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Mathematical aspects of molecular replacement. IV. Measure-theoretic decompositions of motion spaces

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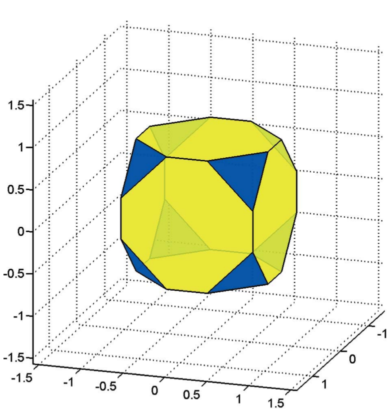
In molecular-replacement (MR) searches, spaces of motions are explored for determining the appropriate placement of rigid-body models of macromolecules in crystallographic asymmetric units. The properties of the space of non-redundant motions in an MR search, called a 'motion space', are the subject of this series of papers. This paper, the fourth in the series, builds on the others by showing that when the space group of a macromolecular crystal can be decomposed into a product of two space subgroups that share only the lattice translation group, the decomposition of the group provides different decompositions of the corresponding motion spaces. Then an MR search can be implemented by trading off between regions of the translation and rotation subspaces. The results of this paper constrain the allowable shapes and sizes of these subspaces. Special choices result when the space group is decomposed into a product of a normal Bieberbach subgroup and a symmorphic subgroup (which is a common occurrence in the space groups encountered in protein crystallography). Examples of Sohncke space groups are used to illustrate the general theory in the three-dimensional case (which is the relevant case for MR), but the general theory in this paper applies to any dimension.



1. Introduction

Molecular replacement (MR) is a computational method to phase macromolecular crystals that was introduced more than half a century ago (Rossmann & Blow, 1962). The output of MR is a set of candidate rigid-body motion parameters to describe how a protein (or other macromolecule) may be positioned and oriented in a crystal, based on information from its diffraction pattern.

This paper is concerned with characterizing the space of non-redundant rigid-body motions in which an MR search can take place, and is the fourth paper in a series. In the first paper of this series (Chirikjian, 2011), it was shown that this 'motion space', when endowed with an appropriate composition operator, forms an algebraic structure called a *quasigroup*, and that this set of motions over which MR searches are performed corresponds to a coset space of the group of proper rigid-body motions by a Sohncke space group. In the second paper of the series (Chirikjian & Yan, 2012), the geometric properties of these spaces were investigated. The third paper of this series (Chirikjian, Sajjadi *et al.*, 2015) examined the subgroup structure of the Sohncke space groups in which proteins crystallize and assessed the frequency of occurrence of these groups in the Protein Data Bank (PDB) (Berman *et al.*, 2002).

The results presented in this fourth paper also build on the previous recent paper (Chirikjian, Ratnayake *et al.*, 2015), where it was shown that most Sohncke space groups in which proteins crystallize can be decomposed as a semi-direct product of a Bieberbach subgroup (*i.e.* one that acts on Euclidean space without fixed points) and a subgroup of the point group.

In order to formulate the problem to be solved in this paper, some notation is first required. Here we summarize notation consistent with those previous works. Let $X = \mathbb{R}^n$, n-dimensional Euclidean space and let $\mathbf{x} \in X$.[1] The inputs to MR computations are then: (i) the electron-density function of a known rigid macromolecule (or fragment thereof) called the reference molecule; and (ii) the diffraction pattern of the protein crystal under investigation, which includes information about the symmetry group of the crystal, Γ, which is a discrete subgroup of $G \doteq \mathrm{SE}(n)$, the (connected) Lie group of proper motions of rigid bodies in n-dimensional Euclidean space. The discrete group Γ includes all information about the symmetry and geometry of the unit cell and asymmetric unit. The group operation for G and Γ is denoted as '$\circ$', and their action on Euclidean space is denoted as '$\cdot$'.

The electron-density function $\rho_X(\mathbf{x})$ takes a positive value on the reference molecule and a zero value away from it. This density can be thought of as defining a rigid body, $B \subset X$, as follows:[2]

$$B = \{\mathbf{x} \in X \,|\, \rho_X(\mathbf{x}) > 0\}.$$

The goal of MR is then to find the $g \in G$ such that the square of the magnitude of the Fourier transform of

$$\rho_{\Gamma\backslash X}(\mathbf{x}; g) \doteq \sum_{\gamma \in \Gamma} \rho_X[(\gamma \circ g)^{-1} \cdot \mathbf{x}]$$

matches the diffraction pattern. Because the summation is over $\gamma \in \Gamma$, there is no need to search over all of G, but rather only over the right coset space $\Gamma\backslash G$, or equivalently, a fundamental domain $F_{\Gamma\backslash G} \subset G$ consisting of one element of G for each right coset $\Gamma g \in \Gamma\backslash G$. This paper describes methods of evaluating integrals over $\Gamma\backslash G$ that use measures on various fundamental domains.

As described in the first two papers in this series, several different functions of the form $f : F_{\Gamma\backslash G} \longrightarrow \mathbb{R}_{\geq 0}$ arise in MR, the most well known of which is the Patterson correlation function and variants thereof. The particular goal of this paper is to describe different representations of the fundamental domain $F_{\Gamma\backslash G} \subset G$ of the coset space $\Gamma\backslash G$. In particular, we use decompositions of the form $\Gamma = K \ltimes N$ (where N is a normal subgroup of Γ and K is a subgroup of Γ consisting of pure rotations) to quantify the tradeoff in searching over translations and rotations in MR searches.

The Patterson correlations discussed in the first two papers in this series are examples of functions on $F_{\Gamma\backslash G}$. In the context of integration, §3 therefore explains what it means for two descriptions of the motion space $F_{\Gamma\backslash G}$ to be equivalent. In particular, a measure-theoretic sense of equivalence (as opposed to a topological sense) is defined, which is the most relevant for MR applications. §§4 and 5 provide a mathematical apparatus for interconverting between equivalent descriptions of a motion space *via* fibered integrals. §6 provides specific examples of these decompositions for some of the space groups in which proteins most frequently crystallize.

The notation and terminology used in this paper are summarized in a glossary at the end of this paper. Any terminology not explicitly defined here can be found in the many excellent books on the topic of space groups that have been published over the years including: Boisen & Gibbs (1990), Burns & Glazer (2013), Engel (1986), Evarestov & Smirnov (1993), Iversen (1990), Janssen (1973), Miller (1972), Senechal (1990). Up-to-date expositions of space groups, including the relationships between space groups, can be found in Hahn (2002), Wondratschek & Müller (2008) and Müller (2013).

2. Motivation

Current MR searches are initiated using a single copy of a known candidate molecule which is placed in a unit cell at *a priori* unknown candidate poses (positions and orientations). The full search space associated with this approach is then the Cartesian product of the unit cell and the full rotation group, each of which is a three-dimensional space. There are some advantages to taking this approach. In particular, the unit cell is the natural periodic object for use in FFT (fast Fourier transform) algorithms, and when there is only one copy of the candidate molecule per unit cell, the translational dependence of the pose appears as a phase factor in Fourier space which vanishes in the Patterson function. This allows a natural decomposition of a six-dimensional search into a search first over rotations, followed by one over translations (wherein a more realistic model of the unit cell including all symmetry mates is constructed). While this has been the standard approach to MR for more than half a century, this series of papers is motivated by a modified view in which the full six-dimensional space is handled from the beginning with a model unit cell consisting of all symmetry mates of the candidate molecule rather than a single isolated one.

A consequence of including all symmetry mates in the unit cell is that the search can no longer be decomposed into two sequential three-dimensional searches. However, there are three main reasons for pursuing this approach. First, as described in previous papers in this series, the total size of this search space is smaller by a factor of $[\Gamma : T]$ than the product of the full unit cell and full rotation group, and such factors can be substantial (*e.g.* 8, 12, or 24 in some cases). Practically, this means that translations can be drawn from only an asymmetric unit rather than the full unit cell. Second, and more importantly, the signal-to-noise ratio will in general be better than in separate searches over orientation and translation because the higher-dimensional models treat all 'cross talk' between all bodies in the unit cell as signal rather than treating cross terms

[1] Our presentation will be kept general, though of course the case $n = 3$ is the one of relevance in MR.
[2] The body B may in fact consist of a union of individual bodies which as a collection populate the crystallographic asymmetric unit $F_{\Gamma\backslash X}$, but only B as a whole under the action of Γ and a specific $g \in G$ replicates an ideal infinite crystal.

as noise. (This strategy is a starting point for a full $6N$-dimensional search when there are N molecules in each asymmetric unit.) Third, and most importantly, with a model unit cell that includes all symmetry mates it is possible to *a priori* assess which poses lead to collisions between symmetry mates. As a consequence, vast regions of the six-dimensional search space need not be searched because they correspond to nonphysical collisions between candidate molecules.

We have made progress in the paradigm of full-dimensional search in our previous paper (Chirikjian & Shiffman, 2016) by illustrating in the planar case how much of the unit cell is covered by 'collision zones' corresponding to candidate two-dimensional molecular models being in collision. We found in the planar case that the collision zones can be characterized as Minkowski sums of symmetry mates of candidate molecules. (The three-dimensional case also involves Minkowski sums, but the details are somewhat involved and are outside of the scope of the present paper.) Whereas proteins are irregular shapes, for the purpose of obtaining conservative estimates of the collision zones, it is possible to replace the original protein shape with an appropriately chosen ellipsoid and use the results in Yan & Chirikjian (2015) to compute these Minkowski sums either exactly or approximately. Ellipsoids are convenient objects to use because it is very easy to assess when a point lies inside or outside of an ellipsoid, and therefore searches that exclude sampling inside of ellipsoidal underestimates of collision zones can efficiently skip sampling there.

Herein lies one of the main motivations for the current paper. As observed in Yan & Chirikjian (2015), when two ellipsoids are close to being spherical, their Minkowski sum is almost ellipsoidal regardless of their orientations, and it is possible to construct ellipsoids that are both contained in the true Minkowski sum and that contain it. In the extreme case when the macromolecular candidates are spherical (as is the case for crystals of some kinds of viral particles), the Minkowski sums are simply spheres. Therefore, when viewing the search space $\Gamma\backslash G$ as being equivalent to $\Gamma\backslash X \times \mathrm{SO}(3)$, we can simply search first over $\Gamma\backslash X$ for positions that do not lead to collision because of the spherical symmetry, and then do rotation searches over rotations with high-fidelity models having first fixed candidate translations. (This would be doing things in opposite order to how MR usually works.) In contrast, at the other extreme when the candidate molecules in MR are either very prolate or oblate, their Minkowski sums can only be approximated well as ellipsoids at orientations that are close to the identity rotation. Therefore, recognizing that the full search space $\Gamma\backslash G$ can not only be described as $\Gamma\backslash X \times \mathrm{SO}(3)$, but also as $T\backslash X \times \mathbb{P}\backslash\mathrm{SO}(3)$, where $\mathbb{P}$ is the point group, allows for a more restricted search over rotations with the tradeoff of a larger search over translations. [Fundamental domains for the quotient $\mathbb{P}\backslash\mathrm{SO}(3)$ were illustrated in Chirikjian & Yan (2012).] The more restricted search over rotations is favorable in justifying the approximation of Minkowski sums of ellipsoids as ellipsoids, which in turn is favorable for rapid exploration of the collision-free part of the full six-dimensional MR search space by 'jumping over' regions known to correspond to symmetry mates being in collision.

In the long run, the goal is to extend the formulation in this paper to the case of full $6N$-dimensional searches in which there are N bodies per asymmetric unit. While that is challenging, there are some near-term problems of intermediate difficulty for which the methodology presented here is also applicable. In particular, for proteins consisting of two large rigid units (body 1 and body 2) connected by a long flexible region consisting of substantial material, it is sometimes the case that current MR approaches partially solve the problem by accurately placing body 1, but failing to place body 2. In this context, the available free space for body 2 to translate (for each candidate orientation) is the complement of the union of two kinds of 'collision zones'. The first is the Minkowski sum of body 2 with each symmetry-related copy of body 1. The second is the collision zone generated from the three-dimensional generalization of the procedure in Chirikjian & Shiffman (2016) which performs a calculation based on the Minkowski sum of body 2 with its own symmetry mates. As with the case of a single body per asymmetric unit, large amounts of the six-dimensional roto-translation space for body 2 are eliminated from consideration by characterizing the space of all possible collisions in this two-body scenario.

This paper formalizes the various ways that the space $\Gamma\backslash G$ can be decomposed. In short, there is a conservation law of sorts in which a tradeoff exists in choosing the volume of the translational and rotational parts of the search space. This tradeoff depends on the structure of the Sohncke space group describing the symmetry of a macromolecular crystal, and the fact that such groups are subgroups of the Special Euclidean group. The decompositions of the roto-translation space derived in this paper directly apply when there is one body per asymmetric unit, and also apply when there are two bodies per asymmetric unit, but with the position and orientation of one of the bodies predetermined.

3. Measure-equivalent fundamental domains

3.1. General fundamental domains

A discrete subgroup Δ of a Lie group $\mathbf{G}$ acts on $\mathbf{G}$ in a 'properly discontinuous' way, so that the orbit space of the left action, $\Delta\backslash\mathbf{G}$, is always a manifold. Discrete groups such as space groups acting on Euclidean space, and finite symmetry groups of the Platonic solids acting on spheres typically do not result in quotients that are manifolds. But they do act in a way that is 'nice enough'. This is reflected in the concept of a *properly discontinuous* action on a smooth Riemannian manifold Y, *e.g.* Euclidean space X or Euclidean motion group G. What this means is that given any compact (closed and bounded) set $\mathcal{S}$ in the manifold Y, there are only a finite number of elements δ in the discrete group Δ such that $(\delta \cdot \mathcal{S}) \cap \mathcal{S}$ is nonempty. All of the actions of discrete groups on continuous spaces of interest in MR have this property. The consequence of the existence of a discrete group Δ acting properly discontinuously on a smooth manifold Y is that one can find 'fundamental domains' $F_{\Delta\backslash Y}$ having the property that their images under the actions of the elements of Δ have closures that cover Y and interiors that do not overlap. To be precise, we give two equivalent descriptions of fundamental domains in the following lemma:

Lemma 3.1. Let Δ be a discrete group acting properly discontinuously on a manifold Y and suppose that Y has a Riemannian metric whose volume measure $d\mu$ is invariant under the Δ action. Let $E \subset Y$ be a measurable set. Then the following two conditions are equivalent:

(i)

$$\mu\left(Y \backslash \bigcup_{\delta\in\Delta} \delta \cdot E\right) = 0, \tag{1}$$

in combination with

$$\mu(\delta \cdot E \cap \delta' \cdot E) = 0 \quad \forall\, \delta \neq \delta'; \tag{2}$$

(ii) For every non-negative measurable function $\varphi : Y \to \mathbb{R}_{\geq 0}$,

$$\int_Y \varphi(y)\,\mathrm{d}\mu(y) = \int_E \sum_{\delta\in\Delta} \varphi(\delta \cdot y)\,\mathrm{d}\mu(y). \tag{3}$$

Proof. First suppose that equations (1)–(2) hold. Then the integral over Y can be divided into integrals over each $\delta \cdot E$ and added as

$$\begin{aligned}\int_Y \varphi(y)\,\mathrm{d}\mu(y) &= \sum_{\delta\in\Delta} \int_{\delta\cdot E} \varphi(y)\,\mathrm{d}\mu(y)\\ &= \sum_{\delta\in\Delta} \int_E \varphi(\delta^{-1} \cdot y)\,\mathrm{d}\mu(y)\\ &= \int_E \sum_{\delta\in\Delta} \varphi(\delta \cdot y)\,\mathrm{d}\mu(y).\end{aligned}$$

Now suppose that, contrary to equation (2), there exist $\delta \neq \delta'$ with

$$0 < \mu(\delta \cdot E \cap \delta' \cdot E) = \mu(E \cap \delta^{-1}\delta' \cdot E).$$

Let $\delta'' = \delta^{-1}\delta' \neq e$ and choose a measurable set $A \subseteq E \cap \delta'' \cdot E$ with $0 < \mu(A) < \infty$, and let $\varphi = \chi_A$. Then

$$\begin{aligned}\int_E \sum_{\lambda\in\Delta} \varphi(\lambda \cdot y)\,\mathrm{d}\mu(y) &= \sum_{\lambda\in\Delta} \int_{\lambda^{-1}\cdot E} \varphi\,\mathrm{d}\mu\\ &\geq \mu(A \cap E) + \mu(A \cap \delta'' \cdot E)\\ &= 2\mu(A) > \mu(A) = \int_Y \varphi\,\mathrm{d}\mu.\end{aligned}$$

Next suppose that $\mu(Y\backslash Y_0) > 0$, where $Y_0 \doteq \bigcup_{\delta\in\Delta} \delta \cdot E$, and consider the function $\varphi = \chi_{Y\backslash Y_0}$. Then the right side of equation (3) equals 0 while $\int_Y \varphi\,\mathrm{d}\mu = \mu(Y\backslash Y_0) > 0$. Thus in both cases, there exists φ for which equation (3) does not hold. □

If E is a closed set, equation (1) becomes

$$Y = \bigcup_{\delta\in\Delta} \delta \cdot E,$$

since $\bigcup_{\delta\in\Delta} \delta \cdot E$ is a closed set, so its complement is an open set of measure 0 and hence empty. Note that equations (1) and (2) do not depend on the choice of Riemannian metric on Y.

Definition 3.2. A fundamental domain for the discrete group Δ acting properly discontinuously on Y is defined to be any measurable set E that satisfies equations (1) and (2), or equivalently equation (3). Fundamental domains for $\Delta\backslash Y$ are denoted $F_{\Delta\backslash Y}$.[3] An exact fundamental domain is a fundamental domain, which we denote as $F'_{\Delta\backslash Y}$, containing exactly one point in each Δ orbit, *i.e.* Y is the disjoint union of the sets $\delta \cdot F'_{\Delta\backslash Y}$, for $\delta \in \Delta$.

For example, choosing a Riemannian metric on Y invariant under the Δ action, we can take as a fundamental domain for $\Delta\backslash Y$ the closed *Voronoi cell*

$$F^{\mathrm{Vor}}_{\Delta\backslash Y} \doteq \{y \in Y : \mathrm{dist}(y, y_0) \leq \mathrm{dist}(y, \delta \cdot y_0) \quad \forall\, \delta \in \Delta\}, \tag{4}$$

for any $y_0 \in Y$ such that $\delta \cdot y_0 \neq y_0\, \forall \delta \in \Delta\backslash\{e\}$.

Corollary 3.3. Let $F_{\Delta\backslash Y}$ be a fundamental domain for a finite group Δ acting on a manifold Y with Δ-invariant volume measure $d\mu$. If $f : Y \to \mathbb{R}_{\geq 0}$ is a measurable function with the symmetry $f(\delta \cdot y) = f(y)$ for all $\delta \in \Delta$, then

$$\int_Y f(y)\,\mathrm{d}\mu(y) = |\Delta| \int_{F_{\Delta\backslash Y}} f(y)\,\mathrm{d}\mu(y). \tag{5}$$

Proof. By equation (3) and the invariance of *f*,

$$\begin{aligned}\int_Y f(y)\,\mathrm{d}\mu(y) &= \sum_{\delta\in\Delta} \int_{F_{\Delta\backslash Y}} f(y)\,\mathrm{d}\mu(y)\\ &= |\Delta| \int_Y f(y)\,\mathrm{d}\mu(y).\end{aligned}$$

□

As an example, suppose that $\mathbf{G}$ is a Lie group with left-invariant measure μ and Δ is a discrete subgroup of $\mathbf{G}$. Then the orbits of the left action of Δ are the right cosets $\{\Delta g\}$ and for an integrable function φ on $\mathbf{G}$, we have by equation (3)

$$\int_{\mathbf{G}} \varphi\,\mathrm{d}\mu = \sum_{\delta\in\Delta} \int_{F_{\Delta\backslash\mathbf{G}}} \varphi(\delta \circ g)\,\mathrm{d}\mu(g).$$

Throughout this paper we use the following application of Lemma 3.1:

Theorem 3.4. Let $F_{\Delta\backslash Y}$ be a fundamental domain for a discrete group Δ acting properly discontinuously on a Riemannian manifold Y with a Δ-invariant volume element

[3] For the results in this paper, fundamental domains are not assumed to be connected, although we are primarily interested in connected fundamental domains.

$d\mu$. Then a measurable set $E \subset Y$ is a fundamental domain for $\Delta\backslash Y$ if and only if

$$\int_{F_{\Delta\backslash Y}} f\,\mathrm{d}\mu = \int_E f\,\mathrm{d}\mu \qquad (6)$$

for all non-negative measurable functions $f : Y \to \mathbb{R}_{\geq 0}$ invariant under the Δ action.

Proof. Suppose E is a fundamental domain and let $f : Y \to \mathbb{R}_{\geq 0}$ such that $f(\delta \cdot y) = f(y)$ for all $\delta \in \Delta$. By equation (3) applied to E with $\varphi = \chi_{F_{\Delta\backslash Y}} f$, we have

$$\begin{aligned}\int_{F_{\Delta\backslash Y}} f\,\mathrm{d}\mu &= \int_Y \varphi\,\mathrm{d}\mu = \int_E \sum_{\delta\in\Delta} \varphi(\delta\cdot y)\,\mathrm{d}\mu(y)\\ &= \sum_{\delta\in\Delta} \int_{E\cap\delta^{-1}\cdot F_{\Delta\backslash Y}} f\,\mathrm{d}\mu = \int_E f\,\mathrm{d}\mu,\end{aligned}$$

where the last equality is by equations (1)–(2).

To show the converse, we suppose that E satisfies equation (6). Let $\varphi : Y \to \mathbb{R}_{\geq 0}$ be an arbitrary non-negative measurable function and define

$$f(y) \doteq \sum_{\delta\in\Delta} \varphi(\delta\cdot y).$$

Then, by equation (6),

$$\begin{aligned}\int_E \sum_{\delta\in\Delta} \varphi(\delta\cdot y)\,\mathrm{d}\mu(y) &= \int_E f\,\mathrm{d}\mu = \int_{F_{\Delta\backslash Y}} f\,\mathrm{d}\mu\\ &= \sum_{\delta\in\Delta} \int_{F_{\Delta\backslash Y}} \varphi(\delta\cdot y)\,\mathrm{d}\mu(y)\\ &= \sum_{\delta\in\Delta} \int_{\delta^{-1}\cdot F_{\Delta\backslash Y}} \varphi\,\mathrm{d}\mu = \int_Y \varphi\,\mathrm{d}\mu,\end{aligned}$$

and thus by Lemma 3.1 E is a fundamental domain. □

3.2. Measure equivalence

The symbol '$\cong$' is used in several different ways in the first two papers in the series (and in mathematics more generally). In group theory, $A \cong B$ means that the groups $(A, \circ)$ and $(B, \hat{\circ})$ are isomorphic (with the group operations $\circ$ and $\hat{\circ}$ not stated explicitly). And in topology, when A and B are topological spaces, $A \cong B$ means that A and B are homeomorphic, *i.e.* there is a bijection from A to B that is continuous with continuous inverse. In order to distinguish between these two concepts, we denote the group-theoretic notion of equivalence as $\cong_{\mathrm{I}}$ and the topological version of equivalence as $\cong_{\mathrm{H}}$. For example,

$$\mathrm{SE}(n) \cong_{\mathrm{H}} \mathrm{SO}(n) \times \mathbb{R}^n,$$

as topological spaces, but as groups

$$\mathrm{SE}(n) = \mathrm{SO}(n) \ltimes \mathbb{R}^n \not\cong_{\mathrm{I}} \mathrm{SO}(n) \times \mathbb{R}^n.$$

We use the corresponding notation $f : A \overset{\approx}{\to}_{\mathrm{I}} B$ to indicate that f is a group isomorphism, and $f : A \overset{\approx}{\to}_{\mathrm{H}} B$ to indicate that f is a homeomorphism. We also write $f : A \overset{\approx}{\to}_{\mathrm{S}} B$ to indicate that f is a bijection (isomorphism of sets).

In what follows, a different sense of equivalence, which we call *equivalence in measure*, is considered. Namely, if $\Phi : (\Omega, \mu) \to (Y, \nu)$ is a measurable map of measure spaces, we write $\Phi : \Omega \overset{\approx}{\to}_{\mathrm{M}} Y$ if there exist negligible sets[4] $\mathcal{N} \subset \Omega$ and $\mathcal{N}' \subset Y$ such that $\Phi|_{\Omega\backslash\mathcal{N}} : \Omega\backslash\mathcal{N} \to Y\backslash\mathcal{N}'$ is a bijection and $\nu = \Phi_*\mu$ (*i.e.* $\int_Y f\,\mathrm{d}\nu = \int_\Omega f\circ\Phi\,\mathrm{d}\mu$ for all integrable functions f on Y). In this case we say that Φ is an equivalence in measure. If in addition Φ is a bijection, we write $\Phi : \Omega \overset{\approx}{\to}_{\mathrm{M,S}} Y$, and we similarly write $\Phi : \Omega \overset{\approx}{\to}_{\mathrm{M,H}} Y$ if φ is a measure-preserving homeomorphism. We also use the shorthand $\Omega \cong_{\mathrm{M}} Y$, $\Omega \cong_{\mathrm{M,S}} Y$, $\Omega \cong_{\mathrm{M,H}} Y$ when there exists a measure equivalence, a measure-preserving bijection or a measure-preserving homeomorphism, respectively, between Ω and Y. This shorthand notation is less precise, since it does not specify the mapping. However, we use it when the mapping is understood by the context.

An elementary example of the concept of measure equivalence is given by the formula for integration over SO(3),

$$\int_{\mathrm{SO}(3)} f(R)\,\mathrm{d}R,$$

which is computed in ZXZ Euler angles as

$$\begin{aligned}&\frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} f(\alpha,\beta,\gamma)\sin\beta\,\mathrm{d}\alpha\,\mathrm{d}\beta\,\mathrm{d}\gamma\\ &= \int_{\mathrm{SO}(2)}\int_{S^2} f(\alpha,\beta,\gamma)\,\mathrm{d}\mathbf{u}(\alpha,\beta)\frac{1}{2\pi}\,\mathrm{d}\gamma,\end{aligned}$$

where (α, β, γ) are ZXZ Euler angles of the rotation R, and where $\mathbf{u} \in S^2$ with β, α serving the roles of polar and azimuthal spherical coordinates. In this interpretation $d\mathbf{u}(\alpha, \beta) = (1/4\pi)\sin\beta\, d\alpha\, d\beta$. Therefore, we have

$$\mathrm{SO}(3) \cong_{\mathrm{M}} \mathrm{SO}(2) \times S^2 = S^1 \times S^2,$$

even though $\mathrm{SO}(3) \not\cong_{\mathrm{H}} \mathrm{SO}(2) \times S^2$.

A common example is when $\mathcal{N}$ is a negligible set in a measure space Ω, then $\Omega\backslash\mathcal{N}$ is measure equivalent to Ω (under the inclusion map). In particular, if Δ acts isometrically without fixed points on a Riemannian manifold Y, then the closed Voronoi fundamental domain $F^{\mathrm{Vor}}_{\Delta\backslash Y}$ given by equation (4) contains a measure-equivalent exact fundamental domain $F'_{\Delta\backslash Y}$.

Using the notation of Theorem 3.4, we define the mapping $\iota : F_{\Delta\backslash Y} \longrightarrow \Delta\backslash Y$ given by $\iota(y) = \Delta y$, which induces the measure $\tilde{\mu}$ on $\Delta\backslash Y$ defined by $\tilde{\mu}(A) = \mu(\iota^{-1}(A))$. Then ι is a measure equivalence:

$$\iota : F_{\Delta\backslash Y} \overset{\approx}{\to}_{\mathrm{M}} \Delta\backslash Y \qquad (7)$$

with respect to the measures μ on Y, $\tilde{\mu}$ on $\Delta\backslash Y$. In other words, if $\tilde{f}$ is a measurable non-negative (or integrable) function on $\Delta\backslash Y$ and f is the Δ-invariant function on Y given by $f(y) = \tilde{f}(\Delta y)$, then equation (7) is equivalent to

$$\int_{F_{\Delta\backslash Y}} f\,\mathrm{d}\mu = \int_{\Delta\backslash Y} \tilde{f}\,\mathrm{d}\tilde{\mu}. \qquad (8)$$

[4] Sets of measure zero.

Theorem 3.4 can then be restated to say that the measure $\tilde{\mu}$ on the orbit space $\Delta\backslash Y$ given by equation (7) is independent of the choice of fundamental domain $F_{\Delta\backslash Y}$. It follows that if $F_{\Delta\backslash Y}$ and $\widetilde{F}_{\Delta\backslash Y}$ are two fundamental domains for $\Delta\backslash Y$, then we have a measure-equivalent map

$$\boxed{\tau : F_{\Delta\backslash Y} \xrightarrow{\approx}_M \widetilde{F}_{\Delta\backslash Y},} \tag{9}$$

given by associating a point in $F_{\Delta\backslash Y}$ with a point of $\widetilde{F}_{\Delta\backslash Y}$ in the same Δ orbit. (This is defined for all points of $F_{\Delta\backslash Y}$ outside a set of measure 0.) Combining equations (7) and (9), we have

$$F_{\Delta\backslash Y} \cong_{\rm M} \widetilde{F}_{\Delta\backslash Y} \cong_{\rm M} \Delta\backslash Y. \tag{10}$$

If Δ is a fixed-point-free action on Y, then equation (9) becomes

$$\boxed{\tau : F'_{\Delta\backslash Y} \xrightarrow{\approx}_{M,S} \widetilde{F}'_{\Delta\backslash Y}} \tag{11}$$

where we recall that $F'_{\Delta\backslash Y}$ denotes an exact fundamental domain. Bijectivity in equation (11) holds since an exact fundamental domain contains exactly one point in each orbit. We then have

$$F'_{\Delta\backslash Y} \cong_{\rm M,S} \widetilde{F}'_{\Delta\backslash Y} \cong_{\rm M,S} \Delta\backslash Y. \tag{12}$$

The measure-equivalent map τ between fundamental domains in equations (9) and (11) can be described as cutting up the first fundamental domain and applying Δ actions on the pieces to re-assemble them inside the second fundamental domain.

4. Fundamental domains for motion spaces

The central theme of this paper is the description of various fundamental domains $F_{\Gamma\backslash G}$ for a crystallographic group Γ acting on the motion group G. The description is based on the representation of $G \doteq {\rm SE}(n)$ as an (external) semi-direct product $G = {\rm SO}(n) \ltimes \mathbb{R}^n$ so that special Euclidean transformations can be written $g = (R, \mathbf{t}) \in {\rm SE}(n)$, which acts on positions as $g \cdot \mathbf{x} = R\mathbf{x} + \mathbf{t}$. The group law in G is then

$$g_1 \circ g_2 = (R_1, \mathbf{t}_1) \circ (R_2, \mathbf{t}_2) = (R_1 R_2, R_1 \mathbf{t}_2 + \mathbf{t}_1).$$

A crystallographic group Γ is a discrete subgroup of G that contains a discrete translation subgroup T of rank n as its maximal normal abelian subgroup. The group T consists of translations by elements of a lattice $\mathbb{L}$ in $X = \mathbb{R}^n$. (We have $\mathbb{L} = T \cdot \mathbf{0}$; $T = \{\mathbb{I}\} \times \mathbb{L}$.) Elements γ of the group $\Gamma < G$ are of the form

$$\gamma = [R_\gamma, \mathbf{t}_\gamma + \mathbf{v}(R_\gamma)], \tag{13}$$

where $\mathbf{t}_\gamma \in \mathbb{L}$ and $\mathbf{v}_\gamma(R_\gamma)$ is a fraction (possibly 0) of an element of $\mathbb{L}$, given uniquely modulo T by equation (13).

In the remainder of this paper, we describe different ways to construct fundamental domains $F_{\Gamma\backslash G}$. Both these and the coset spaces $\Gamma\backslash G$ can be considered motion spaces, since they are measure equivalent, as described earlier. The following observations provide our motivation:

(*a*) The functions encountered in the kinds of MR searches described in earlier papers in this series have the symmetry $f(g) = f(\gamma \circ g)$ for all $\gamma \in \Gamma$ and $g \in G$.

(*b*) It is possible to construct $F_{\Gamma\backslash G}$ and the asymmetric unit $F_{\Gamma\backslash X}$ in such a way that they have useful symmetries.

(*c*) Given a function on Euclidean space with symmetry $\rho(\mathbf{x}) = \rho(\mathbf{x} + \mathbf{t})$ where $\mathbf{t} \in \mathbb{L}$, the integral of this function over *any* unit cell $F_{T\backslash X}$ produces the same outcome. In particular,

$$\int_{F_{T\backslash X}} \rho(\mathbf{x})\,{\rm d}\mathbf{x} = \int_{F_{T\backslash X}} \rho(\mathbf{x} + \mathbf{a})\,{\rm d}\mathbf{x}$$

for any $\mathbf{a} \in X$.

Specializing Lemma 3.1 and Theorem 3.4 to the Euclidean motion group G, we have:

Theorem 4.1. Let H be a subgroup of a crystallographic group $\Gamma < G$ and let E be a measurable set in G. Then the following are equivalent:

(i) E is a fundamental domain for H acting on G.

(ii) For every non-negative measurable function $\varphi : G \to \mathbb{R}_{\geq 0}$,

$$\int_G \varphi(g)\,{\rm d}g = \int_E \sum_{h \in H} \varphi(h \circ g)\,{\rm d}g.$$

(iii) If $F_{H\backslash G}$ is a fundamental domain for $H\backslash G$, then

$$\int_{F_{H\backslash G}} f\,{\rm d}g = \int_E f\,{\rm d}g,$$

for every non-negative measurable function $f : G \to \mathbb{R}_{\geq 0}$ such that $f(\gamma \cdot g) = f(g)$ for all $h \in H$, $g \in G$.

As a consequence, if $F'_{H\backslash G}$ and $\widetilde{F}'_{H\backslash G}$ are fundamental domains for $H\backslash G$, we have measure equivalences

$$F'_{H\backslash G} \cong_{\rm M,S} \widetilde{F}'_{H\backslash G} \cong_{\rm M,S} H\backslash G. \tag{14}$$

Important cases of Theorem 4.1 and equation (14) are $H = \Gamma$ and $H = T$, discussed below.

4.1. The motion space $T\backslash G$

As discussed in §4.2 of Chirikjian & Yan (2012), the left action of T on G given by

$$t' \cdot g = (\mathbb{I}, \mathbf{t}') \circ (R, \mathbf{t}) = (R, \mathbf{t}' + \mathbf{t})$$

has no effect on the rotational part of $g \in G$, and

$$T\backslash G \cong_{\rm H} {\rm SO}(n) \times T\backslash X \tag{15}$$

is a trivial principal ${\rm SO}(n)$ bundle.[5] Moreover,

$$F_{T\backslash G} \cong_{\rm M,H} {\rm SO}(n) \times F_{T\backslash X}$$

(*i.e.* this equivalence is both topological and measure-theoretic).

We can think of $F_{T\backslash X}$ as the unit cell that tiles $\mathbb{R}^n$ under the action of T, and

[5] In §4.2 of Chirikjian & Yan (2012) all instances of $\Gamma\backslash G$ and $\Gamma\backslash X$ should be read as $T\backslash G$ and $T\backslash X$, respectively, if $\cong$ is interpreted as $\cong_{\rm H}$, or can be left as is if $\cong$ is interpreted as $\cong_{\rm M}$.

$$G = \bigcup_{t \in T} t \cdot F_{T\backslash G},$$

where

$$\mu\big[F_{T\backslash G} \cap (t \cdot F_{T\backslash G})\big] = 0, \quad \forall\, t \in T\backslash\{e\}.$$

Any integrable function $\tilde{f} : T\backslash G \to \mathbb{R}$ can be thought of as being equivalent to $f : G \to \mathbb{R}$ together with the constraint that $f(t \circ g) = f(g)$ for all $t \in T$. Then, by equation (7),

$$\mu_{T\backslash G}(\tilde{f}) = \int\limits_{T\backslash G} \tilde{f}(Tg)\,\mathrm{d}(Tg) = \int\limits_{F_{T\backslash G}} f(g)\,\mathrm{d}g.$$

Since $\mathrm{SO}(n) \times F_{T\backslash X}$ is a fundamental domain for $T\backslash G$, we conclude from Theorem 3.4 that

$$\int\limits_{F_{T\backslash G}} f(g)\,\mathrm{d}g = \int\limits_{F_{T\backslash X}} \int\limits_{\mathrm{SO}(n)} f(R, \mathbf{t})\,\mathrm{d}R\,\mathrm{d}\mathbf{t}.$$

4.2. The motion space $\Gamma\backslash G$

In the context of more general motion spaces, we consider measurable functions $f : G = \mathrm{SE}(n) \to \mathbb{R}$ with symmetry

$$f(g) = f(\gamma \circ g), \quad \forall \gamma \in \Gamma < G.$$

Writing $\gamma = [R_\gamma, \mathbf{t}_\gamma + \mathbf{v}(R_\gamma)] \in \Gamma$, we have

$$f(R, \mathbf{t}) = f(R_\gamma R, \gamma \cdot \mathbf{t}) = f[R_\gamma R,\ R_\gamma \mathbf{t} + \mathbf{t}_\gamma + \mathbf{v}(R_\gamma)]. \qquad (16)$$

We are interested in integrals of the form

$$\int\limits_{\Gamma\backslash G} \tilde{f}(\Gamma g)\,\mathrm{d}(\Gamma g) = \int\limits_{F_{\Gamma\backslash G}} f(g)\,\mathrm{d}g$$

where $\tilde{f}(\Gamma g) \doteq f(g)$. Here dg and $d(\Gamma g)$ are the Haar measures for G and $\Gamma\backslash G$, respectively.

Suppose that N is a normal subgroup of Γ. (For example, we can take N to be the pure translation group $T = \{(\mathbb{I}, \mathbf{t}) : \mathbf{t} \in \mathbb{L}\}$.) We then write $\overline{G} \doteq N\backslash G$, $\overline{\Gamma} \doteq \frac{\Gamma}{N}$. The group $\overline{\Gamma}$ acts on $\overline{G}$ by the rule

$$(N\gamma) \cdot (Ng) \doteq N\gamma g. \qquad (17)$$

Any function $\tilde{f} : \Gamma\backslash G \to \mathbb{R}$ can be regarded as a function $\tilde{f} : N\backslash G \to \mathbb{R}$ with additional symmetries of the form

$$\tilde{f}[(N\gamma) \cdot (Ng)] = \tilde{f}(Ng) \qquad (18)$$

whenever $\gamma \in F_{N\backslash\Gamma} \subset \Gamma$.

We show below that equation (17) gives a well defined $\overline{\Gamma}$ action on $\overline{G}$ and there is a natural measure-preserving homeomorphism $\alpha : \overline{\Gamma}\backslash\overline{G} \overset{\approx}{\to}_{\mathrm{H,M}} \Gamma\backslash G$ (see Proposition 4.4). We begin with the following general fact:

Lemma 4.2. Let N be a normal subgroup of a group K acting on the left on a set Ω (for example, K is a subgroup of a group Ω), and let $\overline{K} \doteq \frac{K}{N}$. Then the group $\overline{K}$ acts on the orbit space $\overline{\Omega} \doteq N\backslash\Omega$ by the rule

$$(Nk) \cdot (N\omega) = N(k \cdot \omega),\ \text{for}\ k \in K,\ \omega \in \Omega, \qquad (19)$$

and we have a bijective mapping

$$\alpha : \overline{K}\backslash\overline{\Omega} \overset{\approx}{\to}_{\mathrm{S}} K\backslash\Omega,\ \alpha\big[\overline{K} \cdot (N\omega)\big] = K\omega. \qquad (20)$$

Proof. Equation (19) gives a well defined action since for any $n, n' \in N$,

$$k' = nk,\ \omega' = n' \cdot \omega \Rightarrow$$
$$N(k' \cdot \omega') = N(nkn' \cdot \omega) = N(n''k \cdot \omega) = N(k \cdot \omega),$$

since N is normal in K. The action is a group action since

$$(Nk_1) \cdot [(Nk_2) \cdot (N\omega)] = (Nk_1) \cdot (Nk_2 \cdot \omega) = N(k_1 k_2 \cdot \omega).$$

We use the notation $\overline{k} = Nk \in \overline{K}, \overline{\omega} = N\omega \in \overline{\Omega}$. The mapping α is well defined and bijective since for any two elements $\omega, \omega' \in \omega$,

$$\overline{K\omega} = \overline{K\omega'} \Leftrightarrow \exists k \in K \mathrm{s.t.} \overline{\omega} = \overline{k} \cdot \overline{\omega}' = \overline{k \cdot \omega'}$$
$$\Leftrightarrow \exists n \in N \mathrm{s.t.} \omega = nk \cdot \omega' \Leftrightarrow K\omega = K\omega'.$$

□

For example, given a group H with $N \triangleleft K < H$, we have a natural bijective map

$$\alpha : \left(\frac{K}{N}\right)\backslash(N\backslash H) \overset{\approx}{\to}_{\mathrm{S}} K\backslash H. \qquad (21)$$

If, in addition, $N \triangleleft H$ and $K \triangleleft H$, then equation (21) becomes the 'Third Isomorphism Theorem' of group theory,

$$\left(\frac{K}{N}\right)\backslash\left(\frac{H}{N}\right) \cong_{\mathrm{I}} \frac{H}{K}.$$

Our main interest here is when K is a discrete group acting on a manifold:

Lemma 4.3. Let $N \triangleleft K$ where K is a discrete group acting properly discontinuously on a Riemannian manifold Y and let $\overline{K} = \frac{K}{N}$. Suppose that K preserves the volume measure on Y and let $\overline{Y} = N\backslash Y$ with the volume measure given by equation (7). Then there is a measure-preserving homeomorphism

$$\alpha : \overline{K}\backslash\overline{Y} \overset{\approx}{\to}_{\mathrm{H,M}} K\backslash Y,\ \overline{K} \cdot \overline{y} \mapsto K \cdot y, \qquad (22)$$

where $\overline{y} = Ny \in \overline{Y}$.

Proof. Let $\alpha : \overline{K}\backslash\overline{Y} \overset{\approx}{\to}_{\mathrm{S}} K\backslash Y$ be given as in Lemma 4.2. Now consider the maps π, π' given by

$$N\backslash Y = \overline{Y} \overset{\pi}{\to} \overline{K}\backslash\overline{Y} \overset{\alpha}{\to} K\backslash Y$$

and

$$\pi' = \alpha \circ \pi : N\backslash Y \to K\backslash Y.$$

To show the measure and topological equivalences, suppose $A \subset \overline{K}\backslash\overline{Y}$ and let $A' = \alpha(A) \subset K\backslash Y$. Then

$$A\ \text{is open} \Longleftrightarrow \pi^{-1}(A) = \pi'^{-1}(A')\ \text{is open}$$
$$\Longleftrightarrow A'\ \text{is open},$$

which completes the proof of topological equivalence. To show measure equivalence, we similarly have

$$\mu(A) = \frac{1}{|\overline{K}|}\mu\big[\pi^{-1}(A)\big] = \frac{1}{|\overline{K}|}\mu\big[\pi'^{-1}(A')\big] = \mu(A').$$

Therefore, $\alpha : \overline{K}\backslash\overline{Y} \overset{\approx}{\rightarrow}_{\rm H,M} K\backslash Y$. □

Applying Lemma 4.3 with $K = \Gamma$ and $Y = G$ or X, we obtain:

Proposition 4.4. Suppose that $N \triangleleft \Gamma$ and write $\overline{G} = N\backslash G$, $\overline{\Gamma} = N\backslash\Gamma$. Then there are measure-preserving homeomorphisms

$$\alpha_G : \overline{\Gamma}\backslash\overline{G} \overset{\approx}{\rightarrow}_{\rm H,M} \Gamma\backslash G, \overline{\Gamma}\overline{g} \mapsto \Gamma g, \tag{23}$$

$$\alpha_X : \overline{\Gamma}\backslash\overline{X} \overset{\approx}{\rightarrow}_{\rm H,M} \Gamma\backslash X, \overline{\Gamma}\overline{\mathbf{x}} \mapsto \Gamma\mathbf{x}, \tag{24}$$

where equation (7) is used to define the induced measures on the quotient spaces.

4.3. Fundamental domains for Γ\G

Suppose $F'_{N\backslash G}$ is a fundamental domain for $N\backslash G$, where $N \triangleleft \Gamma$. Since $F'_{N\backslash G} \cong_{\rm M,S} N\backslash G$, it follows from equation (23) that $N\backslash\Gamma$ provides a fixed-point-free group action on $F'_{N\backslash G}$. In fact, we have the following:

Theorem 4.5. Suppose that $N \triangleleft \Gamma$ and let $F'_{N\backslash G}$ be a fundamental domain for $N\backslash G$. Then there is a fundamental domain $F'_{\Gamma\backslash G} \subset F'_{N\backslash G}$ such that each orbit of $\overline{\Gamma} \doteq N\backslash\Gamma$ acting on $F'_{N\backslash G}$ contains exactly one point of $F'_{\Gamma\backslash G}$, and equivalences

$$\overline{\Gamma}\backslash(F'_{N\backslash G}) \cong_{\rm M,S} F'_{\Gamma\backslash G} \cong_{\rm M,S} F'_{\overline{\Gamma}\backslash(F'_{N\backslash G})}. \tag{25}$$

Furthermore, if $[\Gamma : N] < \infty$ (*e.g.* if $T \le N \triangleleft \Gamma$) and $f : F'_{N\backslash G} \to \mathbb{R}$ is a measurable function that is invariant under the $\overline{\Gamma}$ action, then

$$\int_{F'_{\Gamma\backslash G}} f(g)\,{\rm d}g = \frac{1}{[\Gamma : N]}\int_{F'_{N\backslash G}} f(g)\,{\rm d}g. \tag{26}$$

Proof. Let $F'_{\overline{\Gamma}\backslash(F'_{N\backslash G})}$ be a fundamental domain for $\overline{\Gamma}\backslash(F'_{N\backslash G})$. Since

$$\overline{\Gamma}\backslash(F'_{N\backslash G}) \cong_{\rm M,S} \overline{\Gamma}\backslash\overline{G} \cong_{\rm M,S} \Gamma\backslash G$$

by equation (23), it follows that $F'_{\overline{\Gamma}\backslash(F'_{N\backslash G})}$ is also a fundamental domain for $\Gamma\backslash G$, and equation (25) then follows from equation (7). To verify equation (26), we apply Corollary 3.3 with $Y = F'_{N\backslash G}$ and $\Delta = \overline{\Gamma}$ to obtain

$$\int_{F'_{N\backslash G}} f(g)\,{\rm d}g = |\overline{\Gamma}|\int_{F'_{\overline{\Gamma}\backslash(F'_{N\backslash G})}} f(g)\,{\rm d}g = |\overline{\Gamma}|\int_{F'_{\Gamma\backslash G}} f(g)\,{\rm d}g,$$

where the second equality follows from equation (25). Since $|\overline{\Gamma}| = [\Gamma : N]$, equation (26) follows. □

The action of $N\backslash\Gamma$ on $N\backslash G$ that led to equation (26) can be thought of as constructing $F_{N\backslash G}$ from copies of $F_{\Gamma\backslash G}$, as

$$F_{N\backslash G} = \bigcup_{\gamma\in F_{N\backslash\Gamma}} \gamma\cdot F_{\Gamma\backslash G}.$$

If $F_{\Gamma\backslash X} \subset X$ is a fundamental domain for $\Gamma\backslash X$, then $\mathrm{SO}(n) \times F_{\Gamma\backslash X}$ is a fundamental domain for $\Gamma\backslash G$. To see this, let $g = (R, \mathbf{t}) \in G$ be arbitrary. Then for $\gamma = [R_\gamma, \mathbf{t}_\gamma + \mathbf{v}(R_\gamma)]$, we have by equation (16) $\gamma\circ g = (R_\gamma R, \gamma\cdot\mathbf{t})$. Since the sets $\gamma\cdot F_{\Gamma\backslash X}$ tile X (when γ runs through Γ), it follows that the sets $\gamma\cdot[\mathrm{SO}(n) \times F_{\Gamma\backslash X}]$ tile $G = \mathrm{SO}(n) \ltimes X$. Therefore, if $F_{\Gamma\backslash G}$ is an arbitrary fundamental domain for $\Gamma\backslash G$, we have

$$\boxed{F_{\Gamma\backslash G} \cong_M \mathrm{SO}(n) \times F_{\Gamma\backslash X}.} \tag{27}$$

In particular, if f is a measurable function on G, invariant under the left Γ action, then

$$\int_{F_{\Gamma\backslash G}} f(g)\,{\rm d}g = \int_{F_{\Gamma\backslash X}}\int_{\mathrm{SO}(n)} f(R, \mathbf{t})\,{\rm d}R\,{\rm d}\mathbf{t}. \tag{28}$$

Similarly, if $F_{T\backslash X} \subset X$ is a fundamental domain for $T\backslash X$, then $\mathrm{SO}(n) \times F_{T\backslash X}$ is a fundamental domain for $T\backslash G$ (and the same holds for the exact fundamental domain $F'_{T\backslash X} \subset X$). Therefore, by equation (26),

$$\int_{F_{\Gamma\backslash G}} f(g)\,{\rm d}g = \frac{1}{[\Gamma : T]}\int_{F_{T\backslash X}}\int_{\mathrm{SO}(n)} f(R, \mathbf{t})\,{\rm d}R\,{\rm d}\mathbf{t}, \tag{29}$$

where we recall that $[\Gamma : T] = |T\backslash\Gamma|$. Since

$$F'_{T\backslash G} \cong_{\rm M,S} \mathrm{SO}(n) \times F'_{T\backslash X}, \tag{30}$$

it follows from Theorem 4.5 that

$$\boxed{\Gamma\backslash G \cong_{M,S} (T\backslash\Gamma)\backslash\left[\mathrm{SO}(n) \times F'_{T\backslash X}\right].} \tag{31}$$

An alternative to equation (27) is given by the following:

Proposition 4.6. $F'_{\mathbb{P}\backslash\mathrm{SO}(n)} \times F'_{T\backslash X}$ is an exact fundamental domain for $\Gamma\backslash G$.

Proof. Let $F \doteq F'_{\mathbb{P}\backslash\mathrm{SO}(n)} \times F'_{T\backslash X}$. We first show that the sets $\{\gamma\cdot F\}_{\gamma\in\Gamma}$ are disjoint. Since the Γ action is a group action, it suffices to show that $(\gamma\cdot F)\cap F = \emptyset$ for all $\gamma \ne e$. Let $\gamma = [R_\gamma, \mathbf{t}_\gamma + \mathbf{v}(R_\gamma)] \ne (\mathbb{I}, \mathbf{0})$ be arbitrary.

Case (1), $R_\gamma \ne \mathbb{I}$. Since $R_\gamma \in \mathbb{P}$, by the definition of the fundamental domain $F'_{\mathbb{P}\backslash\mathrm{SO}(n)}$, we have

$$F'_{\mathbb{P}\backslash\mathrm{SO}(n)} \cap R_\gamma\cdot F'_{\mathbb{P}\backslash\mathrm{SO}(n)} = \emptyset$$

and thus $(\gamma\cdot F)\cap F = \emptyset$.

Case (2), $R_\gamma = \mathbb{I}$. Then $\gamma = (\mathbb{I}, \mathbf{t}_\gamma)$, where $\mathbf{t}_\gamma \in T\backslash\mathbf{0}$. Since $\gamma \circ (R, \mathbf{t}) = (R, \mathbf{t} + \mathbf{t}_\gamma)$ and $F'_{T\backslash X} \cap (\mathbf{t}_\gamma + F'_{T\backslash X}) = \emptyset$, it follows that $(\gamma \cdot F) \cap F = \emptyset$.

It remains to show that

$$\bigcup_{\gamma\in\Gamma} \gamma \cdot F = G. \tag{32}$$

So suppose that $g = (R, \mathbf{t})$ is an arbitrary element of G. Then there exist $R_\gamma \in \mathbb{P}$ and $\tilde{R} \in F'_{\mathbb{P}\backslash\mathrm{SO}(n)}$ (where $\mathbb{P}$ denotes the point group defined below) such that $\tilde{R} = R_\gamma R$. And there exist $\mathbf{t}_\gamma \in T$ and $\tilde{\mathbf{t}} \in F'_{T\backslash X}$ such that $\tilde{\mathbf{t}} = \mathbf{t}_\gamma + [R_\gamma \mathbf{t} + \mathbf{v}(R_\gamma)]$. Let $\gamma = [R_\gamma, \mathbf{t}_\gamma + \mathbf{v}(R_\gamma)] \in \Gamma$. Then

$$\gamma \circ g = [R_\gamma, \mathbf{t}_\gamma + \mathbf{v}(R_\gamma)] \circ (R, \mathbf{t}) = (\tilde{R}, \tilde{\mathbf{t}}) \in F$$

and therefore $g = \gamma^{-1} \circ (\tilde{R}, \tilde{\mathbf{t}}) \in \gamma^{-1} \circ F$, which verifies equation (32). □

We conclude from equation (11) and Proposition 4.6 that

$$\boxed{F'_{\Gamma\backslash G} \cong_{M,S} F'_{\mathbb{P}\backslash\mathrm{SO}(n)} \times F'_{T\backslash X}} \tag{33}$$

for arbitrary (exact) fundamental domains $F'_{\Gamma\backslash G}$, $F'_{\mathbb{P}\backslash\mathrm{SO}(n)}$, $F'_{T\backslash X}$.

4.4. Voronoi cells as fundamental domains in G

The fundamental domain $F^{\mathrm{Vor}}_{\Gamma\backslash G} \subset G$ was defined in Chirikjian & Yan (2012)[6] as the set of all $g \in G$ such that

$$d(e, g) \le d(g, \gamma) \quad \forall\, \gamma \in \Gamma\backslash\{e\};$$

that is, $F^{\mathrm{Vor}}_{\Gamma\backslash G}$ is the closed *Voronoi cell* for Γ centered at e. The metrics defined in that paper were all left-invariant, and as a consequence $d(\gamma \circ g_1, \gamma \circ g_2) = d(g_1, g_2)$. They were also bi-invariant with respect to pure rotations, *i.e.*

$$d(r_1 \circ g_1 \circ r_2, r_1 \circ g_2 \circ r_2) = d(g_1, g_2) \quad \forall\, r_1, r_2 \in \mathcal{R}.$$

More generally, for any subgroup $H \le \Gamma$, we have the Voronoi cell $F^{\mathrm{Vor}}_{H\backslash G}$ given by equation (4).

We let $\mathbb{P} < \mathrm{SO}(n)$ denote the *point group*:

$$\mathbb{P} \doteq \{R \in \mathrm{SO}(n) : \exists\, \mathbf{v}(R) \in X \text{ such that } [R, \mathbf{v}(R)] \in \Gamma\}.$$

This is well known to be isomorphic with the quotient of Γ by T: $\mathbb{P} \cong_{\mathrm{I}} T\backslash\Gamma$. In contrast, we can define a subgroup $\mathbb{S} \le \mathbb{P}$ defined as

$$\mathbb{S} \doteq \{R \in \mathrm{SO}(n) \text{ such that } (R, \mathbf{0}) \in \Gamma\}.$$

In the case when $\mathbb{S} = \mathbb{P}$, then Γ is symmorphic. Otherwise, $\mathbb{S} < \mathbb{P}$ and Γ is nonsymmorphic.

We let $\mathcal{R} \doteq \mathrm{SO}(n) \times \{\mathbf{0}\}$ denote the rotation subgroup of G. We also let $S \le P < \mathcal{R}$ be given by[7]

$$P \doteq \mathbb{P} \times \{0\} < G, \quad S \doteq \mathcal{R} \cap \Gamma = P \cap \Gamma, \quad S \doteq \mathbb{S} \times \{0\}.$$

Let $N \triangleleft \Gamma$. If $\gamma \in N$ and $s \in S$, then $s \circ \gamma \circ s^{-1} \in N$ and $d(e, s \circ \gamma \circ s^{-1}) = d(e, \gamma)$, and thus

$$d(e, g) \le d(g, \gamma) \Longleftrightarrow d(e, s \circ g \circ s^{-1}) \le d(s \circ g \circ s^{-1}, \gamma'),$$

where $\gamma' = s \circ \gamma \circ s^{-1}$. Therefore, $s \circ g \circ s^{-1} \in F^{\mathrm{Vor}}_{N\backslash G}$ for all $g \in F^{\mathrm{Vor}}_{N\backslash G}$. And so

$$sF^{\mathrm{Vor}}_{N\backslash G}s^{-1} = F^{\mathrm{Vor}}_{N\backslash G} \text{ for all } s \in S. \tag{34}$$

In the symmorphic case, $\mathbb{S} = \mathbb{P}$ and thus equation (34) holds for all $s \in P$.

Moreover, even if Γ is not symmorphic, for the case $N = T$ we have

$$pF^{\mathrm{Vor}}_{T\backslash G}p^{-1} = F^{\mathrm{Vor}}_{T\backslash G} \text{ for all } p \in P. \tag{35}$$

To verify equation (35), we let $p = (R, 0)$, $R \in \mathbb{P}$. Then for $g \in G$ and $t = (\mathbb{I}, a) \in T$, we have

$$d(e, g) \le d(g, t) \Longleftrightarrow d(e, p \circ g \circ p^{-1}) \le d(p \circ g \circ p^{-1}, t'),$$

where

$$t' = p \circ t \circ p^{-1} = (\mathbb{I}, Ra) \in T,$$

as the point group $\mathbb{P}$ preserves the lattice.[8]

We recall from Chirikjian, Sajjadi *et al.* (2015) and Chirikjian, Ratnayake *et al.* (2015) that $\Gamma = \Gamma_{\mathrm{B}}\Gamma_{\mathrm{S}}$ (in at least one way for every Sohncke group, and in more than one way for some) where Γ_{B} is Bieberbach and Γ_{S} is symmorphic. Moreover, when Γ_{B} and Γ_{S} both share the primitive lattice of Γ, this becomes $\Gamma = \Gamma_{\mathrm{B}}S$ where $S < \Gamma_{\mathrm{S}}$ and $S \cong_{\mathrm{I}} \Gamma_{\mathrm{S}}/T$ and $\Gamma_{\mathrm{B}} \cap S = \{e\}$. In most of these cases, $\Gamma_{\mathrm{B}} \triangleleft \Gamma$ and hence $\Gamma = \Gamma_{\mathrm{B}} \rtimes S$. The results in the next section are presented with this in mind, but are not limited to the case when $H = \Gamma_{\mathrm{B}}$ or even $H \triangleleft \Gamma$.

5. Transferring symmetry between translational and rotational parts of motion spaces

Suppose that Γ can be decomposed as KH where $K \le S = P \cap \Gamma$ and H is a space group such that $K \cap H = \{e\}$. Note that this implies that H and Γ both share T as their maximal translation group, and that $K \ltimes T$ is a symmorphic subgroup, also with T as its maximal translation group. We then write

$$(s, h) \doteq h \circ s \in \Gamma, \text{ when } s \in K, h \in H.$$

Explicitly, if $s = (R_s, 0) \in K$ and $h = [R_h, \mathbf{t}_h + \mathbf{v}(R_h)] \in H$, we have $(s, h) = [R_h R_s, \mathbf{t}_h + \mathbf{v}(R_h)]$. Note that if $K = S$, then H is a Bieberbach group.

The following results provide ways to decompose $F_{\Gamma\backslash G}$ as a measure-equivalent product space when $\Gamma = KH$ as above.

In the discussion below, we use the following elementary facts:

(i) If A and B are subgroups of a group H such that $H = AB \doteq \{ab : a \in A, b \in B\}$, then $H = H^{-1} = (AB)^{-1} = B^{-1}A^{-1} = BA$ and thus $AB = BA$ (although neither subgroup may be normal).

(ii) Suppose that A and B are subgroups of H such that $A \cap B = \{e\}$. If $a, a' \in A$, $b, b' \in B$ such that $ab = a'b'$, then $a^{-1}a' = bb'^{-1} \in A \cap B$ and thus $a = a'$, $b = b'$.

[6] The fundamental domain $F^{\mathrm{Vor}}_{\Gamma\backslash G}$ is denoted $\overline{F_{\Gamma\backslash G}}$ in Chirikjian & Yan (2012).
[7] We shall also refer to P as the point group and we call $T\backslash\Gamma$ the *abstract point group* in §6.

[8] To see directly that $(\mathbb{I}, Ra) \in T$, we let $\gamma = [R, \mathbf{v}(R)] \in \Gamma$, and thus $\gamma \circ (\mathbb{I}, a) \circ \gamma^{-1} = (\mathbb{I}, Ra) \in \Gamma \cap (\{\mathbb{I}\} \times \mathbb{R}^n) = T$.

If A and B are discrete groups acting properly discontinuously on a manifold Y, we shall use the notation $F^B_{A\backslash Y}$ to indicate a fundamental domain that is invariant under the action by elements of B. The following lemma describes a general situation where such symmetric groups exist.

Lemma 5.1. Let Δ be a discrete group acting properly discontinuously on a manifold Y. Suppose that A and B are subgroups of Δ such that $\Delta = AB$ and $A \cap B = \{e\}$. Then there exists a fundamental domain $F^B_{A\backslash Y}$ for A acting on Y that is invariant under the B action.

Proof. Let $F_{\Delta\backslash Y}$ be a fundamental domain for the action of Δ on Y. We use the B images of $F_{\Delta\backslash Y}$ as building blocks to construct the set

$$F \doteq \bigcup_{b\in B} b \cdot F_{\Delta\backslash Y},$$

which has the symmetry $b \cdot F = F$ for $b \in B$. Let μ be a volume measure on Y (in any Riemannian metric). The sets $a \cdot F$ cover all of Y except possibly for a set of measure zero, since

$$Y \cong_{\rm M} \bigcup_{\delta\in\Delta} \delta \cdot F_{\Delta\backslash Y} = \bigcup_{a\in A}\bigcup_{b\in B} ab \cdot F_{\Delta\backslash Y} = \bigcup_{a\in A} a \cdot F.$$

Now suppose that $a \in A\backslash\{e\}$. We have

$$F \cap a \cdot F = \bigcup_{b,b'\in B} \big(b' \cdot F_{\Delta\backslash Y} \cap ab \cdot F_{\Delta\backslash Y}\big).$$

We note that $ab \neq b'$ for all pairs $b, b' \in B$ since $A \cap B = \{e\}$, and thus

$$\mu\big(b' \cdot F_{\Delta\backslash Y} \cap ab \cdot F_{\Delta\backslash Y}\big) = 0 \quad \forall\, b, b' \in B.$$

Therefore

$$\mu(F \cap a \cdot F) = 0,$$

so the set $F^B_{A\backslash Y} \doteq F$ is our desired symmetric fundamental domain. □

Theorem 5.2. Suppose that a space group Γ can be decomposed as a product of two space groups as $\Gamma = \Gamma'\Gamma''$ where Γ, Γ' and Γ'' share the same translation group T, and $\Gamma' \cap \Gamma'' = T$. Let $P = P'P''$ denote the point group of Γ with P' and P'' being the point groups of Γ' and Γ'', respectively. Then there exists a fundamental domain $F^{P''}_{P'\backslash\mathcal{R}}$ with the symmetry

$$q \cdot F^{P''}_{P'\backslash\mathcal{R}} = F^{P''}_{P'\backslash\mathcal{R}}, \quad \forall\, q \in P'' \tag{36}$$

and $F^{P''}_{P'\backslash\mathcal{R}} \times F_{\Gamma''\backslash X}$ is a fundamental domain for $\Gamma\backslash G$. Thus we have

$$\boxed{F_{\Gamma\backslash G} \cong_M F^{P''}_{P'\backslash\mathcal{R}} \times F_{\Gamma''\backslash X}\,.} \tag{37}$$

Proof. We note that $P' \cap P'' = \{e\}$ since if $p = (R, \mathbf{0}) \in P' \cap P''$, then $[R, \mathbf{v}(R)] \in \Gamma' \cap \Gamma'' = T$ and therefore $R = \mathbb{I}$. By Lemma 5.1 with $Y = \mathcal{R}$, $\Delta = P$, $A = P'$ and $B = P''$, we obtain a fundamental domain $F^{P''}_{P'\backslash\mathcal{R}}$ having the symmetry (38).

Write $F \doteq F^{P''}_{P'\backslash\mathcal{R}} \times F_{\Gamma''\backslash X}$, where $F^{P''}_{P'\backslash\mathcal{R}}$ satisfies equation (36). We let $\mathcal{R}_0 \doteq P' \cdot F^{P''}_{P'\backslash\mathcal{R}}$, which is a set of full measure in $\mathcal{R}$ by equation (1), and we let

$$X_0 \doteq \bigcap_{k\in\Gamma'} k\Gamma'' \cdot F_{\Gamma''\backslash X} = \bigcap_{k\in F_{T\backslash\Gamma'}} k\Gamma'' \cdot F_{\Gamma''\backslash X},$$

which is also a set of full measure in X, since it is a finite intersection of sets of full measure.

Let $g = (R, \mathbf{t})$ be an arbitrary element of $\mathcal{R}_0 \times X_0$. To show that the sets $\gamma \cdot F$ cover $\mathcal{R}_0 \times X_0$, we must find an element $\gamma \in \Gamma$ such that $\gamma \circ g \in F$. We first select $k = [R_k, \mathbf{t}_k + \mathbf{v}(R_k)] \in \Gamma'$ such that $R' \doteq R_k R \in F^{P''}_{P'\backslash\mathcal{R}}$. Write $k \circ g = (R', \mathbf{t}')$. Since $\mathbf{t}' = k \cdot \mathbf{t} \in k \cdot X_0 = X_0$, we can find $h = [R_h, \mathbf{t} + \mathbf{v}(R_h)] \in \Gamma''$ such that $h \cdot \mathbf{t}' \in F_{\Gamma''\backslash X}$. Let $\gamma = h \circ k$. Then

$$\gamma \circ g = h \circ (R', \mathbf{t}') = (R_h R', h \cdot \mathbf{t}') \in \mathcal{R} \times F_{\Gamma''\backslash X}.$$

Since $R_h \in P''$, $R' = R_k R \in F^{P''}_{P'\backslash\mathcal{R}}$ and $F^{P''}_{P'\backslash\mathcal{R}}$ is invariant under the left P'' action, it follows that $R_h R' \in F^{P''}_{P'\backslash\mathcal{R}}$, and thus $\gamma \circ g \in F$. Therefore, $\bigcup_{\gamma\in\Gamma} \gamma \cdot F$ contains $\mathcal{R}_0 \times X_0$, which has full measure in G.

To complete the proof, we must show that $F \cap \gamma \cdot F$ has zero measure for all $\gamma \in \Gamma\backslash\{e\}$. Let $g \in F$ and $\gamma \in \Gamma\backslash\{e\}$ be arbitrary. We can write $\gamma = h \circ k$, $h \in \Gamma''$, $k \in P'$. First suppose that $k \neq e$. Recalling that $R_h \in P''$, we have

$$\gamma \circ g \in R_h R_k \cdot F_{P'\backslash\mathcal{R}} \times X.$$

We note that $P' \cap P'' = \{e\}$, since if $(R_\alpha, \mathbf{0}) \in P' \cap P''$, then $[R_\alpha, \mathbf{v}(R_\alpha)] \in \Gamma' \cap \Gamma'' = \{e\}$ and thus $R_\alpha = \mathbb{I}$. Since $P'P'' = P''P'$ (although neither P nor P'' may be normal), $R_h R_k = R_{k'} R_q$, $k' \in P'$, $q \in P''$. Furthermore, $k' \neq e$ since $P' \cap P'' = \{e\}$. Since $F^{P''}_{P'\backslash\mathcal{R}}$ is invariant under P'', we then have $\gamma \circ g \in R_{k'} \cdot F^{P''}_{P'\backslash\mathcal{R}} \times X$. Thus

$$F \cap \gamma \cdot F \subset \big(F^{P''}_{P'\backslash\mathcal{R}} \cap R_{k'} \cdot F^{P''}_{P'\backslash\mathcal{R}}\big) \times X,$$

which has measure zero in $\mathcal{R} \times X$.

On the other hand, if $\gamma = h \in \Gamma''\backslash\{e\}$, then the set of $g \in F$ with $\gamma \circ g \in F$ has measure zero since, by definition,

$$\mu\big(F_{\Gamma''\backslash X} \cap h \cdot F_{\Gamma''\backslash X}\big) = 0 \quad \forall\, h \in \Gamma''\backslash\{e\}.$$

□

Corollary 5.3. Let $\Gamma < {\rm SE}(n)$ be a Sohncke group that can be decomposed as a product $\Gamma = KH$ where $K \leq S = \Gamma \cap \mathcal{R}$ is a subgroup of the point group and H is a Sohncke group such that $K \cap H = \{e\}$. If Q denotes the point group of H, then there exists a fundamental domain $F^Q_{K\backslash\mathcal{R}}$ with the symmetry

$$q \cdot F^Q_{K\backslash\mathcal{R}} = F^Q_{K\backslash\mathcal{R}}, \quad \forall\, q \in Q, \tag{38}$$

and $F^{Q}_{K\backslash\mathcal{R}} \times F_{H\backslash X}$ is a fundamental domain for $\Gamma\backslash G$. Thus we have

$$\boxed{F_{\Gamma\backslash G} \cong_M F^{Q}_{K\backslash\mathcal{R}} \times F_{H\backslash X}\,.} \tag{39}$$

Proof. Let T denote the translation group of Γ. Apply Theorem 5.2 with $\Gamma' = K \ltimes T$ and $\Gamma'' = H$. □

When $\Gamma = KH$ as in Corollary 5.3, we can similarly construct fundamental domains by instead requiring symmetry of the second factor in equation (39):

Theorem 5.4. Let $\Gamma = KH$ be as in Corollary 5.3. Then there exists a fundamental domain $F^{K}_{H\backslash X}$ with the symmetry

$$k \cdot F^{K}_{H\backslash X} = F^{K}_{H\backslash X} \quad \forall\, k \in K, \tag{40}$$

and $F_{K\backslash\mathcal{R}} \times F^{K}_{H\backslash X}$ is a fundamental domain for $\Gamma\backslash G$. Thus we have

$$\boxed{F_{\Gamma\backslash G} \cong_M F'_{K\backslash\mathcal{R}} \times F^{K}_{H\backslash X}\,.} \tag{41}$$

Proof. The existence of a fundamental domain in X having the symmetry (40) follows from Lemma 5.1, this time with $Y = X$, $\Delta = \Gamma$, $A = H$ and $B = K$.

Let $X_0 \doteq H \cdot F^{K}_{H\backslash X}$, which has full measure in X, and suppose that $g = (R, \mathbf{t})$ is an arbitrary element of $\mathcal{R} \times X_0$. Then we can find $\mathbf{t}_F \in F^{K}_{H\backslash X}$ and $h \in H$ such that $h \cdot \mathbf{t}_F = \mathbf{t}$. Then

$$g = h \circ (R_h^{-1} R, \mathbf{t}_F).$$

We have a unique decomposition $R_h^{-1} R = R_s R_F$ with $k \in K$, $R_F \in F'_{K\backslash\mathcal{R}}$. Therefore

$$\begin{aligned} g &= h \circ (R_k R_F, \mathbf{t}_F) \\ &= (h \circ k) \circ (R_F, k^{-1} \cdot \mathbf{t}_F) \\ &= \gamma \circ (R_F, \mathbf{t}'), \end{aligned}$$

where $\gamma = h \circ k \in \Gamma$ and $\mathbf{t}' = k^{-1} \cdot \mathbf{t}_F \in F^{K}_{H\backslash X}$ since $F^{K}_{H\backslash X}$ is invariant under the K action. Therefore the Γ images of $F'_{K\backslash\mathcal{R}} \times F^{K}_{H\backslash X}$ cover $\mathcal{R} \times X_0$, which has full measure in G. Since the choice of $k \in K$ is unique, the only way these Γ images can overlap is when there exists another decomposition $\tilde{h} \cdot \tilde{\mathbf{t}}_F = \mathbf{t}$. But this occurs only when $\mathbf{t}$ lies in the intersection $(h \cdot F^{K}_{H\backslash X}) \cap (\tilde{h} \cdot F^{K}_{H\backslash X})$, which is a set of measure zero. □

In the symmorphic case when $\Gamma = P \ltimes T$, it was shown in Chirikjian & Yan (2012) that the Wigner–Seitz cell (*i.e.* the Voronoi cell centered on each lattice point) is a fundamental domain $F_{T\backslash X}$ with the symmetry $p \cdot F_{T\backslash X} = F_{T\backslash X}$ for all $p \in P$. This generalizes to the case where Γ is the product of a symmorphic group and a Bieberbach group (where neither factor need be normal), yielding the following alternative construction of the symmetric fundamental domain in Theorem 5.4:

Proposition 5.5. Suppose that the group $\Gamma < \mathrm{SE}(n)$ can be decomposed as a product $\Gamma = \Gamma_{\rm S}\Gamma_{\rm B}$ of a symmorphic group $\Gamma_{\rm S}$ and a Bieberbach group $\Gamma_{\rm B}$, where Γ, $\Gamma_{\rm S}$ and $\Gamma_{\rm B}$ share the same translation group T, and $\Gamma_{\rm S} \cap \Gamma_{\rm B} = T$. Let $d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|$ denote the Euclidean distance in X from $\mathbf{x}$ to $\mathbf{y}$. Then the Voronoi cell

$$F^{\rm Vor}_{\Gamma_{\rm B}\backslash X} \doteq \{\mathbf{x} \in X | d(\mathbf{x}, \mathbf{0}) \le d(\mathbf{x}, h \cdot \mathbf{0}) \quad \forall\, h \in \Gamma_{\rm B}\} \tag{42}$$

is a fundamental domain for $\Gamma_{\rm B}\backslash X$ and has the symmetry

$$s \cdot F^{\rm Vor}_{\Gamma_{\rm B}\backslash X} = F^{\rm Vor}_{\Gamma_{\rm B}\backslash X} \quad \forall\ s \in S, \tag{43}$$

where $S = \Gamma \cap \mathcal{R}$ is the point group of $\Gamma_{\rm S}$. Thus

$$\boxed{F_{\Gamma\backslash G} \cong_M F_{S\backslash\mathcal{R}} \times F^{\rm Vor}_{\Gamma_B\backslash X}\,.} \tag{44}$$

Proof. We first note that

$$F^{\rm Vor}_{\Gamma_{\rm B}\backslash X} = \{\mathbf{x} \in X | d(\mathbf{x}, \mathbf{0}) \le d(\mathbf{x}, \gamma \cdot \mathbf{0}) \quad \forall\, \gamma \in \Gamma\}, \tag{45}$$

since each $\gamma \in \Gamma = \Gamma_{\rm S}\Gamma_{\rm B} = \Gamma_{\rm B}\Gamma_{\rm S} = \Gamma_{\rm B}S$ can be decomposed as $\gamma = hs$, where $h \in \Gamma_{\rm B}$ and $s \in S$, and thus $\gamma \cdot \mathbf{0} = h \cdot (s \cdot \mathbf{0}) = h \cdot \mathbf{0}$.

Since Euclidean distance has the property that

$$d(R\mathbf{x}, R\mathbf{y}) = d(\mathbf{x}, \mathbf{y}) \quad \forall \mathbf{x}, \mathbf{y} \in X,\ \ R \in \mathrm{SO}(n),$$

we then have that

$$s \cdot F^{\rm Vor}_{\Gamma_{\rm B}\backslash X} = F^{\rm Vor}_{\Gamma_{\rm B}\backslash X}$$

because

$$\begin{aligned} &\{\mathbf{x} \in X | d(s^{-1} \cdot \mathbf{x}, \mathbf{0}) \le d(s^{-1} \cdot \mathbf{x}, \gamma \cdot \mathbf{0}) \quad \forall\, \gamma \in \Gamma\} \\ &\quad = \{\mathbf{x} \in X | d(\mathbf{x}, \mathbf{0}) \le d(\mathbf{x}, s\gamma \cdot \mathbf{0}) \quad \forall\, \gamma \in \Gamma\} \end{aligned}$$

and every $\gamma \in \Gamma$ has the form $s\gamma'$, with $\gamma' = s^{-1}\gamma \in \Gamma$. □

If $K = S = P \cap \Gamma$ in Theorem 5.4, then H must be a Bieberbach group, resulting in a decomposition $\Gamma = \Gamma_{\rm S}\Gamma_{\rm B}$, where $\Gamma_{\rm S}$ is a symmorphic group and $\Gamma_{\rm B}$ is a Bieberbach group. Every Sohncke space group $\Gamma < \mathrm{SE}(3)$ can be written as a product $\Gamma = \Gamma_{\rm S}\Gamma_{\rm B}$ (Chirikjian, Ratnayake *et al.*, 2015), but $\Gamma_{\rm B}$ is not always normal and its maximal translation subgroup is not always T. A list of those groups having a decomposition $\Gamma = S \ltimes \Gamma_{\rm B}$ is provided in Chirikjian, Ratnayake *et al.* (2015). Note that if we let $K = \{e\}$ in equation (39), we recover our basic example [equation (27)].

We now give an interpretation of Theorem 5.4 in terms of integral formulas, which can be used to give an alternative proof of the theorem. Consider an arbitrary non-negative measurable function $f : G \to \mathbb{R}_{\ge 0}$ with $f(\gamma \circ g) = f(g)$ for all $\gamma \in \Gamma$. Then we have

$$f(h \circ g) = f(g) \text{ and } f(k \circ g) = f(g)$$

for all $h = [R_h, \mathbf{t}_h + \mathbf{v}(R_h)] \in H$ and $k = (R_k, \mathbf{0}) \in K$. We have

$$\frac{1}{[H:T]}\int_{F_{T\backslash G}} f(g)\,\mathrm{d}g = \int_{F_{H\backslash G}} f(g)\,\mathrm{d}g = \int_{F_{H\backslash X}}\int_{\mathcal{R}} f(R,\mathbf{t})\,\mathrm{d}R\,\mathrm{d}\mathbf{t}.$$

Moreover, the integral over $\mathcal{R} = \mathrm{SO}(n)$ can be decomposed as

$$\int_{\mathcal{R}} f(R,\mathbf{t})\,\mathrm{d}R = \sum_{k\in K}\int_{F_{K\backslash\mathcal{R}}} f(R_k R,\mathbf{t})\,\mathrm{d}R$$

for each fixed value of $\mathbf{t}\in F_{H\backslash X}$.

If we choose $F_{H\backslash X}$ to have the symmetry of K, so that $R_k\cdot F_{H\backslash X} = F_{H\backslash X}$, and since it is already the case that $f(k\circ g) = f(g)$, which can be written more explicitly as $f(R_kR, R_k\mathbf{t}) = f(R,\mathbf{t})$, then

$$\begin{aligned}\sum_{k\in K}\int_{F_{H\backslash X}}\int_{F_{K\backslash\mathcal{R}}} f(R_kR,\mathbf{t})\,\mathrm{d}R\,\mathrm{d}\mathbf{t} &= \sum_{k\in K}\int_{R_{k-1}\cdot F_{H\backslash X}}\int_{F_{K\backslash\mathcal{R}}} f(R,\mathbf{t})\,\mathrm{d}R\,\mathrm{d}\mathbf{t}\\ &= |K|\cdot\int_{F_{H\backslash X}}\int_{F_{K\backslash\mathcal{R}}} f(R,\mathbf{t})\,\mathrm{d}R\,\mathrm{d}\mathbf{t}. \qquad (46)\end{aligned}$$

Therefore, since $[H:T]\cdot|K| = [\Gamma:T]$,

$$\int_{F_{H\backslash X}}\int_{F_{K\backslash\mathcal{R}}} f(R,\mathbf{t})\,\mathrm{d}R\,\mathrm{d}\mathbf{t} = \frac{1}{[H:T]\cdot|K|}\int_{F_{T\backslash G}} f(g)\,\mathrm{d}g = \int_{F_{\Gamma\backslash G}} f(g)\,\mathrm{d}g.$$

Since f is arbitrary, this provides an independent verification of Theorem 5.4.

As an example of Theorem 5.4, we revisit Chirikjian & Yan (2012). Let Γ_P denote the symmorphic group $P\ltimes T$ and suppose that $K\lhd P$. If we can find $Q<P$ such that $KQ = P$ and $K\cap Q = \{e\}$, then $P = K\rtimes Q$ (and $Q\cong_{\mathrm{I}} K\backslash P$). In this case, H can be taken to be $\Gamma_K = T\rtimes K$, so that $\Gamma_P = Q\ltimes H$ and we have

$$F_{\Gamma_P\backslash G} \cong_{\mathrm{M}} F_{Q\backslash\mathcal{R}}\times F_{\Gamma_K\backslash X}.$$

The following summarizes the results of this section:

Corollary 5.6. Suppose that a space group Γ can be decomposed as a product of two space groups as $\Gamma = \Gamma'\Gamma''$ where Γ, Γ' and Γ'' share the same translation group T, and $\Gamma'\cap\Gamma'' = T$. Let $P = P'P''$ denote the point group of Γ with P' and P'' being the point groups of Γ' and Γ'', respectively, and let $\Gamma_P = P\ltimes T$. Then we have the following measure-equivalent fundamental domains for $\Gamma\backslash G$:

$$F_{\Gamma\backslash G} \cong_{\mathrm{M}} F_{P\backslash\mathcal{R}}\times F_{T\backslash X} \qquad (47)$$

$$\cong_{\mathrm{M}} F_{\Gamma_P\backslash G} \qquad (48)$$

$$\cong_{\mathrm{M}} F^{P''}_{P'\backslash\mathcal{R}}\times F_{\Gamma''\backslash X} \qquad (49)$$

$$\cong_{\mathrm{M}} F^{P'}_{P''\backslash\mathcal{R}}\times F_{\Gamma'\backslash X} \qquad (50)$$

where $F_{Q\backslash\mathcal{R}}$ and $F_{H\backslash X}$ denote arbitrary fundamental domains for $Q\backslash\mathcal{R}$ and $H\backslash X$, respectively (for $Q\le P$, $H\le\Gamma$), and a superscript P' (respectively, P'') signifies that the fundamental domain is invariant under the left P' (respectively, P'') action.

Furthermore, if Γ' is symmorphic, we have

$$F_{\Gamma\backslash G} \cong_{\mathrm{M}} F_{P'\backslash\mathcal{R}}\times F^{P'}_{\Gamma''\backslash X} \qquad (51)$$

and, similarly, if Γ'' is symmorphic, then

$$F_{\Gamma\backslash G} \cong_{\mathrm{M}} F_{P''\backslash\mathcal{R}}\times F^{P''}_{\Gamma'\backslash X}. \qquad (52)$$

Proof. The congruences (47) and (48) follow from Proposition 4.6 and the fact that Γ and Γ_P have the same point group and translation group; (49) and (50) follow from Theorem 5.2; (51) and (52) follow from Theorem 5.4, with $K = P'$ ($K = P''$, respectively) and $H = \Gamma''$ ($H = \Gamma'$, respectively). □

6. Examples

We now apply our results to Sohncke space groups [*i.e.* discrete co-compact subgroups of SE(3)]. Recall that when referring to a space group of type Γ, one is referring to all space groups that are equivalent under orientation-preserving affine transformations. That is, if $\Gamma^\alpha \doteq \alpha\Gamma\alpha^{-1}$ and Γ are both space groups, where $\alpha\in\mathrm{Aff}^+(3) = \mathrm{GL}^+(3)\ltimes\mathbb{R}^3$, then Γ^α and Γ are both instances of the same space-group type. But the motion spaces $\Gamma\backslash G$ and $\Gamma^\alpha\backslash G$ in general will *not* be measure equivalent unless $\alpha\in\mathrm{SE}(3)$, and neither will the fundamental domains $F_{\Gamma\backslash G}$ and $F_{\Gamma^\alpha\backslash G}$. However, for a fixed transformation α, one can decompose motion spaces and their corresponding fundamental domains in multiple measure-equivalent ways.

In the examples illustrated below, for a given space group Γ = 'P#' in the Hermann–Mauguin notation (Hahn, 2002), we let '#' denote the 'abstract point group' $T\backslash\Gamma$ together with its action on the torus $T\backslash\mathbb{R}^3$. For example, the $(T\backslash\Gamma)$ actions for the space groups $P2_12_12_1$, $P222_1$, $P2_12_12$ and $P222$ are denoted $2_12_12_1$, 222_1, 2_12_12 and 222, respectively. They have distinct actions on $T\backslash\mathbb{R}^3$, although as groups they are isomorphic to the same abstract group $\mathbb{Z}_2\oplus\mathbb{Z}_2$. They can also be conjugated by elements of $A\in\mathrm{GL}^+(3)$; although $(2_12_12_1)^A\cong_{\mathrm{I}} 2_12_12_1\cong_{\mathrm{I}} 222$ as abstract groups, the first two are similar to each other in the sense that both act on $T\backslash\mathbb{R}^3$ without fixed points, while $\mathbf{0}$ is a fixed point of the third. And if $A\in\mathrm{SO}(3)$, we go as far as not to distinguish between the first two (since this represents nothing more than a change in perspective) and write $(2_12_12_1)^A = 2_12_12_1$.

We let $\mathbb{T}^3 \doteq T\backslash\mathbb{R}^3 = P1\backslash\mathbb{R}^3$ denote the 3-torus. Furthermore,

$$F_{\Gamma\backslash\mathbb{R}^3} \cong_{\mathrm{M}} F_{(\frac{\Gamma}{T})\backslash\mathbb{T}^3} \cong_{\mathrm{M}} \Gamma\backslash\mathbb{R}^3 \cong_{\mathrm{M,H}} \left(\frac{\Gamma}{T}\right)\backslash\mathbb{T}^3. \qquad (53)$$

Moreover,

$$F'_{\Gamma\backslash\mathrm{SE}(3)} \cong_{\mathrm{M,S}} F'_{(\frac{\Gamma}{T})\backslash[T\backslash\mathrm{SE}(3)]} \cong_{\mathrm{M,S}} \Gamma\backslash\mathrm{SE}(3) \qquad (54)$$

and

$$\Gamma\backslash\mathrm{SE}(3) \cong_{\mathrm{M,H}} \left(\frac{\Gamma}{T}\right)\backslash[T\backslash\mathrm{SE}(3)].$$

Up to isomorphism, there are 65 Sohncke (orientation-preserving) space groups. In most cases, they are either Bieberbach ($\Gamma_{\rm B}$), symmorphic ($\Gamma_{\rm S}$) or a semi-direct product of the form $\Gamma = \Gamma_{\rm B} \rtimes S$ where $S \cong_{\rm I} \Gamma_{\rm S}/T$ with $\Gamma_{\rm B}, \Gamma_{\rm S} < \Gamma$. As a consequence, $\Gamma = \Gamma_{\rm B} S = \Gamma_{\rm B}\Gamma_{\rm S}$ with $\Gamma_{\rm B} \cap S = \{e\}$ and $\Gamma_{\rm B} \cap \Gamma_{\rm S} = T$, and the theorems presented earlier in this paper apply. In all cases it is possible to write $\Gamma = \Gamma_{\rm B}\Gamma_{\rm S}$. In a minority of cases addressed in Chirikjian, Ratnayake *et al.* (2015), $\Gamma_{\rm B} \cap \Gamma_{\rm S} < T$. These are not exemplified here. Some examples of decompositions of motion spaces based on the structure of these space groups are provided below.

6.1. The Bieberbach group $P2_12_12_1$

The most common space group in which proteins crystallize is the Bieberbach group $P2_12_12_1$. We can choose $F_{P2_12_12_1/P1}$ as

$$\{(x, y, z); (-x+1/2, -y, z+1/2); \\ (-x, y+1/2, -z+1/2); (x+1/2, -y+1/2, -z)\}.$$

Here each group element is denoted by its action on the point (x, y, z), where the coordinates are with respect to a basis for $\mathbb{R}^3$ consisting of the generators of the lattice $\mathbb{L}$. As described above, we denote the quotient group $P2_12_12_1/P1$ as $2_12_12_1$, which acts on the 3-torus $P1\backslash\mathbb{R}^3$.

Then the following are measure-equivalent fundamental domains for $P2_12_12_1$ acting on SE(3): $F_{P2_12_12_1\backslash[{\rm SO}(3)\times\mathbb{R}^3]}$, $F_{222\backslash{\rm SO}(3)} \times F_{P1\backslash\mathbb{R}^3}$, ${\rm SO}(3) \times F_{P2_12_12_1\backslash\mathbb{R}^3}$, $F_{P222\backslash{\rm SE}(3)}$. Moreover,

$$\begin{aligned} P2_12_12_1\backslash{\rm SE}(3) &\cong_{\rm M,H} 2_12_12_1\backslash[{\rm SO}(3)\times\mathbb{T}^3] \\ &\cong_{\rm M} {\rm SO}(3)\times 2_12_12_1\backslash\mathbb{T}^3, \end{aligned}$$

with the first being homeomorphic, but the second not.

Note that the quotient space $2_12_12_1\backslash\mathbb{T}^3 \cong_{\rm H} P2_12_12_1\backslash\mathbb{R}^3$ is called the Hantzsche-Wendt flat manifold, which is an example of a 'Euclidean space form' as described in Charlap (1986), Montesinos (1987), Nikulin & Shafarevich (2002) and older references therein.

On the other hand, given $P2_12_12_1$ and $(P2_12_12_1)^\alpha < {\rm SE}(3)$ with $\alpha \in {\rm Aff}^+(3)$, such that the volume of the resulting unit cells are different, then clearly there will be no measure-equivalent map between $P2_12_12_1\backslash{\rm SE}(3)$ and $(P2_12_12_1)^\alpha\backslash{\rm SE}(3)$, and no measure equivalence between their fundamental domains. However,

$$P2_12_12_1\backslash{\rm SE}(3) \cong_{\rm H} (P2_12_12_1)^\alpha\backslash{\rm SE}(3).$$

Whenever Γ is one of the orientation-preserving Bieberbach groups, decompositions analogous to those above can be made.

6.2. The symmorphic group $P2$

$P2 = P1 \rtimes 2$ is a symmorphic group with $P2/P1$ denoted as 2. That is,

$$F_{\frac{P2}{P1}} = \{(x, y, z);\ (-x, y, -z)\} \qquad (55)$$

and '2' is the corresponding abstract point group.

The following fundamental domains are each measure equivalent to the fundamental domain $F_{P2\backslash{\rm SE}(3)}$: $F_{P2\backslash[{\rm SO}(3)\times\mathbb{R}^3]}$, $F_{2\backslash{\rm SO}(3)} \times F_{P1\backslash\mathbb{R}^3}$, ${\rm SO}(3) \times F_{P2\backslash\mathbb{R}^3}$. The spaces $2\backslash\mathbb{T}^3 \cong_{\rm H} P2\backslash\mathbb{R}^3$ are just orbifolds, while the other spaces above are manifolds.

6.3. The symmorphic group $C2$

The space group $\Gamma = C2$ is the most highly represented symmorphic space group in the PDB. In the standard setting, a sublattice $\Sigma < T$ is used instead of the primitive lattice T. Relative to this $\Sigma \lhd \Gamma$, coset representatives are defined according to their actions as

$$\begin{aligned} F_{\frac{\Gamma}{\Sigma}} &= \{(x, y, z); (-x, y, -z); (x+1/2, y+1/2, z); \\ &\quad (-x+1/2, y+1/2, -z)\} \\ &= \{(x, y, z); (-x, y, -z)\}\times \\ &\quad \{(x, y, z); (x+1/2, y+1/2, z)\}. \end{aligned}$$

Here the coordinates are with respect to $\Sigma = P1$, and $T > \Sigma$ is the finest (*i.e.* full/primitive) translational lattice. The group Γ/Σ is generated by a fractional translation relative to the lattice Σ.

Viewing affine transformations (including rigid-body transformations) as 4×4 homogeneous transformation matrices of the form

$$H(A, \mathbf{a}) = \begin{pmatrix} A & \mathbf{a} \\ \mathbf{0}^{\rm T} & 1 \end{pmatrix} \in {\rm Aff}^+(3)$$

and applying the transformation

$$\alpha = \begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

we get $T = \alpha^{-1}\Sigma\alpha > \Sigma$. Thus

$$\frac{\alpha\Gamma\alpha^{-1}}{\Sigma} \cong_{\rm I} \frac{\Gamma}{T} \cong_{\rm I} P, \qquad (56)$$

where

$$P = \{(x, y, z); (-y, -x, -z)\}.$$

Note also that

$$P \cong_{\rm I} \{(x, y, z); (-x, y, -z)\},$$

and even more than this, they are conjugated versions of each other with respect to an element of SO(3). Hence both can be called '2' and their actions on SO(3) are essentially the same. However, their actions on $\mathbb{T}^3$ are different because the conjugation under rotation relating them does not preserve the lattice.

That is, if $P2 = P1 \rtimes 2$, there exists $A \in {\rm SO}(3)$ that is not in the abstract point group 2 such that $C2 = P1 \rtimes (2)^A$ where $(2)^A$ is a conjugated version of 2. And there exists no $\alpha \in {\rm Aff}^+(3)$ such that $C2$ can be written as $(P2)^\alpha$. Hence, when we say that all of the decompositions for $C2$ look like those for $P2$, we mean that the following fundamental domains are each measure equivalent to the fundamental domain $F_{C2\backslash{\rm SE}(3)}$: $F_{C2\backslash[{\rm SO}(3)\times\mathbb{R}^3]}$, $F_{(2)^A\backslash{\rm SO}(3)} \times F_{P1\backslash\mathbb{R}^3}$, ${\rm SO}(3) \times F_{C2\backslash\mathbb{R}^3}$.

6.4. The symmorphic group $P222$

A very uncommon space group for proteins is the symmorphic space group $P222 = P1 \rtimes 222$ with $P222/P1$ denoted as 222. This corresponds to

$$F_{\frac{P222}{P1}} = \{(x, y, z);\ (-x, -y, z);\ (-x, y, -z);\ (x, -y, -z)\}.$$

We nevertheless include this as an example for illustration purposes. The following fundamental domains are measure equivalent to $F_{P222\backslash SE(3)}$: $F_{P222\backslash[SO(3)\times\mathbb{R}^3]}$, $F_{222\backslash SO(3)} \times F_{P1\backslash\mathbb{R}^3}$, $SO(3) \times F_{P222\backslash\mathbb{R}^3}$. Also, $P222 = 2 \ltimes P2$ and so, by Corollary 5.6, we can also write the following:

$$F_{2\backslash SO(3)} \times F_{P2\backslash\mathbb{R}^3}.$$

Recall that, as abstract point groups, 222 and $2_12_12_1$ are the same (isomorphic), but in terms of their actions on $\mathbb{T}^3$ they are quite different. Nevertheless, as a consequence of Proposition 4.6 and the fact that $222 = 2 \times 2 \cong 2_12_12_1$, the above can be used in place of those given in §6.1.

6.5. Example: $P222_1$

This and the following two examples are neither Bieberbach nor symmorphic, but can be decomposed as a semi-direct product of a point group and a normal Beiberbach subgroup, as is the case for all but four of the 65 Sohncke space groups (Chirikjian, Ratnayake *et al.*, 2015). In this case,

$$\begin{aligned} F_{\frac{P222_1}{P1}} &= \{(x, y, z);\ (-x, -y, z + 1/2);\\ &\quad (-x, y, -z + 1/2);\ (x, -y, -z)\}\\ &= \{(x, y, z);\ (-x, -y, z + 1/2)\}\times\\ &\quad \{(x, y, z);\ (x, -y, -z)\}. \end{aligned}$$

Therefore, $P222_1 = 2 \ltimes P2_1$ as in Theorem 5.4, and the following fundamental domains are measure equivalent to $F_{P222_1\backslash SE(3)}$: $F_{P222_1\backslash[SO(3)\times\mathbb{R}^3]}$, $SO(3) \times F_{P222_1\backslash\mathbb{R}^3}$, $F_{2\backslash SO(3)} \times F_{P2_1\backslash\mathbb{R}^3}$. Again, as a consequence of Proposition 4.6 and Corollary 5.6, these can be written using any of the fundamental domains measure equivalent to $F_{P222\backslash[SO(3)\times\mathbb{R}^3]}$ or $F_{P2_12_12_1\backslash[SO(3)\times\mathbb{R}^3]}$.

6.6. Example: $P2_12_12$

This group is also decomposable in the form $P2_12_12 = 2 \ltimes P2_1$, as can be seen from the fact that

$$\begin{aligned} F_{\frac{P2_12_12}{P1}} &= \{(x, y, z); (-x, -y, z);\\ &\quad (-x + 1/2, y + 1/2, -z);\\ &\quad (x + 1/2, -y + 1/2, -z)\}\\ &= \{(x, y, z); (-x, -y, z)\}\times\\ &\quad \{(x, y, z);\ (-x + 1/2, y + 1/2, -z)\} \end{aligned}$$

where $\{(x, y, z);\ (-x + 1/2, y + 1/2, -z)\} = F_{P1\backslash P2_1}$.

Therefore, all of the decompositions for $P2_12_12_1$, $P222$ and $P222_1$ given previously can be used with the understanding that the specific actions of these groups on SE(3) (and on $\mathbb{R}^3$) are all different from each other. Moreover, the groups $2_12_12_1$, 222 and 222_1 each act on the quotient manifold $P1\backslash SE(3)$ (and on the torus $P1\backslash\mathbb{R}^3$) in three different ways. Each of these groups is isomorphic with $\mathbb{P} = 222$, which is a subgroup of SO(3). Therefore an action of 222 on SO(3) can be defined naturally, and this can be used to define actions of $2_12_12_1$ and 222_1 on SO(3) as well, by identifying them through their isomorphism. The same cannot be done for the actions of these groups on SE(3), $\mathbb{R}^3$, $P1\backslash SE(3)$ and $P1\backslash\mathbb{R}^3$.

6.7. Example: $P6_322$

In some cases it is possible to decompose space groups into semi-direct products in multiple ways. For example, using the Bilbao Crystallographic Server (Aroyo *et al.*, 2006, 2011) function *COSETS*, we obtain $F_{P6_322/P1}$ which decomposes as

$$F_{\frac{P6_322}{P1}} = F_{\frac{P2_1}{P1}} \times F_{\frac{P321}{P1}}$$

where

$$\begin{aligned} F_{\frac{P321}{P1}} = \{&(x, y, z);\ (-y, x - y, z);\ (-x + y, -x, z);\\ &(y, x, -z);\ (x - y, -y, -z);\ (-x, -x + y, -z)\} \end{aligned}$$

and

$$F_{\frac{P2_1}{P1}} = \{(x, y, z);\ (-x, -y, z + 1/2)\}.$$

Therefore, $P6_322 = 321 \ltimes P2_1$ and so the following are all measure equivalent to $F_{P6_322\backslash SE(3)}$: $F_{P6_322\backslash[SO(3)\times\mathbb{R}^3]}$, $SO(3) \times F_{P6_322\backslash\mathbb{R}^3}$, $F_{321\backslash SO(3)} \times F_{P2_1\backslash\mathbb{R}^3}$. Alternatively, with the pure translation

$$\alpha_1 = \begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 1/4\\ 0 & 0 & 0 & 1 \end{pmatrix},$$

a similar calculation gives $(P6_322)^{\alpha_1} = 312 \ltimes P2_1$ resulting in similar decompositions as those given above, with 312 in place of 321.

In addition, the following are also measure equivalent to those given above: $F_{P622\backslash[SO(3)\times\mathbb{R}^3]}$, $SO(3) \times F_{P622\backslash\mathbb{R}^3}$, $F_{622\backslash SO(3)} \times F_{P1\backslash\mathbb{R}^3}$. Another decomposition results by observing that

$$\begin{aligned} F_{\frac{P6_322}{P1}} &= \{(x, y, z);\ (-y, x - y, z);\\ &\quad (-x + y, -x, z);\ (-x, -y, z + 1/2);\\ &\quad (y, -x + y, z + 1/2);\ (x - y, x, z + 1/2)\}\\ &\quad \times \{(x, y, z);\ (y, x, -z)\}, \end{aligned}$$

and so

$$P6_322 = 2 \ltimes P6_3.$$

Though $P6_3$ is not Bieberbach, it is nevertheless possible to write the following which is measure equivalent to $F_{P6_322\backslash SE(3)}$: $F_{2\backslash SO(3)} \times F_{P6_3\backslash\mathbb{R}^3}$.

6.8. Example: $P42_12$

This space group cannot be decomposed as a semi-direct product of a point group and a normal Bieberbach group. In this case, $F_{P42_12/P1}$ can be chosen as

$$\begin{aligned}&\{(x,y,z);\ (-x,-y,z);\ (y,x,-z);\ (-y,-x,-z);\\&(-y+1/2,x+1/2,z);\ (y+1/2,-x+1/2,z);\\&(-x+1/2,y+1/2,-z);\ (x+1/2,-y+1/2,-z)\}\\&=\{(x,y,z);\ (-x,-y,z);\ (y,x,-z);\ (-y,-x,-z)\}\\&\times\{(x,y,z);(-x+1/2,y+1/2,-z)\}.\end{aligned}$$

Here the first term is 222 conjugated by a rotation and the second term is 2_1 conjugated by another rotation.

Fundamental domains measure equivalent to $F_{P42_12\backslash\mathrm{SE}(3)}$ include $F_{P42_12\backslash[\mathrm{SO}(3)\times\mathbb{R}^3]}$, $\mathrm{SO}(3)\times F_{P42_12\backslash\mathbb{R}^3}$, $F_{222\backslash\mathrm{SO}(3)}\times F_{P2_1\backslash\mathbb{R}^3}$. Note, however, that $P222$ is *not* a subgroup of index two in $P42_12$.

In contrast, with

$$\alpha'=\begin{pmatrix}1&0&0&0\\0&1&0&1/2\\0&0&1&0\\0&0&0&1\end{pmatrix},$$

$$F_{\frac{(P42_12)^{\alpha'}}{P1}}=F_{\frac{P4}{P1}}\times F_{\frac{P2_1}{P1}}$$

where

$$F_{\frac{P4}{P1}}=\{(x,y,z);\ (-x,-y,z);\ (-y,x,z);(y,-x,z)\}$$

and

$$F_{\frac{P2_1}{P1}}=\{(x,y,z);\ (-x+1/2,y+1/2,-z)\}.$$

Therefore,

$$(P42_12)^{\alpha'}=P4\rtimes 2_1, \tag{57}$$

and fundamental domains measure equivalent to $F_{(P42_12)^{\alpha}\backslash\mathrm{SE}(3)}$ include $F_{(P42_12)^{\alpha'}\backslash[\mathrm{SO}(3)\times\mathbb{R}^3]}$, $\mathrm{SO}(3)\times F_{(P42_12)^{\alpha'}\backslash\mathbb{R}^3}$, $F_{4\backslash\mathrm{SO}(3)}\times F_{P2_1\backslash\mathbb{R}^3}$. Note that equation (57) is an outer semi-direct product and $2_1=P2_1/P1$.

In addition, fundamental domains measure equivalent to $F_{P42_12\backslash\mathrm{SE}(3)}$ include $F_{P422\backslash[\mathrm{SO}(3)\times\mathbb{R}^3]}$, $\mathrm{SO}(3)\times F_{P422\backslash\mathbb{R}^3}$, $F_{422\backslash\mathrm{SO}(3)}\times F_{P1\backslash\mathbb{R}^3}$.

7. Conclusions

Building on the presentation in Chirikjian & Yan (2012), the observations about the structure of space groups in Chirikjian, Sajjadi *et al.* (2015) and the resulting decomposition of space groups in Chirikjian, Ratnayake *et al.* (2015), we have presented here measure-theoretic decompositions of motion spaces. The consequence of these decompositions is that there are many different ways to sample rotations and translations in exhaustive MR searches. For example, at one extreme one can sample all translations in the unit cell and sample rotations in a subset of the rotation group consisting of $1/|\mathbb{P}|$ of its total volume, where $\mathbb{P}$ is the point group of the crystal. At the opposite extreme, one can sample rotations in the full rotation group and restrict the translational search to a single asymmetric unit. If the point group can be decomposed as a product of subgroups that only share the identity element, then the various fundamental domains described in this paper provide for schemes in which full coverage in the MR search is achieved with rotational and translational samples drawn from intermediate-sized subsets of the full rotational and translational subspaces. As a special case, when the space group can be decomposed as a product of a Bieberbach subgroup and a point subgroup, the translation space can be identified with a 'Euclidean space form' and the rotation space can be identified with a 'spherical space form'. In these cases, existing sampling schemes for each of these spaces can be used to benefit MR searches.

8. Glossary

The glossary below, modified from Chirikjian & Shiffman (2016), summarizes the notation and terminology used in this paper.

$\mathbb{R}$, $\mathbb{R}_{>0}$, $\mathbb{R}_{\geq 0}$ – the real numbers, positive and non-negative real numbers, respectively.

X – n-dimensional Euclidean space equipped with the structure of a vector space, *i.e.* $X=\mathbb{R}^n$.

$\mathbf{t},\mathbf{x}\in X$ – an n-dimensional vector.

$R\in\mathrm{SO}(n)$ – an $n\times n$ orthogonal matrix with determinant 1, *i.e.* R is a rotation matrix.

$\mathbf{0}\in X$ – the vector of zeros corresponding to the origin of a coordinate system.

$\mathbb{I}\in\mathrm{SO}(n)$ – the $n\times n$ identity matrix.

$\subset$ – proper subset, *i.e.* $A\subset B$ indicates that A is contained in B and $A\neq B$.

χ_A – the indicator function of a subset A; $\chi_A(y)=1$ if $y\in A$ and equals 0 otherwise.

$<$ – proper subgroup, *i.e.* $K<H$ indicates that K is a subgroup of H and $K\neq H$.

$\lhd$ – normal subgroup, *i.e.* $N\lhd G$ indicates that N is a proper normal subgroup of G.

$|H|$ – the order of a finite group H.

$[H:K]$ – the index of a subgroup K of a group H.

$K\backslash H$ – the set of right cosets of a subgroup K in a group H.

$\frac{H}{N}=N\backslash H=H/N$ – the factor (or quotient) group H modulo N, when $N\lhd H$.

$\times$ – product (either Cartesian product of sets, or direct product of groups, depending on context).

$\rtimes$, $\ltimes$ – semi-direct product (either internal or external, depending on context) of normal N and complement S written as $N\rtimes S$ or $S\ltimes N$.

$\cong_{\mathrm{I}}$, $\cong_{\mathrm{H}}$, $\cong_{\mathrm{M}}$ – equivalence (as isomorphism between groups, homeomorphism between topological spaces or measure-equivalent spaces, as described in §3.2).

$g=(R,\mathbf{t})\in\mathrm{SE}(n)$ – a special Euclidean transformation (*i.e.* a proper rigid-body motion). Mathematically, $\mathrm{SE}(n)=\mathrm{SO}(n)\ltimes\mathbb{R}^n$ (an external semi-direct product) with group law $g_1\circ g_2=(R_1,\mathbf{t}_1)\circ(R_2,\mathbf{t}_2)=(R_1R_2,R_1\mathbf{t}_2+\mathbf{t}_1)$, and which acts on positions as $g\cdot\mathbf{x}=R\mathbf{x}+\mathbf{t}$.

dg – the Haar measure on $\mathrm{SE}(n)=\mathrm{SO}(n)\ltimes\mathbb{R}^n$, $dg=dR\,d\mathbf{t}$, where dR is the normalized Haar measure on $\mathrm{SO}(n)[\int_{\mathrm{SO}(n)}\mathrm{d}R=1]$ and $d\mathbf{t}=dt_1\cdots dt_n$ is the Lebesgue measure; dg is bi-invariant.

G – shorthand for $\mathrm{SE}(n)$.

$\mathcal{R} = \{(R, \mathbf{0}) | R \in \mathrm{SO}(n)\} = \mathrm{SO}(n) \times \{\mathbf{0}\}$ – the rotation subgroup of G. Note that $\mathcal{R} < G$.

Γ – an orientation-preserving (or 'Sohncke') crystallographic group, *i.e.* a discrete subgroup of G that contains a rank-n lattice of translations T.

$\Gamma\backslash G = \{\Gamma g : g \in G\}$ – the set of right cosets of Γ in G. The homogeneous space $\Gamma\backslash G$ is a smooth manifold.

T – the group of lattice translations in Γ. The subgroup $T \triangleleft \Gamma$ is the maximal normal abelian subgroup of Γ.

$T\backslash G = \{Tg : g \in G\}$ – the set of right cosets of T in G. The homogeneous space $T\backslash G$ is a smooth manifold.

$\mathbb{L}$ – the lattice in X of rank n corresponding to T; *i.e.* $T = \{\mathbb{I}\} \times \mathbb{L}$.

γ – an element of a Sohncke crystallographic space group Γ; we write $\gamma = [R_\gamma, \mathbf{t}_\gamma + \mathbf{v}(R_\gamma)]$, where $\mathbf{t}_\gamma$ and $\mathbf{v}_\gamma(R_\gamma)$ are as follows:

$(\mathbb{I}, \mathbf{t}_\gamma) \in T$ – a lattice translation such that $(\mathbb{I}, \mathbf{t}_\gamma) \cdot \mathbb{L} = \mathbb{L} + \mathbf{t}_\gamma = \mathbb{L}$.

$\mathbf{v}(R_\gamma)$ – a translation by a fraction (possibly 0) of an element of $\mathbb{L}$, given (uniquely modulo T) by $\gamma = [R_\gamma, \mathbf{t}_\gamma + \mathbf{v}(R_\gamma)]$, for $\gamma \in \Gamma$.

$\mathbb{P} = \{R_\gamma \in \mathrm{SO}(n) : \exists\, \mathbf{v}(R_\gamma) \in X \text{ such that } [R_\gamma, \mathbf{v}(R_\gamma)] \in \Gamma\}$ – a discrete rotation group, called the *point group*; $\mathbb{P} \cong_{\mathrm{I}} T\backslash\Gamma$. If $\mathbf{v}(R_\gamma) = \mathbf{0}$ for all $\gamma \in \Gamma$ and thus $\mathbb{P} = \{R \in \mathrm{SO}(n) : (R, 0) \in \Gamma\}$, one says that Γ is *symmorphic*.

$P = \mathbb{P} \times \mathbf{0}$ – a subgroup of G such that $P \cong_{\mathrm{I}} \mathbb{P} \cong_{\mathrm{I}} \Gamma/T$.

$S \doteq P \cap \Gamma$ – a subgroup of both Γ and P. Moreover, it can be written as $S = \mathbb{S} \times \{\mathbf{0}\}$ and so $S \cong_{\mathrm{I}} \mathbb{S} < \mathbb{P}$.

$F_{T\backslash X}$ – a crystallographic unit cell (a fundamental domain for T acting on X; the T translates of $\overline{F_{T\backslash X}}$ cover X with all pairwise intersections having measure 0).

$F_{\Gamma\backslash X}$ – a crystallographic asymmetric unit; a fundamental domain for Γ acting on X, *i.e.* the images of $\overline{F_{\Gamma\backslash X}}$ under the action of elements of Γ cover Euclidean space, X, with intersections of measure zero. [Particular choices of asymmetric units can be found in Lučić & Molnár (1991) in the planar case and in Grosse-Kunstleve *et al.* (2011) in $\mathbb{R}^3$.] The space $\Gamma\backslash X$ itself is a *Euclidean orbifold* (Dunbar, 1981).

$F_{\Gamma\backslash G}$ – a fundamental domain for the left action of Γ on G. It is a smallest finite-volume space of rotations and translations in which MR searches need to be performed.

$F'_{\Gamma\backslash G}$ – an 'exact' fundamental domain that contains exactly one point in each Γ orbit. It is measure equivalent to its closure, which is also a fundamental domain for Γ acting on G.

$F'_{T\backslash X}$ – a crystallographic unit cell that is an exact fundamental domain for T acting on X.

Δ – a discrete co-compact subgroup of a general Lie group $\mathbf{G}$, or more generally a discrete group of isometries of a Riemannian manifold acting properly discontinuously.

Y – an arbitrary Riemannian manifold (of which X, G, $T\backslash X$, $T\backslash G$ and $\Gamma\backslash G$ are examples).

$\Delta\backslash Y$ – the space of orbits of a properly discontinuous group action Δ on a manifold Y.

$\mathbb{T}^3$ – the 3-torus $T\backslash\mathbb{R}^3$, where T is the translation lattice of a Sohnke space group $\Gamma < \mathrm{SE}(3)$.

$T\backslash\Gamma$ – the *abstract point group*. It is isomorphic as a group to the point group $\mathbb{P}$, but it acts on $\mathbb{T}^3$ possibly without fixed points.

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