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# Projection method for 4d non-orthogonal hyperlattices

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**Abstract.** The Wigner–Seitz cell of a lattice in *n*-dimensional space displays the complete point group of such a lattice. The vertices of the cell when projected onto pseudo space can serve as the outer shape of acceptance domain or motif. This general procedure leads to acceptance domain or motif identical to those discussed in literature for primitive orthogonal hyperlattices.

Example of 4d non-orthogonal hyperlattices corresponding to 12-fold symmetry will be considered. It will be shown that the first Wigner–Seitz cell degenerates into more than one shape in 2d pseudo space and can serve as a natural partition of the motif. Following a parallel procedure, the consequence of projection of first 4d Brillouin zone will also be discussed.

**Keywords.** Wigner–Seitz cell; quasicrystals; non-orthogonal hyperlattices.

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## 1. Introduction

The two dimensional (d) quasicrystals enjoy a special status in quasicrystalline literature owing to the presence of periodicity parallel to symmetry axis and quasiperiodicity in a plane perpendicular to it. Pentagonal [1, 2], octagonal [3], decagonal [4, 5] and dodecagonal [6, 7] phases belong to this category. The rank of these solids is five and to index their diffraction patterns, one requires five integrally independent basis vectors. There have been attempts to understand the nature of two dimensional (2d) quasiperiodicity by adopting the method of section/projection [8–10]. The 4d lattices corresponding to octagonal, decagonal and dodecagonal symmetry are non-orthogonal [11] and deserve consideration on a different footing. There have been a couple of papers [12, 13] regarding generalization of the procedure of higher dimensional crystallography at the qualitative level. However, the operational details of section/projection seem to be lacking. It is the purpose of this presentation to specify the scheme of choosing an acceptance domain (window) or outer boundary of the motif by determining the Wigner–Seitz cell and then projecting the vertices onto a suitably chosen pseudo space. The criterion of choosing acceptance domain based on the unit cell projection onto a pseudo space is not suitable as the conventional unit cell does not satisfy the geometrical requirements of symmetry for the non-orthogonal situation. We, therefore, believe that the determination of acceptance domain based on Wigner–Seitz cell route to be discussed here should be followed. It will be shown that the vertices of Wigner–Seitz cell on projection degenerate into more than one shape and the outer one may serve as a good starting point for the acceptance domain. Such a procedure when followed in reciprocal space readily gives information about the first Brillouin zone shape in higher dimension and its consequence on physical space projection are explored. We illustrate the steps by taking the example of a 4d dodecagonal lattice.

## 2. Determination of Wigner–Seitz cell and acceptance domain

As indicated earlier, the 4 basis vectors in 2d physical and pseudo space are chosen so as to recover the metric tensor for dodecagonal lattice given by Brown *et al* [11] and they are

$$\begin{bmatrix} V_1 \\ V_2 \\ V_3 \\ V_4 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -\sin\theta & \cos\theta \\ -\cos\theta & -\sin\theta \end{bmatrix} \begin{bmatrix} x^{\|} \\ y^{\|} \end{bmatrix}, \tag{1}$$

$$\begin{bmatrix} W_1 \\ W_2 \\ W_3 \\ W_4 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -\sin\theta & -\cos\theta \\ \cos\theta & -\sin\theta \end{bmatrix} \begin{bmatrix} x^{\perp} \\ y^{\perp} \end{bmatrix}, \tag{2}$$

where $V_i$ s and $W_i$ s (for $i = 1$ to 4) are respectively the physical and pseudo space basis vectors; $\theta = 30°$; $X^{\|}$ and $Y^{\|}$ are Cartesian bases in physical space whereas $X^{\perp}$ and $Y^{\perp}$ are those for pseudo space. The Cartesian bases are complementary with respect to each other. Thus the direct sum of the above two equations gives bases for the 4d space and they are

$$\begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ -\sin\theta & \cos\theta & -\sin\theta & -\cos\theta \\ -\cos\theta & -\sin\theta & \cos\theta & -\sin\theta \end{bmatrix} \begin{bmatrix} x^{\|} \\ y^{\|} \\ x^{\perp} \\ y^{\perp} \end{bmatrix}, \tag{3}$$

where $A_i$s ($i = 1$ to 4) are 4d lattice basis vector. The metric tensor is given by $A_i\, A_j^T$ and has a form similar to that given by Brown *et al* [11].

Any 4d direct lattice vector $R^4$ corresponding to any point given by coordinates $[m_1, m_2, m_3, m_4]$ can be represented by

$$R^4 = t(m_1 A_1 + m_2 A_2 + m_3 A_3 + m_4 A_4), \tag{4}$$

where $t$ is the 4d lattice parameter and can be dropped (being common) for subsequent steps without any loss of generality. The first step in the process of determination of Wigner–Seitz cell involves determination of hyperplanes closest to the origin. This has been achieved by finding those set of $m_i$ s for which $R^4.R^4$ has the minimum magnitude. The $m_i$s are the coordinates of the foot of the plane normal lying on the hyperplane. The intersections of hyperplanes correspond to vertices of the Wigner–Seitz cell. It has been found that there are twelve such hyperplanes whose equations and related $m_i$s are presented in table 1.

**Table 1.** Coordinates of plane normals and equation of hyperplanes.

| $m_1$ | $m_2$ | $m_3$ | $m_4$ | Equation of hyperplane |
|---|---|---|---|---|
| $\pm 1$ | 0 | 0 | 0 | $\pm(x^{\parallel} + x^{\perp}) = 2$ |
| 0 | $\pm 1$ | 0 | 0 | $\pm(y^{\parallel} + y^{\perp}) = 2$ |
| 0 | 0 | $\pm 1$ | 0 | $\pm(-x^{\parallel} + \sqrt{3}y^{\parallel} - x^{\perp} - \sqrt{3}y^{\perp}) = 4$ |
| 0 | 0 | 0 | $\pm 1$ | $\pm(\sqrt{3}x^{\parallel} - y^{\parallel} + \sqrt{3}x^{\perp} - y^{\perp}) = 4$ |
| $\pm 1$ | 0 | $\pm 1$ | 0 | $\pm(-x^{\parallel} + \sqrt{3}y^{\parallel} + x^{\perp} - \sqrt{3}y^{\perp}) = 4$ |
| 0 | $\pm 1$ | 0 | $\pm 1$ | $\pm(-\sqrt{3}x^{\parallel} + y^{\parallel} + \sqrt{3}x^{\perp} + y^{\perp}) = 4$ |

**Table 2.** Coordinate of the vertices of WS cell in terms of 4d cartesian axes in direct and reciprocal space.

| Direct* | | | | Reciprocal* | | | |
|---|---|---|---|---|---|---|---|
| $b_1$ | $b_2$ | $b_2$ | $b_1$ | $b_1$ | $b_1$ | $\bar{b}_2$ | $\bar{b}_2$ |
| $b_3$ | $b_4$ | $b_5$ | $\bar{b}_4$ | $\bar{b}_4$ | $b_3$ | $\bar{b}_4$ | $\bar{b}_5$ |
| $\bar{b}_4$ | $b_5$ | $b_4$ | $b_3$ | $\bar{b}_2$ | $\bar{b}_2$ | $b_1$ | $b_1$ |
| $\bar{b}_6$ | $b_6$ | $b_6$ | $\bar{b}_6$ | $\bar{b}_5$ | $b_3$ | $b_3$ | $\bar{b}_4$ |
| $b_2$ | $b_2$ | $b_1$ | $b_1$ | $b_2$ | $\bar{b}_2$ | $\bar{b}_1$ | $b_1$ |
| $b_1$ | $b_1$ | $b_2$ | $b_2$ | $b_4$ | $\bar{b}_5$ | $b_4$ | $b_3$ |
| $b_2$ | $b_1$ | $b_1$ | $b_2$ | $b_1$ | $\bar{b}_1$ | $\bar{b}_2$ | $b_2$ |
| $b_1$ | $\bar{b}_1$ | $b_2$ | $\bar{b}_2$ | $b_3$ | $b_4$ | $\bar{b}_5$ | $b_4$ |
| $b_1$ | $\bar{b}_2$ | $b_2$ | $\bar{b}_1$ | $b_5$ | $b_4$ | $\bar{b}_3$ | $b_4$ |
| $b_2$ | $\bar{b}_1$ | $b_1$ | $\bar{b}_2$ | $\bar{b}_1$ | $b_2$ | $b_2$ | $\bar{b}_1$ |
| $b_5$ | $b_4$ | $b_3$ | $\bar{b}_4$ | $b_4$ | $b_5$ | $b_4$ | $\bar{b}_3$ |
| $b_2$ | $\bar{b}_2$ | $b_1$ | $\bar{b}_1$ | $b_6$ | $b_6$ | $b_6$ | $\bar{b}_6$ |
| $b_5$ | $\bar{b}_1$ | $b_3$ | $b_1$ | $b_2$ | $b_1$ | $\bar{b}_1$ | $\bar{b}_2$ |
| $\bar{b}_3$ | $\bar{b}_1$ | $b_5$ | $b_1$ | $b_2$ | $b_1$ | $b_1$ | $\bar{b}_2$ |
| $b_1$ | $b_5$ | $b_1$ | $\bar{b}_3$ | $b_4$ | $b_3$ | $b_4$ | $\bar{b}_5$ |
| $\bar{b}_1$ | $b_3$ | $b_1$ | $\bar{b}_5$ | $b_6$ | $\bar{b}_6$ | $b_6$ | $\bar{b}_6$ |
| $b_6$ | $b_6$ | $\bar{b}_6$ | $\bar{b}_6$ | $b_1$ | $b_2$ | $b_2$ | $\bar{b}_1$ |
| $b_4$ | $\bar{b}_3$ | $b_4$ | $\bar{b}_5$ | $b_4$ | $\bar{b}_3$ | $b_4$ | $b_5$ |

$b_1 = \dfrac{3-\sqrt{3}}{6}$ ; $b_2 = \dfrac{3+\sqrt{3}}{6}$ ; $b_3 = \dfrac{3-2\sqrt{3}}{6}$ ; $b_4 = \dfrac{\sqrt{3}}{6}$ ;

$b_5 = \dfrac{3+2\sqrt{3}}{6}$ ; $b_6 = \dfrac{2\sqrt{3}}{6}$ .

*Coordinates of the remaining 18 WS cell vertices can be obtained by a change of sign of the given values. All reciprocal space coordinates have to be multiplied by 2.

The determination of vertices of the Wigner–Seitz cell is accomplished by solving any 4 equations simultaneously to get the intersection of 4 3d-hyperplanes in 4d space. It has been found that the 4d Wigner–Seitz cell has 36 vertices. The vertices are displayed in table 2. The pseudo space projection of these 36 vertices gives rise to three regular dodecagons. It is important to note that these dodecagons will not result if we consider the locus of points in pseudo direct space obtained by projection of the 16 vertices of the 4d unit cell. Thus we see that if any of the three dodecagons is selected as acceptance domain, the resulting quasiperiodic set of points in physical direct space would preserve 12-fold symmetry.

## 3. 4d reciprocal basis and Brillouin zone

The reciprocal basis vectors of the 4d direct counterparts given in equation (3) are obtained by utilizing the criterion $A_i.A_j^* = \delta_{ij}$ (for $i, j = 1$ to 4). The value of Kronecker delta is 1 for $i = j$ otherwise zero. The reciprocal space basis vectors $A_i^*$ ($i = 1$ to 4) is expressed by

$$\begin{bmatrix} A_1^* \\ A_2^* \\ A_3^* \\ A_4^* \end{bmatrix} = \begin{bmatrix} \cos\theta & \sin\theta & \cos\theta & -\sin\theta \\ -\sin\theta & \cos\theta & \sin\theta & \cos\theta \\ 0 & 1 & 0 & -1 \\ -1 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} x^{\|} \\ y^{\|} \\ x^{\perp} \\ y^{\perp} \end{bmatrix} \tag{5}$$

with the identity $[A][A^*]^T = [I]$.

Following a procedure parallel to that explained in the preceding section, the vertices of the first Voronoi cell have been determined. The 36 vertices thus obtained are listed in table 2. The first Brillouin zone hypersurfaces thus obtained degenerate into three dodecagons in physical and pseudo reciprocal spaces. We know that the intensity of reciprocal lattice points (twice of the Brillouin zone vertex vectors) is not identical in physical space. This means that 4d-Brillouin zone boundaries are highly anisotropic and all may not be observable under experimental conditions. This fact has to be kept in mind while considering the Fermi surface and Brillouin zone interaction in these phases for comprehending the behaviour of electronic states near the Fermi level.

## 4. Conclusions

We have presented a method of selecting acceptance domain for non-orthogonal hyperlattices. This has been accomplished by first constructing the Wigner–Seitz cell and then projecting the vertices onto pseudo space. A parallel procedure has been followed to construct the 4d-Brillouin zone boundary. The consequence of projection of vertices onto physical and pseudo space led us to the conclusion that 4d-Wigner–Seitz cell degenerates into three dodecagons. This further meant that the 4d-Brillouin zone faces are anisotropic in view of diffraction. We believe that such a conclusion may be important for understanding the nature of electronic states near the Fermi surface.

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