrt{2+\tau}, \; b = \sqrt{2+\sigma}, \; \tau = \frac{1+\sqrt{5}}{2}, \; \sigma = \frac{1-\sqrt{5}}{2}.
$$
Here we only discuss the projections of two polytopes \((10000)_{B_i} = \pm l_i \ (i = 1, 2, \ldots, 5)\), and \((00001)_{B_i} = \frac{1}{2}(\pm l_1 \pm l_2 \pm l_3 \pm l_4 \pm l_5)\) into the 3D space described by the symmetry group \(W (H_2) \times C_2 \approx D_{5d}\). The group \(D_{5d}\) is generated by the group elements \(R_1 = r_1 r_2, \ R_2 = r_2 r_3, \ R_3 = (r_3 r_2 r_3)^3\) Here \(R_1\) and \(R_2\) generate the dihedral group \(W (H_2) \approx D_5\) of order 10 and \(R_3 = -I\) where \(I\) is the \(5 \times 5\) unit matrix in the \(l_i\) basis. The center of the group \(W (B_5)\) is represented by the elements \(C_2 = \{I, -I\}\) and therefore it commutes with all the elements of the group. Let us choose the 3D space defined by the set of unit vectors \(\hat{x}_1, \hat{x}_4, \hat{x}_5\). The set of vectors \(\pm l_i\) form a single orbit under the group \(D_{5d}\). The polytope \((10000)_{B_i} = \pm l_i\) projected into 3D space represents a pentagonal antiprism as shown in figure 4.

**Figure 4.** The pentagonal Antiprism.

The polytope \((00001)_{B_i} = \frac{1}{2}(\pm l_1 \pm l_2 \pm l_3 \pm l_4 \pm l_5)\) represents the Voronoi cell of the 5D cubic lattice. The 32 vertices decompose under the group \(D_{5d}\) as \(32 = 2 + 10 + 20\). The first orbit of size 2 represents the vectors \(\pm \frac{1}{2}(l_1 + l_2 + l_3 + l_4 + l_5)\). Each vector is invariant under the dihedral group \(D_5\) but changed to each other under the elements of the center \(C_2\). The next orbit of size 10 consists of the vectors like \(\pm \frac{1}{2}(-l_1 + l_2 + l_3 + l_4 + l_5)\) with one or four negative signs. They also constitute a pentagonal antiprism like the one in figure 4. The orbit of size 20 consists of the vectors with two negative and/or three negative signs. The union of two orbits \(2 + 20\) constitutes a rhombic icosahedron as shown in figure 5.

**Figure 5.** The rhombic icosahedron with the symmetry \(D_{5d}\).

### 3.3 Projections of the \(W (B_5)\) polytopes into 3D subspace with \(W (H_2) \approx I_5\) symmetry
The icosahedral symmetry is the one which describes some quasicrystal structures in 3D. Here we first discuss how the icosahedral symmetry, the Coxeter group $W(H_3) \approx I_h$, can be obtained as a subgroup of the Coxeter-Weyl group $W(D_n)$. We have seen in Section 2 that one of the maximal subgroup of the group $W(D_n)$ is the group $W(D_6)$.

We introduce the generators $R_1 = r_1^6, R_2 = r_2^6, R_3 = r_3^6$. They generate the Coxeter group $W(H_3)$ [41, 42, 43] which in turn can be written as $R_1 = r_1^5, R_2 = r_2^5, R_3 = r_3^6$. They satisfy the relations

$$R_1^2 = R_2^2 = R_3^2 = (R_1 R_3)^5 = (R_2 R_3)^5 = 1$$

leading to the usual generation relations of the icosahedral group $W(H_3) \approx A_5 \times C_2 = I_h$. The generators of the icosahedral group are 6×6 matrices in the space of orthonormal vectors $l_i$ and constitute a reducible representation of the icosahedral group. They can be transformed into block-diagonal forms of 3×3 matrices which act on two sets of orthonormal vectors $(\hat{x}_1, \hat{x}_2, \hat{x}_3)$ and $(\hat{x}_1', \hat{x}_2', \hat{x}_3')$. Each block represents a different 3×3 irreducible matrix representation.

The block-diagonal form of the generators of the Coxeter group $W(H_3)$ induces the relation

$$l_i \left( \begin{array}{c} \hat{x}_1 \\ \hat{x}_2 \\ \hat{x}_3 \\ \hat{x}_1' \\ \hat{x}_2' \\ \hat{x}_3' \end{array} \right) = \frac{1}{\sqrt{2(2 + \tau)}} \left( \begin{array}{cccc} -1 & -\tau & 0 & -\tau & 1 & 0 \\ 1 & -\tau & 0 & \tau & 1 & 0 \\ 0 & -1 & -\tau & 0 & -\tau & 1 \\ 0 & -1 & \tau & 0 & -\tau & -1 \\ -\tau & 0 & -1 & 1 & 0 & -\tau \\ \tau & 0 & -1 & -1 & 0 & -\tau \end{array} \right) \left( \begin{array}{c} \hat{x}_1 \\ \hat{x}_2 \\ \hat{x}_3 \\ \hat{x}_1' \\ \hat{x}_2' \\ \hat{x}_3' \end{array} \right)$$

We also note that one can also construct the generators of the Coxeter group $W(H_3)$ as $R_1 = r_1^5, R_2 = r_2^5, R_3 = r_3^5$, which is obtained from the Dynkin diagram symmetry of $D_6$. Therefore two icosahedral groups are conjugate to each other in the group $Aut(D_6) \approx W(B_6)$.

We discuss now the projections of certain $W(B_6)$ polytopes into 3D subspace with a residual icosahedral symmetry. The polytope with 12 vertices (100000)$_{B_6} = \pm l_i$ representing the short roots of the group $W(B_6)$ is projected into an icosahedron represented by the vectors of norm $\frac{1}{\sqrt{2}} \approx 0.707$ as shown in figure 6.

**Figure 6.** An icosahedron projected from the 6D octahedron (100000)$_{B_6}$. 

9
The long roots of the group $W(B_6)$ are the vertices of the polytope $(010000)_{B_6}$ which are given by the 60 vectors $(010000)_{B_6} = \pm l_i \pm l_j \ (i \neq j)$. When they are projected into 3D space they represent two copies of icosidodecahedra with 30 vertices each; one copy is expanded with respect to the other by a factor of $\tau$. Their norms in 3D are $\sqrt{\frac{2}{2+\tau}} \approx 0.743$ and $\sqrt{\frac{2}{2+\sigma}} \approx 1.203$. The icosidodecahedron is a polyhedron with 30 vertices, 32 faces (20 triangles+12 pentagons) and 60 edges. One of the icosidodecahedron is depicted in figure 7.

Figure 7. Icosidodecahedron projected from the 6D polytope $(010000)_{B_6}$.

The polytope $(000001)_{B_6} = \frac{1}{2}(\pm l_1 \pm l_2 \pm l_3 \pm l_4 \pm l_5 \pm l_6)$ represents the Voronoi cell of the 6D cubic lattice with 64 vertices. They decompose into sets with even (−) sign and odd (−) sign representing two orbits of $W(D_6)$ as mentioned in Section 2. One can demonstrate that each orbit of $W(D_6)$ with 32 vertices decomposes as $32 = 20 + 12$. Normally, the orbits of size 20 and 12 represent a dodecahedron and an icosahedron respectively. Therefore we have two copies of dodecahedron and two copies of classified icosahedron as orbit (I), orbit (II), Orbit (III), and orbit (IV). However, the situation here is such that the dodecahedron (orbit I) and icosahedron (orbit III) form a rhombic triacontahedron, a Catalan solid dual to the icosidodecahedron [44] as shown in figure 8. The union of the icosahedron (orbit II) and dodecahedron (orbit IV) represents a star dodecahedron which is displayed in figure 9.

Figure 8. The rhombic triacontahedron obtained as part of the projection of 6D cube.
The vectors representing the vertices of the icosahedra and dodecahedra have the following norms in decreasing order:

\[
\begin{align*}
N(\text{icosahedron III}) &= \frac{\tau}{\sqrt{2}} \approx 1.144, \\
N(\text{dodecahedron I}) &= \sqrt{0.3(2 + \tau)} \approx 1.042, \\
N(\text{dodecahedron IV}) &= \sqrt{0.3(2 + \sigma)} \approx 0.644, \\
N(\text{icosahedron II}) &= \frac{-\sigma}{\sqrt{2}} \approx 0.438.
\end{align*}
\] (20)

These are exactly the same results obtained earlier by Conway and Knowles [45]. Note also that

\[
\begin{align*}
N(\text{icosahedron III})/N(\text{icosahedron II}) &= \tau^2, \\
N(\text{dodecahedron I})/N(\text{dodecahedron IV}) &= \tau.
\end{align*}
\] (21)

Since the icosahedron obtained from the short roots has a norm 0.707 these three icosahedra follow the ratio: \(1: \tau: \tau^2\). Note also that the vectors \(\pm l_i\), when projected into 3D subspace, form rhombohedra when taken in groups of three. For example the sets of vectors \((l_1, l_2, l_3)\) and \((l_4, l_5, l_6)\) form an acute and an obtuse rhombohedra respectively as shown in figure 10.

Figure 10. The acute and obtuse rhombohedra generated by the vectors \(l_i\).

4. Projections of the lattices of the Coxeter-Weyl groups \(W(B_4), W(B_5),\) and \(W(B_6)\) into subspaces

We decompose the \(nD\) space into two subspaces where \(E_r\) represents the subspace into which the lattice points to be projected and the subspace \(E_\perp\) is the complementary orthogonal subspace. The shift of the Voronoi cell \(V(0)\) along the space \(E_\perp\) creates an open strip and the projection of the Voronoi polytope into the subspace \(E_\perp\) determines a region \(K\). It has been shown in a number of examples that the set of lattice points projected from the open strip onto the subspace \(E_\perp\) determines a quasicrystallographic structure [46, 47, 48]. Now we discuss the projections in the flowing subsections.
4.1 Projection of the lattice points of $B_4$ into a 2D space

We will show here that the projected set of lattice points display a quasicrystal with 8-fold symmetry. The components of a lattice vector $p = a_1a_1 + a_2a_2 + a_3a_3 + a_4a_4 \in \mathbb{Z}$ along the unit vectors $\hat{x}_i$ are given as follows:

$$
p_i = \frac{1}{2\sqrt{2(2 - \sqrt{2} + \sqrt{2})}} (\sqrt{2 - \sqrt{2}} a_1 + \sqrt{2} a_2 + \sqrt{2 + \sqrt{2}} a_3 + 2a_4)
$$

$$
p_4 = \frac{1}{2\sqrt{2(2 + \sqrt{2})}} (-\sqrt{2 - \sqrt{2}} a_1 + \sqrt{2} a_2 - \sqrt{2 + \sqrt{2}} a_3 + 2a_4)
$$

$$
p_2 = \frac{1}{2\sqrt{2(2 - \sqrt{2} - \sqrt{2})}} (-\sqrt{2 + \sqrt{2}} a_1 - \sqrt{2} a_2 + \sqrt{2 - \sqrt{2}} a_3 + 2a_4)
$$

$$
p_3 = \frac{1}{2\sqrt{2(2 + \sqrt{2})}} (\sqrt{2 + \sqrt{2}} a_1 - \sqrt{2} a_2 - \sqrt{2 - \sqrt{2}} a_3 + 2a_4)
$$

Assume now that the subspaces are defined by $E_\parallel = (\hat{x}_1, \hat{x}_4)$ and $E_\perp = (\hat{x}_2, \hat{x}_3)$. If Voronoi cell $V(0) = (0001)_{B_4}$ is projected onto the plane $E_\perp = (\hat{x}_2, \hat{x}_3)$ one obtains a disc of radius $R_0 = \max (p_2^2 + p_3^2)$. When the shifted Voronoi cell $V(\omega) = (0001)_{B_4} + \omega$ is projected into the subspace $E_\perp = (\hat{x}_2, \hat{x}_3)$ the components $(p_2, p_3)$ determines the quasicrystal structure with 8-fold symmetry as shown in figure 11. Similar structures are obtained in a recent paper [49]. The quasicrystal structure with 8-fold symmetry was observed in rapidly solidified Cr$_5$Ni$_3$Si$_2$ and V$_{15}$Ni$_{10}$Si$_2$ alloys [50] which can be represented by the quasicrystal structures like in figure 11.

![Figure 11. The quasicrystal structure obtained from 4D cubic lattice.](image)

4.2 Projection of the lattice $B_5$ into a 2D subspace

Projection of the 5D cubic lattice onto a 2D plane with 5-fold symmetry has been discussed earlier [29] with no reference to the Coxeter-Weyl group $W(B_5)$. As we pointed out in Section 2, the Coxeter number of the group $W(B_5)$ is 10 and has a dihedral subgroup $D_{10}$ of order 20. In this section we will study the projections with both symmetries. The 5-fold symmetric projection of the lattice can be obtained by taking the set of orthogonal vectors given by (16). Projection of the Voronoi cell $V(0)$ into the space defined by the unit vectors $(\hat{x}_2, \hat{x}_3, \hat{x}_4)$ determines the window $K$ which constraints the lattice vectors to be projected onto the plane $(\hat{x}_1, \hat{x}_4)$. When the shifted vector $V(\omega) = (00001)_{B_5} + \omega$
is projected into the subspace \((\hat{x}_2, \hat{x}_3, \hat{x}_5)\) the distribution of the quasicrystallographic lattice structure in the Coxeter plane \((\hat{x}_1, \hat{x}_4)\) is depicted in figure 12. The \(\hat{x}_4\) direction in this case preserves the translational invariance.

Figure 12. 5-fold symmetric quasicrystal structure from projection of the \(W(B_3)\) root lattice.

The 10-fold symmetric quasicrystal structure can be obtained by using the orthonormal vectors in (9). The unit vectors in (9) follow the sequence of the Coxeter exponents \(m_1 = 1, m_2 = 3, m_3 = 5, m_4 = 7, m_5 = 9\). Now the pairs of unit vectors \((\hat{x}_1, \hat{x}_4)\) and \((\hat{x}_2, \hat{x}_4)\) determine the principal planes with the first pair being the Coxeter plane; the first one can be taken as \(E_{II}\) and the second pair as \(E_{\perp}\) and the unit vector \(\hat{x}_5\) defines the direction orthogonal to the planes and preserves the translational invariance. The components of the lattice vectors in the planes and the orthogonal direction are given by

\[
E_{II} : \quad p_1 = \frac{1}{\sqrt{10}} \left( -\sigma a_1 + \sqrt{2 + \sigma} a_2 + \tau a_3 + \sqrt{2 + \tau} a_4 + 2 a_5 \right),
\]

\[
p_2 = \frac{1}{\sqrt{10}} \left( -\tau a_1 - \sqrt{2 + \sigma} a_2 + \sigma a_3 + \sqrt{2 + \tau} a_4 + 2 a_5 \right),
\]

\[
p_3 = \frac{1}{\sqrt{10}} \left( -\tau a_1 + \sqrt{2 + \sigma} a_2 + \sigma a_3 - \sqrt{2 + \tau} a_4 + 2 a_5 \right),
\]

\[
p_4 = \frac{1}{\sqrt{10}} \left( \sigma a_1 + \sqrt{2 + \tau} a_2 + \sigma a_3 - \sqrt{2 + \sigma} a_4 + 2 a_5 \right),
\]

\[
p_5 = \frac{1}{\sqrt{5}} (a_1 - a_2 + a_3)
\]

(23)

The quasicrystal structure with 10-fold symmetry from the projection of the root lattice of the Coxeter group \(W(B_3)\) is shown in figure 13.
4.3 Projection of the lattice of $B_6$ into 2D and 3D subspaces

The Coxeter number of the group $W(B_6)$ is 12. In two other publications [27, 28] we have studied projection of the 6D cubic lattice using (9) for the group $W(B_6)$ and obtained the following quasicrystal structure in figure 14.

![Figure 13. 10-fold symmetric quasicrystal structure from 5D cubic lattice.](image)

![Figure 14. 12-fold symmetric quasicrystal structure from 6D cubic lattice.](image)

The figure 14 shows that the tiling displayed here is different than the usual tiling based on the triangle and square tiles only. It also involves rhombi in addition to square and triangle tiles. Such a structure has been recently observed in the dodecagonal quasicrystal formation of BaTiO$_3$ [51].

Earlier, projection of the 6D cubic lattice into 3D subspace has been discussed in various papers but with no reference to the detailed structure of the Coxeter group $W(B_6)$ [12, 45, 47]. An explicit construction of the icosahedral subgroup $W(H_4)$ in terms of the generators of the Coxeter group $W(B_6)$ was given in Section 3.3 and the space was decomposed as $E_\parallel$ and $E_\perp$ defined by the unit vectors $(\hat{x}_1, \hat{x}_2, \hat{x}_3)$ and $(\hat{x}'_1, \hat{x}'_2, \hat{x}'_3)$ respectively. A general root lattice vector can be written as

$$p = \frac{1}{\sqrt{2(2 + \tau)}}[(n_1 + n_2 \tau)\hat{x}_1 + (n_3 + n_4 \tau)\hat{x}_2 + (n_5 + n_6 \tau)\hat{x}_3 + \tau(n_1 + n_2 \sigma)\hat{x}'_1 + \tau(n_3 + n_4 \sigma)\hat{x}'_2 + \tau(n_5 + n_6 \sigma)\hat{x}'_3],$$

where the integers $n_i$ are given by

(24)
\[ n_1 = -a_1, n_2 = -a_5, n_3 = -(a_3 + 2a_4 + 2a_6), \]
\[ n_4 = -(a_1 + 2a_2 + 2a_3 + 2a_4 + 2a_5 + 2a_6), n_5 = -(a_5 + 2a_6), n_6 = -a_3. \]  

(25)

A similar formula to (24) involving just the coefficients of the unit vectors \( \hat{x}_1, \hat{x}_2, \) and \( \hat{x}_3 \) were obtained earlier from another consideration [52].

The root vectors \( \beta_i (i = 1, 2, 3) \) of the Coxeter diagram of \( W(H_3) \) can be determined as

\[ \beta_1 = -\sqrt{2} \hat{x}_1, \beta_2 = \frac{1}{\sqrt{2}} (\hat{x}_1 + \sigma \hat{x}_2 + \tau \hat{x}_3), \beta_3 = -\sqrt{2} \hat{x}_3. \]

The pairs of vectors \( (\beta_1, \beta_1), (\beta_2, \beta_2), \) and \( (\beta_3, \beta_3) \) define 2-fold, 3-fold, and 5-fold symmetry planes respectively. By choosing the vectors in these planes such as \( (\hat{x}_1, \hat{x}_3), (\hat{y}_1, \hat{y}_2), \) and \( (\hat{z}_1, \hat{z}_2) \) where

\[ \hat{y}_1 = \frac{1}{2} (-\hat{x}_1 + \sigma \hat{x}_2 + \tau \hat{x}_3), \hat{y}_2 = -\frac{1}{2\sqrt{3}} (3\hat{x}_1 + \sigma \hat{x}_2 + \tau \hat{x}_3), \]
\[ \hat{z}_1 = \frac{1}{2} (\tau \hat{x}_1 - \hat{x}_2 + \sigma \hat{x}_3), \hat{z}_2 = \frac{1}{2\sqrt{2 + \tau}} (\hat{x}_1 + \sigma \hat{x}_2 + (2 + \tau) \hat{x}_3), \]

(26)

one can project the lattice vectors in (24) onto these planes provided the components of the vectors in \( E_+ \) remain in the window \( K \).

The distribution of the lattice points are displayed in figures 15, 16 and 17.

**Figure 15.** 2-fold symmetry from projection of \( B_6 \) lattice.

**Figure 16.** 3-fold symmetry from projection of \( B_6 \) lattice.
5. Conclusions
A systematic analysis of the higher dimensional lattice projection technique has been presented by emphasizing on the group theoretical structure of the nD cubic lattices. We note that the Coxeter number $h$ of the Coxeter-Weyl group $W(B_n)$ plays a crucial role. The dihedral subgroup $D_h$ of the group $W(B_n)$ determines the symmetry of the quasicrystal structure in the Coxeter plane. The eigenvalues and eigenvectors of the Cartan matrix (Gramm matrix) lead to the correct choice of the Coxeter plane onto which the lattice is projected. In two cases we obtained new results: the 10-fold symmetric quasicrystallography from $W(B_5)$ and the 12-fold symmetric quasicrystal structure from $W(B_6)$ lead to some novel structures. In particular, the tiling displayed in figure 14 is compatible with a recent experiment with 12-fold symmetry [51].

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