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THE COINCIDENCE PROBLEM FOR SHIFTED LATTICES AND MULTILATTICES

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Abstract. A coincidence site lattice is a sublattice formed by the intersection of a lattice Γ in $\mathbb{R}^d$ with the image of Γ under a linear isometry. Such a linear isometry is referred to as a linear coincidence isometry of Γ. Here, we consider the more general case allowing any affine isometry. Consequently, general results on coincidence isometries of shifted copies of lattices, and of multilattices are obtained. In particular, we discuss the shifted square lattice and the diamond packing in detail.

1. Introduction and Outline

It was Friedel in 1911 who first recognized the usefulness of coincidence site lattices (CSLs) in describing and classifying grain boundaries of crystals [11]. Since then, CSLs have been an indispensable tool in the study of grain boundaries, twins, and interfaces [24, 6, 35]. This prompted various authors to examine the CSLs of cubic and hexagonal crystals [30, 17, 14, 18].

The advent of quasicrystals in 1984 triggered a renewed interest in CSLs. This is because experimental evidence showed that quasicrystals, like ordinary crystals, exhibit multiple grains, twin relationships, and coincidence quasilattices [34, 36]. This led to a more general and mathematical treatment of the coincidence problem for lattices in [1].

Various results are now known about the coincidences of lattices and modules in dimensions at most four. The coincidence problem for certain planar lattices and modules was solved in [28, 1] using factorization properties of cyclotomic integers. For lattices and modules in dimensions three and four, quaternions have proven to be an appropriate tool [1, 38, 4, 31, 39, 5, 2, 20, 21].

However, the mathematical treatment of the coincidence problem has been mostly restricted to linear coincidence isometries, whereas isometries containing a translational part are usually ignored. Nevertheless, general (affine) isometries are important in crystallography. Indeed, the situation where one shifts the two component crystals against each other was investigated in [12, 10] and references therein.

Even though the idea of introducing a shift after applying a linear coincidence isometry has already been dealt with in the physical literature, not much can be found in the mathematical literature where a systematic treatment of the subject is still missing. Initial steps in this general direction have actually been made in the appendix of [28]. There, the authors considered coincidence isometries about certain points that are not lattice or

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module points. For example, they determined the set of coincidence isometries about the center of a Delauney cell of the square lattice and calculated the corresponding indices.

In this paper, the notion of a CSL is extended to intersections of two lattices that are related by any isometry. Such intersections are referred to as affine coincidence site lattices (ACSLs), and the isometries that generate these intersections as affine coincidence isometries. Theorem 3.3 identifies the affine coincidence isometries of a lattice, while Equation (3.1) gives the resulting intersections.

The succeeding discussion covers a related and special case: the coincidence problem for shifted lattices. That is, after translating the lattice Γ by some vector x, and upon application of a linear isometry R to the shifted lattice $x+\Gamma$, its intersection with $x+\Gamma$ is considered. Theorem 4.3 asserts that the linear coincidence isometries of $x+\Gamma$ are precisely those coincidence isometries R of Γ that satisfy $Rx-x \in \Gamma+R\Gamma$. Moreover, the CSLs of the shifted lattice are merely translates of CSLs of the original lattice. Hence, no new values of coincidence indices are obtained by shifting the lattice, with some values disappearing or their multiplicity being changed.

Similar to the approach in [28, 1], an extensive analysis of the coincidences of a shifted square lattice in Section 5 is achieved by identifying the square lattice with the ring of Gaussian integers. The coincidence problem for a shifted square lattice is completely solved when the shift consists of an irrational component (Theorem 5.9). For the remaining case, that is, when the shift may be written as a quotient of two Gaussian integers that are relatively prime, one can compute for the set of coincidence rotations of the shifted square lattice using a divisibility condition involving the denominator of the shift (Lemma 5.11). In both instances, the set of coincidence rotations of a shifted square lattice forms a group. An example is given where the set of coincidence isometries of a shifted square lattice is not a group.

The latter part of this contribution is concerned with the coincidences of sets of points formed by the union of a lattice with a finite number of shifted copies of the lattice. Such sets are referred to as multilattices (see [27] and references therein). This idea should be useful for crystals having multiple atoms per primitive unit cell [13, 29]. Theorem 6.3 gives the solution of the coincidence problem for multilattices. Simply put, the linear coincidence isometries of a multilattice are exactly the coincidence isometries of the lattice that generates the multilattice - only the resulting intersections and corresponding indices may vary. This paves the way for the solution of the coincidence problem for the diamond packing given in Theorem 7.3.

2. Linear coincidences of lattices

We start with the basic definitions and some known results on linear coincidence isometries of lattices.

A discrete subset Γ of $\mathbb{R}^d$ is a *lattice* (of *rank* and *dimension* d) if it is the $\mathbb{Z}$-span of d linearly independent vectors $v_1, \ldots, v_d \in \mathbb{R}^d$ over $\mathbb{R}$. The set $\{v_1, \ldots, v_d\}$ is called a *basis* of Γ, and $\Gamma = \mathbb{Z}v_1 \oplus \cdots \oplus \mathbb{Z}v_d$. As a group, Γ is isomorphic to the free abelian group of rank d. Alternatively, one can characterize a lattice in $\mathbb{R}^d$ as a discrete co-compact subgroup of $\mathbb{R}^d$. A subset Γ' of Γ is a *sublattice* of Γ if Γ' is a subgroup of Γ of finite (group) index. Hence, Γ' is itself a lattice of the same rank and dimension as Γ. The index of Γ' in Γ may be interpreted geometrically – $[\Gamma : \Gamma']$ is the quotient of the volume of a fundamental domain of Γ' by the volume of a fundamental domain of Γ.

For a lattice Γ in $\mathbb{R}^d$, its *dual lattice* or *reciprocal lattice* Γ^* is defined by

$$\Gamma^* := \left\{ x \in \mathbb{R}^d : \langle x, y \rangle \in \mathbb{Z} \text{ for all } y \in \Gamma \right\},$$

where $\langle \cdot, \cdot \rangle$ denotes the standard scalar product in $\mathbb{R}^d$. Given a sublattice Γ' of Γ, Γ^* is a sublattice of $(\Gamma')^*$ with $[(\Gamma')^* : \Gamma^*] = [\Gamma : \Gamma']$ and $(\Gamma')^*/\Gamma^* \cong \Gamma/\Gamma'$ [1, Lemma 2.3].

Two lattices Γ_1 and Γ_2 are said to be *commensurate*, denoted $\Gamma_1 \sim \Gamma_2$, if $\Gamma_1 \cap \Gamma_2$ is a sublattice of both Γ_1 and Γ_2. Commensurateness between lattices defines an equivalence relation [1, Proposition 2.1]. Given two commensurate lattices Γ_1 and Γ_2, their *sum* $\Gamma_1 + \Gamma_2 := \{x_1 + x_2 : x_1 \in \Gamma_1, x_2 \in \Gamma_2\}$ is also a lattice. In fact, the following equations hold: $(\Gamma_1 \cap \Gamma_2)^* = \Gamma_1^* + \Gamma_2^*$ and $(\Gamma_1 + \Gamma_2)^* = \Gamma_1^* \cap \Gamma_2^*$ [1, Proposition 2.2].

An orthogonal transformation $R \in O(d) := O(d, \mathbb{R})$ is a *linear coincidence isometry* of the lattice Γ in $\mathbb{R}^d$ if $\Gamma \sim R\Gamma$. The sublattice $\Gamma(R) := \Gamma \cap R\Gamma$ is called the *coincidence site lattice* (CSL) of Γ generated by R, while the index of $\Gamma(R)$ in Γ, $\Sigma_\Gamma(R) := [\Gamma : \Gamma(R)] = [R\Gamma : \Gamma(R)]$, is referred to as the *coincidence index of R with respect to Γ*. If no confusion arises, we simply write $\Sigma(R)$ to denote the coincidence index of R. Clearly, symmetries in the point group of Γ, $P(\Gamma) = \{R \in O(d) : R\Gamma = \Gamma\}$, are precisely those linear coincidence isometries R of Γ with $\Sigma(R) = 1$.

The set of linear coincidence isometries of a lattice Γ in $\mathbb{R}^d$ is denoted by $OC(\Gamma)$ while the set of coincidence rotations of Γ, that is, $OC(\Gamma) \cap SO(d)$, is written as $SOC(\Gamma)$. Since commensurateness of lattices is an equivalence relation, the set $OC(\Gamma)$ forms a group having $SOC(\Gamma)$ as a subgroup [1, Theorem 2.1].

3. Affine coincidences of lattices

Let Γ be a lattice in $\mathbb{R}^d$. A subset of Γ will be called a *cosublattice of* Γ if it is a coset $\ell + \Gamma'$ of some sublattice Γ' of Γ. The *index of a cosublattice $\ell + \Gamma'$ of Γ*, denoted by $[\Gamma : \ell + \Gamma']$, is defined as the index of the sublattice Γ' in Γ. This definition of index makes sense geometrically: a translation does not change the volume of the fundamental domains of Γ and Γ'.

Denote by $E(d)$ the group of isometries of $\mathbb{R}^d$. An element of $E(d)$ shall be written as (v, R), where $(v, R) : x \mapsto v + R(x)$, with $R \in O(d)$ (the linear part of f) and $v \in \mathbb{R}^d$ (the translational part of f). The definition below generalizes the concept of a linear coincidence isometry to an affine coincidence isometry.

Definition 3.1. Let Γ be a lattice in $\mathbb{R}^d$ and $(v, R) \in E(d)$. Then (v, R) is an *affine coincidence isometry* of Γ if $\Gamma \cap (v, R)\Gamma$ contains a cosublattice of Γ.

The set of affine coincidence isometries of Γ shall be denoted by $AC(\Gamma)$. It is easy to see that $AC(\Gamma)$ contains the group $OC(\Gamma) = AC(\Gamma) \cap O(d) = \{(v, R) \in AC(\Gamma) : v = 0\}$.

The following lemma describes the intersection of two lattices that are related by some isometry.

Lemma 3.2. *Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice and $(v, R) \in E(d)$. If $v \in \ell + R\Gamma$ for some $\ell \in \Gamma$, then $\Gamma \cap (v, R)\Gamma = \ell + (\Gamma \cap R\Gamma)$.*

Proof. Since $v \in \ell + R\Gamma$, we have $(v, R)\Gamma = (\ell, R)\Gamma$. It remains to show that $\Gamma \cap (\ell, R)\Gamma = \ell + (\Gamma \cap R\Gamma)$. Take $x \in \Gamma \cap (\ell, R)\Gamma$ and write $x = \ell + R\ell'$ for some $\ell' \in \Gamma$. Then $x \in \ell + (\Gamma \cap R\Gamma)$ because $R\ell' = x - \ell \in \Gamma \cap R\Gamma$. The opposite inclusion is clear. □

Lemma 3.2 brings about the following characterization of an affine coincidence isometry of a lattice.

Theorem 3.3. *Let Γ be a lattice in $\mathbb{R}^d$. Then $(v,R) \in E(d)$ is an affine coincidence isometry of Γ if and only if $R \in OC(\Gamma)$ and $v \in \Gamma + R\Gamma$.*

Proof. It follows from Lemma 3.2 that if $R \in OC(\Gamma)$ and $v \in \Gamma + R\Gamma$ then $\Gamma \cap (v,R)\Gamma$ is a coset of $\Gamma(R)$. Hence, $(v,R) \in E(d)$ is an affine coincidence isometry of Γ.

In the other direction, let $(v,R) \in AC(\Gamma)$. Because $\Gamma \cap (v,R)\Gamma \neq \varnothing$, there exist $\ell, \ell' \in \Gamma$ with $\ell = v + R\ell'$, and so $v = \ell - R\ell' \in \Gamma + R\Gamma$. By Lemma 3.2, one obtains $[\Gamma : \Gamma \cap R\Gamma] = [\Gamma : \ell + (\Gamma \cap R\Gamma)] = [\Gamma : \Gamma \cap (v,R)\Gamma] < \infty$. This implies that $\Gamma \sim R\Gamma$ and $R \in OC(\Gamma)$. □

Therefore, the set of affine coincidence isometries of Γ is given by

$$AC(\Gamma) = \{(v,R) \in E(d) : R \in OC(\Gamma) \text{ and } v \in \Gamma + R\Gamma\}.$$

Moreover, if $(v,R) \in AC(\Gamma)$ with $v \in \ell + R\Gamma$ for some $\ell \in \Gamma$, then

$$\Gamma \cap (v,R)\Gamma = \ell + \Gamma(R) \tag{3.1}$$

by Lemma 3.2. Thus, $\Gamma \cap (v,R)\Gamma$ is a coset of $\Gamma(R)$. This means that the intersection $\Gamma \cap (v,R)\Gamma$ does not only contain a cosublattice of Γ but is in fact a cosublattice of Γ. For this reason, we shall refer to $\Gamma \cap (v,R)\Gamma$ as an *affine coincidence site lattice* (ACSL) of Γ. In addition, each $R \in OC(\Gamma)$ corresponds to $\Sigma(R)$ distinct possible ACSLs.

Remark 3.4. Another lattice of interest in the study of grain boundaries is the *displacement shift complete* (DSC) *lattice*. It is the lattice formed by all possible displacement vectors that preserve the structure of the grain boundary. In this setting, given a linear coincidence isometry R of the lattice Γ, the corresponding DSC lattice is $\{v : (v,R) \in AC(\Gamma)\} = \Gamma + R\Gamma$ by Theorem 3.3. This conclusion is in agreement with the main result of [15], which states that the DSC lattice generated by R is the dual lattice of the CSL of Γ^* obtained from R, that is, $(\Gamma^* \cap R\Gamma^*)^* = \Gamma + R\Gamma$.

Now, the identity isometry $\mathbb{1}_d \in AC(\Gamma)$ for any lattice Γ in $\mathbb{R}^d$. In addition, it follows from Theorem 3.3 that the inverse of every isometry in $AC(\Gamma)$ is also in $AC(\Gamma)$. However, the product of two affine coincidence isometries of Γ may or may not be an element of $AC(\Gamma)$. Thus, the set $AC(\Gamma)$ does not always form a group. The next proposition tells us exactly when $AC(\Gamma)$ is a group.

Proposition 3.5. *Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice. Then $AC(\Gamma)$ is a group if and only if it is the symmetry group G of Γ.*

Proof. Suppose $AC(\Gamma)$ is a group and take $(v,R) \in AC(\Gamma)$. By Theorem 3.3, $R^{-1} \in OC(\Gamma) \subseteq AC(\Gamma)$. Thus, the product $(v,R)(0,R^{-1}) = (v,\mathbb{1}_d) \in AC(\Gamma)$. It follows then from Theorem 3.3 that $v \in \Gamma$. Furthermore, $\Gamma + R\Gamma = \Gamma$ and hence, $R \in P(\Gamma)$. Since G is symmorphic, that is, G is the semidirect product of $P(\Gamma)$ with its translation subgroup $T(G) = \Gamma$, one obtains $(v,R) \in G$. □

4. Linear coincidences of shifted lattices

We now turn our attention to shifted copies $x + \Gamma$ of a lattice Γ in $\mathbb{R}^d$ obtained by translating all the points of Γ by the vector $x \in \mathbb{R}^d$. By a *cosublattice of the shifted lattice* $x + \Gamma$, we mean a subset of $x + \Gamma$ of the form $x + (\ell + \Gamma')$ where $\ell + \Gamma'$ is a cosublattice of Γ. In addition, the *index of the cosublattice* $x + (\ell + \Gamma')$ *in* $x + \Gamma$ is understood to be $[x + \Gamma : x + (\ell + \Gamma')] := [\Gamma : \Gamma']$. There is no ambiguity here - relabeling x as the origin gives back the original lattice Γ and cosublattice $\ell + \Gamma'$. Of particular interest in this section are intersections of the form $(x + \Gamma) \cap R(x + \Gamma)$, where $R \in O(d)$.

Definition 4.1. Let Γ be a lattice in $\mathbb{R}^d$ and $x \in \mathbb{R}^d$. An $R \in O(d)$ is said to be a *linear coincidence isometry of the shifted lattice* $x+\Gamma$ if $(x+\Gamma) \cap R(x+\Gamma)$ is a cosublattice of $x+\Gamma$.

The intersection $(x+\Gamma) \cap R(x+\Gamma)$ will also be referred to as a *CSL of the shifted lattice* $x+\Gamma$. The *coincidence index of* R *with respect to* $x+\Gamma$ is taken to be $\Sigma_{x+\Gamma}(R) := [x+\Gamma : (x+\Gamma) \cap R(x+\Gamma)]$. The set of all linear coincidence isometries of $x+\Gamma$ shall be denoted by $OC(x+\Gamma)$. Likewise, we take $SOC(x+\Gamma) := OC(x+\Gamma) \cap SO(d)$.

Remark 4.2. Observe that applying a linear isometry R on the shifted lattice $x+\Gamma$ is equivalent to applying the same isometry R but with center at $-x$ on the original lattice Γ. Hence, just as $OC(\Gamma)$ is an extension of $P(\Gamma)$, one may interpret $OC(x+\Gamma)$ as a generalization of the stabilizer of the point $-x$.

The following theorem characterizes a linear coincidence isometry R of a shifted lattice $x+\Gamma$ and identifies the CSL of $x+\Gamma$ generated by R. The result lies on the fact that taking the intersection of $x+\Gamma$ and $R(x+\Gamma)$ corresponds to a shift of the intersection of Γ and $(Rx-x, R)\Gamma$ by x. It is a special case of Lemma 6.1 which will be stated and proved in Section 6.

Theorem 4.3. *Let* Γ *be a lattice in* $\mathbb{R}^d$ *and* $x \in \mathbb{R}^d$. *Then*

$$OC(x+\Gamma) = \{R \in OC(\Gamma) : Rx - x \in \Gamma + R\Gamma\}.$$

In addition, if $R \in OC(x+\Gamma)$ *with* $Rx - x \in \ell + R\Gamma$ *for some* $\ell \in \Gamma$, *then*

$$(x+\Gamma) \cap R(x+\Gamma) = (x+\ell) + \Gamma(R). \tag{4.1}$$

Equation (4.1) indicates that the CSL of the shifted lattice $x+\Gamma$ generated by $R \in OC(x+\Gamma)$ is obtained by translating some coset of $\Gamma(R)$ in Γ by x. Consequently,

$$\Sigma_{x+\Gamma}(R) = \Sigma_\Gamma(R) \tag{4.2}$$

for all $R \in OC(x+\Gamma)$. This means that shifting a lattice does not yield any new values of coincidence indices.

Let $S \in P(\Gamma)$. If $R \in OC(\Gamma)$ then $RS \in OC(\Gamma)$ and the CSLs generated by R and RS are the same, that is, $\Gamma(RS) = \Gamma(R)$. The corresponding statement for linear coincidence isometries of shifted lattices reads as follows. It will prove to be useful when counting the number of CSLs of a shifted lattice for a given index.

Proposition 4.4. *Let* $x+\Gamma \subseteq \mathbb{R}^d$ *be a shifted lattice,* $S \in P(\Gamma)$, *and suppose that* $R, RS \in OC(x+\Gamma)$. *Then* $(x+\Gamma) \cap RS(x+\Gamma) = (x+\Gamma) \cap R(x+\Gamma)$ *if and only if* $S \in OC(x+\Gamma)$. *In particular, if* $OC(x+\Gamma)$ *forms a group, then* $(x+\Gamma) \cap RS(x+\Gamma) = (x+\Gamma) \cap R(x+\Gamma)$.

Proof. It follows from Theorem 4.3 that $Rx - x \in \ell_1 + R\Gamma$ and $RSx - x \in \ell_2 + R\Gamma$ for some $\ell_1, \ell_2 \in \Gamma$. Equation (4.1) yields that $(x+\Gamma) \cap RS(x+\Gamma) = (x+\Gamma) \cap R(x+\Gamma)$ if and only if $\ell_2 - \ell_1 \in R\Gamma$. However, $R(Sx-x) = RSx - Rx \in (\ell_2 - \ell_1) + R\Gamma$. This implies that $\ell_2 - \ell_1 \in R\Gamma$ if and only if $Sx - x \in \Gamma$. Applying Theorem 4.3 proves the claim. □

Note that for an $S \in P(\Gamma)$, the condition $S \in OC(x+\Gamma)$ in Proposition 4.4 is equivalent to saying that S is an element of the stabilizer of $-x$ (see Remark 4.2).

Proposition 4.5. *Let* $\Gamma \subseteq \mathbb{R}^d$ *be a lattice and* $x \in \mathbb{R}^d$. *If* $S \in P(\Gamma)$ *then*

$$OC(Sx+\Gamma) = S[OC(x+\Gamma)]S^{-1}.$$

Proof. This is a consequence of Theorem 4.3 because $SRS^{-1}(Sx) - Sx \in \Gamma + SRS^{-1}\Gamma$ if and only if $Rx - x \in \Gamma + R\Gamma$ for all $R \in OC(\Gamma)$. □

For a given lattice $\Gamma \subseteq \mathbb{R}^d$, it is enough to consider values of x in a fundamental domain of Γ to compute for all the different possible sets $OC(x+\Gamma)$. Proposition 4.5 asserts even more: it suffices to look at values of x in a fundamental domain of the symmetry group of Γ.

Furthermore, the following inclusion property follows immediately from Theorem 4.3.

Lemma 4.6. *If Γ is a lattice in $\mathbb{R}^d$ and $x, y \in \mathbb{R}^d$, then for all $a, b \in \mathbb{Z}$,*

$$OC(x+\Gamma) \cap OC(y+\Gamma) \subseteq OC[(ax+by)+\Gamma].$$

Corollary 4.7. *Let Γ be a lattice in $\mathbb{R}^d$ and $x = \frac{1}{n}\ell$, where $\ell \in \Gamma$ and $n \in \mathbb{N}$. If $a \in \mathbb{Z}$ with a and n relatively prime, then $OC(ax+\Gamma) = OC(x+\Gamma)$.*

Proof. The inclusion $OC(x+\Gamma) \subseteq OC(ax+\Gamma)$ follows directly from Lemma 4.6. Since a is relatively prime to n, there exist integers b and c such that $ab + nc = 1$. Applying again Lemma 4.6 yields $OC(ax+\Gamma) \subseteq OC[(ab+nc)\frac{1}{n}\ell + \Gamma] = OC(x+\Gamma)$. □

The next proposition compares the sets of linear coincidence isometries of shifts of similar lattices and is the analogue of Lemma 2.5 in [1] for shifted lattices.

Proposition 4.8. *Let Γ be a lattice in $\mathbb{R}^d$ and $x \in \mathbb{R}^d$.*

(i) *If $\lambda \in \mathbb{R}^+$ then $OC(\lambda x + \lambda\Gamma) = OC(x+\Gamma)$ with $\Sigma_{\lambda x+\lambda\Gamma}(R) = \Sigma_\Gamma(R)$ for all $R \in OC(\lambda x + \lambda\Gamma)$.*

(ii) *If $S \in O(d)$ then $OC(Sx+S\Gamma) = S[OC(x+\Gamma)]S^{-1}$ with $\Sigma_{Sx+S\Gamma}(R) = \Sigma_\Gamma(S^{-1}RS)$ for all $R \in OC(Sx+S\Gamma)$.*

Proof. Both statements follow from Theorem 4.3 and Equation (4.2). □

Now, it is evident from Theorem 4.3 that $OC(x+\Gamma)$ is a subset of $OC(\Gamma)$. The set $OC(x+\Gamma)$ is certainly nonempty because it contains the identity isometry. It also follows from Theorem 4.3 that $OC(x+\Gamma)$ is closed under inverses, that is, $R^{-1} \in OC(x+\Gamma)$ whenever $R \in OC(x+\Gamma)$. However, given R_1, $R_2 \in OC(x+\Gamma)$, the product R_2R_1 is not necessarily in $OC(x+\Gamma)$. Thus, one obtains the following result.

Proposition 4.9. *For a given lattice $\Gamma \subseteq \mathbb{R}^d$ and $x \in \mathbb{R}^d$, the set $OC(x+\Gamma)$ is a group if and only if it is closed under composition.*

We shall see in Example 5.25 an instance when $OC(x+\Gamma)$ fails to form a group. In any case, the product of two linear coincidence isometries of $x+\Gamma$ whose coincidence indices are relatively prime turns out to be again a linear coincidence isometry of $x+\Gamma$. This result is stated in the next proposition.

Proposition 4.10. *Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice and $x \in \mathbb{R}^d$. If $R_1, R_2 \in OC(x+\Gamma)$ with $\Sigma(R_1)$ and $\Sigma(R_2)$ relatively prime, then $R_2R_1 \in OC(x+\Gamma)$.*

Proof. From Theorem 4.3, $R_j \in OC(\Gamma)$ and $R_jx - x \in \Gamma + R_j\Gamma$ for $j \in \{1,2\}$. Thus, the product $R_2R_1 \in OC(\Gamma)$. In addition,

$$R_2R_1x - x = (R_2R_1x - R_2x) + (R_2x - x) \in \Gamma + R_2\Gamma + R_2R_1\Gamma.$$

However, $R_2\Gamma = \Gamma(R_2) + R_2\Gamma(R_1)$ because $\Sigma(R_1)$ and $\Sigma(R_2)$ are relatively prime (see [40, Figure 2]). Since $\Gamma(R_2) \subseteq \Gamma$ and $R_2\Gamma(R_1) \subseteq R_2R_1\Gamma$, $R_2R_1x - x \in \Gamma + R_2R_1\Gamma$. The claim now follows from Theorem 4.3. □

5. Linear coincidences of a shifted square lattice

This entire section is devoted to the solution of the coincidence problem for a shifted square lattice. Some of the results here can be found in [26].

5.1. **Solution of the coincidence problem for the square lattice.** Let us recall first the coincidences of the square lattice $\mathbb{Z}^2$ (see [1, 28] for details). Since $O(2)$ is the semidirect product of $SO(2)$ and the cyclic group C_2 generated by the reflection in the x-axis, we restrict our discussion to coincidence rotations at the outset and later on extend it to include coincidence reflections.

The group of coincidence rotations of $\mathbb{Z}^2$ is $SOC(\mathbb{Z}^2) = SO(2,\mathbb{Q})$. To determine the structure of this group, the square lattice is identified with the ring of Gaussian integers $\Gamma = \mathbb{Z}[i] = \{m + ni : m, n \in \mathbb{Z}, i^2 = -1\}$ embedded in $\mathbb{C}$. It can be shown that every coincidence rotation in $SOC(\Gamma)$ by an angle of θ in the counterclockwise direction corresponds to multiplication by the complex number $e^{i\theta} = \varepsilon\frac{z}{\overline{z}}$ on the unit circle, where $\varepsilon \in \{\pm 1, \pm i\}$ is a unit in $\mathbb{Z}[i]$ and z is a Gaussian integer with z relatively prime to $\overline{z}$. Since the ring $\mathbb{Z}[i]$ is a Euclidean domain and thus a unique factorization domain, z can be uniquely factored into powers of primes. Hence, a coincidence rotation R of Γ is equivalent to multiplication by the complex number

$$\varepsilon \cdot \prod_{p\equiv 1(4)} \left(\frac{\omega_p}{\overline{\omega_p}}\right)^{n_p}, \tag{5.1}$$

where $n_p \in \mathbb{Z}$ and only a finite number of $n_p \neq 0$, p runs over all rational primes $p \equiv 1 \pmod 4$ (called splitting primes in $\mathbb{Z}[i]$), and ω_p, and its complex conjugate $\overline{\omega_p}$, are the Gaussian prime factors of $p = \omega_p \cdot \overline{\omega_p}$. Then z reads

$$z = \prod_{\substack{p\equiv 1(4)\\ n_p>0}} {\omega_p}^{n_p} \cdot \prod_{\substack{p\equiv 1(4)\\ n_p<0}} \left(\overline{\omega_p}\right)^{-n_p}, \tag{5.2}$$

and the coincidence index of R is equal to the number theoretic norm of z, $\Sigma(R) = N(z) := z \cdot \overline{z} = |z|^2$. In addition, the CSL obtained from R is the principal ideal $\Gamma(R) = (z) := z\mathbb{Z}[i]$. Consequently, the group of coincidence rotations of the square lattice is given by $SOC(\mathbb{Z}^2) = SO(2,\mathbb{Q}) \cong C_4 \times \mathbb{Z}^{(\aleph_0)}$, where C_4 is the cyclic group of order 4 generated by i, and $\mathbb{Z}^{(\aleph_0)}$ is the direct sum of countably many infinite cyclic groups each of which is generated by $\frac{\omega_p}{\overline{\omega_p}}$.

Every coincidence reflection T of $\mathbb{Z}^2$ can be written as $T = R \cdot T_r$, where $R \in SOC(\Gamma)$ and T_r is the reflection along the real axis (corresponding to complex conjugation). Since T_r leaves Γ invariant, $\Sigma(T) = \Sigma(R)$ and $\Gamma(T) = \Gamma(R)$. Finally, one obtains that $OC(\mathbb{Z}^2) = O(2,\mathbb{Q}) = SOC(\mathbb{Z}^2) \rtimes \langle T_r \rangle$ (where $\rtimes$ stands for semidirect product).

The coincidence indices and the number of CSLs of $\mathbb{Z}^2$ for a given index m are described by means of a generating function. If $f_{\mathbb{Z}^2}(m)$ denotes the number of CSLs of $\mathbb{Z}^2$ of index m, then $f_{\mathbb{Z}^2}$ is *multiplicative* (that is, $f_{\mathbb{Z}^2}(1) = 1$ and $f_{\mathbb{Z}^2}(mn) = f_{\mathbb{Z}^2}(m) f_{\mathbb{Z}^2}(n)$ whenever m and n are relatively prime), and for primes p and $r \in \mathbb{N}$,

$$f_{\mathbb{Z}^2}(p^r) = \begin{cases} 2, & \text{if } p \equiv 1 \pmod 4 \\ 0, & \text{otherwise.} \end{cases}$$

The generating function for $f_{\mathbb{Z}^2}$ as a Dirichlet series $\Phi_{\mathbb{Z}^2}(s)$ is given by

$$\begin{aligned}\Phi_{\mathbb{Z}^2}(s) &= \sum_{m=1}^{\infty} \frac{f_{\mathbb{Z}^2}(m)}{m^s} = \prod_{p\equiv 1(4)} \frac{1+p^{-s}}{1-p^{-s}} = \frac{1}{1+2^{-s}} \cdot \frac{\zeta_{\mathbb{Q}(i)}(s)}{\zeta(2s)} \\ &= 1 + \tfrac{2}{5^s} + \tfrac{2}{13^s} + \tfrac{2}{17^s} + \tfrac{2}{25^s} + \tfrac{2}{29^s} + \tfrac{2}{37^s} + \tfrac{2}{41^s} + \tfrac{2}{53^s} + \tfrac{2}{61^s} + \tfrac{4}{65^s} + \tfrac{2}{73^s} + \cdots,\end{aligned} \tag{5.3}$$

where $\zeta_{\mathbb{Q}(i)}(s)$ is the Dedekind zeta function of the quadratic field $\mathbb{Q}(i)$ and $\zeta(s) = \zeta_{\mathbb{Q}}(s)$ is Riemann's zeta function (see [7, 37]). Observe from (5.3) that the coincidence indices of the square lattice are positive integers all of whose prime factors are splitting primes in $\mathbb{Z}[i]$. As the rightmost pole of $\Phi_{\mathbb{Z}^2}(s)$ is located at $s = 1$, we can infer from Delange's theorem (see for instance, [3, Theorem 5 of Appendix]) that the summatory function $\sum_{m\le N} f_{\mathbb{Z}^2}(m)$ grows asymptotically as $\frac{N}{\pi}$. In other words, the number of CSLs of $\mathbb{Z}^2$ of index at most N is asymptotically given by $\frac{N}{\pi}$.

The number of coincidence rotations of $\mathbb{Z}^2$ for a given index m is given by $\hat{f}_{\mathbb{Z}^2}(m) = 4f_{\mathbb{Z}^2}(m)$, where the factor 4 stems from the fact that $\mathbb{Z}^2$ has four symmetry rotations. Consequently, the Dirichlet series generating function for $\hat{f}_{\mathbb{Z}^2}$ is $4\Phi_{\mathbb{Z}^2}(s)$.

Remark 5.1. Observe from the complex number in (5.1) and Equation (5.2) that each coincidence rotation R of $\Gamma = \mathbb{Z}^2$ can be associated to a numerator z and unit ε, and this shall be written as $R_{z,\varepsilon}$. Note however that this correspondence is not unique: one can take any associate of z as numerator and the unit ε will change accordingly. Nonetheless, throughout this section, $R_{z,\varepsilon} \in SOC(\Gamma)$ stands for multiplication by the complex number $\varepsilon\frac{z}{\overline{z}}$. Furthermore, the fraction $\frac{z}{\overline{z}}$ is assumed to be reduced, that is, z and $\overline{z}$ have no common prime factors. Also, we set $z = 1$ whenever $R_{z,\varepsilon} \in P(\Gamma)$.

Similarly, $T_{z,\varepsilon} \in OC(\Gamma) \setminus SOC(\Gamma)$ is understood to be the coincidence reflection $T_{z,\varepsilon} = R_{z,\varepsilon} \cdot T_r$.

5.2. **The sets $SOC(x+\Gamma)$ and $OC(x+\Gamma)$.** The following lemma gives a criterion when $R_{z,\varepsilon} \in SOC(\Gamma)$ and $T_{z,\varepsilon} \in OC(\Gamma) \setminus SOC(\Gamma)$ are coincidence isometries of the shifted square lattice $x + \Gamma$.

Lemma 5.2. *Let $\Gamma = \mathbb{Z}[i]$, $x \in \mathbb{C}$, $R = R_{z,\varepsilon} \in SOC(\Gamma)$, and $T = R \cdot T_r$.*

(i) *$R \in SOC(x+\Gamma)$ if and only if $(\varepsilon z - \overline{z})x \in \Gamma$.*
(ii) *$T \in OC(x+\Gamma)$ if and only if $\varepsilon z\overline{x} - \overline{z}x \in \Gamma$.*

Proof. Since $z, \overline{z}$ are relatively prime and $\mathbb{Z}[i]$ is a principal ideal domain, one has

$$\Gamma + R\Gamma = \Gamma + \varepsilon\tfrac{z}{\overline{z}}\Gamma = \tfrac{1}{\overline{z}}\gcd(z,\overline{z})\Gamma = \tfrac{1}{\overline{z}}\Gamma.$$

By Theorem 4.3, $R \in SOC(x+\Gamma)$ if and only if $\varepsilon\frac{z}{\overline{z}}x - x \in \frac{1}{\overline{z}}\Gamma$, that is, whenever $(\varepsilon z - \overline{z})x \in \Gamma$.

Because T_r leaves Γ invariant, $\Gamma + T\Gamma = \frac{1}{\overline{z}}\Gamma$. Applying again Theorem 4.3 proves the corresponding result for T. □

It turns out that the set of coincidence rotations of $x + \Gamma$ forms a group.

Theorem 5.3. *If $\Gamma = \mathbb{Z}[i]$ then $SOC(x+\Gamma)$ is a subgroup of $SOC(\Gamma)$ for all $x \in \mathbb{C}$.*

Proof. By Proposition 4.9, it is enough to show that $SOC(x+\Gamma)$ is closed under composition to prove the claim. Let $R_j = R_{z_j,\varepsilon_j} \in SOC(x+\Gamma)$ for $j \in \{1,2\}$. Then $(\varepsilon_j z_j - \overline{z_j})x \in \Gamma$

from Lemma 5.2. Take $g := \gcd(\overline{z_1}, z_2)$, and express $\overline{z_1} = \overline{h_1}g$ and $z_2 = h_2 g$. One has

$$\begin{aligned}\big(\varepsilon_2\varepsilon_1 h_2 h_1 - \overline{h_2 h_1}\big)x &= \tfrac{1}{g}\big(\varepsilon_2\varepsilon_1 z_2 h_1 - \overline{h_2 z_1}\big)x \\ &= \tfrac{1}{g}\big[\varepsilon_1 h_1(\varepsilon_2 z_2 - \overline{z_2})x + \overline{h_2}(\varepsilon_1 z_1 - \overline{z_1})x\big] \in \tfrac{1}{g}\Gamma.\end{aligned}$$

In the same manner, one obtains that $\big(\varepsilon_2\varepsilon_1 h_2 h_1 - \overline{h_2 h_1}\big)x \in \frac{1}{\overline{g}}\Gamma$. Together, they imply that

$$\big(\varepsilon_2\varepsilon_1 h_2 h_1 - \overline{h_2 h_1}\big)x \in \tfrac{1}{g}\Gamma \cap \tfrac{1}{\overline{g}}\Gamma = \tfrac{1}{g\overline{g}}\operatorname{lcm}(g, \overline{g})\Gamma = \Gamma.$$

This is because $\mathbb{Z}[i]$ is a principal ideal domain and g is relatively prime to $\overline{g}$. Thus, $R_2 R_1 = R_{h_2 h_1, \varepsilon_2\varepsilon_1} \in SOC(x+\Gamma)$ by Lemma 5.2. □

However, the situation is more complicated for $OC(x+\Gamma)$. One has the following results.

Lemma 5.4. *Let $\Gamma = \mathbb{Z}[i]$ and $x \in \mathbb{C}$. Then $OC(x+\Gamma)$ is a subgroup of $OC(\Gamma)$ if and only if for any coincidence reflections T_1, $T_2 \in OC(x+\Gamma)$, the coincidence rotation $T_2 T_1 \in SOC(x+\Gamma)$.*

Proof. It follows from Proposition 4.9 and Theorem 5.3 that it suffices to show that the product of a coincidence reflection and a coincidence rotation of $x+\Gamma$ is again a coincidence reflection of $x+\Gamma$. Applying the same techniques employed in the proof of Theorem 5.3 yields the claim. □

Remark 5.5. Let $x \in \mathbb{C}$ and $T_j = T_{z_j, \varepsilon_j} \in OC(x+\Gamma)\setminus SOC(x+\Gamma)$ for $j \in \{1,2\}$. Applying the procedure used in the proof of Theorem 5.3 to the product $T_2 T_1$ only leads to

$$\big(\varepsilon_2\overline{\varepsilon_1} h_2 \overline{h_1} - \overline{h_2} h_1\big)x \in \tfrac{1}{\overline{g}}\Gamma, \tag{5.4}$$

where $g := \gcd(z_1, z_2)$ and $z_j = h_j g$ for $j \in \{1,2\}$. It follows then from Lemma 5.2 that if z_1 were relatively prime to z_2, then $T_2 T_1 = R_{h_2\overline{h_1}, \varepsilon_2\overline{\varepsilon_1}} \in (S)OC(x+\Gamma)$. This fact can also be deduced from Proposition 4.10, because if z_1 and z_2 were relatively prime, then so are $N(z_1) = \Sigma(R_1)$ and $N(z_2) = \Sigma(R_2)$.

Proposition 5.6. *Let $\Gamma = \mathbb{Z}[i]$ and $x \in \mathbb{C}$. If $OC(x+\Gamma)$ contains a reflection symmetry $T \in P(\Gamma)$ then $OC(x+\Gamma) = SOC(x+\Gamma) \rtimes \langle T\rangle$ and is a subgroup of $OC(\Gamma)$. Otherwise, the coincidence reflection $T_{z,\varepsilon} \notin OC(x+\Gamma)$ for all units ε of Γ whenever $R = R_{z,\varepsilon'} \in SOC(x+\Gamma)$ for some unit ε'.*

Proof. Because $T \in P(\Gamma)$, $T = T_{1,\varepsilon}$ for some unit ε of $\mathbb{Z}[i]$. Thus, $\overline{x} \in \overline{\varepsilon}x + \Gamma$ by Lemma 5.2. Let $T_j = T_{z_j,\varepsilon_j} \in OC(x+\Gamma) \setminus SOC(x+\Gamma)$ for $j \in \{1,2\}$. If $g := \gcd(z_1, z_2)$ and $z_j = h_j g$ for $j \in \{1,2\}$, then it follows from Lemma 5.2 that

$$g\big(\varepsilon_2\overline{\varepsilon_1} h_2 \overline{h_1} - \overline{h_2} h_1\big)\overline{x} = \overline{\varepsilon_1 h_1}(\varepsilon_2 z_2 \overline{x} - \overline{z_2}x) - \overline{\varepsilon_1 h_2}(\varepsilon_1 z_1 \overline{x} - \overline{z_1}x) \in \Gamma.$$

Since $\overline{x} \in \overline{\varepsilon}x + \Gamma$, we have $\big(\varepsilon_2\overline{\varepsilon_1} h_2 \overline{h_1} - \overline{h_2} h_1\big)x \in \frac{1}{g}\Gamma$. This, together with (5.4), implies that $\big(\varepsilon_2\overline{\varepsilon_1} h_2 \overline{h_1} - \overline{h_2} h_1\big)x \in \frac{1}{g}\Gamma \cap \frac{1}{\overline{g}}\Gamma = \Gamma$, and thus $T_2 T_1 \in OC(x+\Gamma)$. From Lemma 5.4, $OC(x+\Gamma)$ is a subgroup of $OC(\Gamma)$.

In addition, any coincidence reflection $T' = T_{z',\varepsilon'}$ of $x+\Gamma$ can be written as $T' = R' \cdot T$ where $R' = R_{z', \overline{\varepsilon}\varepsilon'} \in SOC(x+\Gamma)$. Hence, $OC(x+\Gamma)$ is the semidirect product of $SOC(x+\Gamma)$ and $\langle T\rangle$.

Suppose $OC(x+\Gamma)$ does not contain any reflection symmetry and $T_{z,\varepsilon} \in OC(x+\Gamma)$ for some unit ε of $\mathbb{Z}[i]$. Since $R \in SOC(x+\Gamma)$, $R^{-1} \cdot T_{z,\varepsilon} \in OC(x+\Gamma)$ by Lemma 5.4. This is a contradiction because $R^{-1} \cdot T_{z,\varepsilon} = T_{1,\overline{\varepsilon'}\varepsilon} \in P(\Gamma)$. □

Proposition 5.6 tells us that when computing for $OC(x+\Gamma)$, it is advantageous to determine at the outset whether there is a reflection symmetry T that is in $OC(x+\Gamma)$. If such a T exists, then $OC(x+\Gamma)$ is a group and it is the semidirect product of $SOC(x+\Gamma)$ and $\langle T\rangle$. Otherwise, once $SOC(x+\Gamma)$ has already been identified, only those coincidence reflections $T_{z,\varepsilon} \in OC(\Gamma)$ for which $R_{z,\varepsilon'} \notin SOC(x+\Gamma)$ for all units ε' of Γ may be elements of $OC(x+\Gamma)$.

The following corollary describes exactly when a reflection symmetry is a coincidence isometry of $x+\Gamma$, and thus, gives an explicit version of Proposition 5.6.

Corollary 5.7. *Let $\Gamma = \mathbb{Z}[i]$ and $x \in \mathbb{C}$. If one of the following conditions on x is satisfied:* $\operatorname{Re}(x) \in \frac{1}{2}\mathbb{Z}$, $\operatorname{Im}(x) \in \frac{1}{2}\mathbb{Z}$, *or* $\operatorname{Re}(x) \pm \operatorname{Im}(x) \in \mathbb{Z}$, *then $OC(x+\Gamma) = SOC(x+\Gamma) \rtimes \langle T_{1,\varepsilon}\rangle$ and is a subgroup of $OC(\Gamma)$, where*

$$\varepsilon = \begin{cases} 1, & \text{if } \operatorname{Im}(x) \in \frac{1}{2}\mathbb{Z} \\ -1, & \text{if } \operatorname{Re}(x) \in \frac{1}{2}\mathbb{Z} \\ i, & \text{if } \operatorname{Re}(x) - \operatorname{Im}(x) \in \mathbb{Z} \\ -i, & \text{if } \operatorname{Re}(x) + \operatorname{Im}(x) \in \mathbb{Z}. \end{cases}$$

Proof. Apply Lemma 5.2 and Proposition 5.6. □

5.3. **Determination of $SOC(x+\Gamma)$ and $OC(x+\Gamma)$.** We now turn to the actual computation of $OC(x+\Gamma)$ for specific values of x. Given $R_{z,\varepsilon} \in SOC(\Gamma)$, one sees from Lemma 5.2 the significance of the expression

$$\varepsilon z - \overline{z} = \begin{cases} 2i\operatorname{Im}(z), & \text{if } \varepsilon = 1 \\ -2\operatorname{Re}(z), & \text{if } \varepsilon = -1 \\ -[\operatorname{Re}(z) + \operatorname{Im}(z)](1-i), & \text{if } \varepsilon = i \\ -[\operatorname{Re}(z) - \operatorname{Im}(z)](1+i), & \text{if } \varepsilon = -i\,. \end{cases} \tag{5.5}$$

Since $\varepsilon z\overline{x} - \overline{z}x = \varepsilon(z\overline{x}) - \overline{(z\overline{x})}$, (5.5) can also be used to compute for $\varepsilon z\overline{x} - \overline{z}x$ for a given $T_{z,\varepsilon} \in OC(\Gamma) \setminus SOC(\Gamma)$.

Remark 5.8. Let $\Gamma = \mathbb{Z}[i]$. Given an $R_{z,\varepsilon} \in SOC(\Gamma)$ or $T_{z,\varepsilon} \in OC(\Gamma) \setminus SOC(\Gamma)$, the following holds on account of the choice of z (see (5.2) and Remark 5.1):

(i) The rational integers $\operatorname{Re}(z)$ and $\operatorname{Im}(z)$ are relatively prime and are of different parity (that is, one is odd while the other is even).
(ii) $\operatorname{Re}(z)$ is nonzero while $z = 1$ if $\operatorname{Im}(z) = 0$.

The following theorem states the complete solution of the coincidence problem for $x+\Gamma$ whenever x has an irrational component.

Theorem 5.9. *Let $\Gamma = \mathbb{Z}[i]$ and $x = a + bi$, with $a, b \in \mathbb{R}$. If a or b is irrational then $OC(x+\Gamma)$ is a group of at most two elements. In particular, if*

(i) *a is irrational and b is rational then* $OC(x+\Gamma) = \begin{cases} \langle T_r\rangle, & \text{if } 2b \in \mathbb{Z} \\ \{\mathbb{1}\}, & \text{otherwise.} \end{cases}$

(ii) *a is rational and b is irrational then* $OC(x+\Gamma) = \begin{cases} \langle T_{1,-1}\rangle, & \text{if } 2a \in \mathbb{Z} \\ \{\mathbb{1}\}, & \text{otherwise.} \end{cases}$

(iii) *both a and b are irrational, and*
  (a) *1, a, and b are rationally independent then $OC(x+\Gamma) = \{\mathbb{1}\}$.*

(b) $a = \frac{p_1}{q_1} + \frac{p_2}{q_2} b$ *where* p_j, $q_j \in \mathbb{Z}$, *and* p_j *is relatively prime to* q_j *for* $j \in \{1, 2\}$, *with*

(1) $p_2 q_2$ *even, then* $OC(x+\Gamma) = \begin{cases} \langle T_{p_2+q_2 i, 1} \rangle, & \text{if } q_1 \mid 2q_2 \\ \{\mathbb{1}\}, & \text{otherwise.} \end{cases}$

(2) $p_2 q_2$ *odd, then* $OC(x+\Gamma) = \begin{cases} \left\langle T_{\frac{p_2+q_2}{2} - \frac{p_2-q_2}{2} i, i} \right\rangle, & \text{if } q_1 \mid q_2 \\ \{\mathbb{1}\}, & \text{otherwise.} \end{cases}$

Proof. Suppose either a or b is irrational, that is, $x \notin \mathbb{Q}(i)$. If $R_{z,\varepsilon} \in SOC(x+\Gamma)$ then it follows from Lemma 5.2 that $\varepsilon z - \overline{z} = 0$. Thus, $\varepsilon \frac{z}{\overline{z}} = 1$ which means that $SOC(x+\Gamma) = \{\mathbb{1}\}$, where $\mathbb{1}$ is the identity isometry.

Assume $OC(x+\Gamma)$ includes two distinct reflections $T_1 = T_{h_1 g, \varepsilon_1}$ and $T_2 = T_{h_2 g, \varepsilon_2}$, with h_1 and h_2 relatively prime. Since $\frac{1}{g}\Gamma \subseteq \mathbb{Q}(i)$, one obtains from (5.4) that $\varepsilon_2 \overline{\varepsilon_1} h_2 \overline{h_1} - \overline{h_2} h_1 = 0$. This implies that $T_2 T_1 = \mathbb{1}$, and hence, $T_1 = T_2$. Therefore, either $OC(x+\Gamma) = \{\mathbb{1}\}$ or $OC(x+\Gamma) = \langle T \rangle$ for some coincidence reflection T.

Let $T_{z,\varepsilon} \in OC(\Gamma) \setminus SOC(\Gamma)$. It follows from Remark 5.8 that if a is irrational and b is rational, then $2\mathrm{Re}\,(z\overline{x}), \mathrm{Re}\,(z\overline{x}) \pm \mathrm{Im}\,(z\overline{x}) \notin \mathbb{Z}$. This means that $\varepsilon z\overline{x} - \overline{z}x \in \mathbb{Z}[i]$ if and only if $\varepsilon = 1$ and $2\mathrm{Im}\,(z\overline{x}) \in \mathbb{Z}$, that is, if $\varepsilon = z = 1$ by (5.5) and Remark 5.8. If $z = 1$, one has $2\mathrm{Im}\,(\overline{x}) = -2b \in \mathbb{Z}$ and (i) now follows from Lemma 5.2. The proof of (ii) proceeds analogously.

Suppose now that both a and b are irrational. From (5.5) and Lemma 5.2, one obtains that a coincidence reflection $T_{z,\varepsilon} \in OC(x+\Gamma)$ if and only if

$$a = \begin{cases} \frac{t}{2\mathrm{Im}(z)} + \frac{\mathrm{Re}(z)}{\mathrm{Im}(z)} b, & \text{if } \varepsilon = 1 \\ \frac{t}{2\mathrm{Re}(z)} - \frac{\mathrm{Im}(z)}{\mathrm{Re}(z)} b, & \text{if } \varepsilon = -1 \\ \frac{t}{\mathrm{Re}(z)+\mathrm{Im}(z)} + \frac{\mathrm{Re}(z)-\mathrm{Im}(z)}{\mathrm{Re}(z)+\mathrm{Im}(z)} b, & \text{if } \varepsilon = i \\ \frac{t}{\mathrm{Re}(z)-\mathrm{Im}(z)} - \frac{\mathrm{Re}(z)+\mathrm{Im}(z)}{\mathrm{Re}(z)-\mathrm{Im}(z)} b, & \text{if } \varepsilon = -i, \end{cases} \tag{5.6}$$

for some $t \in \mathbb{Z}$. In each case, one is able to write a uniquely as $a = c + d \cdot b$ where $c, d \in \mathbb{Q}$.

Assume that $a = \frac{p_1}{q_1} + \frac{p_2}{q_2} b$ where p_j, $q_j \in \mathbb{Z}$ with p_j and q_j relatively prime for $j \in \{1, 2\}$. If $p_2 q_2$ is even then a is expressible in the form (5.6) if and only if $\varepsilon = \pm 1$ and $q_1 \mid 2q_2$. Then, one can simply take $\varepsilon = 1$ and $z = p_2 + q_2 i$ so that $T_{z,\varepsilon} \in OC(x+\Gamma)$. Similarly, if $p_2 q_2$ is odd, a solution exists if and only if $\varepsilon = \pm i$ and $q_1 \mid q_2$. In particular, $\varepsilon = i$ and $z = \frac{p_2+q_2}{2} - \frac{p_2-q_2}{2} i$ gives the unique $T_{z,\varepsilon} \in OC(x+\Gamma)$. This completes the proof. □

Remark 5.10. Note that for $T_{\frac{p_2+q_2}{2} - \frac{p_2-q_2}{2} i, i} = R \cdot T_r$ in Theorem 5.9(iii), R actually corresponds to multiplication by the complex number $\frac{z}{\overline{z}}$ with $z = p_2 + q_2 i$. However, in such a representation, z and $\overline{z}$ are not relatively prime.

It only remains to consider the case when both components of x are rational. Suppose that $x = a + bi \in \mathbb{Q}(i)$ and write $x = \frac{p}{q}$, where p, $q \in \mathbb{Z}[i]$ with p and q relatively prime. The following lemma indicates that $SOC(x+\Gamma)$ ultimately depends on the denominator q of x.

Lemma 5.11. *Let $\Gamma = \mathbb{Z}[i]$, $x = \frac{p}{q}$ where p, $q \in \Gamma$ with p and q relatively prime, and $R = R_{z,\varepsilon} \in SOC(\Gamma)$. Then $R \in SOC(x+\Gamma)$ if and only if q divides $\varepsilon z - \overline{z}$. Consequently, $SOC(x+\Gamma) = SOC(\frac{1}{q}+\Gamma)$.*

Proof. It follows from Lemma 5.2 that $R \in SOC(x+\Gamma)$ if and only if $\frac{(\varepsilon z - \overline{z})p}{q} \in \Gamma$. The latter is equivalent to $q \mid (\varepsilon z - \overline{z})$, because p and q are relatively prime. □

The following properties that relate $SOC(x+\Gamma)$ for different rational values of x are obtained as a result of the divisibility condition set forth in Lemma 5.11.

Corollary 5.12. *If $q_1, q_2 \in \mathbb{Z}[i]$ such that $q_1 \mid q_2$, then $SOC(\frac{1}{q_2}+\Gamma) \subseteq SOC(\frac{1}{q_1}+\Gamma)$.*

Corollary 5.13. *Suppose $q_1, q_2 \in \mathbb{Z}[i]$. Then*

$$SOC(\tfrac{1}{q_1}+\Gamma) \cap SOC(\tfrac{1}{q_2}+\Gamma) = SOC\big(\tfrac{1}{\operatorname{lcm}(q_1,q_2)}+\Gamma\big).$$

In particular, if q_1 is relatively prime to q_2 then

$$SOC(\tfrac{1}{q_1}+\Gamma) \cap SOC(\tfrac{1}{q_2}+\Gamma) = SOC\big(\tfrac{1}{q_1 q_2}+\Gamma\big).$$

Proof. The backward inclusion follows from Corollary 5.12. Suppose that $R = R_{z,\varepsilon} \in SOC(\Gamma)$ is a coincidence isometry of $\frac{1}{q_1}+\Gamma$ and $\frac{1}{q_2}+\Gamma$. Then, by Lemma 5.11, $q_j \mid (\varepsilon z - \overline{z})$ for $j \in \{1,2\}$. Since $\mathbb{Z}[i]$ is a principal ideal domain, $\operatorname{lcm}(q_1,q_2) \mid (\varepsilon z - \overline{z})$ and so $R \in SOC\big(\frac{1}{\operatorname{lcm}(q_1,q_2)}+\Gamma\big)$. □

One can easily generalize Corollary 5.13. That is, if the denominator q of x factorizes as $q = \prod_j q_j^{r_j}$ where the q_j's are primes in $\Gamma = \mathbb{Z}[i]$ that are pairwise relatively prime, then

$$SOC(\tfrac{1}{q}+\Gamma) = \bigcap_j SOC\left(\tfrac{1}{q_j^{r_j}}+\Gamma\right).$$

Corollary 5.14. *If $q \in \mathbb{Z}[i]$ then $SOC(\frac{1}{q}+\Gamma) = SOC(\frac{1}{\overline{q}}+\Gamma) = SOC\big(\frac{1}{\operatorname{lcm}(q,\overline{q})}+\Gamma\big)$.*

Proof. Since $\overline{\varepsilon z - \overline{z}} = -\overline{\varepsilon}(\varepsilon z - \overline{z})$, $q \mid (\varepsilon z - \overline{z})$ if and only if $\overline{q} \mid (\varepsilon z - \overline{z})$. The equalities then follow from Lemma 5.11 and Corollary 5.13. □

The next proposition provides additional sufficient conditions when $OC(x+\Gamma)$ forms a group.

Proposition 5.15. *Let $x = \frac{p}{q}$ where $p, q \in \mathbb{Z}[i]$ with p and q relatively prime. If none of the prime factors of $N(q)$ is a splitting prime of $\mathbb{Z}[i]$, then $OC(x+\Gamma)$ is a group.*

Proof. From Lemma 5.4, it suffices to show that the product of any two coincidence reflections $T_1 = T_{z_1,\varepsilon_1}$ and $T_2 = T_{z_2,\varepsilon_2}$ of $x+\Gamma$ is in $SOC(x+\Gamma)$ to prove the claim.

Since none of the prime factors of $N(q)$ splits in $\mathbb{Z}[i]$, $\overline{q} = \overline{u}q$ for some unit u of $\mathbb{Z}[i]$. It follows from Lemma 5.2 that for $j \in \{1,2\}$, $q \mid (u\varepsilon_j z_j \overline{p} - \overline{z_j} p)$. Set $g := \gcd(z_1, z_2)$ and write $z_j = h_j g$ for $j \in \{1,2\}$. Then q divides $u\varepsilon_2 z_2 \overline{z_1 p} - u\varepsilon_1 \overline{z_2} z_1 \overline{p} = u\varepsilon_1 g\overline{gp}\big(\varepsilon_2 \overline{\varepsilon_1} h_2 \overline{h_1} - \overline{h_2} h_1\big)$, and hence, $q \mid \big(\varepsilon_2 \overline{\varepsilon_1} h_2 \overline{h_1} - \overline{h_2} h_1\big)$. Finally, because $T_2 T_1 = R_{h_2\overline{h_1}, \varepsilon_2\overline{\varepsilon_1}} \in SOC(\Gamma)$, the product $T_2 T_1 \in SOC(x+\Gamma)$ by Lemma 5.11. □

The next proposition renders useful results about coincidence rotations of $x+\Gamma$ and their corresponding coincidence indices whenever the denominator q of x is an odd rational integer.

Proposition 5.16. *Let $\Gamma = \mathbb{Z}[i]$ and $q > 1$ be an odd rational integer. If $R = R_{z,\varepsilon} \in SOC(\frac{1}{q} + \Gamma)$ then the following holds.*

(i) *For all other units $\varepsilon' \neq \varepsilon$, $R_{z,\varepsilon'} \notin SOC(\frac{1}{q} + \Gamma)$.*
(ii) *The coincidence index $\Sigma(R)$ is not divisible by q.*

Proof. By Lemma 5.11, $q \mid (\varepsilon z - \overline{z})$.

(i) Assume to the contrary that $R_{z,\varepsilon'} \in SOC(\frac{1}{q} + \Gamma)$ for some unit $\varepsilon' \neq \varepsilon$ of $\mathbb{Z}[i]$. Then $q \mid (\varepsilon' z - \overline{z})$ from Lemma 5.11 which implies that q divides z. However, q is a rational integer, and so q divides both real and imaginary parts of z. This is impossible by the choice of z (see Remark 5.8(i)).
(ii) Suppose q divides $\Sigma(R) = N(z) = z\overline{z}$. Since q divides $z(\varepsilon z - \overline{z}) = \varepsilon z^2 - z\overline{z}$, the rational integer q also divides z^2. This contradicts Remark 5.8(i). □

It is a well-known fact that $\mathbb{Z}[i]$ is a Euclidean domain. That is, for any $a, b \in \mathbb{Z}[i]$ with $b \neq 0$, there exist $k, r \in \mathbb{Z}[i]$ such that $a = kb + r$ and $N(r) \leq \frac{1}{2}N(b)$ (see for instance, [19, Theorem 215]). The next proposition makes use of this fact.

Proposition 5.17. *Let $q > 1$ be an odd rational integer and write $z = kq + r$ where $k, r \in \mathbb{Z}[i]$ and $N(r) < \frac{1}{2}N(q)$. Then $R = R_{z,\varepsilon} \in SOC(\frac{1}{q} + \Gamma)$ if and only if $\overline{r} = \varepsilon r$, that is, when r and $\overline{r}$ are associates in $\mathbb{Z}[i]$.*

Proof. Note that $\varepsilon z - \overline{z} = \left(\varepsilon k - \overline{k}\right)q + (\varepsilon r - \overline{r})$.

Suppose $R \in SOC(\frac{1}{q} + \Gamma)$. Then by Lemma 5.11, $q \mid (\varepsilon z - \overline{z})$ and hence, $q \mid (\varepsilon r - \overline{r})$. Since q is odd, $(1-i)q$ still divides $\varepsilon r - \overline{r}$ from (5.5). Thus, $N((1-i)q) = 2N(q) \mid N(\varepsilon r - \overline{r})$. However, (5.5) indicates that $N(\varepsilon r - \overline{r}) \leq 4N(r) < 2N(q)$. Therefore, $N(\varepsilon r - \overline{r}) = 0$ and so $\overline{r} = \varepsilon r$.

Conversely, suppose $\overline{r} = \varepsilon r$ for some unit ε of $\mathbb{Z}[i]$. Then $q \mid (\varepsilon z - \overline{z})$ and $R \in SOC(\frac{1}{q} + \Gamma)$ by Lemma 5.11. □

Observe that r and $\overline{r}$ are associates in $\mathbb{Z}[i]$ if and only if r is a rational integer multiple of 1, i, $1 + i$, or $1 - i$. Hence, for all odd rational integers $q > 1$,

$$SOC\left(\tfrac{1}{q} + \Gamma\right) = \left\{R_{z,1} \in SOC(\Gamma) : z = kq + r; k \in \mathbb{Z}[i], r \in \mathbb{Z}, 0 < r < \tfrac{1}{2}q\right\} \cup \left\{R_{z,i} \in SOC(\Gamma) : z = kq + (1+i)r; k \in \mathbb{Z}[i], r \in \mathbb{Z}, 0 < r < \tfrac{1}{2}q\right\}.$$

Let $\mathcal{V}$ be the set of *visible* (or *primitive*) points of $\mathbb{Z}[i]$, that is,

$$\mathcal{V} = \{z \in \mathbb{Z}[i] : \gcd(\mathrm{Re}\,(z), \mathrm{Im}\,(z)) = 1\}$$

and let $\mathcal{V}' = \{z \in \mathcal{V} : (1+i) \nmid z\}$ be the set of visible points that are not divisible by $1 + i$. If $f_{1/q+\Gamma}(m)$ denotes the number of CSLs for a given index m of the shifted lattice $\frac{1}{q} + \Gamma$, then the Dirichlet series generating function for $f_{1/q+\Gamma}(m)$ is given by

$$\begin{aligned}\Phi_{1/q+\Gamma}(s) &= \sum_{m=1}^{\infty} \frac{f_{1/q+\Gamma}(m)}{m^s} \\ &= \sum_{\substack{0<r<\frac{q}{2} \\ \gcd(r,q)=1}} \left(\sum_{\substack{k \in \mathbb{Z}[i] \\ kq+r \in \mathcal{V}'}} \frac{1}{N(kq+r)^s} + \sum_{\substack{k \in \mathbb{Z}[i] \\ kq+(1+i)r \in \mathcal{V}'}} \frac{1}{N(kq+(1+i)r)^s} \right). \end{aligned} \tag{5.7}$$

To visualize the set that the sum in (5.7) runs over, consider the grid

$$L_q = q\mathbb{Z}[i] + \{r, ir, (1+i)r, (1-i)r : r \in \mathbb{R}\}$$

(see Figure 1). Observe that the sum is taken over one-fourth of the points of $\mathcal{V}'$ lying on the grid L, that is, one point out of the four points of $\mathcal{V}' \cap L$ that are equivalent under the action of C_4 appears in the sum.

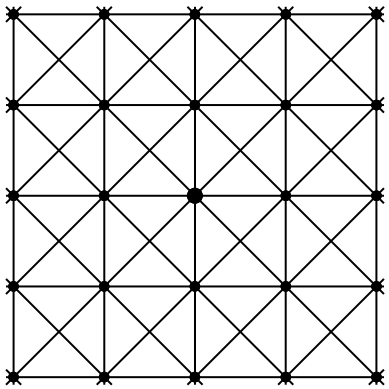

FIGURE 1. The grid L_q. The black dots are points of $q\mathbb{Z}[i]$.

Proposition 5.17 also gives the following lower bound on the coincidence index of a coincidence rotation of $\frac{1}{q} + \Gamma$.

Corollary 5.18. *Let $\Gamma = \mathbb{Z}[i]$ and $q > 1$ be an odd rational integer. If $R = R_{z,\varepsilon} \in SOC(\frac{1}{q} + \Gamma) \setminus P(\Gamma)$ then $\Sigma(R) > \frac{1}{2}q^2$.*

Proof. Write $z = kq + r$ where $k, r \in \mathbb{Z}[i]$ and $N(r) < \frac{1}{2}N(q)$. If $\Sigma(R) = N(z) \leq \frac{1}{2}q^2 = \frac{1}{2}N(q)$, then $r = z$. However, $\frac{z}{\bar{z}}$ is not a unit, contradicting Proposition 5.17. □

5.4. **Specific examples.** We now explicitly compute $OC(x + \Gamma)$ for certain values of $x \in \mathbb{Q}(i)$. Other examples can be found in [26, 25]. It follows from Proposition 4.5 that it suffices to compute $OC(x+\Gamma)$ for values of x in some fundamental domain of the symmetry group G of Γ (a crystallographic group of type $p4m$ or $*442$ in orbifold notation). We choose this fundamental domain to be the triangular region $\left\{x \in \mathbb{C} : 0 \leq \operatorname{Im}(x) \leq \operatorname{Re}(x) \leq \frac{1}{2}\right\}$ shown in Figure 2.

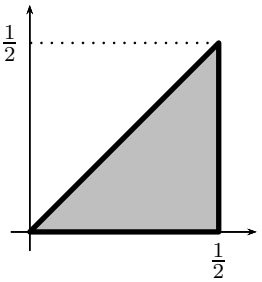

FIGURE 2. A fundamental domain of the symmetry group of $\mathbb{Z}[i]$

Remark 5.19. Let $\Gamma = \mathbb{Z}[i]$, G the symmetry group of Γ, and $x \in \mathbb{C}$.

(i) It follows from Corollary 5.7 that for values of x in the fundamental domain of G in Figure 2, $OC(x+\Gamma)$ is a subgroup of $OC(\Gamma)$ whenever x lies on the boundary of the fundamental domain, that is, when $\mathrm{Re}\,(x) = \frac{1}{2}$, $\mathrm{Im}\,(x) = 0$, or $\mathrm{Re}\,(x) = \mathrm{Im}\,(x)$.

(ii) The number of coincidence rotations and CSLs for a given index m of the shifted lattice $x+\Gamma$ shall be denoted by $\hat{f}_{x+\Gamma}(m)$ and $f_{x+\Gamma}(m)$, respectively.

Example 5.20. $x = \frac{1}{2} + \frac{1}{2}i = \frac{1}{1-i}$
We obtain that the denominator of x is $q = 1 - i$. One sees from (5.5) that $q \mid (\varepsilon z - \overline{z})$ for all numerators z and for all units ε of $\mathbb{Z}[i]$. Lemma 5.11 and Corollary 5.7 imply that $(S)OC(x+\Gamma) = (S)OC(\Gamma)$. Moreover, $\hat{f}_{x+\Gamma}(m) = \hat{f}_{\mathbb{Z}^2}(m)$ and $f_{x+\Gamma}(m) = f_{\mathbb{Z}^2}(m)$ by Proposition 4.4.

The results in Example 5.20 agree with those obtained in [28, Appendix A] (simply shift the center of a Delaunay cell into the origin, see also Remark 4.2).

Example 5.21. $x = \frac{1}{2}$
The denominator of x is $q = 2$. One obtains from Remark 5.8(i) and (5.5) that for all numerators z, $q \mid (\varepsilon z - \overline{z})$ if and only if $\varepsilon = \pm 1$. Hence, by Lemma 5.11,

$$SOC(x+\Gamma) = \{R_{z,\varepsilon} \in SOC(\Gamma) : \varepsilon = \pm 1\} \cong C_2 \times \mathbb{Z}^{(\aleph_0)}.$$

By Corollary 5.7, $OC(x+\Gamma) = SOC(x+\Gamma) \rtimes \langle T_r \rangle$ is a subgroup of $OC(\Gamma)$ of index 2. By Proposition 4.4, $f_{x+\Gamma}(m) = f_{\mathbb{Z}^2}(m)$ but $\hat{f}_{x+\Gamma}(m) = 2f_{x+\Gamma}(m) = \frac{1}{2}\hat{f}_{\mathbb{Z}^2}(m)$.

Example 5.22. $x = \frac{1}{3} + \frac{1}{3}i$
Here, x has denominator $q = 3$. Observe that if $r \in \Gamma$ lies inside the disk with center at 0 and radius $\sqrt{\frac{1}{2}N(q)} = \frac{3}{2}\sqrt{2}$, then r and $\overline{r}$ are associates in Γ. Hence, by Propositions 5.16 and 5.17, there is a unique unit ε of $\mathbb{Z}[i]$ for a numerator z such that $R_{z,\varepsilon} \in SOC(x+\Gamma)$. Thus, $SOC(x+\Gamma) \cong \mathbb{Z}^{(\aleph_0)}$. Furthermore, by Corollary 5.7, $OC(x+\Gamma) = SOC(x+\Gamma) \rtimes \langle T_{1,i} \rangle$ is a subgroup of $OC(\Gamma)$ of index 4. Finally, $\hat{f}_{x+\Gamma}(m) = f_{x+\Gamma}(m) = f_{\mathbb{Z}^2}(m)$.

Example 5.23. $x = \frac{1}{2} + \frac{1}{4}i$
The denominator of x is $q = 4$. Note that 2 divides q and so $SOC(x+\Gamma) \subseteq SOC(\frac{1}{2}+\Gamma)$. Lemma 5.11, together with (5.5), yields

$$SOC(x+\Gamma) = \left\{R_{z,\varepsilon} \in SOC(\Gamma) : \varepsilon = (-1)^{\mathrm{Im}(z)}\right\} \cong \mathbb{Z}^{(\aleph_0)}.$$

It follows from Corollary 5.7 that $OC(x+\Gamma) = SOC(x+\Gamma) \rtimes \langle T_{1,-1} \rangle$ is again a subgroup of index 4 in $OC(\Gamma)$. Moreover, $\hat{f}_{x+\Gamma}(m) = f_{x+\Gamma}(m) = f_{\mathbb{Z}^2}(m)$.

Example 5.24. $x = \frac{1}{5}, \frac{2}{5}$
Here, the denominator is $q = 5$. Write $z = 5k + r$ where $k, r \in \mathbb{Z}[i]$ and $N(r) < \frac{25}{2}$. For all possible remainders r, $\overline{r}$ is not an associate of r if and only if $5 \mid N(z)$, because $N(z) = 25N(k) + 10\mathrm{Re}\,(k\overline{r}) + N(r)$. It follows then from Propositions 5.16 and 5.17 that for all numerators z, there is a (unique) unit ε of $\mathbb{Z}[i]$ for which $R_{z,\varepsilon} \in SOC(x+\Gamma)$ if and only if $5 \nmid N(z)$. This means that $SOC(x+\Gamma) \cong \mathbb{Z}^{(\aleph_0)}$. Moreover, $OC(x+\Gamma)$ is a subgroup of $OC(\Gamma)$ with $OC(x+\Gamma) = SOC(x+\Gamma) \rtimes \langle T_r \rangle$ by Corollary 5.7. Furthermore,

$$\hat{f}_{x+\Gamma}(m) = f_{x+\Gamma}(m) = \begin{cases} f_{\mathbb{Z}^2}(m), & \text{if } 5 \nmid m \\ 0, & \text{otherwise.} \end{cases}$$

The function $f_{x+\Gamma}$ is still multiplicative and the Dirichlet series generating function for $f_{x+\Gamma}(m)$ is given by

$$\begin{aligned}\Phi_{x+\Gamma}(s) &= \sum_{m=1}^{\infty} \frac{f_{x+\Gamma}(m)}{m^s} = \frac{1-5^{-s}}{1+5^{-s}} \cdot \Phi_{\mathbb{Z}^2}(s) \\ &= 1 + \tfrac{2}{13^s} + \tfrac{2}{17^s} + \tfrac{2}{29^s} + \tfrac{2}{37^s} + \tfrac{2}{41^s} + \tfrac{2}{53^s} + \tfrac{2}{61^s} + \tfrac{2}{73^s} + \tfrac{2}{89^s} + \tfrac{2}{97^s} + \tfrac{2}{101^s} \\ &\quad + \tfrac{2}{109^s} + \tfrac{2}{113^s} + \tfrac{2}{137^s} + \tfrac{2}{149^s} + \tfrac{2}{157^s} + \tfrac{2}{169^s} + \tfrac{2}{173^s} + \tfrac{2}{181^s} + \tfrac{2}{193^s} + \tfrac{2}{197^s} \\ &\quad + \tfrac{4}{221^s} + \tfrac{2}{229^s} + \cdots .\end{aligned}$$

One can show using a specific case of Delange's theorem (see for instance, [3, Theorem 5 of Appendix]) that the number of CSLs of $x+\Gamma$ with index at most N is asymptotically $\frac{2N}{3\pi}$.

The next example gives an instance when the set of coincidence isometries of a shifted lattice fails to form a group.

Example 5.25. $x = \frac{2}{5} + \frac{1}{5}i = \frac{i}{1+2i}$
In this case, the denominator of x is $q = 1+2i$. Since $5 = \operatorname{lcm}(q, \overline{q})$,

$$SOC(x+\Gamma) = SOC(\tfrac{1}{5}+\Gamma) \cong \mathbb{Z}^{(\aleph_0)}$$

by Corollary 5.14. Observe that x lies in the interior of the fundamental domain of G in Figure 2 (see Remark 5.19(i)) and $OC(x+\Gamma)$ does not include a reflection symmetry by Lemma 5.2. Recall from Example 5.24 that there is a (unique) unit ε of $\mathbb{Z}[i]$ for a numerator z with $R_{z,\varepsilon} \in SOC(\frac{1}{5}+\Gamma)$ if and only if $5 \nmid N(z)$. This fact, together with Proposition 5.6, implies that $5 \mid N(z)$ whenever $T_{z,\varepsilon} = R_{z,\varepsilon} \cdot T_r \in OC(x+\Gamma)$.

Given a numerator z whose norm is divisible by 5, either $1+2i$ or $1-2i$ (and not both) appears in the factorization of z into primes of Γ. If $(1-2i) \mid z$, then $z\overline{x} \in \Gamma$ which means that $\varepsilon z\overline{x} - \overline{z}x \in \Gamma$ for all units ε of $\mathbb{Z}[i]$. On the other hand, if $(1+2i) \mid z$ then $\varepsilon z\overline{x} - \overline{z}x = \frac{i(-\varepsilon y - \overline{y})}{5}$, where $y = (1+2i)z$. This implies that $\varepsilon z\overline{x} - \overline{z}x \notin \Gamma$ for all units ε of $\mathbb{Z}[i]$, since otherwise, $R_{y,-\varepsilon} \in SOC(\frac{1}{5}+\Gamma)$ by Lemma 5.11 which is impossible because $5 \mid N(y)$.

Therefore, by Lemma 5.2,

$$OC(x+\Gamma) = SOC(x+\Gamma) \cup \{T_{z,\varepsilon} \in OC(\Gamma) : (1-2i) \mid z\}.$$

We claim that $OC(x+\Gamma)$ is not a group. Indeed, let $T_j = T_{z,\varepsilon_j} \in OC(x+\Gamma) \setminus SOC(x+\Gamma)$ for $j \in \{1,2\}$ with $\varepsilon_1 \neq \varepsilon_2$. Then $T_2T_1 = R_{1,\varepsilon_2\overline{\varepsilon_1}} \in P(\Gamma)$ with $\varepsilon_2\overline{\varepsilon_1} \neq 1$, which means that $T_2T_1 \notin SOC(x+\Gamma)$. Hence, $OC(x+\Gamma)$ is not a subgroup of $OC(\Gamma)$.

Since $SOC(x+\Gamma) = SOC(\frac{1}{5}+\Gamma)$, one concludes that $\hat{f}_{x+\Gamma}(m) = \hat{f}_{\frac{1}{5}+\Gamma}(m)$. Denote by $\hat{F}_{x+\Gamma}(m)$ the number of linear coincidence isometries of $x+\Gamma$ of index m. Since each non-identity rotation symmetry is not a coincidence rotation of $x+\Gamma$, by Proposition 4.4, $f_{x+\Gamma}(m) = \hat{F}_{x+\Gamma}(m)$. Here, $f_{x+\Gamma}$ is also multiplicative and is given by

$$f_{x+\Gamma}(p^r) = \begin{cases} 2, & \text{if } p \equiv 1 \pmod 4 \text{ and } p \neq 5 \\ 4, & \text{if } p = 5 \\ 0, & \text{otherwise,} \end{cases}$$

for primes p and $r \in \mathbb{N}$. The Dirichlet series generating function for $f_{x+\Gamma}(m)$ reads

$$\begin{aligned}\Phi_{x+\Gamma}(s) &= \sum_{m=1}^{\infty} \frac{f_{x+\Gamma}(m)}{m^s} = \frac{1+3\cdot 5^{-s}}{1+5^{-s}} \cdot \Phi_{\mathbb{Z}^2}(s) \\ &= 1 + \tfrac{4}{5^s} + \tfrac{2}{13^s} + \tfrac{2}{17^s} + \tfrac{4}{25^s} + \tfrac{2}{29^s} + \tfrac{2}{37^s} + \tfrac{2}{41^s} + \tfrac{2}{53^s} + \tfrac{2}{61^s} + \tfrac{8}{65^s} + \tfrac{2}{73^s} + \cdots .\end{aligned}$$

Looking at $\Phi_{x+\Gamma}(s)$, we have that the number of CSLs of $x+\Gamma$ of index at most N is asymptotically given by $\frac{4N}{3\pi}$.

Example 5.26. $x = \frac{1}{3} + \frac{1}{6}i$
The denominator of x is $q = 6 = 2 \cdot 3$. Hence, by Corollary 5.13,

$$SOC(x+\Gamma) = SOC(\tfrac{1}{2}+\Gamma) \cap SOC(\tfrac{1}{3}+\Gamma).$$

From Example 5.21, $R_{z,\varepsilon} \in SOC(\frac{1}{2}+\Gamma)$ if and only if $\varepsilon = \pm 1$. Write $z = 3k + r$, where $k, r \in \mathbb{Z}[i]$ and $N(r) < \frac{9}{2}$. Note that $N(z) \equiv N(r) \pmod 3$, and for all possible remainders r, $\varepsilon = \frac{\overline{r}}{r} = \pm 1$ if and only if $N(r) \equiv 1 \pmod 3$. It follows then from Proposition 5.17 that $R_{z,\varepsilon} \in SOC(x+\Gamma)$ for some (unique) $\varepsilon \in \{1,-1\}$ if and only if $N(z) \equiv 1 \pmod 3$. Thus, $SOC(x+\Gamma) \cong \mathbb{Z}^{(\aleph_0)}$ and

$$\hat{f}_{x+\Gamma}(m) = \begin{cases} f_{\mathbb{Z}^2}(m), & \text{if } m \equiv 1 \pmod 3 \\ 0, & \text{otherwise.} \end{cases}$$

Here, $\hat{f}_{x+\Gamma}$ is not multiplicative anymore. As $\hat{f}_{x+\Gamma}(m) = \frac{1}{2}\big(1+\chi_{-3}(m)\big) f_{\mathbb{Z}^2}(m)$ is the sum of two multiplicative functions, we can still explicitly calculate its Dirichlet series generating function to be

$$\begin{aligned}\hat{\Phi}_{x+\Gamma}(s) = \sum_{m=1}^{\infty} \frac{\hat{f}_{x+\Gamma}(m)}{m^s} &= \tfrac{1}{2}\Phi_{\mathbb{Z}^2}(s) + \frac{1}{1-2^{-s}} \cdot \frac{1}{1-3^{-2s}} \cdot \frac{L(s,\chi_{-3})L(s,\chi_{12})}{2\zeta(2s)} \\ &= 1 + \tfrac{2}{13^s} + \tfrac{2}{25^s} + \tfrac{2}{37^s} + \tfrac{2}{61^s} + \tfrac{2}{73^s} + \tfrac{4}{85^s} + \tfrac{2}{97^s} + \cdots ,\end{aligned}$$

where $L(s,\chi_{-3})$ and $L(s,\chi_{12})$ are the L-series of the primitive Dirichlet characters

$$\chi_{-3}(m) = \begin{cases} 1, & \text{if } m \equiv 1 \pmod 3 \\ -1, & \text{if } m \equiv 2 \pmod 3 \\ 0, & \text{otherwise} \end{cases} \quad \text{and} \quad \chi_{12}(m) = \begin{cases} 1, & \text{if } m \equiv 1, 11 \pmod{12} \\ -1, & \text{if } m \equiv 5, 7 \pmod{12} \\ 0, & \text{otherwise,} \end{cases}$$

respectively. One obtains that the number of coincidence rotations of $x+\Gamma$ of index at most N is asymptotically $\frac{N}{2\pi}$.

Again, x lies in the interior of the fundamental domain of G in Figure 2 and so $OC(x+\Gamma)$ does not contain a reflection symmetry. Proposition 5.6 indicates that if the coincidence reflection $T_{z,\varepsilon} \in OC(x+\Gamma)$ then $N(z) \equiv 2 \pmod 3$. Conversely, suppose that z is a numerator with $N(z) \equiv 2 \pmod 3$. Observe that the numerator of the shift x, $p = 2+i$, is a factor of 5 which is a splitting prime in Γ. This means that if $p \nmid z$, $y := z\overline{p}$ is still a numerator corresponding to some coincidence rotation of Γ. In fact, because $N(y) \equiv 1 \pmod 3$, $R_{y,\varepsilon} \in SOC(x+\Gamma)$ for some (unique) $\varepsilon \in \{1,-1\}$. Hence, $6 \mid (\varepsilon y - \overline{y})$ by Lemma 5.11, and one obtains that $\varepsilon z\overline{x} - \overline{z}x = \frac{1}{6}(\varepsilon y - \overline{y}) \in \Gamma$. The case where $p \mid z$ yields the same result, since $\varepsilon z\overline{x} - \overline{z}x = \frac{5}{6}(\varepsilon y - \overline{y}) \in \Gamma$ where $y := \frac{z}{p}$. Thus, $T_{z,\varepsilon} \in OC(x+\Gamma)$ by Lemma 5.2. Altogether

one has

$$OC(x+\Gamma) = SOC(x+\Gamma) \cup \left\{ T_{z,\varepsilon} : N(z) \equiv 2 \pmod 3 \text{ and } \varepsilon = \begin{cases} 1, & \text{if } 3\nmid \mathrm{Re}(z\overline{p}) \\ -1, & \text{if } 3 | \mathrm{Re}(z\overline{p}) \end{cases} \right\}.$$

Since $N(q) = 2^2 \cdot 3^2$, $OC(x+\Gamma)$ forms a group by Proposition 5.15. Lastly, $\hat{F}_{x+\Gamma}(m) = f_{x+\Gamma}(m) = f_{\mathbb{Z}^2}(m)$, where $\hat{F}_{x+\Gamma}(m)$ counts the number of linear coincidence isometries of $x+\Gamma$ of a given index m.

6. Linear coincidences of multilattices

We now take a step further and consider the coincidence problem this time for sets of points formed by finite unions of shifted lattices. Such sets are of particular interest in crystallography because they are a standard model for ideal crystals. We briefly recall the notion of multilattices here and refer for further reading to [27] and references therein.

A subset L of $\mathbb{R}^d$ shall be called a *multilattice generated by the lattice* Γ *in* $\mathbb{R}^d$ if L is the union of Γ and a finite number of translated copies of Γ, that is, $L = \bigcup_{k=0}^{m-1}(x_k+\Gamma)$ where $x_k \in \mathbb{R}^d$, $m \in \mathbb{N}$, and $x_0 = 0$. In general, a multilattice is not a lattice. An orthogonal transformation $R \in O(d)$ will be called a *linear coincidence isometry of* L if $L(R) := L \cap RL$ includes a cosublattice of some shifted lattice $x_k+\Gamma$, $0 \le k \le m-1$. The intersection $L(R)$ shall be referred to as the *coincidence site multilattice* (CSML) of L generated by R. The density of $L(R)$ in L, by this we mean the ratio of the density of points in L by the density of points in $L(R)$, is the *coincidence index of* R *with respect to* L, which is denoted by $\Sigma_L(R)$. Note that $\Sigma_L(R)$ is not necessarily an integer.

The next lemma describes exactly when the intersection of the shifted lattice $x_k+\Gamma$ and the image of the shifted lattice $x_j+\Gamma$ under a linear isometry forms a cosublattice of $x_k+\Gamma$.

Lemma 6.1. *Suppose* Γ *is a lattice in* $\mathbb{R}^d$, $R \in O(d)$, *and* $x_j, x_k \in \mathbb{R}^d$. *Then* $(x_k+\Gamma) \cap R(x_j+\Gamma)$ *contains a cosublattice of* $x_k+\Gamma$ *if and only if* $R \in OC(\Gamma)$ *and* $Rx_j - x_k \in \Gamma + R\Gamma$. *Moreover, if* $Rx_j - x_k \in \ell_{j,k} + R\Gamma$ *with* $\ell_{j,k} \in \Gamma$, *then*

$$(x_k+\Gamma) \cap R(x_j+\Gamma) = (x_k+\ell_{j,k}) + \Gamma(R). \tag{6.1}$$

Proof. Write $(x_k+\Gamma) \cap R(x_j+\Gamma) = (x_k, \mathbb{1}_d)[\Gamma \cap (Rx_j - x_k, R)\Gamma]$. Then the intersection $(x_k+\Gamma) \cap R(x_j+\Gamma)$ contains a cosublattice of $x_k+\Gamma$ if and only if $(Rx_j - x_k, R) \in AC(\Gamma)$. By Theorem 3.3, the latter is equivalent to saying that $R \in OC(\Gamma)$ and $Rx_j - x_k \in \Gamma + R\Gamma$. It follows from (3.1) that

$$(x_k+\Gamma) \cap R(x_j+\Gamma) = (x_k, \mathbb{1}_d)[\ell_{j,k} + \Gamma(R)] = (x_k+\ell_{j,k}) + \Gamma(R). \qquad \square$$

Theorem 4.3 now follows directly from Lemma 6.1 by taking $x_k = x_j = x$.

Equation (6.1) tells us that given an $R \in OC(\Gamma)$ satisfying $Rx_j - x_k \in \Gamma + R\Gamma$, then the intersection $(x_k+\Gamma) \cap R(x_j+\Gamma)$ does not only contain a cosublattice of $x_k+\Gamma$, but is itself a cosublattice of $x_k+\Gamma$. In addition, the index of the cosublattice $(x_k+\Gamma) \cap R(x_j+\Gamma)$ in $x_k+\Gamma$ is $\Sigma(R)$.

Remark 6.2. Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice, $R \in O(d)$, and $x_j, x_k \in \mathbb{R}^d$. The intersection $(x_k+\Gamma) \cap R(x_j+\Gamma)$ is a cosublattice of $x_k+\Gamma$ if and only if it is a cosublattice of $Rx_j + R\Gamma$. Indeed, if $Rx_j - x_k \in Rt_{j,k} + \Gamma$ with $t_{j,k} \in \Gamma$ then

$$(x_k+\Gamma) \cap R(x_j+\Gamma) = (Rx_j - Rt_{j,k}) + \Gamma(R). \tag{6.2}$$

The cosublattice $(x_k+\Gamma) \cap R(x_j+\Gamma)$ is also of index $\Sigma(R)$ in $Rx_j + R\Gamma$.

The following theorem gives the solution of the coincidence problem for a multilattice.

Theorem 6.3. *Let $L = \bigcup_{k=0}^{m-1}(x_k + \Gamma)$ be a multilattice generated by the lattice Γ in $\mathbb{R}^d$, where $x_k \in \mathbb{R}^d$ for $0 \leq k \leq m-1$, $x_0 = 0$, and $x_k - x_j \notin \Gamma$ whenever $k \neq j$.*

(i) *The set of linear coincidence isometries of L is $OC(\Gamma)$.*
(ii) *Given an $R \in OC(\Gamma)$, let $\sigma = \{(x_j, x_k) : Rx_j - x_k \in \Gamma + R\Gamma\}$. Then*

$$\Sigma_L(R) = \tfrac{m}{|\sigma|}\Sigma(R).$$

In addition, if $Rx_j - x_k = \ell_{j,k} + Rt_{j,k}$ with $\ell_{j,k}, t_{j,k} \in \Gamma$, then

$$L(R) = \bigcup_{(x_j,x_k)\in\sigma} [(x_k + \ell_{j,k}) + \Gamma(R)] = \bigcup_{(x_j,x_k)\in\sigma} [(Rx_j - Rt_{j,k}) + \Gamma(R)]. \tag{6.3}$$

Proof. The intersection $L(R)$ can be expressed as the disjoint union

$$L(R) = L \cap RL = \bigcup_{j=0}^{m-1} \bigcup_{k=0}^{m-1} [(x_k + \Gamma) \cap R(x_j + \Gamma)]. \tag{6.4}$$

(i) Suppose R is a linear coincidence isometry of L. Then there is some shifted lattice $x_k + \Gamma$ for which $(x_k + \Gamma) \cap RL$ contains a cosublattice of $x_k + \Gamma$. Thus, $(x_k + \Gamma) \cap R(x_j + \Gamma) \neq \varnothing$ for some j with $0 \leq j \leq m-1$. However, the number of shifted copies of Γ in L is finite. This implies that the intersection $(x_k+\Gamma)\cap R(x_j+\Gamma)$ must be also a cosublattice of $x_k + \Gamma$. It now follows from Lemma 6.1 that $R \in OC(\Gamma)$. Conversely, if $R \in OC(\Gamma)$ then the sublattice $\Gamma(R)$ of Γ appears in $L(R)$. Thus, R is a linear coincidence isometry of L.
(ii) Since $(x_0, x_0) \in \sigma$, $|\sigma| \neq 0$. One sees from Lemma 6.1 that $(x_k+\Gamma)\cap R(x_j+\Gamma) \neq \varnothing$ whenever $(x_j, x_k) \in \sigma$. Applying (6.1) and (6.2) to each intersection of the disjoint union in (6.4) yields (6.3). Now, each $(x_j, x_k) \in \sigma$ contributes a different shifted copy of $\Gamma(R)$ to $L(R)$. This means that $L(R)$ is made up of $|\sigma|$ distinct shifted copies of $\Gamma(R)$, each of which is of index $\Sigma(R)$ in the respective shifted copy of Γ (or $R\Gamma$). Because L consists of m separate shifted copies of Γ, the formula for $\Sigma_L(R)$ follows. □

Therefore, the set of linear coincidence isometries of the multilattice L generated by Γ is still $OC(\Gamma)$, albeit the coincidence indices of an $R \in OC(\Gamma)$ with respect to Γ and L are not necessarily equal. Moreover, $L(R)$ consists of cosublattices of shifted lattices in L, one of which must always be $\Gamma(R)$.

7. Linear coincidences of the diamond packing

The *diamond packing* or *tetrahedral packing* is made up of two face-centered cubic (f.c.c.) lattices, wherein one of the f.c.c. lattices is a translate of the other by $\frac{1}{4}(a, a, a)$, with a being the length of the edges of a conventional unit cell of the f.c.c. lattice (see Figure 3). It is also known as the packing D_3^+ and is not a lattice [8]. An equivalent way of constructing the diamond packing as a motif of vertices of tetrahedrons and their barycenters can be found in [32]. Here, we use the results of Section 6 to identify the linear coincidence isometries, coincidence indices, and the resulting intersections of the diamond packing. To this end, we first recall the corresponding results for cubic lattices.

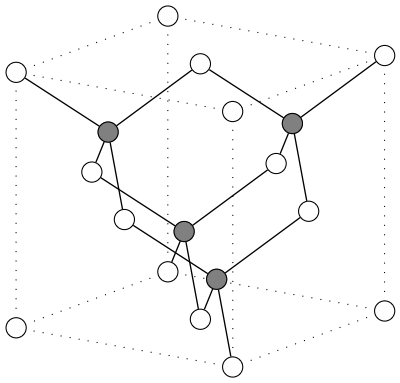

FIGURE 3. A conventional unit cell of the diamond packing. The white dots are part of the f.c.c. lattice while the gray dots belong to the shifted f.c.c. lattice

7.1. **Solution of the coincidence problem for the cubic lattices.** We see from Section 6 that it is imperative that we familiarize ourselves with the coincidences of the f.c.c. lattice (see [14, 17, 16, 1, 38]) before we even consider the coincidences of the diamond packing. Let $\Gamma_P = \mathbb{Z}^3$, $\Gamma_B = \Gamma_P \cup [(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) + \Gamma_P]$, and $\Gamma_F = \Gamma_B^*$ denote the primitive cubic (p.c.), body-centered cubic (b.c.c.), and f.c.c. lattice, respectively. Then $OC(\Gamma_P) = OC(\Gamma_B) = OC(\Gamma_F) = O(3, \mathbb{Q})$, and if $R \in O(3, \mathbb{Q})$, then $\Sigma_{\Gamma_P}(R) = \Sigma_{\Gamma_B}(R) = \Sigma_{\Gamma_F}(R)$ [17, 1]. Therefore, it is enough to look at the coincidences of the p.c. lattice.

Take $\Gamma = \mathbb{Z}^3$. As in the planar case, the analysis of $OC(\Gamma)$ starts with the set of coincidence rotations of Γ, $SO(3, \mathbb{Q})$, since anyway $O(3)$ is the direct product of $SO(3)$ and $\{\pm \mathbb{1}_3\}$, where $\mathbb{1}_3$ is the 3×3-identity matrix. To this end, Cayley's parametrization of matrices in $SO(3)$ by quaternions is used [1]. Let us first recall some results about quaternions and introduce some notations. Extensive treatments on quaternions can be found in [23, 9, 22, 19].

Let $\{\mathbf{e}, \mathbf{i}, \mathbf{j}, \mathbf{k}\}$ be the standard basis of $\mathbb{R}^4$ where $\mathbf{e} = (1,0,0,0)^T$, $\mathbf{i} = (0,1,0,0)^T$, $\mathbf{j} = (0,0,1,0)^T$, and $\mathbf{k} = (0,0,0,1)^T$. The *quaternion algebra over* $\mathbb{R}$ is the associative division algebra $\mathbb{H} := \mathbb{H}(\mathbb{R}) = \mathbb{R}\mathbf{e} + \mathbb{R}\mathbf{i} + \mathbb{R}\mathbf{j} + \mathbb{R}\mathbf{k} \cong \mathbb{R}^4$ where multiplication is defined by the relations

$$\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = \mathbf{ijk} = -\mathbf{e}.$$

Elements of $\mathbb{H}$ are called quaternions, and a quaternion q is written as either $q = q_0\mathbf{e} + q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k}$ or $q = (q_0, q_1, q_2, q_3)$. Given two quaternions q and p, their *inner product* is defined as the standard scalar product of q and p as vectors in $\mathbb{R}^4$.

The *conjugate* of a quaternion $q = (q_0, q_1, q_2, q_3)$ is $\overline{q} = (q_0, -q_1, -q_2, -q_3)$, and its *norm* is $|q|^2 = q\,\overline{q} = q_0^2 + q_1^2 + q_2^2 + q_3^2 \in \mathbb{R}$. It is easy to verify that $\overline{qp} = \overline{p}\,\overline{q}$ and $|q\,p|^2 = |q|^2|p|^2$ for any $q, p \in \mathbb{H}$.

A quaternion whose components are all integers is called a *Lipschitz quaternion* or *Lipschitz integer*. The set $\mathbb{L}$ of Lipschitz quaternions shall be denoted by

$$\mathbb{L} = \{(q_0, q_1, q_2, q_3) \in \mathbb{H} : q_0, q_1, q_2, q_3 \in \mathbb{Z}\}.$$

A *primitive quaternion* q is a quaternion in $\mathbb{L}$ whose components are relatively prime. On the other hand, a *Hurwitz quaternion* or *Hurwitz integer* is a quaternion whose components

are all integers or all half-integers. The set $\mathbb{J}$ of Hurwitz quaternions is given by

$$\mathbb{J} = \left\{(q_0, q_1, q_2, q_3) \in \mathbb{H} : q_0, q_1, q_2, q_3 \in \mathbb{Z} \text{ or } q_0, q_1, q_2, q_3 \in \tfrac{1}{2} + \mathbb{Z}\right\} = \mathbb{L} \cup [(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}) + \mathbb{L}].$$

Given a quaternion $q = (q_0, q_1, q_2, q_3)$, its *real part* and *imaginary part* are defined as $\mathrm{Re}\,(q) = q_0$ and $\mathrm{Im}\,(q) = q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k}$, respectively. The *imaginary space of* $\mathbb{H}$ is the three-dimensional vector subspace $\mathrm{Im}\,(\mathbb{H}) = \{\mathrm{Im}\,(q) : q \in \mathbb{H}\} \cong \mathbb{R}^3$ of $\mathbb{H}$.

An $R \in SOC(\Gamma) = SO(3, \mathbb{Q})$ can be parametrized by a primitive quaternion q so that for all $x \in \mathbb{R}^3$ viewed as an element of $\mathrm{Im}\,(\mathbb{H})$, $R(x) = qxq^{-1}$. In such a case, we denote R by R_q. As a matrix in $SO(3)$, R_q, with $q = (q_0, q_1, q_2, q_3)$ primitive, corresponds to

$$R_q = \frac{1}{|q|^2}\begin{pmatrix} q_0^2 + q_1^2 - q_2^2 - q_3^2 & -2q_0q_3 + 2q_1q_2 & 2q_0q_2 + 2q_1q_3 \\ 2q_0q_3 + 2q_1q_2 & q_0^2 - q_1^2 + q_2^2 - q_3^2 & -2q_0q_1 + 2q_2q_3 \\ -2q_0q_2 + 2q_1q_3 & 2q_0q_1 + 2q_2q_3 & q_0^2 - q_1^2 - q_2^2 + q_3^2 \end{pmatrix}.$$

However, observe that each element of $SO(3, \mathbb{Q})$ is encountered twice in Cayley's parametrization because $R_{-q} = R_q$. The coincidence index of $R_q \in SOC(\Gamma)$ is equal to the odd part of $|q|^2$, that is, $\Sigma(R_q) = \frac{|q|^2}{2^\ell}$, where ℓ is the largest power of 2 that divides $|q|^2$ [17, 16, 1].

Similarly, a primitive quaternion q can be associated to every $T \in OC(\Gamma) \setminus SOC(\Gamma)$ so that $T(x) = -qxq^{-1} = q\bar{x}q^{-1}$ for all $x \in \mathrm{Im}\,(\mathbb{H})$, in which case, T shall be written as T_q. Since $T_q = R_q \cdot (-\mathbb{1}_3)$ where $R_q \in SOC(\Gamma)$, $\Gamma(T_q) = \Gamma(R_q)$ and $\Sigma(T_q) = \Sigma(R_q)$.

Let $f_{\mathbb{Z}^3}(m)$ be the number of CSLs of $\mathbb{Z}^3$ of index m. Once again, $f_{\mathbb{Z}^3}$ is multiplicative and is given by

$$f_{\mathbb{Z}^3}(p^r) = \begin{cases} 0, & \text{if } p = 2 \\ (p+1)p^{r-1}, & \text{otherwise,} \end{cases}$$

where p is prime and $r \in \mathbb{N}$ [16, 1]. From this, one obtains the Dirichlet series generating function for $f_{\mathbb{Z}^3}$, namely,

$$\begin{aligned} \Phi_{\mathbb{Z}^3}(s) &= \sum_{m=1}^{\infty} \frac{f_{\mathbb{Z}^3}(m)}{m^s} = \prod_{p \neq 2} \frac{1 + p^{-s}}{1 - p^{1-s}} = \frac{1}{1 + 2^{-s}} \cdot \frac{\zeta_{\mathbb{J}}(s/2)}{\zeta(2s)} \\ &= 1 + \tfrac{4}{3^s} + \tfrac{6}{5^s} + \tfrac{8}{7^s} + \tfrac{12}{9^s} + \tfrac{12}{11^s} + \tfrac{14}{13^s} + \tfrac{24}{15^s} + \tfrac{18}{17^s} + \tfrac{20}{19^s} + \tfrac{32}{21^s} + \tfrac{24}{23^s} + \cdots, \end{aligned} \tag{7.1}$$

where $\zeta_{\mathbb{J}}(s) = \left(1 - 2^{1-2s}\right)\zeta(2s)\zeta(2s-1)$ is the zeta function of $\mathbb{J}$ or the Dirichlet series generating function for the number of nonzero right ideals of $\mathbb{J}$, compare [33]. One sees from (7.1) that all the coincidence indices of the cubic lattices are odd. Since $\mathbb{Z}^3$ has twenty-four symmetry rotations, the number of coincidence rotations of $\mathbb{Z}^3$ for a given index m is given by $\hat{f}_{\mathbb{Z}^3}(m) = 24 f_{\mathbb{Z}^3}(m)$. Consequently, the Dirichlet series generating function for $\hat{f}_{\mathbb{Z}^3}(m)$ is $24\Phi_{\mathbb{Z}^3}(s)$.

7.2. **The diamond packing viewed as a multilattice.** Take Γ to be an f.c.c. lattice. We identify $\mathbb{R}^3$ with $\mathrm{Im}\,(\mathbb{H})$, and associate Γ with

$$\Gamma = 2\mathrm{Im}\,(\mathbb{L}) \cup [(1,1,0) + 2\mathrm{Im}\,(\mathbb{L})] \cup [(0,1,1) + 2\mathrm{Im}\,(\mathbb{L})] \cup [(1,0,1) + 2\mathrm{Im}\,(\mathbb{L})].$$

The dual lattice of Γ is the b.c.c. lattice $\Gamma^* = \mathrm{Im}\,(\mathbb{J})$, and the diamond packing is identified with $D_3^+ = \Gamma \cup (x + \Gamma)$, where $x = \frac{1}{2}(1,1,1)$. It follows from Theorem 6.3 that the group of linear coincidence isometries of D_3^+ is $OC(\Gamma) = OC(\Gamma^*)$.

Theorem 6.3 suggests that it is necessary that we compute for $OC(x + \Gamma)$ to ascertain the coincidence index of a linear coincidence isometry R of D_3^+. To this end, note that

$\Gamma + R\Gamma = [\Gamma^*(R)]^*$, that is, $\Gamma + R\Gamma$ is the dual lattice of the CSL $\Gamma^*(R)$ of Γ^*. The next lemma, stated in [38], gives a spanning set for $\Gamma^*(R)$ over $\mathbb{Z}$.

Lemma 7.1. *Let* $\Gamma^* = \mathrm{Im}\,(\mathbb{J})$ *and* $R = R_q \in SOC(\Gamma^*)$ *where* $q = (q_0, q_1, q_2, q_3)$ *is a primitive quaternion. Let*

$$\begin{aligned} \mathbf{r_0} &:= \mathrm{Im}\,(q) = (q_1, q_2, q_3), & \mathbf{r_2} &:= \mathrm{Im}\,(q\mathbf{j}) = (-q_3, q_0, q_1), \\ \mathbf{r_1} &:= \mathrm{Im}\,(q\mathbf{i}) = (q_0, q_3, -q_2), & \mathbf{r_3} &:= \mathrm{Im}\,(q\mathbf{k}) = (q_2, -q_1, q_0). \end{aligned} \tag{7.2}$$

Then the CSL $\Gamma^*(R)$ *of* Γ^* *is the* $\mathbb{Z}$*-span of the following vectors:*

(i) $\mathbf{r_0}$, $\mathbf{r_1}$, $\mathbf{r_2}$, $\mathbf{r_3}$, $\frac{1}{2}(\mathbf{r_0} + \mathbf{r_1} + \mathbf{r_2} + \mathbf{r_3})$ *if* $|q|^2$ *is odd,*
(ii) $\mathbf{r_0}$, $\frac{1}{2}(\mathbf{r_0} + \mathbf{r_1})$, $\frac{1}{2}(\mathbf{r_0} + \mathbf{r_2})$, $\frac{1}{2}(\mathbf{r_0} + \mathbf{r_3})$ *if* $|q|^2 \equiv 2 \pmod 4$,
(iii) $\frac{1}{2}\mathbf{r_0}$, $\frac{1}{2}\mathbf{r_1}$, $\frac{1}{2}\mathbf{r_2}$, $\frac{1}{2}\mathbf{r_3}$ *if* $|q|^2 \equiv 0 \pmod 4$.

We now proceed to determine $OC(x+\Gamma)$. In the succeeding calculations, we embed $\mathrm{Im}\,(\mathbb{H})$ in $\mathbb{H}$ via the canonical projection so that vectors in $\mathrm{Im}\,(\mathbb{H})$ are treated as quaternions whose real part is 0.

Observe that for $u \in \{\mathbf{e}, \mathbf{i}, \mathbf{j}, \mathbf{k}\}$, $R = R_q \in SOC(\Gamma)$, and $x \in \mathrm{Im}\,(\mathbb{H})$, $\langle Rx - x, \mathrm{Im}\,(qu)\rangle = \langle uq - qu, x\rangle$. Denote by $\times$ the usual vector (cross) product of two vectors in $\mathrm{Im}\,(\mathbb{H}) \cong \mathbb{R}^3$. Given $a, b, c \in \mathrm{Im}\,(\mathbb{H})$, one has $a \times b = \frac{1}{2}(ab - ba)$ and $\langle a \times b, c\rangle = \langle a, b \times c\rangle$ (see for instance, [23]). Together, they imply that $\langle Rx - x, \mathrm{Im}\,(qu)\rangle = -2\langle q, u \times x\rangle$ whenever $u \in \{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$. Therefore, substituting the vectors in (7.2) yields

$$\begin{aligned} \langle Rx - x, \mathbf{r_0}\rangle &= 0, & \langle Rx - x, \mathbf{r_2}\rangle &= -2\langle q, \mathbf{j} \times x\rangle, \\ \langle Rx - x, \mathbf{r_1}\rangle &= -2\langle q, \mathbf{i} \times x\rangle, & \langle Rx - x, \mathbf{r_3}\rangle &= -2\langle q, \mathbf{k} \times x\rangle. \end{aligned} \tag{7.3}$$

From now on, let $x = \frac{1}{2}(0, 1, 1, 1)$. Keeping in mind that $Rx - x \in \Gamma + R\Gamma$ if and only if $\langle Rx - x, \mathbf{t}\rangle \in \mathbb{Z}$ for all $\mathbf{t} \in \Gamma^*(R)$, we consider the following three possibilities:

`Case I:` $|q|^2$ is odd

By Lemma 7.1, $\mathbf{t} = a\mathbf{r_0} + b\mathbf{r_1} + c\mathbf{r_2} + d\mathbf{r_3} + \frac{1}{2}e(\mathbf{r_0} + \mathbf{r_1} + \mathbf{r_2} + \mathbf{r_3})$, for some $a, b, c, d, e \in \mathbb{Z}$. It follows from (7.3) that

$$\langle Rx - x, \mathbf{t}\rangle = -\langle q, (0, b, c, d) \times (0, 1, 1, 1)\rangle \in \mathbb{Z}$$

for all $a, b, c, d, e \in \mathbb{Z}$. Thus, by Theorem 4.3, $R_q \in SOC(x + \Gamma)$ whenever $|q|^2$ is odd.

`Case II:` $|q|^2 \equiv 2 \pmod 4$

Write $\mathbf{t} = a\mathbf{r_0} + \frac{1}{2}b(\mathbf{r_0} + \mathbf{r_1}) + \frac{1}{2}c(\mathbf{r_0} + \mathbf{r_2}) + \frac{1}{2}d(\mathbf{r_0} + \mathbf{r_3})$, for some $a, b, c, d \in \mathbb{Z}$. Since $|q|^2 \equiv 2 \pmod 4$, $q = r + 2s$ for some $s \in \mathbb{J}$ and $r \in \{(1, 1, 0, 0), (1, 0, 1, 0), (1, 0, 0, 1)\}$. Then

$$\langle Rx - x, \mathbf{t}\rangle = -\tfrac{1}{2}\langle r, (0, b, c, d) \times (0, 1, 1, 1)\rangle - \langle s, (0, b, c, d) \times (0, 1, 1, 1)\rangle \notin \mathbb{Z}$$

for some values of $b, c, d \in \mathbb{Z}$. This means that $R_q \notin SOC(x + \Gamma)$ if $|q|^2 \equiv 2 \pmod 4$.

`Case III:` $|q|^2 \equiv 0 \pmod 4$

One can express $\mathbf{t}$ as $\mathbf{t} = \frac{1}{2}a\mathbf{r_0} + \frac{1}{2}b\mathbf{r_1} + \frac{1}{2}c\mathbf{r_2} + \frac{1}{2}d\mathbf{r_3}$ for some $a, b, c, d \in \mathbb{Z}$. Write $q = r + 2s$ where $s \in \mathbb{L}$ and $r = (1, 1, 1, 1)$, which is possible because $|q|^2 \equiv 0 \pmod 4$. This yields

$$\langle Rx - x, \mathbf{t}\rangle = -\langle s, (0, b, c, d) \times (0, 1, 1, 1)\rangle \in \mathbb{Z},$$

for all $a, b, c, d \in \mathbb{Z}$. Consequently, $R_q \in SOC(x + \Gamma)$ whenever $|q|^2 \equiv 0 \pmod 4$.

The following lemma summarizes the results for $OC(x + \Gamma)$.

Lemma 7.2. *Let Γ be the f.c.c. lattice*

$$\Gamma = 2\mathrm{Im}\,(\mathbb{L}) \cup [(1,1,0) + 2\mathrm{Im}\,(\mathbb{L})] \cup [(0,1,1) + 2\mathrm{Im}\,(\mathbb{L})] \cup [(1,0,1) + 2\mathrm{Im}\,(\mathbb{L})],$$

and $x = \frac{1}{2}(1,1,1)$. Then $(S)OC(x+\Gamma)$ is a subgroup of $(S)OC(\Gamma)$ of index 2 given by

$$SOC(x+\Gamma) = \left\{ R_q \in SOC(\Gamma) : |q|^2 \not\equiv 2 \pmod 4 \right\}, \text{ and}$$
$$OC(x+\Gamma) = SOC(x+\Gamma) \cup \left\{ T_q : |q|^2 \equiv 2 \pmod 4 \right\}.$$

If $f_{x+\Gamma}(m)$, $\hat{f}_{x+\Gamma}(m)$, and $\hat{F}_{x+\Gamma}(m)$ denote the number of CSLs, coincidence rotations, and linear coincidence isometries of $x+\Gamma$ of index m, respectively, then $f_{x+\Gamma}(m) = f_{\mathbb{Z}^3}(m)$, $\hat{f}_{x+\Gamma}(m) = 12 f_{x+\Gamma}(m)$, and $\hat{F}_{x+\Gamma}(m) = 24 f_{x+\Gamma}(m)$.

Proof. The explicit expression for $SOC(x+\Gamma)$ was obtained from the computations preceding the lemma. Similar calculations yield $OC(x+\Gamma)$.

Now, $R \in SOC(x+\Gamma)$ if and only if R is parametrized by a quaternion q with $|q|^2 = 2^m\alpha$, where m is an even integer and α is odd. Similarly, the coincidence reflection $T \in OC(x+\Gamma)$ if and only if T is parametrized by a quaternion q with $|q|^2 = 2^n\beta$, where n and β are odd integers. With these two criteria, one concludes by going through all the possible cases that $(S)OC(x+\Gamma)$ is closed under composition. Hence, by Proposition 4.9, $(S)OC(x+\Gamma)$ is a group.

It follows then from Proposition 4.4 that $f_{x+\Gamma}(m) = f_{\mathbb{Z}^3}(m)$. Furthermore, expressions for $\hat{f}_{x+\Gamma}(m)$ and $\hat{F}_{x+\Gamma}(m)$ follow from the fact that there are 12 symmetry rotations R_q with $|q|^2 \not\equiv 2 \pmod 4$, and 12 rotoreflection symmetries T_q with $|q|^2 \equiv 2 \pmod 4$, respectively. □

Finally, applying the same technique used in computing for $SOC(x+\Gamma)$, one can show that both x and Rx are not in $\Gamma + R\Gamma$ for all $R \in OC(\Gamma)$. Theorem 6.3, together with Lemma 7.2, brings about the following solution of the coincidence problem for the diamond packing.

Theorem 7.3. *Let Γ be the f.c.c. lattice*

$$\Gamma = 2\mathrm{Im}\,(\mathbb{L}) \cup [(1,1,0) + 2\mathrm{Im}\,(\mathbb{L})] \cup [(0,1,1) + 2\mathrm{Im}\,(\mathbb{L})] \cup [(1,0,1) + 2\mathrm{Im}\,(\mathbb{L})],$$

and D_3^+ be the diamond packing $D_3^+ = \Gamma \cup (x+\Gamma)$, where $x = \frac{1}{2}(1,1,1)$. Then the group of linear coincidence isometries of D_3^+ is $OC(\Gamma)$. In particular, $R = R_q \in SOC(\Gamma)$ is a coincidence rotation of D_3^+ with

(i) $D_3^+(R) = \Gamma(R)$ *and* $\Sigma_{D_3^+}(R) = 2\Sigma_\Gamma(R) = |q|^2$ *if* $|q|^2 \equiv 2 \pmod 4$.

(ii) $D_3^+(R) = \Gamma(R) \cup [(x+\ell) + \Gamma(R)]$, *where* $\ell \in (Rx - x + R\Gamma) \cap \Gamma$, *and*

$$\Sigma_{D_3^+}(R) = \Sigma_\Gamma(R) = \begin{cases} |q|^2, & \text{if } |q|^2 \text{ is odd} \\ \frac{1}{4}|q|^2, & \text{if } |q|^2 \equiv 0 \pmod 4. \end{cases}$$

Also, $T = T_q \in OC(\Gamma) \setminus SOC(\Gamma)$ is a coincidence rotoreflection of D_3^+ with

(i) $D_3^+(T) = \Gamma(T)$ *and* $\Sigma_{D_3^+}(T) = 2\Sigma_\Gamma(T) = \begin{cases} 2|q|^2, & \text{if } |q|^2 \text{ is odd} \\ \frac{1}{2}|q|^2, & \text{if } |q|^2 \equiv 0 \pmod 4. \end{cases}$

(ii) $D_3^+(T) = \Gamma(T) \cup [(x+\ell) + \Gamma(T)]$, *where* $\ell \in (Tx - x + T\Gamma) \cap \Gamma$, *and* $\Sigma_{D_3^+}(T) = \Sigma_\Gamma(T) = \frac{1}{2}|q|^2$ *if* $|q|^2 \equiv 2 \pmod 4$.

If $f_{D_3^+}(m)$ is the number of CSMLs of D_3^+ of index m, then $f_{D_3^+}$ is multiplicative and for primes p and $r \in \mathbb{N}$,

$$f_{D_3^+}(p^r) = \begin{cases} 1, & \text{if } p^r = 2 \\ 0, & \text{if } p = 2 \text{ and } r > 1 \\ (p+1)p^{r-1}, & \text{otherwise.} \end{cases}$$

The Dirichlet series generating function for $f_{D_3^+}(m)$ reads

$$\begin{aligned} \Phi_{D_3^+}(s) &= \sum_{m=1}^{\infty} \frac{f_{D_3^+}(m)}{m^s} = (1+2^{-s}) \cdot \Phi_{\mathbb{Z}^3}(s) = \frac{\zeta_{\mathbb{J}}(s/2)}{\zeta(2s)} \\ &= 1 + \tfrac{1}{2^s} + \tfrac{4}{3^s} + \tfrac{6}{5^s} + \tfrac{4}{6^s} + \tfrac{8}{7^s} + \tfrac{12}{9^s} + \tfrac{6}{10^s} + \tfrac{12}{11^s} + \tfrac{14}{13^s} + \tfrac{8}{14^s} + \tfrac{24}{15^s} + \tfrac{18}{17^s} + \cdots . \end{aligned}$$

Finally, the number of CSMLs of D_3^+ with index at most N is asymptotically $\frac{9N^2}{2\pi^2}$.

8. Outlook

In this paper, the idea of linear coincidence isometries of lattices was extended to include affine isometries. Moreover, the coincidence problem for shifted lattices and for multilattices was formulated in a mathematical setting and was solved for some important examples. Considering further lattices and crystal structures would be interesting. For applications to quasicrystals, the ideas in this paper should be extended to the $\mathbb{Z}$-module case. In particular, techniques implemented and results obtained in Section 5 on the coincidences of a shifted square lattice may be generalized to planar modules by identifying these modules with rings of cyclotomic integers. Initial results in this direction can be found in [25].

The set of affine coincidence isometries of a lattice and the set of linear coincidence isometries of a shifted lattice do not form a group in general. An investigation of their algebraic structure should prove worthwhile. It has been shown in [25] that both sets are groupoids if and only if they are groups. An example where the set of coincidence rotations of a shifted lattice fails to form a group is still lacking. Such an example might be found in three-dimensions, where $O(d)$ is not abelian anymore.

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