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A unified approach to the topological origin of Wigner–Seitz cells

Xiaoxia Yang(杨晓霞)[1], Qihou Liu(刘启后)[1,2,†], Dier Zhang(张笛儿)[3,‡], and Xiao Gu(顾晓)[1,§]

[1] *School of Physical Science and Technology, Ningbo University, Ningbo* 315211, *China*
[2] *Department of Mathematical Sciences, Xi'an Jiaotong-Liverpool University, Suzhou* 215123, *China*
[3] *Zhuguangya Institute of Advanced Science and Technology, Shanghai* 201306, *China*

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While Wigner–Seitz cells of different Bravais lattices exhibit distinct geometric features, their topological formation follows a unified fundamental principle. This study explores the topological origins of Wigner–Seitz cells. We demonstrate that a finite set of lattice vectors, termed root vectors, can universally and fully characterize these cells in n-dimensional Euclidean space ($\mathbb{R}^n$) via half-space representations. The configuration of root vectors determines the topological shapes of the corresponding Wigner–Seitz cells. Specifically, the number of orthogonal pairs within the base vectors dictates the degeneracy of codimension-1 faces. For general lattices with no orthogonal pairs, the Wigner–Seitz cell possesses the maximum possible number of codimension-1 faces.

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1. Introduction

Space partitioning is a classic and persistent problem. As a special class of Voronoi polytopes, Wigner–Seitz cells have wide applications, especially in quantum chemistry, crystal physics, and astrophysics.[1–4] In crystal physics, the determination of the space occupied by atoms in periodic crystal lattices is not straightforward. Accordingly, Wigner and Seitz introduced the so-called Wigner–Seitz polyhedron in body-centered cubic sodium.[5] This construction preserves translational invariance and provides a practical method to define the space occupied by atoms in crystals.[5,6] With such occupied volumes, they also defined the Wigner–Seitz radius, which has found applications in crystallography and in the modeling of ultra-dense neutron-star matter.[7–11] In quantum chemistry, Wigner–Seitz cells also arise naturally for atoms and molecules with confined boundaries.[12] Wigner–Seitz cells also underlie approaches to analyzing charge distributions in crystals and molecules.[13] In *ab initio* calculations, the first Brillouin zone of a reciprocal lattice is a Wigner–Seitz polytope. Their geometric features enable computations in momentum space without explicit real-space descriptions of local potentials or charge densities.[14] Wigner–Seitz cells also play a role in the success of density functional methods in condensed matter physics.[15,16] The Wigner–Seitz cell of the displacement-shift-complete lattice is used to characterize grain boundary microstates via a translation vector.[17]

It is well known that the choice of a Bravais lattice basis influences the shape of the corresponding Wigner–Seitz cell. Wigner–Seitz cells of Bravais lattices have been discussed in detail in crystallography.[18] Background on lattices, Voronoi polytopes, and reduction theory can be found in standard references.[19–22] Recently, Voronoi and Delone cells of root/weight lattices for $W(A_n)$ and $W(D_n)$ have been systematically constructed, revealing their facet topology and aperiodic tilings.[23] Much of the literature focuses on highly symmetric cases, while low-symmetry Wigner–Seitz cells have received comparatively less attention. From a topological point of view, natural questions include: which polytopes can arise as Wigner–Seitz cells, how many topological types occur, and what relations exist among them.[24–26] Addressing these questions requires rigorous criteria and proofs.

This paper studies the topological shapes of Wigner–Seitz cells. In general, Wigner–Seitz cells are convex polytopes. Two convex polytopes are considered topologically equivalent if there is a one-to-one correspondence between their vertices, edges, and faces that preserves the incidence relation.

2. Results and discussion

A lattice Γ is generic if for any lattice Γ' sufficiently close to Γ, the Wigner–Seitz cell of Γ' is topologically equivalent to that of Γ.

A finite half-space description is now introduced. For a

†Corresponding author. E-mail: gibbs.grassmann@gmail.com
‡Corresponding author. E-mail: diorland_xh@163.com
§Corresponding author. E-mail: guxiao@nbu.edu.cn

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lattice Γ in $\mathbb{R}^n$, the Wigner–Seitz cell $\mathbb{W}_n$ of Γ is a polytope obtained as the intersection of half spaces[1,2]

$$\mathbb{W}_n(\Gamma) = \bigcap_{\boldsymbol{c}\in\Gamma} \mathcal{P}_+(\boldsymbol{c}), \tag{1}$$

where $\mathcal{P}_+(\boldsymbol{c})$ is a half space carved by a vector $\boldsymbol{c}$: $\mathcal{P}_+(\boldsymbol{c}) = \{\boldsymbol{v}\in\mathbb{R}^n | (\boldsymbol{v}-\boldsymbol{c}/2)\cdot\boldsymbol{c}\le 0\}$.

In this equation, $\mathbb{W}_n(\Gamma)$ is the intersection of infinite half spaces. The goal is to express $\mathbb{W}_n(\Gamma)$ as a finite intersection by carefully choosing a minimal finite subset $\Omega_n(\Gamma)\subset\Gamma$, called the set of root vectors, such that[1,22]

$$\mathbb{W}_n(\Gamma) = \bigcap_{\boldsymbol{c}\in\Omega_n(\Gamma)} \mathcal{P}_+(\boldsymbol{c}). \tag{2}$$

The description of the topological shapes of $\mathbb{W}_n(\Gamma)$ then follows from the study of the geometry of the configuration $\Omega_n(\Gamma)$.

To construct $\Omega_n(\Gamma)$, the concept of flat basis is introduced. A flat basis is a basis of $\mathbb{R}^n$, $\{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\ldots,\boldsymbol{\alpha}_n\}$, such that

$$\begin{cases} \boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_j < 0, & i\neq j, \\ \boldsymbol{\alpha}_i\cdot(\boldsymbol{\alpha}_1+\boldsymbol{\alpha}_2+\cdots+\boldsymbol{\alpha}_n) > 0. \end{cases} \tag{3}$$

When the above inequalities are not strict ($\boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_j\le 0$; $\boldsymbol{\alpha}_i\cdot(\boldsymbol{\alpha}_1+\boldsymbol{\alpha}_2+\cdots+\boldsymbol{\alpha}_n)\ge 0$), $\{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\ldots,\boldsymbol{\alpha}_n\}$ is called a weakly flat basis. In particular, every flat basis is a weakly flat basis.

Given a lattice Γ in $\mathbb{R}^n$ and a weakly flat basis (flat basis) $\{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\ldots,\boldsymbol{\alpha}_n\}\subset\Gamma$, if any $\boldsymbol{c}\in\Gamma$ can be uniquely expressed as a linear combination of $\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\ldots,\boldsymbol{\alpha}_n$ with integer coefficients, then $\{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\ldots,\boldsymbol{\alpha}_n\}$ is called a weakly flat basis (flat basis) of Γ. A key technical input is that a weakly flat basis exists for every lattice in dimensions 2 and 3 (see the discussion below). By contrast, in higher dimensions there exist lattices without a weakly flat basis.

In the construction of $\Omega_2(\Gamma)$ in dimension 2, let $\{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2\}$ be a weakly flat basis of Γ and define $\Omega_2(\Gamma) = \{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\boldsymbol{\alpha}_1+\boldsymbol{\alpha}_2,-\boldsymbol{\alpha}_1,-\boldsymbol{\alpha}_2,-\boldsymbol{\alpha}_1-\boldsymbol{\alpha}_2\}$. By relabeling $\boldsymbol{\alpha}_1$ as $\boldsymbol{a}$ and $\boldsymbol{\alpha}_1+\boldsymbol{\alpha}_2$ as $\boldsymbol{b}$, one may write $\Omega_2(\Gamma) = \{\boldsymbol{a},\boldsymbol{b},\boldsymbol{b}-\boldsymbol{a},-\boldsymbol{a},-\boldsymbol{b},\boldsymbol{a}-\boldsymbol{b}\}$ (see Fig. 1). Therefore, the corresponding Wigner–Seitz cell is $\mathbb{W}_2(\Gamma) = \bigcap_{\boldsymbol{c}\in\Omega_2(\Gamma)} \mathcal{P}_+(\boldsymbol{c})$.

All degenerate (non-generic) cases in dimensions 2 and 3 are listed, yielding a complete classification of the possible topological shapes of Wigner–Seitz cells in these dimensions. This classification recovers the classical results on crystal systems and suggests analogous investigations for higher-dimensional lattices and related settings. Motivated by the low-dimensional classification, it is conjectured that for any generic lattice in $\mathbb{R}^n$, the number of codimension-1 faces of the Wigner–Seitz cell equals $2\cdot(2^n-1)$. In contrast to the cases $n=2,3$, generic types need not be unique when $n\ge 4$.

Let Π_2 denote the set of all unordered pairs $\{\boldsymbol{r}_1,\boldsymbol{r}_2\}$ of distinct root vectors in $\Omega_2(\Gamma)$. As shown in Fig. 1, in the case of $\boldsymbol{a}\cdot\boldsymbol{b}>0$, $\boldsymbol{b}\cdot(\boldsymbol{b}-\boldsymbol{a})>0$, and $\boldsymbol{a}\cdot(\boldsymbol{a}-\boldsymbol{b})>0$, no pair in Π_2 is orthogonal, and $\mathbb{W}_2$ is a polygon of 6 edges and 6 vertices, namely a parallel hexagon. In the degenerate cases, where one of $\boldsymbol{a}\cdot\boldsymbol{b}$, $\boldsymbol{b}\cdot(\boldsymbol{b}-\boldsymbol{a})$, and $\boldsymbol{a}\cdot(\boldsymbol{a}-\boldsymbol{b})$ is 0 (one element of Π_2 is orthogonal), $\mathbb{W}_2$ is a rectangle. It follows that there can be at most one orthogonal pair in Π_2. Ultimately, two-dimensional Wigner–Seitz cells are either parallel hexagons or rectangles.

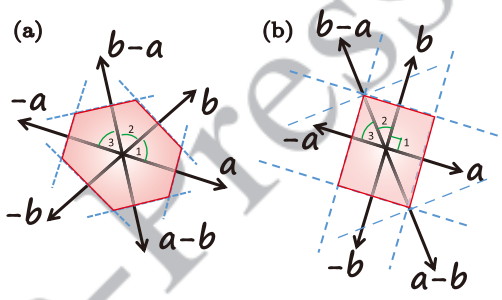


Fig. 1. Wigner–Seitz cells in 2D. Vectors $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{b}-\boldsymbol{a}$, $-\boldsymbol{a}$, $-\boldsymbol{b}$, and $\boldsymbol{a}-\boldsymbol{b}$ form a set of root vectors. Dashed lines are perpendicular bisectors of the corresponding vectors. (a) It contains no right angles (generic case), and the Wigner–Seitz cell is a parallel hexagon. (b) One of the angles is a right angle, $\angle 1=\pi/2$, and the Wigner–Seitz cell is a rectangle.

Similarly, in dimension 3, one may define the set of root vectors by

$$\begin{aligned}\Omega_3(\Gamma) = \Big\{&\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\boldsymbol{\alpha}_3,\boldsymbol{\alpha}_1+\boldsymbol{\alpha}_2,\boldsymbol{\alpha}_2+\boldsymbol{\alpha}_3,\boldsymbol{\alpha}_3+\boldsymbol{\alpha}_1,\\ &\boldsymbol{\alpha}_1+\boldsymbol{\alpha}_2+\boldsymbol{\alpha}_3,-\boldsymbol{\alpha}_1,-\boldsymbol{\alpha}_2,-\boldsymbol{\alpha}_3,-\boldsymbol{\alpha}_1-\boldsymbol{\alpha}_2,\\ &-\boldsymbol{\alpha}_2-\boldsymbol{\alpha}_3,-\boldsymbol{\alpha}_3-\boldsymbol{\alpha}_1,-\boldsymbol{\alpha}_1-\boldsymbol{\alpha}_2-\boldsymbol{\alpha}_3\Big\},\end{aligned} \tag{4}$$

where Γ is a lattice in $\mathbb{R}^3$, and $\{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\boldsymbol{\alpha}_3\}$ is a weakly flat basis of Γ. As shown in Fig. 2, by relabeling $\boldsymbol{\alpha}_1$ as $\boldsymbol{\alpha}'$, $\boldsymbol{\alpha}_2$ as $\boldsymbol{\beta}'$, $-\boldsymbol{\alpha}_3$ as $\boldsymbol{\beta}$, and $\boldsymbol{\alpha}_1+\boldsymbol{\alpha}_2+\boldsymbol{\alpha}_3$ as $\boldsymbol{\alpha}$, with $\boldsymbol{\gamma_1}=\boldsymbol{\alpha}-\boldsymbol{\alpha}'$; $\boldsymbol{\gamma_2}=\boldsymbol{\beta}-\boldsymbol{\alpha}'$; $\boldsymbol{\gamma_3}=\boldsymbol{\alpha}+\boldsymbol{\beta}$, one may write $\Omega_3(\Gamma)$ as

$$\begin{aligned}\Omega_3(\Gamma) = \{&\boldsymbol{\alpha},\boldsymbol{\beta},\boldsymbol{\alpha}',\boldsymbol{\beta}',-\boldsymbol{\alpha},-\boldsymbol{\beta},-\boldsymbol{\alpha}',-\boldsymbol{\beta}',\\ &\boldsymbol{\gamma_1},-\boldsymbol{\gamma_1},\boldsymbol{\gamma_2},-\boldsymbol{\gamma_2},\boldsymbol{\gamma_3},-\boldsymbol{\gamma_3}\}.\end{aligned} \tag{5}$$

Weakly flat bases and their associated graphs are introduced next, and degeneracy is characterized by counting right angles. The corresponding Wigner–Seitz cell in 3D is $\mathbb{W}_3(\Gamma) = \bigcap_{\boldsymbol{c}\in\Omega_3(\Gamma)} \mathcal{P}_+(\boldsymbol{c})$. Since $\Omega_3(\Gamma)$ contains 14 root vectors, $\mathbb{W}_3(\Gamma)$ is the intersection of 14 half spaces. Hence $\mathbb{W}_3(\Gamma)$ has at most 14 faces.

1. Let $\alpha = \{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\ldots,\boldsymbol{\alpha}_n\}$ be a weakly flat basis of $\mathbb{R}^n$, and denote $\boldsymbol{\alpha}_0 = \boldsymbol{\alpha}_1+\boldsymbol{\alpha}_2+\cdots+\boldsymbol{\alpha}_n$. Then $\{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\ldots,\boldsymbol{\alpha}_n\}$ is defined as the base vectors ($\mathbb{V}_n$). The associated graph of α is the graph $\mathbb{G}(\alpha)$ defined as follows:

(i) the set of vertices of $\mathbb{G}(\alpha)$ is $\widetilde{\mathbb{V}}_n = \{\boldsymbol{\alpha}_0,\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_n\}$.

(ii) there is an edge between $\boldsymbol{\alpha}_i$ and $\boldsymbol{\alpha}_j$ (with $i\neq j$) if $\boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_j = 0$.

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Definition 1 Two weakly flat bases $\alpha = \{\alpha_1, \alpha_2, \ldots, \alpha_n\}$ and $\beta = \{\beta_1, \beta_2, \ldots, \beta_n\}$ are equivalent if the lattices generated by α and β have topologically equivalent Wigner–Seitz cells. The associated graph can be used to classify weakly flat bases up to equivalence.

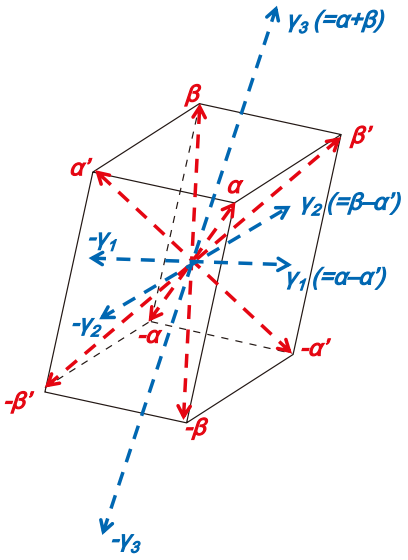


Fig. 2. A set of root vectors in $\mathbb{R}^3$: $\Omega_3(\Gamma) = \{\boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\alpha'}, \boldsymbol{\beta'}, -\boldsymbol{\alpha}, -\boldsymbol{\beta}, -\boldsymbol{\alpha'}, -\boldsymbol{\beta'}, \boldsymbol{\gamma_1}, -\boldsymbol{\gamma_1}, \boldsymbol{\gamma_2}, -\boldsymbol{\gamma_2}, \boldsymbol{\gamma_3}, -\boldsymbol{\gamma_3}\}$

2. The case of $\mathbb{R}^3$. Let $\mathbb{G}(\alpha)$ be the associated graph of a weakly flat basis, $\alpha = \{\alpha_1, \alpha_2, \alpha_3\}$. Then

(i) For each vertex α_i of $\mathbb{G}(\alpha)$, $\deg(\alpha_i) \leq 2$.

To show $\deg(\alpha_i) \leq 2$, suppose for contradiction that $\deg(\alpha_1) \geq 3$. Since there are only four vertices $\alpha_0, \alpha_1, \alpha_2, \alpha_3$, the vertex α_1 must be adjacent to at least three of the others. Without loss of generality, assume α_1 is adjacent to α_2, α_3, and α_0. Then by definition of adjacency, $\alpha_1 \cdot \alpha_2 = 0$, $\alpha_1 \cdot \alpha_3 = 0$, and $\alpha_1 \cdot \alpha_0 = 0$. But $\alpha_0 = \alpha_1 + \alpha_2 + \alpha_3$, so $\alpha_1 \cdot \alpha_0 = |\alpha_1|^2 + \alpha_1 \cdot \alpha_2 + \alpha_1 \cdot \alpha_3 = |\alpha_1|^2$. Setting this to zero gives $|\alpha_1|^2 = 0$, a contradiction. Hence $\deg(\alpha_i) \leq 2$.

(ii) $\mathbb{G}(\alpha)$ contains no cycle of length 4.

Indeed, if $\alpha_1 \cdot \alpha_2 = 0$, $\alpha_2 \cdot \alpha_0 = 0$, $\alpha_0 \cdot \alpha_3 = 0$, and $\alpha_3 \cdot \alpha_1 = 0$, then $0 = \alpha_0 \cdot (\alpha_2 + \alpha_3) = \alpha_1 \cdot (\alpha_2 + \alpha_3) + (\alpha_2 + \alpha_3)^2 = (\alpha_2 + \alpha_3)^2$, a contradiction.

Hence, $\mathbb{G}(\alpha)$ is one of the following: (a) no edges, (b) exactly 1 edge, (c) exactly 2 disjoint edges, (d) exactly 2 edges sharing a vertex, (e) exactly 3 edges forming a path of length 3, as shown in Fig. 3.

Let α_1, α_2, α_3 be a weakly flat basis and let $\alpha_0 = \alpha_1 + \alpha_2 + \alpha_3$. Among the 6 angles $\angle(\alpha_i, \alpha_j)$, $0 \leq i < j \leq 3$, some of them might be $\pi/2$. Let N be the number of right angles among these 6 angles. Degeneracy occurs when $N > 0$.

Case (0) $N = 0$ In this case, none of the six angles is $\pi/2$, hence no degeneracy occurs. Equivalently, $\alpha_i \cdot \alpha_j \neq 0$ for all $0 \leq i < j \leq 3$. The corresponding polyhedron is in the generic topological type T_{14}.

Case (1) $N = 1$ The basic situation is

$$\alpha_1 \cdot \alpha_2 = 0,$$

and the shape of the polyhedron is T_{12a}.

Case (2) $N = 2$**.**

$$\alpha_i \cdot \alpha_j = \alpha_k \cdot \alpha_l = 0 \quad (i, j, k, l \in \{0, 1, 2, 3\}).$$

Subcase (1)

$$\{\alpha_i, \alpha_j\} \cap \{\alpha_k, \alpha_l\} = \emptyset.$$

It may be assumed

$$\alpha_1 \cdot \alpha_2 = 0, \quad \alpha_0 \cdot \alpha_3 = 0.$$

The shape of the polyhedron is T_{12b}.

Subcase (2)

$$\{\alpha_i, \alpha_j\} \cap \{\alpha_k, \alpha_l\} \neq \emptyset.$$

The basic situation is

$$\alpha_1 \cdot \alpha_2 = 0 = \alpha_1 \cdot \alpha_3,$$

and the shape of the polyhedron is T_8.

Subcase (3) Other configurations with $N = 2$ can be reduced to Subcase (1) or Subcase (2) by changing the weakly flat basis:

(i) If $\alpha_1 \cdot \alpha_2 = 0$ and $\alpha_1 \cdot \alpha_0 = 0$, one may choose $\{-\alpha_1, -\alpha_2, \alpha_0\}$ as a basis, which is still weakly flat; this reduces to the previous basic situation.

(ii) If $\alpha_0 \cdot \alpha_1 = 0$ and $\alpha_0 \cdot \alpha_2 = 0$, one may choose $\{\alpha_0, -\alpha_1, -\alpha_2\}$ as a basis.

Case (3) $N = 3$ The basic situation is

$$\alpha_1 \cdot \alpha_2 = \alpha_1 \cdot \alpha_3 = \alpha_2 \cdot \alpha_3 = 0.$$

(one verifies that there are no other right angles in this situation). The shape of the polyhedron is T_6. Other possibilities are considered next and reduced to the basic situation.

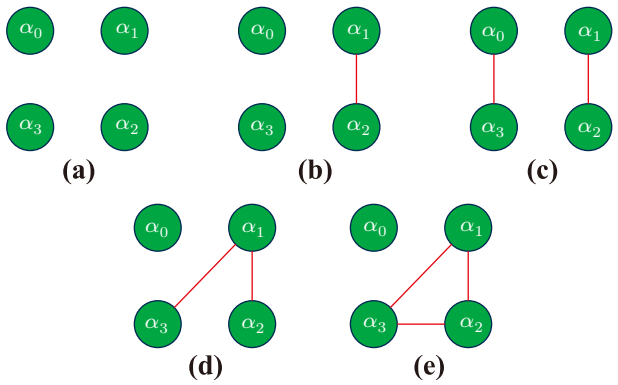


Fig. 3. Orthogonality of the $\mathbb{V}_3$ base vectors; red lines represent orthogonal pairs. (a) No right angles. (b) One right angle. (c) Two separated right angles. (d) Two adjacent right angles. (e) Three right angles.

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Subcase (1)

$$\alpha_1\cdot\alpha_2=\alpha_1\cdot\alpha_3=0,\quad \alpha_0\cdot\alpha_j=0,$$

for some $j\in\{1,2,3\}$. Then $\alpha_0\cdot\alpha_1\neq 0$; otherwise

$$\alpha_1\cdot\alpha_1=\alpha_1\cdot(\alpha_0-\alpha_2-\alpha_3)=\alpha_1\cdot\alpha_0-\alpha_1\cdot\alpha_2-\alpha_1\cdot\alpha_3=0,$$

which is impossible. So $\alpha_0\cdot\alpha_2=0$ or $\alpha_0\cdot\alpha_3=0$. Suppose $\alpha_0\cdot\alpha_2=0$; then

$$\alpha_2\cdot(\alpha_2+\alpha_3)=\alpha_2\cdot\alpha_0-\alpha_2\cdot\alpha_1=0.$$

In this subcase, we have $\alpha_0\cdot\alpha_2=0$. Together with $\alpha_0=\alpha_1+\alpha_2+\alpha_3$, this implies

$$0=\alpha_0\cdot\alpha_2=(\alpha_1+\alpha_2+\alpha_3)\cdot\alpha_2=\alpha_1\cdot\alpha_2+|\alpha_2|^2+\alpha_3\cdot\alpha_2.$$

Since $\alpha_1\cdot\alpha_2=0$, we obtain $\alpha_2\cdot\alpha_3=-|\alpha_2|^2<0$.

Now observe that the original basis $\{\alpha_1,\alpha_2,\alpha_3\}$ itself already satisfies the basic situation of Case (3): we have $\alpha_1\cdot\alpha_2=0$, $\alpha_1\cdot\alpha_3=0$, and $\alpha_2\cdot\alpha_3<0$. The weak flatness condition $\alpha_i\cdot(\alpha_1+\alpha_2+\alpha_3)\geq 0$ for each i follows from the fact that $\{\alpha_1,\alpha_2,\alpha_3\}$ is a weakly flat basis of the original lattice. Thus, no basis change is needed; the basic situation is already attained with the original basis. The problematic basis $\{\alpha_1,\alpha_2,\alpha_2+\alpha_3\}$ is therefore not used.

Subcase (2)

$$\alpha_1\cdot\alpha_2=0,\quad \alpha_0\cdot\alpha_j=\alpha_0\cdot\alpha_k=0,$$

for some $j,k\in\{1,2,3\}$, $j\neq k$.

(i) If $\alpha_0\cdot\alpha_1=\alpha_0\cdot\alpha_2=0$, choose $\{-\alpha_1,-\alpha_2,\alpha_0\}$ as a basis.

(ii) If $\alpha_0\cdot\alpha_1=\alpha_0\cdot\alpha_3=0$, then

$$\alpha_1\cdot(\alpha_1+\alpha_3)=\alpha_1\cdot(\alpha_0-\alpha_2)=\alpha_1\cdot\alpha_0-\alpha_1\cdot\alpha_2=0.$$

Choose $\{\alpha_0,\alpha_1,\alpha_1+\alpha_3\}$ as a basis.

It remains to verify that this new basis is weakly flat. The pairwise inner products are

$$\alpha_0\cdot\alpha_1=0,\quad \alpha_0\cdot(\alpha_1+\alpha_3)=0,$$
$$\alpha_1\cdot(\alpha_1+\alpha_3)=|\alpha_1|^2+\alpha_1\cdot\alpha_3=0,$$

where the last equality follows from $\alpha_0\cdot\alpha_1=0$, which implies $\alpha_1\cdot\alpha_3=-|\alpha_1|^2$. Hence all off-diagonal inner products of the new basis are non-positive.

Furthermore, let the total sum of the new basis vectors be

$$S=\alpha_0+\alpha_1+(\alpha_1+\alpha_3)=\alpha_0+2\alpha_1+\alpha_3.$$

We compute

$$\alpha_0\cdot S=|\alpha_0|^2>0,\quad \alpha_1\cdot S=|\alpha_1|^2>0,$$

and

$$(\alpha_1+\alpha_3)\cdot S=\alpha_1\cdot\alpha_3+|\alpha_3|^2=-|\alpha_1|^2+|\alpha_3|^2.$$

Since the original basis is weakly flat, we have $\alpha_2\cdot\alpha_3\leq 0$. From $\alpha_0\cdot\alpha_3=0$ and $\alpha_0=\alpha_1+\alpha_2+\alpha_3$, together with $\alpha_0\cdot\alpha_1=0$, one obtains

$$\alpha_2\cdot\alpha_3=|\alpha_1|^2-|\alpha_3|^2.$$

Thus $\alpha_2\cdot\alpha_3\leq 0$ gives $|\alpha_3|^2\geq|\alpha_1|^2$, so $(\alpha_1+\alpha_3)\cdot S\geq 0$. Therefore, all weak flatness conditions are satisfied.

Subcase (3)

$$\alpha_0\cdot\alpha_1=\alpha_0\cdot\alpha_2=\alpha_0\cdot\alpha_3=0.$$

Then

$$\alpha_0\cdot\alpha_0=\alpha_0\cdot\alpha_1+\alpha_0\cdot\alpha_2+\alpha_0\cdot\alpha_3=0,$$

which is impossible.

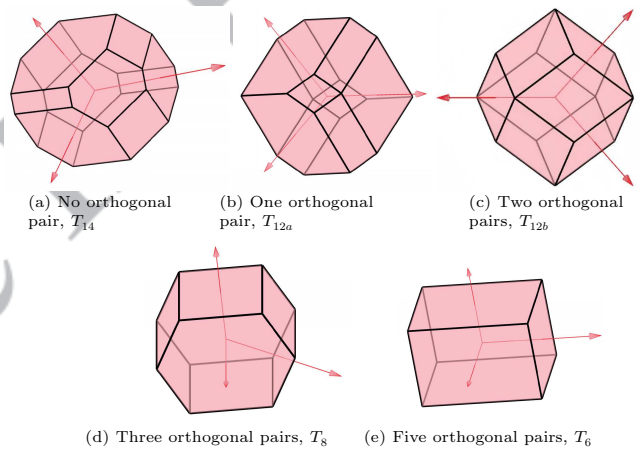


Fig. 4. Topological shapes of Wigner–Seitz cells in $\mathbb{R}^3$, cataloged according to the number of orthogonal pairs among the $\mathbb{V}_3$ base vectors. Red lines represent the basis.

The above arguments enumerate the topological shapes of Wigner–Seitz cells in dimensions 2 and 3, each of which has a unique generic case (Fig. 1 and Fig. 4). This uniqueness need not persist in higher dimensions ($n\geq 4$). In every dimension, explicit generic lattices can be constructed whose Wigner–Seitz cells attain $2\cdot(2^n-1)$ codimension-1 faces.

Assume that $\{\boldsymbol{\beta}_1,\boldsymbol{\beta}_2,\ldots,\boldsymbol{\beta}_{n-1}\}$ is a *flat basis* of $\mathbb{R}^{n-1}$. Define $\boldsymbol{\alpha}_n=(0,0,\ldots,0,1)$ and $\boldsymbol{\alpha}_i=\boldsymbol{\beta}_i-\varepsilon\boldsymbol{\alpha}_n$ for $1\leq i\leq n-1$, where $\varepsilon>0$. If ε is sufficiently small, then $\{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\ldots,\boldsymbol{\alpha}_n\}$ is a *flat basis* of $\mathbb{R}^n$. Let $\Gamma=\Gamma(\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\ldots,\boldsymbol{\alpha}_n)$ denote the lattice in $\mathbb{R}^n$ generated by $\{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\ldots,\boldsymbol{\alpha}_n\}$, namely

$$\Gamma(\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\ldots,\boldsymbol{\alpha}_n)=\Big\{\sum_{i=1}^{n}\lambda_i\boldsymbol{\alpha}_i\,\Big|\,\lambda_i\in\mathbb{Z}\Big\}.$$

Define the corresponding root vectors by

$$\Omega_n(\Gamma)=\{\boldsymbol{\alpha}_s\mid s\subseteq\{1,2,\ldots,n\},s\neq\varnothing\}\cup\{-\boldsymbol{\alpha}_s\mid s\subseteq\{1,2,\ldots,n\},s\neq\varnothing\},\tag{6}$$

where $s\subseteq\{1,2,\ldots,n\},s\neq\varnothing$, $\boldsymbol{\alpha}_s=\sum_{i\in s}\boldsymbol{\alpha}_i$, and (i) for $s,s'\subseteq\{1,2,\ldots,n\}$, $s\cap s'=\varnothing$, $\boldsymbol{\alpha}_s\cdot\boldsymbol{\alpha}_{s'}<0$; (ii) for $s,s'\subseteq\{1,2,\ldots,n\}$, $s\subseteq s'$, $\boldsymbol{\alpha}_s\cdot\boldsymbol{\alpha}_{s'}>0$.

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As in the low-dimensional case, by decomposing $\mathbb{R}^n$ into suitable cones, the intersection of infinitely many half spaces can be reduced to a finite intersection. For the lattice Γ, the Wigner–Seitz cell satisfies

$$\mathbb{W}_n(\Gamma) = \bigcap_{\boldsymbol{c}\in\Gamma} \mathcal{P}_+(\boldsymbol{c}) = \bigcap_{\boldsymbol{c}\in\Omega_n(\Gamma)} \mathcal{P}_+(\boldsymbol{c}).$$

Since $\#\Omega_n(\Gamma) = 2\cdot(2^n-1)$, the Wigner–Seitz cell $\mathbb{W}_n(\Gamma)$ has at most $2\cdot(2^n-1)$ codimension-1 faces.

On the other hand, one verifies that for any $s,s'\subseteq\{1,2,\ldots,n\}$ with $s,s'\neq\varnothing$ and $s\neq s'$, the following hold: (i) $(\boldsymbol{\alpha}_s-\boldsymbol{\alpha}_{s'})\cdot\boldsymbol{\alpha}_{s'}<0$; (ii) $(\boldsymbol{\alpha}_s+\boldsymbol{\alpha}_{s'})\cdot(-\boldsymbol{\alpha}_{s'})<0$; (iii) $(-\boldsymbol{\alpha}_s-\boldsymbol{\alpha}_{s'})\cdot\boldsymbol{\alpha}_{s'}<0$; (iv) $(-\boldsymbol{\alpha}_s+\boldsymbol{\alpha}_{s'})\cdot(-\boldsymbol{\alpha}_{s'})<0$. These inequalities imply that for any $\boldsymbol{r},\boldsymbol{r'}\in\Omega_n(\Gamma)$ with $\boldsymbol{r}\neq\boldsymbol{r'}$, the point $\boldsymbol{r}/2$ lies in the interior of $\mathcal{P}_+(\boldsymbol{r'})$. Consequently, $\partial\mathcal{P}_+(\boldsymbol{r})\cap\partial\mathbb{W}_n(\Gamma)$ is non-degenerate for each $\boldsymbol{r}\in\Omega_n(\Gamma)$, and therefore $\mathbb{W}_n(\Gamma)$ has exactly $2\cdot(2^n-1)$ codimension-1 faces. Furthermore, any lattice Γ' sufficiently close to Γ is also generated by a *flat basis* of $\mathbb{R}^n$, and its Wigner–Seitz cell $\mathbb{W}_n(\Gamma')$ has the same topological shape as $\mathbb{W}_n(\Gamma)$. In particular, Γ is generic.

For example, one can construct a generic lattice $\Gamma(\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\boldsymbol{\alpha}_3,\boldsymbol{\alpha}_4)$ in dimension 4 with the following flat basis:

$$\begin{cases}\boldsymbol{\alpha}_1=(1,1,1,-\varepsilon),\\ \boldsymbol{\alpha}_2=(1,-1,-1,-\varepsilon),\\ \boldsymbol{\alpha}_3=(-1,-1,1,-\varepsilon),\\ \boldsymbol{\alpha}_4=(0,0,0,1).\end{cases} \tag{7}$$

When ε is sufficiently small, $\{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\boldsymbol{\alpha}_3,\boldsymbol{\alpha}_4\}$ is a *flat basis* of $\mathbb{R}^4$. Therefore, the *root vectors* and the Wigner–Seitz cell are $\Omega=\{\boldsymbol{\alpha}_s\mid s\subseteq\{1,2,3,4\},s\neq\varnothing\}\cup\{-\boldsymbol{\alpha}_s\mid s\subseteq\{1,2,3,4\},s\neq\varnothing\}$, $\mathbb{W}(\Gamma)=\bigcap_{\boldsymbol{c}\in\Omega}\mathcal{P}_+(\boldsymbol{c})$, respectively. Here, $\mathbb{W}(\Gamma)$ has exactly 30 faces, each having either 12 or 24 vertices. However, in higher dimensions ($n\geq4$), such a generic case is not unique.

3. Conclusion

In conclusion, the topological origin of Wigner–Seitz cell shapes has been investigated, and it has been shown that a finite set of lattice vectors (the root vectors) suffices to describe the corresponding Wigner–Seitz cell in $\mathbb{R}^n$ as a finite intersection of half spaces. In particular, the number of half spaces needed is bounded above by the number of *root vectors*. Orthogonality within base vectors leads to degeneracies that reduce the number of codimension-1 faces; in the generic case, where no such orthogonality occurs, the Wigner–Seitz cell attains the maximal number of codimension-1 faces, $2(2^n-1)$. In dimensions 2 and 3, this yields a complete classification: there are only two (resp. five) topological types of polytopes that occur as Wigner–Seitz cells in $\mathbb{R}^2$ (resp. $\mathbb{R}^3$), and all degeneracies of vertices, edges, and faces are enumerated.

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References

[1] Voronoï G F 1908 *J. Reine Angew. Math.* **134** 198
[2] Voronoï G F 1909 *J. Reine Angew. Math.* **136** 67
[3] Aurenhammer F 1991 *ACM Comput. Surv.* **23** 345
[4] Okabe A, Boots B, Sugihara K and Chiu S N 2000 *Spatial Tessellations: Concepts and Applications of Voronoi Diagrams* 2nd ed (Wiley)
[5] Wigner E and Seitz F 1933 *Phys. Rev.* **43** 804
[6] Wigner E and Seitz F 1934 *Phys. Rev.* **46** 509
[7] Keister B D 1984 *J. Phys. C: Solid State Phys.* **17** 1833
[8] Than H S, Khan E and Giai N V 2011 *J. Phys. G: Nucl. Part. Phys.* **38** 025201
[9] Negele J W and Vautherin D 1973 *Nucl. Phys. A* **207** 298
[10] Pethick C J and Ravenhall D G 1995 *Annu. Rev. Nucl. Part. Sci.* **45** 429
[11] Zou P F and Bader R F W 1994 *Acta Cryst. A* **50** 714
[12] Sabin J R and Brandas E J 2009 *Theory of Confined Quantum Systems Parts I and II* (Elsevier)
[13] Bader R 1994 *Atoms in Molecules: A Quantum Theory* (Oxford University Press)
[14] Chadi D J and Cohen M L 1973 *Phys. Rev. B* **8** 5747
[15] Kresse G and Furthmüller J 1996 *Comput. Mater. Sci.* **6** 15
[16] Kresse G and Furthmüller J 1996 *Phys. Rev. B* **54** 11169
[17] Winter I S and Frolov T 2025 *Acta. Mater.* **291** 120968
[18] Kittel C 2005 *Introduction to Solid State Physics* 8th ed (Wiley)
[19] Gruber P M and Lekkerkerker C G 1987 *Geometry of Numbers* 2nd ed (North-Holland)
[20] Conway J H and Sloane N J A 1999 *Sphere Packings, Lattices and Groups* 3rd ed (Springer)
[21] Martinet J 2003 *Perfect Lattices in Euclidean Spaces* (Springer)
[22] Schürmann A 2009 *Computational Geometry of Positive Definite Quadratic Forms: Polyhedral Reduction Theories, Algorithms, and Applications* (American Mathematical Society)
[23] Koca M, Koca N O, Al-Siyabi A and Koc R 2018 *Acta Cryst.* **A74** 499
[24] Deza M M, Grishukhin V P and Shtogrin M I 2004 *Scale-Isometric Polytopal Graphs in Hypercubes and Cubic Lattices: Polytopes in Hypercubes and* $\mathbb{Z}^n$ (Imperial College Press)
[25] Erdahl R M 1999 *Eur. J. Comb.* **20** 527
[26] Deza M and Dutour Sikiríc M 2014 arXiv:1401.0040
[27] Cassels J W S 1959 *An Introduction to the Geometry of Numbers* (Springer-Verlag)
[28] Rogers C A 1964 *Packing and Covering* (Cambridge University Press)
[29] Grünbaum B 1967 *Convex Polytopes* (Wiley-Interscience)
[30] Ziegler G M 1995 *Lectures on Polytopes* (Springer)
[31] Zong C 1999 *Sphere Packings* (Springer)

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