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Collision-free configuration-spaces in macromolecular crystals

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SUMMARY

Molecular replacement (MR) is a well-established computational method for phasing in macromolecular crystallography. In MR searches, spaces of motions are explored for determining the appropriate placement of rigid single-body (or articulated multi-rigid-body) models of macromolecules. By determining *a priori* which portions of motion space correspond to non-physical packing arrangements with symmetry mates in collision, it becomes feasible to construct more efficient MR techniques which avoid searching in these non-realizable regions of motion space. This paper investigates which portion of the motion space is physically realizable, given that packing of protein molecules in a crystal are subject to the constraint that they cannot interpenetrate, and gives explicit expressions for the volume of the non-realizable regions for crystals in two-dimensions.

1. Introduction

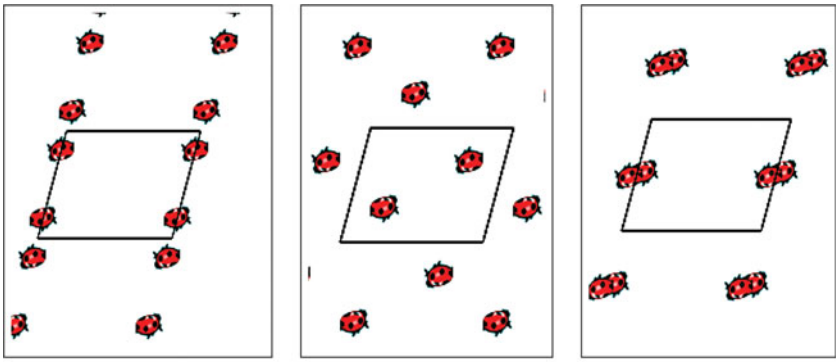
Imagine an ideal crystal composed of an infinite number of identical copies of a solid body. Although a true crystal is always finite in its extent, it consists of such a large number of copies that the idealization does not introduce too much discrepancy from the reality. With knowledge of the shape and pose (position and orientation) of one of the bodies in the crystal, and knowledge of the crystallographic symmetry group, it is possible to reconstruct the whole crystal. This is essentially the situation that arises in macromolecular crystallography (MX), where the solid body may be a protein, nucleic acid, or complex composed of both. And information about the crystal symmetry is provided by an X-ray diffraction experiment.

This symmetry information, together with prior information about the shape of the bodies obtained from the Protein Data Bank (PDB),[1] can be used to assist in solving the so-called "phase problem" in X-ray crystallography in a purely computational way using a modified version of the method of MR.[14,15] In doing so, it becomes feasible to phase large biomolecular structures that currently require expensive experimental methods. The subject of this paper is to describe the regions of the space of candidate poses ("C-space") corresponding to configurations that put the bodies in non-physical collisions/overlaps. By excluding those poses at the beginning of an MR search, one can make MR searches more efficient by sampling only in the collision-free regions of C-space. C-space searches are by their very nature a robot motion planning problem, and an MR search is akin to the coordination of multiple robots moving in formation, with C-space obstacles describing when members of the formation collide with each other. (This is somewhat different than traditional robot motion planning problems in which there are static obstacles and moving robots.)

The infinite number of bodies[(2)] that fill Euclidean space in an ideal crystal form a highly symmetrical pattern described by a crystallographic space group. For simple (inorganic) molecules, the number of allowable space groups is quite large. But for macromolecules, which are chiral (i.e.,

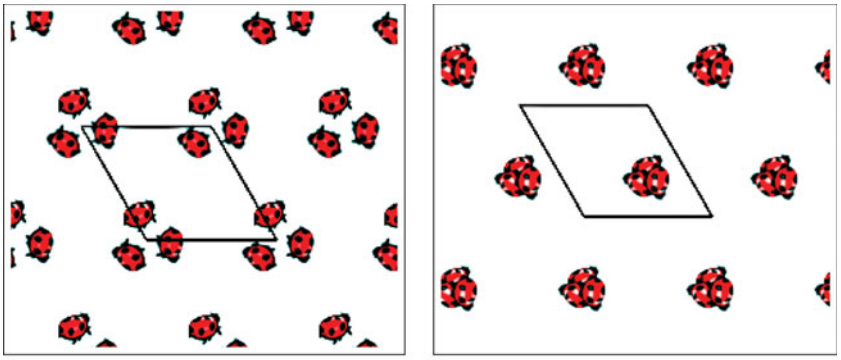
* Corresponding author.
(1) This paper is an expanded version of a paper delivered at the Workshop on Robotics Methods for Structural and Dynamic Modeling of Molecular Systems in July 2014 at Berkeley, CA (cs.unm.edu/amprg/rss14workshop/PAPERS/Chirikjian.pdf).
(2) In our figures generated using ref. [13], the bodies are represented by ladybugs.

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(a) (b) (c)

Fig. 1. Three configurations of solid bodies with $p2$ symmetry.



(a) (b)

Fig. 2. Two configurations of solid bodies with $p3$ symmetry.

they have handedness), far fewer symmetries are allowed, since mirror reflections and glide planes are not possible. For this reason, there are only five isomorphism classes of planar crystallographic groups for which patterns composed of solid planar bodies can exist (out of a total of 17 isomorphism classes of planar wallpaper groups), and only 65 are allowable in the spatial case (out of 230).[9] Figure 1 shows three configurations of a planar pattern with $p2$ symmetry generated using the free iphone app "Eschermobile" developed by ref. [13]. These figures all have the same wallpaper group symmetry, called $p2$, but differ by translational degrees of freedom. It is also possible to construct configurations with $p2$ symmetry for which each solid body rotates in concert with the others. In Figs. 1(a) and (b), the bodies are not in collision, but in Fig. 1(c), the bodies are in collision. Obviously, if these bodies were physical, such collisions would not be allowed. Figure 2 (generated using the iphone app "Eschermobile"[13]) shows two configurations of a planar pattern with $p3$ symmetry. In Fig. 2(a), the bodies are not in collision, while in Fig. 2(b), the bodies are in collision. In all of these figures, the parallelogram in the middle is the crystallographic unit cell, which can be viewed as a tile that reproduce the whole infinite crystal under the action of a discrete lattice translation group. Illustrations with $p4$ and $p6$ symmetries are given in Sections 3.3–3.4 below.

This paper characterizes the subset of motions that will cause bodies to collide with their symmetry mates. In so doing, the complement of this space, the free space, is naturally characterized. These results are directly applicable to accelerate MR searches. In the remainder of this section, the mathematical aspects of the MR problem are reviewed, and terminology used throughout the rest of the paper is established. Section 2 formulates the general problem in n-dimensional space and shows how the collision space for an infinite crystal corresponds to when several coordinated bodies moving in a torus overlap, and the resulting C-space obstacles can be characterized as Minkowski sums in the torus. Proposition 2.3 gives an explicit general formula for the collision space. When specialized to a specific 3D crystallographic group, the formula can be used to limit the location search in the MR method by avoiding unproductive searches of the positions where collisions occur. Section 3

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works out the details for the planar case, with a view toward the 3D problem. This formulation is demonstrated with elliptical bodies in Section 4. We conclude with some numerical results concerning the volumes of the collision space (expressed as probabilities) for elliptical bodies. These results show that a significant portion of the motion space is in fact inaccessible due to collisions in this 2D analog of the MR method.

In order to understand our formulation, the following glossary of symbols is provided below.

1.1. Glossary

X - n-dimensional Euclidean space, $\mathbb{R}^n$.

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

$\mathcal{R}(\theta) \in \mathrm{SO}(2)$ - rotation in $\mathbb{R}^2$ by an angle θ.

$\mathbf{t}, \mathbf{x} \in X$ - an n-dimensional translation vector or position on which this translation acts by vector addition.

$g = (R, \mathbf{t}) \in \mathrm{SE}(n)$ - a special-Euclidean transformation (i.e., a proper rigid-body motion). Mathematically, $\mathrm{SE}(n) = \mathrm{SO}(n) \ltimes \mathbb{R}^n$ (a semi-direct product) which acts on positions as $g \cdot \mathbf{x} = R\mathbf{x} + \mathbf{t}$.

G - shorthand for $\mathrm{SE}(n)$.

$\mathbb{L}$ - a lattice in X of rank n.

T - a lattice translation subgroup of G consisting of elements identified with the set $\mathbb{L}$.

$T\backslash G = \{Tg : g \in G\}$ - the set of right cosets of T in G.

Γ - a chiral crystallographic group, i.e., a discrete subgroup of G that contains a rank-n lattice of translations T as the maximal normal Abelian subgroup.

γ - an element of a chiral 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 described below.

$\mathbf{t}_\gamma \in T$ - a lattice translation such that $\mathbf{t}_\gamma \cdot \mathbb{L} = \mathbb{L}$.

$\mathbf{v}(R_\gamma)$ - 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 $\gamma \in \Gamma$.[10]

$\mathbb{P} = \{R_\gamma \in \mathrm{SO}(n) : \exists\ \mathbf{v}(R_\gamma) \in X$ such that $(R_\gamma, \mathbf{v}(R_\gamma)) \in \Gamma\}$ - a discrete rotation group, called the point group; $\mathbb{P} \cong T\backslash\Gamma$. 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*.

$p : X \to T\backslash X$ - the projection from X to its quotient $T\backslash X$ given by $p(\mathbf{x}) \doteq T \cdot \mathbf{x} = \mathbb{L} + \mathbf{x} \in T\backslash X$.

$\mathbf{v}_1, \ldots, \mathbf{v}_n$ - generators of the Bravais lattice $\mathbb{L}$.

$F_{T\backslash X}$ - a (closed) crystallographic unit cell (a fundamental domain for T acting on X). We define the crystallographic unit cell by

$$F_{T\backslash X} \doteq \{c_1\mathbf{v}_1 + \cdots + c_n\mathbf{v}_n : 0 \le c_j \le 1, \text{ for } j = 1, \ldots, n\},$$

so that the restriction of p to $F_{T\backslash X}$ gives a surjective map $p : F_{T\backslash X} \to T\backslash X$ (which is injective on the interior of $F_{T\backslash X}$).

$F_{\Gamma\backslash X}$ - a crystallographic asymmetric unit (a fundamental domain for Γ acting on X, i.e., a closed tile whose images under the action of elements of Γ form a tiling of X; i.e, its Γ-symmetry mates cover Euclidean space, X, without gaps and with non-intersecting interiors, as computed in ref. [12] in the planar case and in ref. [8] in 3D). The space $\Gamma\backslash X$ itself is called a Euclidean orbifold.[7]

$B_1 + B_2 = \{\mathbf{x}_1 + \mathbf{x}_2 : \mathbf{x}_1 \in B_1, \mathbf{x}_2 \in B_2\}$ - the Minkowski sum of two bodies B_1,B_2 in X.

$p(B_1) \boxplus p(B_2) = p(B_1 + B_2)$ - the Minkowski sum of $p(B_1)$ and $p(B_2)$ in the Abelian group $T\backslash X$.

$F_{\Gamma\backslash G} = \mathrm{SO}(n) \times F_{\Gamma\backslash X}$ - a smallest finite-volume space of rotations and translations in which MR searches need to be performed; this is a fundamental domain for Γ in G; its images under Γ form a tiling of G, filling G without gaps or overlapping interiors. The homogeneous space $\Gamma\backslash G$ is a smooth manifold.

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$F_{T\backslash G} = \mathrm{SO}(n) \times F_{T\backslash X}$ - a fundamental domain for T in G; its images under T form a tiling of G.

$V_n(B)$ - the volume of an n-dimensional body $B \subset X$.

$vol(S)$ - the invariant ($\frac{n^2+n}{2}$-dimenional) volume measure of a set S in $G = \mathrm{SE}(n)$; it is invariant under the left and right actions of G.

MR is a computational method to phase macromolecular crystals that has been in use for more than half a century.[15] We briefly review the mathematical formulation of this method.

Let $X = \mathbb{R}^n$, n-dimensional Euclidean space, where of course the most practical case is $n = 3$. The inputs to MR computations are then: (1) the electron density, $\rho_X(\mathbf{x})$, of a known rigid macromolecule (or fragment thereof) called the reference molecule; and (2) the symmetry group of the crystal, Γ, which is a discrete subgroup of $G = \mathrm{SE}(n)$, the (continuous) Lie group of proper motions of rigid-bodies in n-dimensional Euclidean space. The group operation for G and Γ is denoted as "$\circ$", and their action on Euclidean space is denoted as "$\cdot$".

The reference molecule should be similar in structure to the one to be determined in order for the MR method to work. Such knowledge for proteins may come from prior knowledge of the similarity of the amino acid sequences of the reference and actual molecules, and the many tens of thousands of existing structures in the PDB.[1]

In MR, the goal is to position and orient copies of the electron densities of the reference molecule in the crystallographic unit cell by some $g \in G$ to form a model density of the form

$$\rho_{\Gamma\backslash X}(\mathbf{x}; g) = \sum_{\gamma\in\Gamma} \rho_X\left((\gamma \circ g)^{-1} \cdot \mathbf{x}\right). \tag{1}$$

(This can be viewed as a function of $\mathbf{x}$ indexed by g.) The density function $\rho_X(\mathbf{x})$, takes a non-negative value on the reference molecule and a zero value away from it.

Suppose that all of the dimensions of the reference molecule are smaller than all of the dimensions of the fundamental domain $F_{\Gamma\backslash X} \subset X$, which is identified with the asymmetric unit of the crystal. Then, if the reference frame in which $\rho_X(\mathbf{x})$ is defined is centered at the origin of X, and $F_{\Gamma\backslash X}$ is defined to have its center at the origin of X, and if g is a small motion, the body will still be fully contained in $F_{\Gamma\backslash X}$. In such a circumstance, the sum in Eq. (1) will only have non-zero contribution from $\gamma = e$.

For each fixed $g \in G$, $\rho_{\Gamma\backslash X}(\mathbf{x}; g)$ can be viewed either as a function on the asymmetric unit $F_{\Gamma\backslash X}$, or as function on the unit cell $F_{T\backslash X}$. In the latter case, the function will have symmetry within the unit cell described by the finite factor group $F_{T\backslash\Gamma} = F_{\Gamma/T} \cong \mathbb{P}$. Here and throughout this paper, $F_{A\backslash Y} \subset Y$ denotes a fundamental domain from which a space Y can be tiled or reconstructed by the left action of a group A acting on Y.

To describe our motivation, we let $\rho_X \doteq \rho_X^B : X \to \{0, 1\}$ denote the indicator function for a body $B \subset X$ (which takes a value of one on the body, and zero otherwise), and we let $\rho_{\Gamma\backslash X} \doteq \rho^B_{\Gamma\backslash X} : \Gamma\backslash X \to \mathbb{Z}_{\geq 0}$ denote the density function for a crystal composed of bodies $\gamma \cdot B$ with density $\sum_{\gamma\in\Gamma} \rho_X \circ \gamma^{-1}$. (The density $\rho_{\Gamma\backslash X}$ is an indicator function if the bodies do not collide. Otherwise $\rho_{\Gamma\backslash X}(\mathbf{x})$ equals the number of the bodies $\gamma \cdot B$ containing $\mathbf{x}$.) As established in ref. [5], all candidate poses, $g \in G$, can be chosen without loss of generality to be of the form $g \in F_{\Gamma\backslash G}$, or equivalently, each g can be viewed as a distinguished representative of the coset $\Gamma g \in \Gamma\backslash G$. These candidate poses can be evaluated and ranked according to the value of a cost function such as

$$C(g) = \sum_{\mathbf{k}\in\hat{F}_{T\backslash X}} \left(|\hat{\rho}_{\Gamma\backslash X}(\mathbf{k}; g)|^2 - \hat{P}(\mathbf{k})\right)^2, \tag{2}$$

where $P(\mathbf{x})$ is the real-space *Patterson function* for the crystal, and $\hat{P}(\mathbf{k})$ is the experimentally measured diffraction intensity. In general, $\hat{f}$ denotes the Fourier transform of a function f, and $\hat{F}_{T\backslash X} \cong \mathbb{Z}^3$ is the unitary dual (Fourier space) corresponding to $F_{T\backslash X}$.

The main goal of MR is to obtain a list of physically realizable candidate poses $\{g\}$ rank-ordered by the value of $C(g)$. To this end, this paper seeks to characterize the set of all $g \in F_{\Gamma\backslash G}$ when reference

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molecules and their symmetry mates are in collision, in order that such regions of motion space can be circumvented in MR searches, thereby speeding up computations.

2. Room-to-Move for Bodies in Crystallographic Environments

Let $\mathbb{L} \subset X = \mathbb{R}^n$ denote a lattice. The corresponding lattice translation group is $T = \mathbb{L} \rtimes \{\mathbb{I}\}$, where $\mathbb{I} \in \mathrm{SO}(n)$ is the identity rotation. The distinction between T and $(\mathbb{L}, +)$ is often blurred, but it is T defined in this way which forms a normal subgroup of any crystallographic space group, Γ, with Bravais lattice $\mathbb{L}$.

As discussed in ref. [6], we can take

$$F_{\Gamma\backslash G} = \mathrm{SO}(n) \times F_{\Gamma\backslash X}.$$

The action of any $g \in F_{\Gamma\backslash G}$ on any $\mathbf{x} \in F_{\Gamma\backslash X}$ will in general not produce a result that is in $F_{\Gamma\backslash X}$. But, as discussed in ref. [5], it is always possible to find a $\gamma \in \Gamma$ such that $\gamma \circ g \cdot \mathbf{x} \in F_{\Gamma\backslash X}$ and this "equivalent point" in $F_{\Gamma\backslash X}$ can be thought of as a "quasigroup action."

Let $B \subset F_{\Gamma\backslash X}$ denote an open set (i.e., a body without its boundary points) that can be fully contained in the chosen crystallographic asymmetric unit. In particular, let

$$\delta \doteq \min\{\, \|\mathbf{t}_\gamma\| \,:\, \mathbf{t}_\gamma \in \mathbb{L},\ \mathbf{t}_\gamma \neq \mathbf{0}\}\,. \tag{3}$$

Let

$$S \doteq \left\{ g \in F_{\Gamma\backslash G} \,:\, (g \cdot B) \cap \bigcup_{\gamma \in \Gamma \setminus \{e\}} (\gamma \circ g) \cdot B \neq \emptyset \right\}. \tag{4}$$

Here, "$\setminus$" denotes the difference of sets, and "e" denotes the identity in Γ. This set corresponds to all motions $g = (R, \mathbf{t}) \in F_{\Gamma\backslash G}$ of the body B so that the resulting body $g \cdot B$ will collide with (intersect) at least one of its symmetry mates $(\gamma \circ g) \cdot B$. As we shall see below, we only need to consider finitely many of the γ in Eq. (4), as the rest are redundant. This condition is equivalent to the motion g causing a collision between any two symmetry mates, since $(\gamma_1 \circ g) \cdot B \cap (\gamma_2 \circ g) \cdot B = \gamma_1 \cdot \left[(g \cdot B) \cap (\gamma_1^{-1} \circ \gamma_2 \circ g) \cdot B\right]$.

Definition 2.1. The collision probability for a body $B \subset X$ is given by

$$P_c(B) \doteq \frac{vol(S)}{vol(F_{\Gamma\backslash G})}, \tag{5}$$

where S is the set of motions resulting in a collision as defined in Eq. (4), and "vol" denotes a bi-invariant volume on G (which is unique up to a scalar multiple).

We define this quantity because it is a measure of how much of the motion space corresponds to bodies in collision. To compute the collision probability, we find it easier to work with the crystallographic unit cell (fundamental domain) $F_{T\backslash X}$ in X and the corresponding fundamental domain $F_{T\backslash G} = \mathrm{SO}(n) \times F_{T\backslash X}$ in G (rather than the fundamental domains $F_{\Gamma\backslash X}$, $F_{\Gamma\backslash G}$). Indeed, we have

Lemma 2.2.

$$P_c(B) = \frac{vol(S^*)}{vol(F_{T\backslash G})}, \tag{6}$$

where

$$S^* \doteq \left\{ g \in F_{T\backslash G} \,:\, (g \cdot B) \cap \bigcup_{\gamma \in \Gamma \setminus \{e\}} (\gamma \circ g) \cdot B \neq \emptyset \right\}.$$

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Proof. Let $k = |\mathbb{P}|$, the order of the point group. Since $\mathbb{P} \cong T\backslash\Gamma$, the fundamental domain, or tile, $F_{T\backslash G}$ is the union of k fundamental domains for Γ acting on G that fill $F_{T\backslash G}$ without gaps or positive-measure overlaps. Since the volume is invariant under the action of Γ, it then follows that $vol(F_{T\backslash G}) = k \cdot vol(F_{\Gamma\backslash G})$. Furthermore, S^* is the union of k disjoint images of S under the action of elements of Γ, so we also have $vol(S^*) = k \cdot vol(S)$. □

Fix the orientation $R \in \mathrm{SO}(n)$ of the moving version of body B, and define

$$B_R \doteq \{R\mathbf{x} \,:\, \mathbf{x} \in B\}.$$

Then, let

$$\begin{aligned} S_R^* &= \{\mathbf{t} \in F_{T\backslash X} \,:\, (R,\mathbf{t}) \in S^*\} \\ &= \left\{ \mathbf{t} \in F_{T\backslash X} \,:\, (B_R + \mathbf{t}) \cap \bigcup_{\gamma\in\Gamma\smallsetminus\{e\}} \gamma\cdot(B_R+\mathbf{t}) \neq \emptyset \right\}. \end{aligned} \tag{7}$$

The "slice" S_R^* of the collision space S^* consists of those translations (in a unit cell $F_{T\backslash X}$) that cause the rotated body B_R to collide with a symmetry mate. Thus, the spaces S_R^* (where R ranges over all rotations $R \in \mathrm{SO}(n)$) give a description of the full collision space S^*.

Note that any $\gamma \in \Gamma$ can be written as $\gamma = (R_\gamma, \mathbf{t}_\gamma + \mathbf{v}(R_\gamma))$, where $R_\gamma \in \mathbb{P}$, $\mathbf{t}_\gamma \in T$; only in the symmorphic case is $\mathbf{v}(R_\gamma) = \mathbf{0}$ for all values of R_γ. Suppose that $\mathbf{t} \in F_{T\backslash X}$. Then by Eq. (7),

$$\mathbf{t} \in S_R^* \iff \exists\, \mathbf{a},\mathbf{b} \in B_R,\ \gamma \in \Gamma$$

such that

$$\mathbf{a} + \mathbf{t} = R_\gamma(\mathbf{b} + \mathbf{t}) + \mathbf{t}_\gamma + \mathbf{v}(R_\gamma). \tag{8}$$

This can be rearranged as

$$(\mathbb{I} - R_\gamma)\mathbf{t} = R_\gamma\mathbf{b} - \mathbf{a} + \mathbf{t}_\gamma + \mathbf{v}(R_\gamma). \tag{9}$$

To summarize, we have

Proposition 2.3. The collision space S^* for a body $B \subset \mathbb{R}^n$ with crystallographic group $\Gamma \subset \mathrm{SO}(n)$ is given by

$$S^* = \bigcup_{\gamma\in\Gamma\smallsetminus\{e\}} \left\{(R,\mathbf{t}) \in \mathrm{SO}(n) \times F_{T\backslash X} : (\mathbb{I} - R_\gamma)\mathbf{t} \in (R_\gamma B_R) + (-B_R) + \mathbf{t}_\gamma + \mathbf{v}(R_\gamma)\right\}.$$

Here, $-B_R = (-\mathbb{I})\cdot B_R$, and $(R_\gamma B_R) + (-B_R)$ is a Minkowski sum of bodies. The collision space S^* can be decomposed into two sets:

$$\begin{aligned} &S^* = S_{\mathbb{P}}^* \cup S_{\mathbb{L}}^*, \qquad \text{where} \\ &S_{\mathbb{P}}^* \doteq \bigcup_{R_\gamma\in\mathbb{P}\smallsetminus\{\mathbb{I}\}} \left\{(R,\mathbf{t}) \in \mathrm{SO}(n) \times F_{T\backslash X} : (\mathbb{I} - R_\gamma)\mathbf{t} \in (R_\gamma B_R) + (-B_R) + \mathbb{L} + \mathbf{v}(R_\gamma)\right\}, \\ &S_{\mathbb{L}}^* = S_{\mathbb{L}}^\sharp \times F_{T\backslash X}, \quad S_{\mathbb{L}}^\sharp \doteq \{R \in \mathrm{SO}(n) : [B_R + (-B_R)] \cap (\mathbb{L} \smallsetminus \{\mathbf{0}\}) \neq \emptyset\}. \end{aligned} \tag{10}$$

The set $S_{\mathbb{L}}^*$ corresponds to collisions of a body with its translates across different unit cells, whereas the set $S_{\mathbb{P}}^*$ corresponds to collisions with symmetry mates other than its translates. Equation (10) reflects the fact that if a given pose of the body collides with one of its lattice translates, then the same holds for all poses of the same orientation no matter how they are translated. The set $S_{\mathbb{L}}^\sharp \subset \mathrm{SO}(n)$ is the set of orientations resulting in these collisions of lattice translates.

Thus, we have the following alternative description of the collision space:

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Proposition 2.4. The collision space S^* for a body $B \subset \mathbb{R}^n$ with crystallographic group $\Gamma \subset \mathrm{SO}(n)$ is given by $S^* = S^*_{\mathbb{P}} \cup (S^\sharp_{\mathbb{L}} \times F_{T\setminus X})$, where

$$S^*_{\mathbb{P}} = \bigcup_{R_\gamma \in \mathbb{P}\setminus\{\mathbb{I}\}} \left\{(R,\mathbf{t}) \in \mathrm{SO}(n) \times F_{T\setminus X} : (\mathbb{I} - R_\gamma)\mathbf{t} \in (R_\gamma B_R) + (-B_R) + \mathbb{L} + \mathbf{v}(R_\gamma)\right\}, \tag{11}$$

and

$$S^\sharp_{\mathbb{L}} = \bigcup_{\mathbf{t}_\gamma \in \mathbb{L},\ 0<\|\mathbf{t}_\gamma\|<\mathrm{diam}(B)} \{R \in \mathrm{SO}(n) : R^{-1}\mathbf{t}_\gamma \in B + (-B)\}. \tag{12}$$

Proof. It suffices to verify Eq. (12). Since

$$R^{-1} \cdot \left\{ [B_R + (-B_R)] \cap (\mathbb{L} \setminus \{\mathbf{0}\})\right\} = [B + (-B)] \cap (R^{-1} \cdot \mathbb{L} \setminus \{\mathbf{0}\}),$$

it follows from Eq. (10) that

$$S^\sharp_{\mathbb{L}} = \bigcup_{\mathbf{t}_\gamma \in \mathbb{L}\setminus\{\mathbf{0}\}} \{R \in \mathrm{SO}(n) : R^{-1}\mathbf{t}_\gamma \in B + (-B)\}. \tag{13}$$

(Note that $S^\sharp_{\mathbb{L}}$ depends only on the body B and the Bravais lattice $\mathbb{L}$.)

Since

$$\mathrm{diam}(B) = \sup_{\mathbf{x}_1,\mathbf{x}_2 \in B} \|\mathbf{x}_1 - \mathbf{x}_2\| = \sup_{\mathbf{x} \in B+(-B)} \|\mathbf{x}\|, \tag{14}$$

Eq. (12) is equivalent to Eq. (13). (Note that we are assuming that B is an open set so that the supremum in Eq. (14) is never attained and thus $\|\mathbf{x}\| < \mathrm{diam}(B)$ for all $\mathbf{x} \in B + (-B)$.) □

As a consequence of Proposition 2.4, we have the following formula for the slices S^*_R of the collision space.

Corollary 2.5. For $R \in \mathrm{SO}(n) \setminus S^\sharp_{\mathbb{L}}$, we have

$$S^*_R = \bigcup_{R_\gamma \in \mathbb{P}\setminus\{\mathbb{I}\}} \left\{\mathbf{t} \in F_{T\setminus X} : (\mathbb{I} - R_\gamma)\mathbf{t} \in (R_\gamma B_R) + (-B_R) + \mathbb{L} + \mathbf{v}(R_\gamma)\right\}. \tag{15}$$

Note that $S^*_R = F_{T\setminus X}$ for $R \in S^\sharp_{\mathbb{L}}$ by definition.

Equation (12) provides a formula for $S^*_{\mathbb{L}}$ that is amenable to computation and does not depend on the isomorphism class of the crystallographic group Γ. In Section 3, we shall describe $S^*_{\mathbb{P}}$ for each of the isomorphism classes of planar chiral crystallographic groups.

Note that it follows from Eq. (12) that if

$$\mathrm{diam}(B) \le \delta, \tag{16}$$

then $S^\sharp_{\mathbb{L}}$ is vacuous, and hence $S^* = S^*_{\mathbb{P}}$. Condition (16) means that the bodies are small enough that they can freely rotate without colliding with copies that are pure translates located in other unit cells; i.e., all rotations B_R of the body cannot collide with any of its lattice translates $B_R + \mathbf{t}_\gamma$.

On the other hand, in the $p1$ case, where $\mathbb{P} = \{\mathbb{I}\}$, $S^*_{\mathbb{P}}$ is vacuous and hence $S^* = S^*_{\mathbb{L}}$.

Remark 2.6. When using Eq. (11) to compute $S^*_{\mathbb{P}}$, we need to consider only finitely many $\mathbf{t}_\gamma \in \mathbb{L}$; e.g., it suffices to consider those $\mathbf{t}_\gamma$ satisfying the weak bound obtained from (9):

$$\begin{aligned}\|\mathbf{t}_\gamma\| &\le \|\mathbf{t}\| + \|R_\gamma\mathbf{t}\| + \|R_\gamma\mathbf{b}\| + \|\mathbf{a}\| + \|\mathbf{v}(R_\gamma)\| \\ &\le 3\ \sup_{\mathbf{t}\in F_{T\setminus X}} \|\mathbf{t}\| + 2\ \sup_{\mathbf{x}\in B} \|\mathbf{x}\|.\end{aligned}$$

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Proposition 2.4 can be restated to give a description of the admissible search region where collisions do not occur.

Proposition 2.7. Let $A^* \doteq (F_{T\backslash G}) \smallsetminus S^*$ denote the admissible search space for a body $B \subset \mathbb{R}^n$ with crystallographic group $\Gamma \subset \mathrm{SO}(n)$. Then,

$$A^* = \bigcup_{R_\gamma \in \mathbb{P} \smallsetminus \{\mathbb{I}\}} \left\{ (R, \mathbf{t}) \in \left[\mathrm{SO}(n) \smallsetminus S^\sharp_{\mathbb{L}} \right] \times F_{T\backslash X} : (\mathbb{I} - R_\gamma)\mathbf{t} \notin (R_\gamma B_R) + (-B_R) + \mathbb{L} + \mathbf{v}(R_\gamma) \right\},$$

where $S^\sharp_{\mathbb{L}}$ is given by Eq. (12).

Remark 2.8. It appears that the problem of computing $P_c(B)$ has not been studied either in the mathematics or the crystallography literature. The closest work to this that we are aware of originates in the field of integral geometry and geometric probability. In this field, the so-called Principal Kinematic Formula computes the volume in G corresponding to collisions of one moving body and one fixed body (both convex).[2,4,11,16–18] Some work has generalized this to the case when the bodies are in a homogenous space other than Euclidean space[3] or when instead of a single fixed body, a periodic array of fixed bodies is present.[19] But neither of these works apply directly to our problem.

3. Characterization of Collision Space for the Planar Case

Since all chiral space groups in the plane are symmorphic, $\mathbf{v}(R_\gamma) = 0$ in Eq. (8) in the planar case ($n = 2$). Thus, we have by Proposition 2.4,

$$S^* = \{(R, \mathbf{t}) \in \mathrm{SO}(n) \times F_{T\backslash X} : \mathbf{t} \in S^*_R\}, \tag{17}$$

where

$$S^*_R = \begin{cases} \displaystyle\bigcup_{R_\gamma \in \mathbb{P} \smallsetminus \{\mathbb{I}\}} \left\{ \mathbf{t} \in F_{T\backslash X} : (\mathbb{I} - R_\gamma)\mathbf{t} \in (R_\gamma B_R) + (-B_R) + \mathbb{L}) \right\}, & \text{for } R \notin S^\sharp_{\mathbb{L}} \\ F_{T\backslash X}, & \text{for } R \in S^\sharp_{\mathbb{L}} \end{cases}$$

We let

$$B^\gamma = B^{R_\gamma} \doteq (\mathbb{I} - R_\gamma)^{-1} \left[(R_\gamma B) + (-B) \right], \tag{18}$$

where $B_1 + B_2$ denotes the Minkowski sum of bodies B_1 and B_2, $R_\gamma B = \{R_\gamma \cdot \mathbf{b} : \mathbf{b} \in B\}$ and $-B = (-\mathbb{I}) \cdot B$. Since rotations commute in the planar case, $(B^\gamma)_R = (B_R)^\gamma$, which we now write as B^γ_R.

Then,

$$S^*_R = F_{T\backslash X} \cap \bigcup_{R_\gamma \in \mathbb{P} \smallsetminus \{\mathbb{I}\}} \left\{ (\mathbb{I} - R_\gamma)^{-1}\mathbb{L} + B^\gamma_R \right\}, \quad \text{for } R \in \mathrm{SO}(2) \smallsetminus S^\sharp_{\mathbb{L}}. \tag{19}$$

We let $p : X \to T\backslash X$ denote the covering map given by

$$p(\mathbf{x}) \doteq T \cdot \mathbf{x} = \mathbb{L} + \mathbf{x} \in T\backslash X\,. \tag{20}$$

(Here, $T \cdot \mathbf{x}$ denotes the T-orbit of $\mathbf{x}$, which is identical to the coset $\mathbb{L} + \mathbf{x}$ in the Abelian group X.) Since p is injective on the interior of $F_{T\backslash X}$, we have

$$V_2(S^*_R) = V_2(p(S^*_R))\,. \tag{21}$$

Since the point group leaves $\mathbb{L}$ invariant, we have $R_\gamma \mathbb{L} = \mathbb{L}$, and therefore for all $\mathbf{t}_\gamma \in \mathbb{L}$,

$$(\mathbb{I} - R_\gamma)^{-1}\mathbb{L} + \mathbf{t}_\gamma = (\mathbb{I} - R_\gamma)^{-1}[\mathbb{L} + \mathbf{t}_\gamma - R_\gamma \mathbf{t}_\gamma] = (\mathbb{I} - R_\gamma)^{-1}\mathbb{L}\,.$$

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Therefore, the sets $(\mathbb{I} - R_\gamma)^{-1}\mathbb{L} + B_R^\gamma$ are invariant under the action of T. Since each element of the space X has a T-translate in the fundamental domain $F_{T\backslash X}$, it follows that the image of S_R^* in the torus $T\backslash X$ is given by

$$p(S_R^*) = \bigcup_{R_\gamma \in \mathbb{P} \smallsetminus \{\mathbb{I}\}} \left\{ p([\mathbb{I} - R_\gamma]^{-1}\mathbb{L}) \boxplus p(B_R^\gamma) \right\} \subset T\backslash X \quad \text{for } R \in \mathrm{SO}(2) \smallsetminus S_{\mathbb{L}}^\sharp. \tag{22}$$

(Recall that "$\boxplus$" denotes the Minkowski sum in $T\backslash X$.)

For each $R_\gamma \in \mathbb{P} \smallsetminus \{\mathbb{I}\}$, we let n_γ denote the number of distinct points of the form $p([\mathbb{I} - R_\gamma]^{-1}\mathbf{t}_\gamma) \in T\backslash X$, where $\mathbf{t}_\gamma$ runs through the points of the lattice $\mathbb{L}$, i.e.,

$$n_\gamma \doteq \#\left\{ p([\mathbb{I} - R_\gamma]^{-1}\mathbb{L}) \right\}. \tag{23}$$

If Eq. (16) holds so that $S_{\mathbb{L}}^\sharp$ is empty, then by Eq. (22), the collision probabilities $P_c(B)$ depend only on the areas of B^γ and the cardinalities n_γ. We shall determine the sets $p([\mathbb{I} - R_\gamma]^{-1}\mathbb{L})$ and their cardinalities n_γ explicitly and compute $P_c(B)$ for bodies with small diameter in the four chiral cases separately.

Remark 3.1. The numbers n_γ can also be obtained from the Lefschetz fixed point formula, as follows: We note that $p([\mathbb{I} - R_\gamma]^{-1}\mathbb{L})$ is the fixed point set of R_γ acting on $T\backslash X$, and each fixed point has index 1 (since R_γ is a rotation about the fixed point). Identifying $\mathbb{L}$ with $H_1(T\backslash X, \mathbb{Z})$ via the covering map $X \to T\backslash X$, we see that the action of R_γ on $H_1(T\backslash X, \mathbb{Z})$ is just the action of R_γ on $\mathbb{L}$. Therefore, by the Lefschetz formula

$$\begin{aligned} n_\gamma &= 1 - \mathrm{Trace}\big[R_{\gamma *} : H_1(T\backslash X, \mathbb{Z}) \to H_1(T\backslash X, \mathbb{Z})\big] + 1 \\ &= 2 - \mathrm{Trace}(R_\gamma) = 2 - 2\cos\theta_\gamma, \end{aligned}$$

where R_γ is a rotation by the angle θ_γ. Note that θ_γ is always a multiple of either $\pi/2$ or $\pi/3$, and thus n_γ takes the values 1, 2, 3, or 4, depending on the symmetry.

We now consider each isomorphism class separately. Recall that for crystallographic groups in the $p1$ class, $S_{\mathbb{P}}^* = \emptyset$ and hence $S^* = S_{\mathbb{L}}^*$, which is described in Proposition 2.4. In particular in the $p1$ class, if Eq. (16) holds, then $S^* = \emptyset$. Hence, we shall begin with $p2$.

In the following, we shall let $\mathbf{v}_1, \mathbf{v}_2$ denote generators of the Bravais lattice $\mathbb{L}$.

3.1. p2 symmetry

For crystallographic groups Γ in the $p2$ isomorphism class, $\mathbb{P} = \{\mathbb{I}, -\mathbb{I}\}$ and $\mathbb{L}$ is arbitrary. Then, Eq. (22) becomes

$$p(S_R^*) = p\left(\tfrac{1}{2}\mathbb{L}\right) \boxplus p\left(B_R^\gamma\right), \quad \text{for } R \in \mathrm{SO}(2) \smallsetminus S_{\mathbb{L}}^\sharp, \tag{24}$$

where by (18) with $R_\gamma = -\mathbb{I}$

$$B^\gamma = -\tfrac{1}{2}(B + B). \tag{25}$$

We have the following description of the collision space:

Theorem 3.2. Let $\Gamma \subset \mathrm{SE}(2)$ be a crystallographic group in the isomorphism class $p2$ acting on a body $B \subset \mathbb{R}^2$, and let $\mathbf{v}_1, \mathbf{v}_2$ be generators of the Bravais lattice $\mathbb{L}$. Then,

$$p(S_R^*) = \bigcup_{j=1}^{4} p\left(-\tfrac{1}{2}[B_R + B_R] + \mathbf{w}_j\right) \quad \text{for } R \in \mathrm{SO}(2) \smallsetminus S_{\mathbb{L}}^\sharp,$$

where

$$\mathbf{w}_1 \doteq \mathbf{0}, \quad \mathbf{w}_2 \doteq \tfrac{1}{2}\mathbf{v}_1, \quad \mathbf{w}_3 \doteq p\big(\tfrac{1}{2}\mathbf{v}_1 + \tfrac{1}{2}\mathbf{v}_2\big), \quad \mathbf{w}_4 \doteq \tfrac{1}{2}\mathbf{v}_2.$$

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Proof. One easily sees that $p(\frac{1}{2}\mathbb{L})$ consists of the four points $p(\mathbf{w}_j) \in T\backslash X,\ 1 \le j \le 4$. The result then follows from Eqs. (24)–(25). □

Now, suppose that $\mathrm{diam}(B) \le \frac{1}{2}\delta$. Then, for distinct points $\mathbf{t}_\gamma, \mathbf{t}_{\gamma'} \in \mathbb{L}$,

$$\mathrm{diam}(B_R^\gamma) = \mathrm{diam}\left[\tfrac{1}{2}(B+B)\right] = \mathrm{diam}(B) \le \left\| \tfrac{1}{2}\mathbf{t}_\gamma - \tfrac{1}{2}\mathbf{t}_{\gamma'} \right\|, \tag{26}$$

and thus the (open) bodies $B_R^\gamma + \frac{1}{2}\mathbf{t}_\gamma$ and $B_R^\gamma + \frac{1}{2}\mathbf{t}_{\gamma'}$ are disjoint. Then, $S_{\mathbb{L}}^\sharp = \emptyset$ and

$$p(S_R^*) = \bigsqcup_{j=1}^{4} p(B_R^\gamma + \mathbf{w}_j) = \bigsqcup_{j=1}^{4} \left[p(B_R^\gamma) \boxplus \alpha_j\right] \tag{27}$$

for all $R \in \mathrm{SO}(2)$, where $\bigsqcup$ denotes a disjoint union.

Therefore,

$$V_2(S_R^*) = V_2\left(p(S_R^*)\right) = 4\,V_2\left(B^\gamma\right) = V_2(B+B)\,. \tag{28}$$

We can now give a formula for the collision probability.

Theorem 3.3. For a crystallographic group Γ in the isomorphism class p2, the collision probability for a body B is given by

$$P_c(B) = \frac{V_2(B+B)}{V_2(F_{T\backslash X})}, \tag{29}$$

when $\mathrm{diam}(B) \le \frac{1}{2}\delta$.

Proof. Rewriting Eq. (7) and recalling that $F_{T\backslash G} = F_{T\backslash X} \times \mathrm{SO}(2)$, we have

$$S^* \;=\; \{(R,\mathbf{t}) \in F_{T\backslash G} \;:\; \mathbf{t} \in S_R^*\}. \tag{30}$$

Since the invariant volume measure on $G = \mathrm{SO}(2) \ltimes \mathbb{R}^2$ is (up to a scalar factor) the product of the area measure in $\mathbb{R}^2$ and $d\theta$ on SO(2), we have

$$vol(F_{T\backslash G}) = 2\pi\ V_2(F_{T\backslash X}),$$
$$vol(S^*) = \int_0^{2\pi} V_2(S^*_{\mathcal{R}(\theta)})\,d\theta \;=\; 2\pi\ V_2(B+B),$$

where the last equality follows from Eq. (28). Formula (29) then follows from Lemma 2.2. □

Corollary 3.4. For a crystallographic group Γ in the isomorphism class $p2$, the collision probability for a convex body B of diameter at most $\frac{1}{2}\delta$ is given by

$$P_c(B) = 4\,V_2(B)/V_2(F_{T\backslash X})\,.$$

Proof. $B + B = 2B$ for a convex body B. □

3.2. p3 symmetry

For a crystallographic group Γ in the $p3$ isomorphism class, $\mathbb{P} \equiv \{\mathbb{I}, \mathcal{R}(\eta), \mathcal{R}(2\eta)\}$, where $\eta = 2\pi/3$. We can assume without loss of generality that the lattice $\mathbb{L}$ is generated by

$$\mathbf{v}_1 \doteq (\delta, 0), \qquad \mathbf{v}_2 \doteq \mathcal{R}(\eta)\cdot\mathbf{v}_1 = \left(-\frac{1}{2}\,\delta,\ \frac{\sqrt{3}}{2}\,\delta\right),$$

for some $\delta > 0$.

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Since $\mathcal{R}(\eta)\mathbb{L} = \mathbb{L}$, if $g \cdot B$ intersects $\mathcal{R}(\eta)(g \cdot B) + \mathbf{t}_\gamma$, then $\mathcal{R}(\eta)(g \cdot B)$ intersects

$$\mathcal{R}(\eta)[\mathcal{R}(\eta)(g \cdot B) + \mathbf{t}_\gamma] = \mathcal{R}(2\eta)(g \cdot B) + \mathbf{t}_{\gamma'},$$

and similarly $\mathcal{R}(2\eta)(g \cdot B)$ intersects $(g \cdot B) + \mathbf{t}_{\gamma''}$, for some $\gamma', \gamma'' \in \mathbb{L}$. Therefore to find the slices S_R^* of the collision space, we only need to consider $R_\gamma = \mathcal{R}(\eta)$ in Eq. (22), so we have

$$p(S_R^*) = p([\mathbb{I} - \mathcal{R}(\eta)]^{-1}\mathbb{L}) \boxplus p(B_R^\gamma) \quad \text{for } R \in \mathrm{SO}(2) \setminus S_{\mathbb{L}}^\sharp. \tag{31}$$

To determine the summands in Eq. (31), we note that

$$[\mathbb{I} - \mathcal{R}(\eta)]^{-1} = \frac{1}{\sqrt{3}}\,\mathcal{R}\left(\frac{\pi}{6}\right). \tag{32}$$

It follows that $n_{\mathcal{R}(\eta)} = 3$ and

$$\begin{aligned} p([\mathbb{I} - \mathcal{R}(\eta)]^{-1}\mathbb{L}) &= \{p(\mathbf{z}_1),\, p(\mathbf{z}_2),\, p(\mathbf{z}_3)\} \\ &= \{p(\mathbf{0}),\, p(\mathbf{z}_2),\, p(-\mathbf{z}_2)\}, \end{aligned} \tag{33}$$

where[3]

$$\mathbf{z}_1 = [\mathbb{I} - \mathcal{R}(\eta)]^{-1}\mathbf{0} = (0, 0), \tag{34}$$

$$\mathbf{z}_2 = [\mathbb{I} - \mathcal{R}(\eta)]^{-1}(\mathbf{v}_1 + \mathbf{v}_2) = (0, \tfrac{\sqrt{3}}{3}\delta), \tag{35}$$

$$\mathbf{z}_3 = [\mathbb{I} - \mathcal{R}(\eta)]^{-1}\mathbf{v}_1 = (\tfrac{1}{2}\delta, \tfrac{\sqrt{3}}{6}\delta)\,. \tag{36}$$

By Eqs. (18) and (32),

$$B_R^\gamma = \frac{1}{\sqrt{3}}\,\mathcal{R}\left(\frac{\pi}{6}\right)\left[\mathcal{R}\left(\frac{2\pi}{3}\right)B_R + (-B_R)\right] = \frac{1}{\sqrt{3}}\left[\mathcal{R}\left(\frac{5\pi}{6}\right)B_R + \mathcal{R}\left(\frac{7\pi}{6}\right)B_R\right]. \tag{37}$$

Therefore,

$$p(S_R^*) = \bigcup_{j=1}^{3} p(B_R^\gamma + \mathbf{z}_j) \quad \text{for } R \in \mathrm{SO}(2) \setminus S_{\mathbb{L}}^\sharp\,. \tag{38}$$

To summarize, we have

Theorem 3.5. Let $\Gamma \subset \mathrm{SE}(2)$ be a crystallographic group in the isomorphism class $p3$ acting on a body $B \subset \mathbb{R}^2$, and suppose that $\mathbf{v}_1 = (\delta, 0),\ \mathbf{v}_2 = (-\frac{1}{2}\,\delta, \frac{\sqrt{3}}{2}\,\delta)$ generate the Bravais lattice $\mathbb{L}$. Then,

$$p(S_R^*) = \bigcup_{j=1}^{3} p\left(\frac{1}{\sqrt{3}}\left[\mathcal{R}\left(\frac{5\pi}{6}\right)B_R + \mathcal{R}\left(\frac{7\pi}{6}\right)B_R\right] + \mathbf{z}_j\right) \quad \text{for } R \in \mathrm{SO}(2) \setminus S_{\mathbb{L}}^\sharp,$$

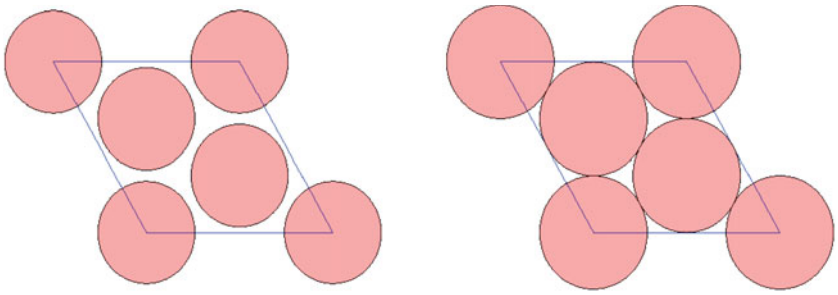
where $\mathbf{z}_1, \mathbf{z}_2, \mathbf{z}_3$ are given by Eqs. (34)–(36).

We note that

$$\mathrm{diam}(B_R^\gamma) = \frac{1}{\sqrt{3}}\,\mathrm{diam}\left[B + \mathcal{R}\left(\frac{\pi}{3}\right)B\right] \le \frac{2}{\sqrt{3}}\,\mathrm{diam}(B),$$

[3] It is convenient to make the identification $\mathbb{R}^2 \leftrightarrow \mathbb{C}$ when doing these computations. Then, $\mathcal{R}(\eta) \leftrightarrow e^{i\eta}$, $\mathbb{I} - \mathcal{R}(\eta) \leftrightarrow \sqrt{3}\,e^{-i\pi/6}$, $\mathbf{v}_1 \leftrightarrow \delta$, $\mathbf{v}_2 \leftrightarrow e^{i2\pi/3}\delta$, etc.

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(a) $r < \frac{\delta}{4}$ (b) $r = \frac{\delta}{4}$

Fig. 3. Disjoint circular collision zones in the $p3$ case.

and for distinct points $\mathbf{t}, \mathbf{t}' \in \mathbb{L}$,

$$\|(\mathbb{I} - \mathcal{R}(\eta))^{-1}\mathbf{t} - (\mathbb{I} - \mathcal{R}(\eta))^{-1}\mathbf{t}'\| \geq \frac{\delta}{\sqrt{3}}\,.$$

Hence it follows as before that if $\mathrm{diam}(B) < \delta/2$, then $S^*_{\mathbb{L}} = \emptyset$ and $\mathrm{diam}(RB^\gamma) \leq \delta/\sqrt{3}$, and the three collision zones $p(B^\gamma_R + \mathbf{z}_j)$ (for $j = 1, 2, 3$) in Eq. (38) will be disjoint. For example, when B is a disk of radius r, the collision zones will be circular. Figure 3(a) shows the three disjoint circular collision zones (in the torus $T\backslash X$) when B is a disk of radius $r < \delta/4$, and Fig. 3(b) shows the circular collision zones touching when B is a disk of radius $r = \delta/4$. (Since we defined the bodies as open sets, they also do not intersect as sets in this case). In Fig. 3 and the following figures, the outline represents the boundary of the crystallographic unit cell $F_{T\backslash\mathbb{R}^2}$.

Thus, if $\mathrm{diam}(B) \leq \delta/2$, it follows from Eqs. (37)–(38) that

$$V_2\left(p(S^*_R)\right) = 3\,V_2\left(B^\gamma\right) = V_2\left[B + \mathcal{R}\left(\frac{\pi}{3}\right)B\right]. \tag{39}$$

Since Eq. (39) is independent of the rotation R, Eq. (39) together with the argument from the proof of Theorem 3.3 yields the following formula for the collision probability.

Theorem 3.6. For a crystallographic group Γ in the isomorphism class $p3$, the collision probability for a body B is given by

$$P_c(B) = \frac{V_2\left[B + \mathcal{R}\left(\frac{\pi}{3}\right)B\right]}{V_2(F_{T\backslash X})} = \frac{2}{\sqrt{3}\,\delta^2}\,V_2\left[B + \mathcal{R}\left(\frac{\pi}{3}\right)B\right], \tag{40}$$

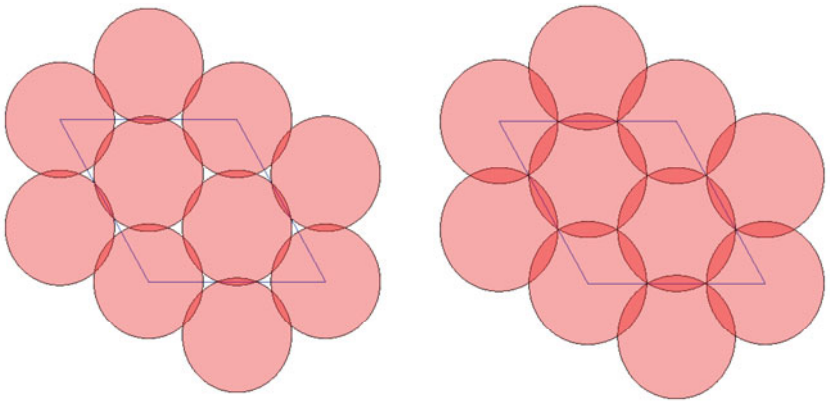
when $\mathrm{diam}(B) \leq \frac{1}{2}\delta$.

Remark 3.7. In fact, the above argument shows that if $\mathrm{diam}\left[B + \mathcal{R}(\frac{\pi}{3})B\right] \leq \delta$, then the collision zones will be disjoint, and thus the collision probability will still be given by Eq. (40). We shall use this observation in the discussion of collision probabilities for elliptical bodies in Section 4.

If B is a disk of radius $> \delta/4$, then the circular collision zones will intersect in pairs. Figure 4 shows two cases in which the circular collision zones intersect in pairs. In Fig. 4(a), the circular collision zones intersect in pairs leaving very little allowable room for the bodies to move; in Fig. 4(b), the circular collision zones cover the entire crystallographic unit cell, so no configurations are possible.[4]

[4] In Fig. 4(b), there are no triple intersections of the (open) circular collision zones, but the closures of the circular collision zones have six triple intersection points in the crystallographic unit cell: $(\frac{1}{3}\delta, 0)$, $(\frac{2}{3}\delta, 0)$, $(\frac{1}{6}\delta, \pm\frac{\sqrt{3}}{6}\delta)$, $(\frac{1}{3}\delta, \pm\frac{\sqrt{3}}{3}\delta)$.

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(a) $\frac{\delta}{4} < r < \frac{\delta}{3}$ (b) $r = \frac{\delta}{3}$

Fig. 4. Intersecting circular collision zones in the $p3$ case.

3.3. p4 symmetry

For a crystallographic group Γ in the $p4$ isomorphism class, $\mathbb{P}$ is generated by a 90° rotation: $\mathbb{P} = \{\mathbb{I}, \mathcal{R}(\frac{1}{2}\pi), -\mathbb{I}, \mathcal{R}(\frac{3}{2}\pi)\}$. The lattice $\mathbb{L}$ is a square, so we can assume without loss of generality that it is generated by $\mathbf{v}_1 = (\delta, 0)$, $\mathbf{v}_2 = (0, \delta)$. By the argument in the $p3$ case above, if $g \cdot B$ collides with $\mathcal{R}(\frac{1}{2}\pi)(g \cdot B) + \mathbb{L}$, it must also collide with $\mathcal{R}(\frac{3}{2}\pi)(g \cdot B) + \mathbb{L}$ (and conversely). Suppose that $g \cdot B$ collides with $R_\gamma \cdot B + \mathbf{t}_\gamma$ and $R_\gamma \neq \mathbb{I}$. Then, there are only two possiblities: $g \cdot B$ collides with $\mathcal{R}(\frac{1}{2}\pi)(g \cdot B) + \mathbb{L}$, or $g \cdot B$ collides with $(-\mathbb{I})(g \cdot B) + \mathbb{L}$. (Both can also occur simultaneously.) Figure 5 (generated using the iphone app "Eschermobile"[13]) shows three configurations of a pattern with $p4$ symmetry. In Fig. 5(a), the bodies are not in collision; in Fig. 5(b), $(g \cdot B)$ collides with $(-\mathbb{I})(g \cdot B) + \mathbb{L}$, and consequently $\mathcal{R}(\frac{1}{2}\pi)(g \cdot B)$ collides with $\mathcal{R}(\frac{3}{2}\pi)(g \cdot B) + \mathbb{L}$; in Fig. 5(c), $g \cdot B$ collides with $\mathcal{R}(\frac{1}{2}\pi)(g \cdot B) + \mathbb{L}$, which collides with $(-\mathbb{I})(g \cdot B) + \mathbb{L}$, which collides with $\mathcal{R}(\frac{3}{2}\pi)(g \cdot B) + \mathbb{L}$, which in turn collides with $g \cdot B + \mathbb{L}$.

Thus, letting $R_\gamma = \mathcal{R}(\frac{1}{2}\pi)$ and recalling from Eq. (25) that $B^{-\mathbb{I}} = -\frac{1}{2}(B + B)$, we have

$$p(S_R^*) = \left\{p([\mathbb{I} - \mathcal{R}(\tfrac{1}{2}\pi)]^{-1}\mathbb{L}) \boxplus p(B_R^\gamma)\right\} \cup \left\{p\left(\tfrac{1}{2}\,\mathbb{L}\right) \boxplus p\left[-\tfrac{1}{2}(B_R + B_R)\right]\right\}, \tag{41}$$

for $R \in \mathrm{SO}(2) \setminus S_{\mathbb{L}}^\sharp$. From the $p2$ case, $p(\frac{1}{2}\mathbb{L}) = \{\alpha_1, \alpha_2, \alpha_3, \alpha_4\}$, where

$$\alpha_1 = p(0, 0), \quad \alpha_2 = p(\tfrac{\delta}{2}, 0), \quad \alpha_3 = p(\tfrac{\delta}{2}, \tfrac{\delta}{2}), \quad \alpha_4 = p(0, \tfrac{\delta}{2}). \tag{42}$$

We note that[(5)]

$$(\mathbb{I} - R_\gamma)^{-1} = \frac{1}{\sqrt{2}}\,\mathcal{R}\left(\frac{\pi}{4}\right).$$

Thus,

$$B^\gamma = \frac{1}{\sqrt{2}}\mathcal{R}(\frac{\pi}{4})\left[\mathcal{R}(\frac{\pi}{2})B + (-1)B\right] = \frac{1}{\sqrt{2}}\left[\mathcal{R}(\frac{3\pi}{4})B + \mathcal{R}(\frac{5\pi}{4})B\right]$$

and

$$p([\mathbb{I} - \mathcal{R}(\tfrac{1}{2}\pi)]^{-1}\mathbb{L}) = \{\alpha_1, \alpha_3\}.$$

Thus, we have the following result:

[(5)] Identifying $\mathbb{R}^2 \leftrightarrow \mathbb{C}$, we have $R_\gamma \leftrightarrow i$, $(\mathbb{I} - R_\gamma)^{-1} \leftrightarrow \frac{1}{2} + \frac{1}{2}i = \frac{1}{\sqrt{2}}\,e^{i\pi/4}$.

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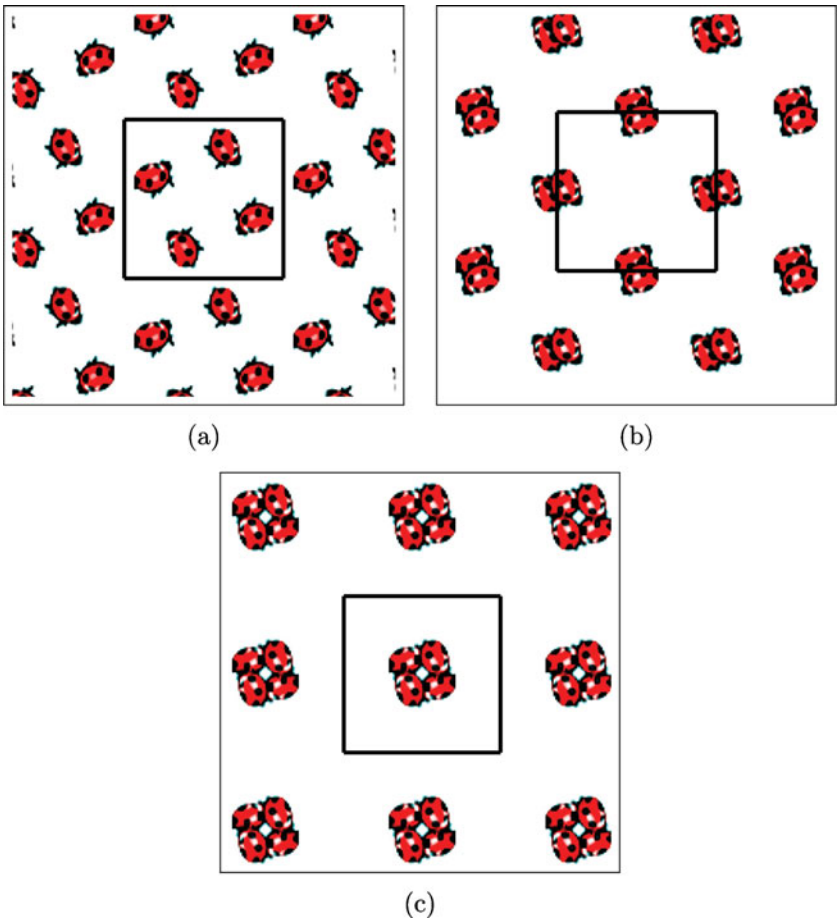


Fig. 5. Three configurations of solid bodies with $p4$ symmetry.

Theorem 3.8. Let $\Gamma \subset \mathrm{SE}(2)$ be a crystallographic group in the isomorphism class $p4$ acting on a body $B \subset \mathbb{R}^2$, and suppose that $\mathbf{v}_1 = (\delta, 0)$, $\mathbf{v}_2 = (0, \delta)$ generate the Bravais lattice $\mathbb{L}$. Then,

$$p(S_R^*) = \left(p\left[-\frac{1}{2}(B_R + B_R) \right] \boxplus \{\alpha_2, \alpha_4\} \right) \cup \left(p\left\{ \frac{1}{\sqrt{2}} \left[\mathcal{R}\left(\frac{3\pi}{4}\right) B_R + \mathcal{R}\left(\frac{5\pi}{4}\right) B_R \right] \cup \left(-\frac{1}{2}\right)(B_R + B_R) \right\} \boxplus \{\alpha_1, \alpha_3\} \right),$$

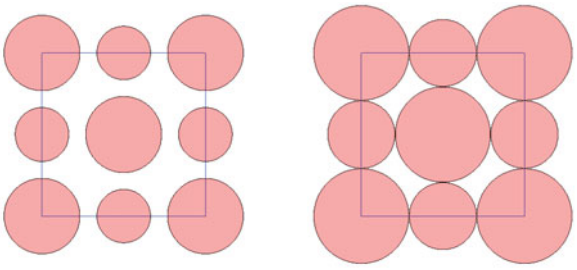
for $R \in \mathrm{SO}(2) \setminus S_{\mathbb{L}}^{\sharp}$, where $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ are given by Eq. (42).

Definition 3.9. For a body $B \subset \mathbb{R}^2$, we let r_B denote the circumradius of B, which is the radius of the smallest closed disk containing B.

Replacing B by a translate, we can assume that B is contained in a disk of radius r_B centered at 0. Therefore, B^{γ} is contained in a disk of radius of radius $\sqrt{2}\, r_B$ about 0, and $\frac{1}{2}(B + B)$ is contained in a disk of radius r_B about 0. Let $D(\mathbf{x}, r) = \{\mathbf{t} \in \mathbb{R}^2 : \|\mathbf{t} - \mathbf{x}\| < r\}$ denote the disk of radius r about $\mathbf{x}$, and write $p\big(D(\mathbf{x}, r)\big) = \widetilde{D}(p(\mathbf{x}), r)$. We have

$$p(S_R^*) = A_1 \cup A_2 \cup A_3 \cup A_4 \quad \text{for } R \in \mathrm{SO}(2) \setminus S_{\mathbb{L}}^{\sharp},$$

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(a) $r < \frac{\delta}{2(1+\sqrt{2})}$ (b) $r = \frac{\delta}{2(1+\sqrt{2})}$

Fig. 6. Disjoint circular collision zones in the $p4$ case.

where

$$\begin{array}{lll} A_1 = p\left\{\left[B_R^\gamma \cup (-\frac{1}{2})(B_R + B_R)\right]\right\} \boxplus \alpha_1 & \subset & \widetilde{D}(\alpha_1, \sqrt{2}\, r_B), \\ A_2 = \quad p\left[-\frac{1}{2}(B_R + B_R)\right] \boxplus \alpha_2 & \subset & \widetilde{D}(\alpha_2, r_B), \\ A_3 = p\left\{\left[B_R^\gamma \cup (-\frac{1}{2})(B_R + B_R)\right]\right\} \boxplus \alpha_3 & \subset & \widetilde{D}(\alpha_3, \sqrt{2}\, r_B), \\ A_4 = \quad p\left[-\frac{1}{2}(B_R + B_R)\right] \boxplus \alpha_4 & \subset & \widetilde{D}(\alpha_4, r_B)\,. \end{array} \tag{43}$$

Then, for the case $\mathrm{diam}(B) \le \delta$, the collision space $p(S_R^*)$ is contained in a union of four disks

$$\widetilde{D}(\alpha_1, \sqrt{2}\, r_B) \,\cup\, \widetilde{D}(\alpha_2, r_B) \,\cup\, \widetilde{D}(\alpha_3, \sqrt{2}\, r_B) \,\cup\, \widetilde{D}(\alpha_4, r_B) \tag{44}$$

in the torus $T \backslash X$. We see from Eq. (42) and Fig. 6 below that the four disks will be disjoint, and therefore the sets A_j will be disjoint, if

$$r_B \le \frac{\delta}{2(1+\sqrt{2})}\,. \tag{45}$$

For example, when B is a disk of radius r, the collision zones will consist of the four disks in Eq. (44), as illustrated in Figs. 6–7.

Thus, if r_B satisfies the bound (45), then

$$\begin{aligned} V_2(p(S_R^*)) &= \sum_{j=1}^{4} V_2(A_j) \;=\; \sum_{j=1}^{4} V_2([-1]A_j) \\ &= 2\, V_2\left(\frac{1}{\sqrt{2}}\left[\mathcal{R}(\frac{\pi}{4})B + \mathcal{R}(-\frac{\pi}{4})B\right] \cup \frac{1}{2}\,(B+B)\right) + 2\, V_2\left(\frac{1}{2}(B+B)\right) \\ &= V_2\left(\left[\mathcal{R}(\frac{\pi}{4})B + \mathcal{R}(-\frac{\pi}{4})B\right] \cup \frac{1}{\sqrt{2}}\,(B+B)\right) + \frac{1}{2}\, V_2(B+B)\,. \end{aligned}$$

Again using the argument from the proof of Theorem 3.3, we obtain a formula for the collision probability in the $p4$ case.

Theorem 3.10. For a crystallographic group Γ in the isomorphism class $p4$, the collision probability for a body B is given by

$$P_c(B) = \frac{1}{\delta^2}\left\{V_2\left(\left[\mathcal{R}\left(\frac{\pi}{4}\right)B + \mathcal{R}\left(-\frac{\pi}{4}\right)B\right] \cup \frac{1}{\sqrt{2}}\,(B+B)\right) + \frac{1}{2}\, V_2(B+B)\right\}, \tag{46}$$

when $r_B \le \frac{\delta}{2(1+\sqrt{2})}$.

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Corollary 3.11. For a crystallographic group Γ in the isomorphism class $p4$, the collision probability for a **convex** body B is given by

$$P_c(B) = \frac{1}{\delta^2}\left\{V_2\left[B + \mathcal{R}\left(\frac{\pi}{2}\right)B\right] + 2\,V_2(B)\right\}, \tag{47}$$

when $r_{B^\gamma} + r_B \le \delta/2$, in particular when $r_B \le \frac{\delta}{2(1+\sqrt{2})}$.

Proof. If B is convex, then

$$B + B = 2\,B \subset \sqrt{2}\left[\mathcal{R}\left(\frac{\pi}{4}\right)B + \mathcal{R}\left(-\frac{\pi}{4}\right)B\right],$$

where the inclusion follows from the identity $2\,\mathbf{x} = \sqrt{2}\left[\mathcal{R}(\frac{\pi}{4})\mathbf{x} + \mathcal{R}(-\frac{\pi}{4})\mathbf{x}\right]$. Therefore using the notation of Eq. (43), $A_1 \subset \widetilde{D}(\alpha_1, r_{B^\gamma})$ and similarly for A_3. The conclusion then follows from Eqs. (44) (see Fig. 6) and (46). □

Corollary 3.12. For a crystallographic group Γ in the isomorphism class $p4$, the collision probability for a body B is given by Eq. (46) (or (47) if B is convex) when

$$\mathrm{diam}(B) \le \frac{\sqrt{3}\,\delta}{2(1+\sqrt{2})}\,.$$

Proof. By Jung's theorem in $\mathbb{R}^2$, which states that $r_B \le \mathrm{diam}(B)/\sqrt{3}$. □

It follows that if Γ is a crystallographic group in the isomorphism class $p4$ and B is a disk of radius $r \le \frac{\sqrt{3}\,\delta}{4(1+\sqrt{2})}$, then

$$P_c(B) = \frac{6\,\pi\,r^2}{\delta^2}\,. \tag{48}$$

In Section 4.1, we give an explicit formula (using an elliptic integral) for the collision probability when B is an ellipse with major semi-axis length $\le \frac{\sqrt{3}\,\delta}{4(1+\sqrt{2})}$. This gives a lower and an upper bound for the collision probability of any body B of diameter $\le \frac{\sqrt{3}\,\delta}{2(1+\sqrt{2})}$ if r is the inradius and the circumradius, repectively, of B. (The upper bound holds for any value of the circumradius.)

Remark 3.13. In the above derivation, we replaced B by a translate contained in a disk about $\mathbf{0}$. However, formula (46) holds for B in any position. Indeed, if $C = B + \mathbf{t}$, then

$$\left[\mathcal{R}\left(\frac{\pi}{4}\right)C + \mathcal{R}\left(-\frac{\pi}{4}\right)C\right] \cup \frac{1}{\sqrt{2}}(C + C) = \left(\left[\mathcal{R}\left(\frac{\pi}{4}\right)B + \mathcal{R}\left(-\frac{\pi}{4}\right)B\right] \cup \frac{1}{\sqrt{2}}(B + B)\right) + \sqrt{2}\,\mathbf{t},$$

and thus translations (as well as rotations) of B leave the areas in Eq. (46) invariant.

Figure 7 shows three cases in which the circular collision zones intersect in pairs. In Figs. 7(a)–(b), the circular collision zones about α_1 and α_3 both intersect the circular collision zones about α_2 and α_4. When $r > \delta/4$, the circular collision zone about α_1 also intersects the circular collision zone about α_3, and finally in Fig. 7(c), the circular collision zones cover the entire crystallographic unit cell, so all configurations are unrealizable.[6]

[6] In Fig. 7(c), there are no triple intersections of the (open) circular collision zones, but the closures of the circular collision zones have eight triple intersection points: $(\frac{3-\sqrt{3}}{4}\delta,\ \frac{\sqrt{3}-1}{4}\delta)$,$(\frac{\sqrt{3}-1}{4}\delta,\ \frac{3-\sqrt{3}}{4}\delta)$, and their images under Γ.

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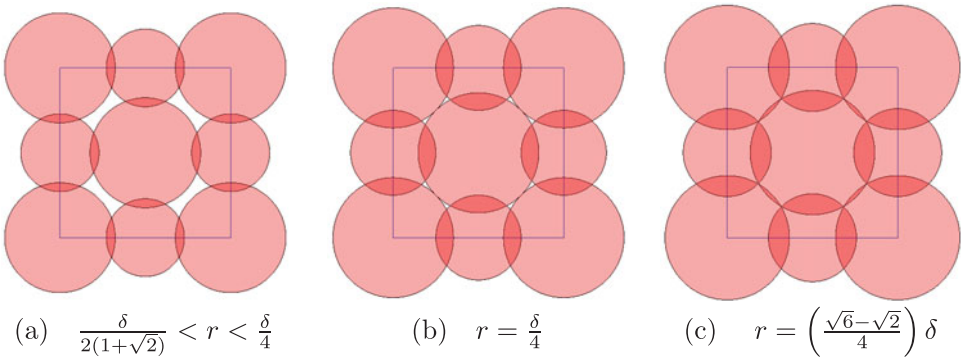


Fig. 7. Intersecting circular collision zones in the $p4$ case.

3.4. p6 symmetry

Finally, we consider crystallographic groups Γ in the $p6$ isomorphism class. As in the $p3$ case, we can assume without loss of generality that the lattice $\mathbb{L}$ is generated by $\mathbf{v}_1 = (\delta, 0)$, $\mathbf{v}_2 = (-\frac{1}{2}\delta, \frac{\sqrt{3}}{2}\delta)$. To simplify notation, we write $B_j = \mathcal{R}(j\pi/3)(g \cdot B)$, for $0 \le j \le 5$.

Figure 8 below, generated using the iphone app "Eschermobile",[13] shows several patterns with $p6$ symmetry. Figure 8(a) shows a pattern where the bodies are not in collision. There are three possible ways that $g \cdot B$ can collide with $R_\gamma(g \cdot B) + \mathbf{t}_\gamma$ with $R_\gamma \neq \mathbb{I}$:

- $g \cdot B = B_0$ collides with $B_3 + \mathbb{L}$, and by successively applying $\mathcal{R}(\pi/3)$, it follows that, B_1 collides with $B_4 + \mathbb{L}$, and B_2 collides with $B_5 + \mathbb{L}$. This case is illustrated in Fig. 8(b).
- B_0 collides with $B_2 + \mathbb{L}$, which collides with $B_4 + \mathbb{L}$, which in turn collides with $B_0 + \mathbb{L}$; also B_1 collides with $B_3 + \mathbb{L}$, which collides with $B_5 + \mathbb{L}$, which in turn collides with $B_1 + \mathbb{L}$. This case is illustrated in Fig. 8(c).
- B_0 collides with $B_1 + \mathbb{L}$, which collides with $B_2 + \mathbb{L}$ which collides with $B_3 + \mathbb{L}$, which collides with $B_4 + \mathbb{L}$, which collides with $B_5 + \mathbb{L}$, which in turn collides with $B_0 + \mathbb{L}$, as illustrated in Fig. 8(d).

Let $\omega = \mathcal{R}(\pi/3) \in \mathbb{P}$. Letting R_γ take the values ω, ω^2 and $\omega^3 = -\mathbb{I}$ in Eq. (19), we then have

$$\begin{aligned} p(S_R^*) &= S_1 \cup S_2 \cup S_3 \quad \text{for } R \in \mathrm{SO}(2) \setminus S_{\mathbb{L}}^\sharp, \\ S_1 &= p([\mathbb{I} - \omega]^{-1}\mathbb{L}) \boxplus p(B_R^\omega), \\ S_2 &= p([\mathbb{I} - \omega^2]^{-1}\mathbb{L}) \boxplus p(B_R^{\omega^2}), \\ S_3 &= p\left(\tfrac{1}{2}\,\mathbb{L}\right) \boxplus p\left[-\tfrac{1}{2}(B_R + B_R)\right]. \end{aligned}$$

Here, we used the fact from the $p2$ case that $B^{-\mathbb{I}} = -\frac{1}{2}(B + B)$.

Again from the $p2$ case, we have $p(\frac{1}{2}\mathbb{L}) = \{\beta_1, \beta_2, \beta_3, \beta_4\}$ where

$$\beta_1 = p(\mathbf{0}), \quad \beta_2 = p(\tfrac{1}{2}\delta, 0), \quad \beta_3 = p(-\tfrac{1}{4}\delta, \tfrac{\sqrt{3}}{4}\delta), \quad \beta_4 = p(\tfrac{1}{4}\delta, \tfrac{\sqrt{3}}{4}\delta). \tag{49}$$

Thus, we have

$$S_3 = p\left[-\tfrac{1}{2}(B_R + B_R)\right] \boxplus \{\beta_1, \beta_2, \beta_3, \beta_4\}. \tag{50}$$

To determine S_2, we note that $\omega^2 = \mathcal{R}(\eta)$, where $\eta = 2\pi/3$ as in Section 3.2. Thus by Eq. (37),[7]

$$B^{\omega^2} = \left[\mathcal{R}(2\pi/3) - \mathbb{I}\right]^{-1}\left[B + \mathcal{R}\left(-\frac{\pi}{3}\right)B\right] = \frac{1}{\sqrt{3}}\left[\mathcal{R}\left(\frac{7\pi}{6}\right)B + \mathcal{R}\left(\frac{5\pi}{6}\right)B\right]. \tag{51}$$

[7] Identifying $\mathbb{R}^2$ with $\mathbb{C}$, we have $B^{\omega^2} = \frac{2}{-3+\sqrt{3}i}(B + e^{-i\pi/3}B) = \frac{1}{\sqrt{3}}\,e^{i7\pi/6}(B + e^{-i\pi/3}B)$.

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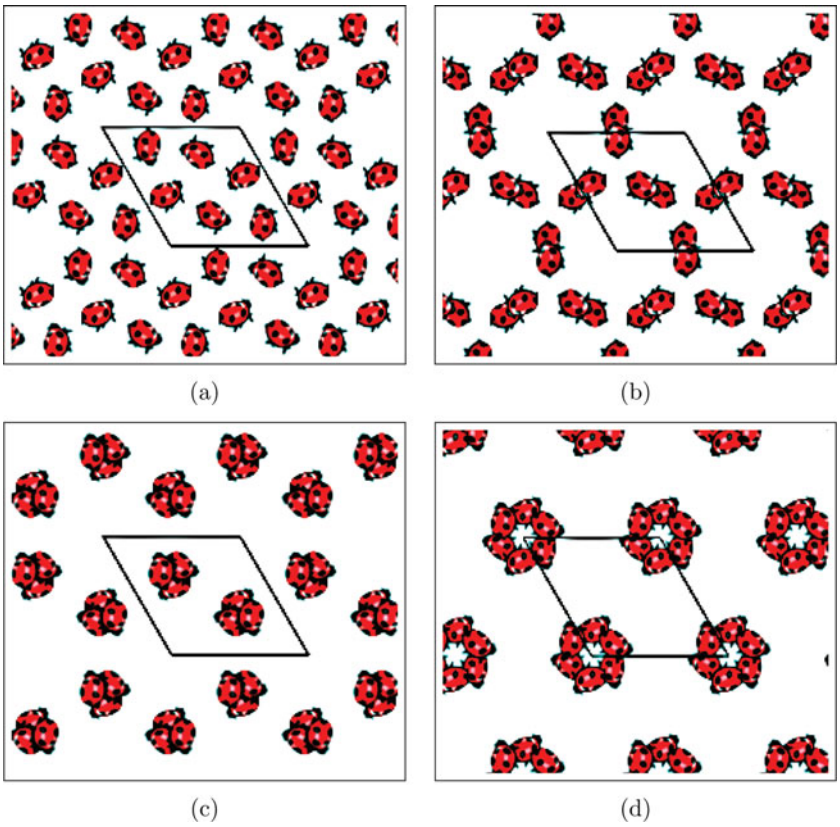


Fig. 8. Four configurations of solid bodies with $p6$ symmetry.

Recalling Eq . (33), we then have

$$S_2 = p\left\{\frac{1}{\sqrt{3}}\left[\mathcal{R}\left(\frac{7\pi}{6}\right)B_R + \mathcal{R}\left(\frac{5\pi}{6}\right)B_R\right]\right\} \boxplus \{p(\mathbf{0}), \beta_5, \beta_6\}, \tag{52}$$

where

$$\beta_5 = p(0, \tfrac{\sqrt{3}}{3}\delta), \quad \beta_6 = p(\tfrac{1}{2}\delta, \tfrac{\sqrt{3}}{6}\delta)\,. \tag{53}$$

The computation of S_1 is similar. We have $[\mathbb{I} - \omega]^{-1} = \mathcal{R}(\pi/3)$ and hence by Eq. (18),

$$B^{\omega} = [\mathbb{I} - \omega]^{-1}\left[\mathcal{R}\left(\frac{\pi}{3}\right)B + (-B)\right] = \mathcal{R}\left(\frac{2\pi}{3}\right)B + \mathcal{R}\left(\frac{4\pi}{3}\right)B\,. \tag{54}$$

We now notice that

$$[\mathbb{I} - \omega]^{-1}\mathbb{L} = \mathcal{R}(\pi/3)\,\mathbb{L} = \mathbb{L}\,.$$

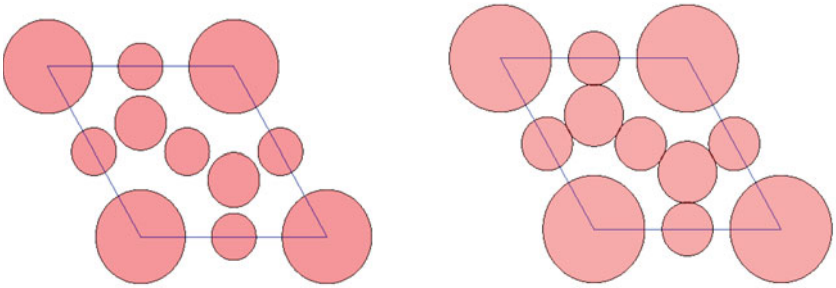
Therefore,

$$S_1 = p\left[\mathcal{R}\left(\frac{2\pi}{3}\right)B_R + \mathcal{R}\left(\frac{4\pi}{3}\right)B_R\right]. \tag{55}$$

Thus, we have the following description of the collision space:

Theorem 3.14. Let $\Gamma \subset \mathrm{SE}(2)$ be a crystallographic group in the isomorphism class $p6$ acting on a body $B \subset \mathbb{R}^2$, and suppose that $\mathbf{v}_1 = (\delta, 0)$, $\mathbf{v}_2 = (-\frac{1}{2}\,\delta, \frac{\sqrt{3}}{2}\,\delta)$ generate the Bravais lattice $\mathbb{L}$.

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(a) $r < \frac{\delta}{4+2\sqrt{3}}$ (b) $r = \frac{\delta}{4+2\sqrt{3}}$

Fig. 9. Disjoint circular collision zones in the $p6$ case.

Then,

$$p(S_R^*) = C_1 \cup (C_2 \boxplus \{\beta_5, \beta_6\}) \cup (C_3 \boxplus \{\beta_2, \beta_3, \beta_4\}) \quad \text{for } R \in \mathrm{SO}(2) \setminus S_{\mathbb{L}}^{\sharp},$$

where

- $C_1 \doteq p\left\{\left[\mathcal{R}\left(\frac{2\pi}{3}\right) B_R + \mathcal{R}\left(\frac{4\pi}{3}\right) B_R\right] \cup \frac{1}{\sqrt{3}}\left[\mathcal{R}\left(\frac{7\pi}{6}\right) B_R + \mathcal{R}\left(\frac{5\pi}{6}\right) B_R\right] \cup \left[-\frac{1}{2}(B_R + B_R)\right]\right\}$,
- $C_2 \doteq p\left\{\frac{1}{\sqrt{3}}\left[\mathcal{R}\left(\frac{7\pi}{6}\right) B_R + \mathcal{R}\left(\frac{5\pi}{6}\right) B_R\right]\right\}$,
- $C_3 \doteq p\left[-\frac{1}{2}(B_R + B_R)\right]$,

and $\beta_2, \ldots, \beta_6$ are given by Eqs. (49) and (53).

To find the probability of collision, we can assume that B is contained in a disk of radius r_B about the origin. We now assume that

$$r_B \leq \frac{\delta}{4 + 2\sqrt{3}}. \tag{56}$$

It then follows from Theorem 3.14 that $p(S_R^*)$ is contained in the union of six circular collision zones

$$\widetilde{D}(\beta_1, 2\, r_B) \cup \widetilde{D}(\beta_2, r_B) \cup \widetilde{D}(\beta_3, r_B) \cup \widetilde{D}(\beta_4, r_B) \cup \widetilde{D}\left(\beta_5, \frac{2}{\sqrt{3}} r_B\right) \cup \widetilde{D}\left(\beta_6, \frac{2}{\sqrt{3}} r_B\right)$$

in the torus $T\backslash\mathbb{R}^2$, for all rotations $R \in \mathrm{SO}(2)$. One can check that the bound (56) implies that these six circular collision zones are disjoint and therefore C_1, the two translates of C_2, and the three translates of C_3 are mutually disjoint subsets of the torus $T\backslash X$. (See Fig. 9.)

In this case,

$$V_2(\widetilde{S}_R^*) = [V_2(C_1) + 2\, V_2(C_2) + 3\, V_2(C_3)]\,, \tag{57}$$

which is independent of R. Therefore, we obtain

Theorem 3.15. For a crystallographic group Γ in the isomorphism class $p6$, the collision probability for a body B is given by

$$P_c(B) = \frac{2}{\sqrt{3}\,\delta^2}\left\{\frac{3}{4} V_2(B + B) + \frac{2}{3} V_2\left[\mathcal{R}\left(\frac{\pi}{6}\right) B + \mathcal{R}\left(-\frac{\pi}{6}\right) B\right] + V_2(C)\right\}, \tag{58}$$

when $r_B \leq \frac{\delta}{4+2\sqrt{3}}$, where

$$C = \frac{1}{2}\Big[B + B\Big] \cup \frac{1}{\sqrt{3}}\left[\mathcal{R}\left(\frac{\pi}{6}\right) B + \mathcal{R}\left(-\frac{\pi}{6}\right) B\right] \cup \left[\mathcal{R}\left(\frac{\pi}{3}\right) B + \mathcal{R}\left(-\frac{\pi}{3}\right) B\right]. \tag{59}$$

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Corollary 3.16. For a crystallographic group Γ in the isomorphism class $p6$, the collision probability for a convex body B is given by

$$P_c(B) = \frac{2}{\sqrt{3}\,\delta^2}\left\{3\,V_2(B) + \frac{2}{3}\,V_2\left[B + \mathcal{R}\left(\frac{\pi}{3}\right)B\right] + V_2\left[B + \mathcal{R}\left(\frac{2\pi}{3}\right)B\right]\right\}, \tag{60}$$

when $r_{[B+\mathcal{R}(\frac{\pi}{3})B]} + \sqrt{3}\,r_B \le \frac{\delta}{2}$, in particular when $r_B \le \frac{\delta}{4+2\sqrt{3}}$.

Proof. Since B is convex, $\frac{1}{2}(B+B) = B$. Since $\mathcal{R}\left(\frac{\pi}{6}\right)\mathbf{x} + \mathcal{R}\left(-\frac{\pi}{6}\right)\mathbf{x} = \sqrt{3}\,\mathbf{x}$, we then have

$$\tfrac{1}{2}(B+B) = B \subset \frac{1}{\sqrt{3}}\left[\mathcal{R}\left(\frac{\pi}{6}\right)B + \mathcal{R}\left(-\frac{\pi}{6}\right)B\right].$$

We furthermore claim that

$$\frac{1}{\sqrt{3}}\left[\mathcal{R}\left(\frac{\pi}{6}\right)B + \mathcal{R}\left(-\frac{\pi}{6}\right)B\right] \subset \left[\mathcal{R}\left(\frac{\pi}{3}\right)B + \mathcal{R}\left(-\frac{\pi}{3}\right)B\right], \tag{61}$$

for B convex. To verify Eq. (61), we let $\mathbf{x}, \mathbf{y} \in B$ be arbitrary and note that

$$\frac{1}{\sqrt{3}}\left[\mathcal{R}\left(\frac{\pi}{6}\right)\mathbf{x} + \mathcal{R}\left(-\frac{\pi}{6}\right)\mathbf{y}\right] = \mathcal{R}\left(\frac{\pi}{3}\right)\left(\frac{2}{3}\mathbf{x} + \frac{1}{3}\mathbf{y}\right) + \mathcal{R}\left(-\frac{\pi}{3}\right)\left(\frac{1}{3}\mathbf{x} + \frac{2}{3}\mathbf{y}\right).$$

Therefore, the set C in Eq. (59) is given by

$$C = \mathcal{R}\left(\frac{\pi}{3}\right)B + \mathcal{R}\left(-\frac{\pi}{3}\right)B, \tag{62}$$

when B is convex. Formula (60) follows from Eqs. (58) and (62). Sufficiency of the bound $r_{[B+\mathcal{R}(\frac{\pi}{3})B]} + \sqrt{3}\,r_B \le \frac{\delta}{2}$ is left to the reader. □

Remark 3.17. In Corollary 3.16, if we assume in addition that $B = -B$ (for example, if B is an ellipse), then we have

$$P_c(B) = \frac{2}{\sqrt{3}\,\delta^2}\left\{3\,V_2(B) + \frac{5}{3}\,V_2\left[B + \mathcal{R}\left(\frac{\pi}{3}\right)B\right]\right\}. \tag{63}$$

Corollary 3.18. For a crystallographic group Γ in the isomorphism class $p6$, the collision probability for a body B is given by Eqs. (58)–(59) when

$$\operatorname{diam}(B) \le \frac{\sqrt{3}\,\delta}{4+2\sqrt{3}}.$$

For example, if B is a disk of radius $r \le \frac{\delta}{4+2\sqrt{3}}$, then

$$P_c(B) = \frac{2\,\pi}{\sqrt{3}\,\delta^2}\left[3\,r^2 + \frac{2}{3}(4r^2) + 4\,r^2\right] = \frac{58\,\pi}{3\sqrt{3}}\,\frac{r^2}{\delta^2}.$$

Figure 10 shows four cases in which the circular collision zones intersect in pairs. Figure 10(c) illustrates all possible intersections in pairs, leaving little allowable room for the bodies to move. In Fig. 10(d), there are no triple intersections of the (open) circular collision zones, but the closures of the circular collision zones have 12 triple intersection points, and the closed circular collision zones cover the entire crystallographic unit cell, so essentially all configurations are unrealizable.

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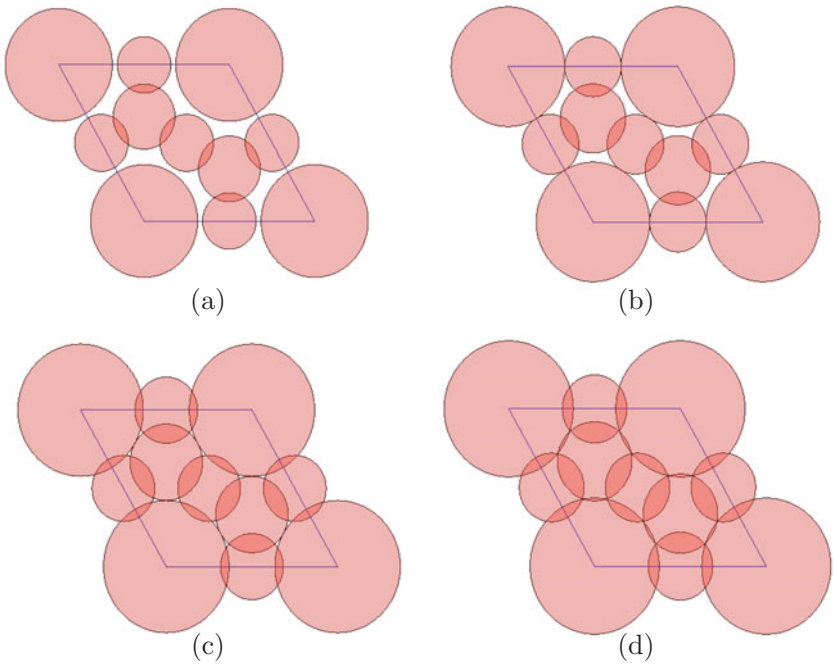


Fig. 10. Intersecting circular collision zones in the $p6$ case.

4. Demonstration with Elliptical Bodies

In this section, we evaluate the collision probabilities (29), (40), (46), (58) for elliptical bodies that are small enough so that the smallest open disks that enclose them have non-intersecting circular collision zones.

4.1. Parameterizing the collision-space boundary and computing volume for the case of ellipsoidal bodies

Suppose that E_1, E_2 are two solid ellipsoids centered at the origin in $\mathbb{R}^n$. We denote their semi-axis lengths by the row vectors $\mathbf{a}_1 = (a_1, \ldots, a_n)$, $\mathbf{a}_2 = (a'_1, \ldots, a'_n)$, respectively. Following the notation in ref. [20], we can represent the ellipsoids implicitly by

$$\{\mathbf{x} \in \mathbb{R}^n : \mathbf{x}^T A_i^{-2} \mathbf{x} \leq 1\},$$

where $A_i = A_i^T = R_i\, \Lambda(\mathbf{a}_i)\, R_i^T$ is an $n \times n$ real symmetric positive-definite matrix, with $R_i \in SO(n)$, for $i = 1, 2$. Here, $\Lambda(\mathbf{a}_i)$ denotes the diagonal matrix with $\Lambda_{kk}(\mathbf{a}_1) = a_k$, $\Lambda_{kk}(\mathbf{a}_2) = a'_k$. Let $\mathbf{x}_i(\mathbf{q}) = A_i \mathbf{u}(\mathbf{q})$ denote the parametric equations of the boundary ellipsoid ∂E_i, where $\mathbf{u}(\mathbf{q}) \in S^{n-1}$ is any parameterization of the unit $(n-1)$-sphere. The boundary of the Minkowski sum of E_1 and E_2, $\partial(E_1 + E_2)$, is given as in ref. [20] by first applying the transformation A_2^{-1}, which transforms E_2 to the unit ball B^n. Let $\widetilde{A}_1 = A_2^{-1} A_1$ and let $\widetilde{E}_1 = A_2^{-1} \cdot E_1 = \widetilde{A}_1 \cdot B^n$. Then, $\widetilde{E}_1 = \{\Phi(\mathbf{x}) \leq 1\}$, where

$$\Phi(\mathbf{x}) = \mathbf{x}^T (\widetilde{A}_1^{-1})^T \widetilde{A}_1^{-1} \mathbf{x} = \mathbf{x}^T A_2 A_1^{-2} A_2 \mathbf{x}\,. \tag{64}$$

It follows that $\partial(\widetilde{E}_1 + B^n)$ is given parametrically by

$$\widetilde{A}_1 \mathbf{u}(\mathbf{q}) + \frac{\nabla\Phi(\widetilde{A}_1 \mathbf{u}(\mathbf{q}))}{\|\nabla\Phi(\widetilde{A}_1 \mathbf{u}(\mathbf{q}))\|} = A_2^{-1} A_1 \mathbf{u}(\mathbf{q}) + \frac{A_2 A_1^{-1} \mathbf{u}(\mathbf{q})}{\|A_2 A_1^{-1} \mathbf{u}(\mathbf{q})\|}.$$

Therefore, $\partial(E_1 + E_2) = A_2 \cdot \partial(\widetilde{E}_1 + B^n)$ can be parameterized in closed form by

$$\mathbf{x}_{1\oplus 2}(\mathbf{q}) = A_1 \mathbf{u}(\mathbf{q}) + \frac{A_2^2 A_1^{-1} \mathbf{u}(\mathbf{q})}{\|A_2 A_1^{-1} \mathbf{u}(\mathbf{q})\|}\,. \tag{65}$$

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To find the n-dimensional volume of the domain $E_1 + E_2$ enclosed by this $(n-1)$-dimensional hypersurface, we again apply the transformation A_2^{-1}. We can then apply Steiner's formula to obtain

$$V_n(E_1 + E_2) = \det A_2 \cdot V_n(\widetilde{E}_1 + B^n) = \det A_2 \cdot \sum_{k=0}^{n} \binom{n}{k} W_k(\widetilde{E}_1)\,, \tag{66}$$

where W_k denotes the k^{th} *quermassintegral*.[16–18]

4.2. The planar case: Elliptical bodies

In the planar case (when $n = 2$), $W_2(\cdot) = \pi$, $2\,W_1(\cdot) = L(\cdot)$ (the perimeter), and

$$W_0(\widetilde{E}_1) = \ V_2(\widetilde{E}_1) = \pi \det A_1 / \det A_2\,.$$

Therefore,

$$V_2(E_1 + E_2) = \pi(\det A_1 + \det A_2) + \det A_2 \cdot L(\widetilde{E}_1)\,. \tag{67}$$

By Eq. (64), $\widetilde{E}_1$ is an ellipse with semi-axis lengths equal to the eigenvalues of the positive definite, symmetric matrix $\sqrt{A_2^{-1}A_1^2A_2^{-1}}$ (or equivalently, the square roots of the eigenvalues of $A_2^{-1}A_1^2A_2^{-1}$). Denote the eigenvalues of $\sqrt{A_2^{-1}A_1^2A_2^{-1}}$ by λ_1, λ_2, ordered so that $\lambda_1 \le \lambda_2$. Then, the perimeter is given by an elliptic integral

$$L(\widetilde{E}_1) = 4\,\lambda_2\,E(1,\epsilon) \doteq 4\,\lambda_2 \int_0^1 \left(\frac{1-\epsilon^2 t^2}{1-t^2}\right)^{1/2} dt,$$

where $\epsilon \doteq (1 - \lambda_1^2/\lambda_2^2)^{1/2}$ is the eccentricity of $\widetilde{E}_1$.

We give formulas below for the collision probabilities for an elliptical body B with semi-axis lengths $a \le b$. In the case of a crystal with $p2$ symmetry, Corollary 3.4 already gives us the formula

$$P_c(B) = \frac{4\,\pi\,a\,b}{V_2(F_{T\setminus X})}, \tag{68}$$

when $b \le \delta/4$.

Now we suppose that the crystal has $p4$ symmetry, and the major semi-axis $b \le \frac{\delta}{2(1+\sqrt{2})}$. Recalling Eq. (47), we apply the above with $E_1 = B$, $E_2 = \mathcal{R}(\frac{\pi}{2})B$. Then, we can take $A_i = \Lambda(\mathbf{a}_i)$, with $\mathbf{a}_1 = (a, b)$, $\mathbf{a}_2 = (b, a)$. Hence, $\sqrt{A_2^{-1}A_1^2A_2^{-1}}$ is a diagonal matrix with eigenvalues $\lambda_1 = a/b$, $\lambda_2 = b/a$, and the ellipse $\widetilde{E}_1$ has eccentricity $\epsilon = (1 - a^4/b^4)^{1/2}$. Therefore by Eq. (67),

$$V_2\left[\mathcal{R}\left(\frac{\pi}{4}\right)B + \mathcal{R}\left(-\frac{\pi}{4}\right)B\right] = V_2(E_1 + E_2) = 2\pi ab + ab \cdot 4\,\frac{b}{a}\,E\left(1,\ [1 - a^4/b^4]^{1/2}\right).$$

Corollary 3.11 then yields the collision probability for (sufficiently small) ellipses in a crystal with $p4$ symmetry:

$$P_c(B) = \frac{1}{\delta^2}\left\{4\pi ab + 4b^2\,E\left(1,\ [1 - a^4/b^4]^{1/2}\right)\right\}, \tag{69}$$

provided that

$$\frac{1}{\sqrt{2}} r_M + r_B \le \frac{\delta}{2}, \qquad M = \mathcal{R}\left(\frac{\pi}{4}\right)B + \mathcal{R}\left(-\frac{\pi}{4}\right)B\,.$$

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To compute the circumradius of the Minkowski sum M, suppose that the major axis of B is horizontal and parametrize the ellipse $\mathcal{R}(\frac{\pi}{4})(\partial B)$:

$$\mathbf{x}(\theta) = \begin{pmatrix} \frac{b}{\sqrt{2}}\,\cos(\theta) - \frac{a}{\sqrt{2}}\,\sin(\theta) \\ \frac{b}{\sqrt{2}}\,\cos(\theta) + \frac{a}{\sqrt{2}}\,\sin(\theta) \end{pmatrix}.$$

One can then show that

$$r_M = 2 \sup_\theta \left[\frac{b}{\sqrt{2}}\,\cos(\theta) - \frac{a}{\sqrt{2}}\,\sin(\theta) \right] = \sqrt{2\,a^2 + 2\,b^2}\,. \tag{70}$$

Therefore, Eq. (69) holds if $\sqrt{a^2+b^2} + b \le \delta/2$. Setting $a = b = r$, we also obtain the collision probability (48) for disks.

Next suppose that the crystal has $p3$ symmetry. Recalling Eq. (40), we need to compute $V_2(E_1 + E_2)$ with $E_1 = B$, $E_2 = \mathcal{R}(\frac{\pi}{3})B$. Hence, we take $A_1 = \Lambda(\mathbf{a}_1)$, with $\mathbf{a}_1 = (a, b)$, and $A_2 = \mathcal{R}(\frac{\pi}{3})\Lambda(\mathbf{a}_1)\mathcal{R}(-\frac{\pi}{3})$. Then,

$$\widetilde{A}_1 = A_2^{-1} A_1 = \begin{pmatrix} \dfrac{b+3a}{4b} & \sqrt{3}\,\dfrac{b-a}{4a} \\ \sqrt{3}\,\dfrac{b-a}{4b} & \dfrac{3b+a}{4a} \end{pmatrix}.$$

As above, we let $\lambda_1^2 \le \lambda_2^2$ denote the eigenvalues of $A_2^{-1} A_1^2 A_2^{-1}$. Then, $\lambda_1^2 = \frac{1}{2}(T - \sqrt{\Delta})$, $\lambda_2^2 = \frac{1}{2}(T + \sqrt{\Delta})$, where

$$T = \mathrm{Trace}(A_2^{-1} A_1^2 A_2^{-1}) = \sum_{j,k} \left[(\widetilde{A}_1)_{jk}\right]^2 = \frac{3\,a^4 + 2\,a^2 b^2 + 3\,b^4}{4\,a^2 b^2}, \tag{71}$$

$$\begin{aligned} \Delta &= T^2 - 4\,\det(A_2^{-1} A_1)^2 = T^2 - 4 \\ &= \frac{3}{16}\,\frac{\left(3\,a^2 + b^2\right)\left(a^2 + 3\,b^2\right)(a+b)^2\,(b-a)^2}{a^4\,b^4}\,. \end{aligned} \tag{72}$$

Then, the eccentricity of the ellipse $A_2^{-1} \cdot E_1$ is given by

$$\begin{aligned} \epsilon &= \frac{\sqrt{2}\,\Delta^{1/4}}{(T + \Delta^{1/2})^{1/2}} \\ &= \frac{\sqrt{2}\left[3(3a^2+b^2)(a^2+3b^2)\right]^{1/4}(b^2-a^2)^{1/2}}{\left\{3a^4 + 2a^2b^2 + 3b^4 + \left[3(3a^2+b^2)(a^2+3b^2)\right]^{1/2}(b^2-a^2)\right\}^{1/2}}\,. \end{aligned} \tag{73}$$

Therefore by Eq. (67),

$$V_2\left[B + \mathcal{R}(\frac{\pi}{3})B\right] = V_2(E_1 + E_2) = 2\pi\,a\,b + 2\sqrt{2}\,a\,b\,(T + \sqrt{\Delta})^{1/2}\,E(1,\epsilon), \tag{74}$$

where T, Δ, ϵ are given by Eqs. (71)–(73). Therefore, by Eq. (40) and Remark 3.7, the collision probability is given by

$$P_c(B) = \frac{4\,a\,b}{\sqrt{3}\,\delta^2}\left[\pi + \sqrt{2}\,\left(T + \sqrt{\Delta}\right)^{1/2} E(1,\epsilon)\right], \tag{75}$$

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Table I. Formulas for collision probabilities.

	Collision probability	
Symmetry	Ellipse with semi-axis lengths $a \le b$	Disk of radius r
$p2$	$\frac{4\pi a b}{V_2(F_{T\setminus X})}$ when $b \le \delta/4$	$\frac{4\pi r^2}{V_2(F_{T\setminus X})}$ when $r \le \delta/4$
$p3$	$\frac{2}{\sqrt{3}\,\delta^2}\left[2\pi a b + \sqrt{2}\,Q(a,b)E(1,\epsilon)\right]$ when $\sqrt{a^2+3b^2} \le \delta/2$	$\frac{8\pi}{\sqrt{3}}\frac{r^2}{\delta^2}$ when $r \le \delta/4$
$p4$	$\frac{1}{\delta^2}\left\{4\pi a b + 4b^2\,E\left(1,\,[1-a^4/b^4]^{1/2}\right)\right\}$ when $\sqrt{a^2+b^2}+b \le \delta/2$	$6\pi\,\frac{r^2}{\delta^2}$ when $r \le \frac{\delta}{2(1+\sqrt{2})}$
$p6$	$\frac{2}{3\sqrt{3}\,\delta^2}\left[19\pi a b + 5\sqrt{2}\,Q(a,b)E(1,\epsilon)\right]$ when $\sqrt{a^2+3b^2}+\sqrt{3}\,b \le \delta/2$	$\frac{58\pi}{3\sqrt{3}}\frac{r^2}{\delta^2}$ when $r \le \frac{\delta}{4+2\sqrt{3}}$

where $Q(a,b) = 2ab\,(T+\sqrt{\Delta})^{1/2}$
$= \left\{3a^4 + 2a^2b^2 + 3b^4 + \left[3(3a^2+b^2)(a^2+3b^2)\right]^{1/2}(b^2-a^2)\right\}^{1/2}$
and ϵ is given by Eq. (73).

provided that the circumradius of the Mikowski sum $\mathcal{R}(\frac{\pi}{6})B + \mathcal{R}(-\frac{\pi}{6})B$ is at most $\delta/2$. One can show by the argument in the $p4$ case above that this circumradius equals $\sqrt{a^2+3\,b^2}$, and hence Eq. (75) holds if $a^2+3\,b^2 \le \frac{\delta^2}{4}$.

Finally, we suppose that the crystal is in the isomorphism class $p6$. Then, Eqs. (63) and (74) yields the collision probability

$$P_c(B) = \frac{2\,a\,b}{3\sqrt{3}\,\delta^2}\left[19\pi + 10\sqrt{2}\left(T+\sqrt{\Delta}\right)^{1/2}E(1,\epsilon)\right], \tag{76}$$

provided that

$$r_{B+\mathcal{R}(\frac{\pi}{3})B} \;+\; \sqrt{3}\,r_B = \sqrt{a^2+3\,b^2}+\sqrt{3}\,b \le \frac{\delta}{2}\,.$$

For example, if we set $a = b = r$ in Eq. (76), we obtain the collision probability for a disk, $\frac{58\pi}{3\sqrt{3}}\frac{r^2}{\delta^2}$, computed in Section 3.4.

Table I summarizes the collision probabilities for elliptical bodies in 2D crystals. Note that the formulas in the second column of Table I remain valid when $a = 0$; i.e., when the body B is a line segment of length $2b$. (When $a = 0$, the collision probabilities can be obtained immediately from Eqs. (40), (47), and (60) since the Minkowski sum in the corresponding formula is a square of area $4b^2$ in the $p4$ case and a rhombus of area $2\sqrt{3}b^2$ in the $p3$ and $p6$ cases.)

4.3. Numerical demonstration

Here, we use the above table and *Maple 18* to give numerical collision probabilities for crystals in the isomorphism classes $p3$, $p4$, and $p6$ with the following bodies:

- disks,
- ellipses with $b = \frac{4}{3}\,a$,
- ellipses with $b = 2a$,
- ellipses with $b = 10a$,
- line segments of length $2b$ (degenerate ellipses with $a = 0$).

Numerical values for these collision probabilities are given in Table II.

The values of b/δ in Table II are the largest values such that the circular collision zones do not intersect when the bodies are disks. (Collision probabilities for $p2$ symmetry are not given here, since they depend on additional parameters and are easily computed using Eq. (68).) Table II shows that,

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Table II. Numerical values.

		Collision probabilities				
sym.	b/δ	$a = 0$ (line)	$a = \frac{1}{10}\,b$	$a = \frac{1}{2}\,b$	$a = \frac{3}{4}\,b$	$a = b$ (disk)
$p3$	0.2500	0.2500	0.2963	0.5175	0.6961	0.9069
$p4$	0.2071	0.1716	0.2255	0.4535	0.6190	0.8085
$p6$	0.1340	0.1197	0.1613	0.3454	0.4797	0.6294

even for the case of bodies with relatively small diameter, a significant fraction of the motion space need not be searched because it will place bodies in non-physical collision.

The edge cases where the bodies (proteins) are touching are the most interesting and relevant because protein crystals consist of tightly packed molecules. As the size of the bodies becomes smaller, so too do the collision zones. The smaller cases in the above tables can be made relevant by inscribing an ellipsoid inside of a protein, which will necessarily make the size of the collision zone smaller than for the true protein, for the sake of tractability using our analysis.

5. Conclusions

The subset of a motion space corresponding to collision-free motions of rigid models of macromolecular structures arranged with crystallographic symmetry has been analyzed. Methods from integral geometry in Euclidean space have been combined with new formulas specific to motion spaces to describe free space as well as to quantify the amount of free space of translations when a test molecule is oriented in a specific way. The two-dimensional case is analyzed in detail, as a prelude to implementation on real crystals in 3D. In the 3D case, the rotation matrix always has a unit eigenvalue, and as a result the collision zones become extruded/cylindrical versions of the planar collision zones described in detail here. In particular, when the bodies are small enough, simple formulas are given for computing the volume of C-space obstacles. The condition for these formulas to work is that the smallest open disks that can contain them must have corresponding non-intersecting circular collision zones in each fixed-orientation slice of C-space. We note as well that inscribing the largest disk inside of an arbitrary body can be used as a tool to easily characterize circular collision regions that need not be searched in C-space. An inscribed disk also provides a lower bound on the volume in C-space occupied by collision zones. By partitioning a motion space into feasible and infeasible regions, MR searches can be limited to only the feasible regions, the volume of which can be small in comparison to the volume of the whole motion space.

Of course, the ultimate goal is to sample from the collision-free region of C-space. There are several possible approaches to this that build on the results of this paper. First, since the collision-space boundaries are parameterized curves in the planar case (or surfaces in the 3D case), it is possible to parametrically define offset curves/surfaces from them and to restrict the parameter range so that we get complete coverage of the free space. Alternatively, from the circular case, we can construct minimal-area polygonal regions that cover the free space while overlapping minimally with the collision zones. The details of exactly how to do this efficiently in the 3D case represent challenging computational geometry questions that we plan to address in a follow-on paper.

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