# On the Computation of Fundamental Domains

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Let $\Gamma$ be an $n$-dimensional space group. One known method for computing a fundamental domain of $\Gamma$ uses the Dirichlet–Voronoi region. Choose $a \in \mathbb{R}^n$. The Dirichlet–Voronoi region $DV(a)$ is defined by

$$DV(a) := \{x \in \mathbb{R}^n \mid d(x,a) < d(x,\gamma(a)) \text{ for all } \gamma \in \Gamma \setminus \mathrm{Stab}_\Gamma(a)\}. \tag{1}$$

See [1, Theorem 1.2.1]. The following facts hold:

- $DV(a)$ is the interior of a convex region.
- If the stabilizer is trivial, $\mathrm{Stab}_\Gamma(a) = \{1\}$, then $DV(a)$ is a fundamental domain of $\Gamma$.

When computing $DV(a)$, only the points of the orbit $\Gamma(a)$ near $a$ matter. Write a translation in the space group as $\tau = \{I, t\} \in \Gamma$. Introduce the slab

$$S_a(\tau) := \{x \in \mathbb{R}^n \mid (a-t,t) < (x,t) < (a+t,t)\}. \tag{2}$$

These inequalities are equivalent to $|x-a| < |x-(a+2t)|$ and $|x-a| < |x-(a-2t)|$. Let $\tau_i$, $i = 1,\dots,n$, be a basis of the translation subgroup $T$ of $\Gamma$. Then [1, Lemma B.2] says:

- To compute $DV(a)$, it is enough to consider the point set

$$\mathcal{O} = \left(\Gamma(a) \cap \bigcap_{i=1}^n S_a(\tau_i)\right) \cup \{\pm\tau_1(a), \pm\tau_2(a), \dots, \pm\tau_n(a)\}. \tag{3}$$

An efficient computation of the Dirichlet–Voronoi region can be organized as follows.[1]

- For a representative $\{p_g, \boldsymbol{t}_g\}$ of the quotient $\Gamma/T$, use the ambiguity by translations in $T$ to choose the translation part $t_g$ so that its components lie inside the unit cell spanned by the lattice vectors. Concretely, writing $\tau_i = \{I, t_i\}$ and

$$t_g = \sum_{i=1}^n x_i t_i, \tag{4}$$

replace

$$x_i \mapsto [x_i] := x_i \bmod 1, \quad t_g \mapsto \sum_{i=1}^n [x_i] t_i. \tag{5}$$

[1] I thank Wataru Ishizaki for explaining the sorting and updating procedure.

- In this standard form, when constructing the set $\Gamma(a) \cap \bigcap_{i=1}^{n} S_a(\tau_i)$, it is enough, for each representative $g = \{p_g | t_g\} \in \Gamma/T$, to consider the finite point set

$$\left\{ p_g a + t_g + \sum_{i=1}^{n} n_i t_i \mid n_i \in \{-1, 0, 1\} \right\}. \tag{6}$$

  Points with $|n_i| = 2$ lie outside the slab $S_a(\tau_i)$.

- First compute the region $DV(a)_0$ using only the lattice translations

$$\mathcal{S} = \{\pm\tau_1(a), \pm\tau_2(a), \ldots, \pm\tau_n(a)\}. \tag{7}$$

- Sort the points in

$$\mathcal{O}' = \Gamma(a) \cap \bigcap_{i=1}^{n} S_a(\tau_i) \tag{8}$$

  by increasing distance from $a$.

- For the ordered points $p_1, p_2, \ldots$ of $\mathcal{O}'$, proceed iteratively:
  - If all boundary points of $DV(a)_j$ lie inside the perpendicular bisector between $a$ and $p_{j+1}$, do not update the region and set $DV(a)_{j+1} = DV(a)_j$.
  - If some boundary point of $DV(a)_j$ lies outside that perpendicular bisector, add $p_{j+1}$ to the point set $\mathcal{S}$ and recompute the region $DV(a)_{j+1}$.

# References


[1] Moritz W. Schmitt, *On Space Groups and Dirichlet-Voronoi Stereohedra*, Thesis, url.