Coincidences of Hypercubic Lattices in 4 dimensions

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Abstract

We consider the CSLs of 4–dimensional hypercubic lattices. In particular, we derive the coincidence index Σ and calculate the number of different CSLs as well as the number of inequivalent CSLs for a given Σ. The hypercubic face centered case is dealt with in detail and it is sketched how to derive the corresponding results for the primitive hypercubic lattice.

1 Introduction

Coincidence site lattices (CSL) for three–dimensional lattices have been studied intensively since they are an important tool to characterize and analyze the structure of grain boundaries in crystals ([1, 2] and references therein). For quasicrystals these concepts have to be adapted. Since a lot of quasiperiodic structures can be obtained by the well–known cut and projection scheme [3, 4] from a periodic structure in superspace, it is natural to also investigate CSLs in higher dimension. An important example are the four–dimensional hypercubic lattices, which shall be discussed here. Four–dimensional lattices are particularly interesting since they are the first ones that allow 5–fold, 8–fold, 10–fold and 12–fold symmetries which are actually observed in quasicrystals. In particular the four–dimensional hypercubic lattices allow 8–fold symmetries, from which we can obtain e.g. the prominent Ammann–Beenker tiling [4].

Since rotations in four–dimensional space can be parameterized by quaternions, one has a strong tool to investigate the CSLs of the hypercubic lattices. In particular, one knows all coincidence rotations [5] and thus all CSLs can be characterized. But one can go much further and this will be done in the present paper. We first calculate the coincidence index Σ and then we try to find all CSLs for a given index Σ. It turns out that one can calculate the total number of different CSLs for a given Σ and furthermore, we can derive even the number of inequivalent CSLs and for each CSL we can calculate the number of equivalent CSLs.

These calculations are facilitated by the fact that the four–dimensional rotations are closely related to the their three–dimensional counterparts. In particular we exploit the fact that $SO(4) \simeq SU(2) \times SU(2)/C_2$, i.e. we can make use of the results of the three–dimensional cubic case that have been published recently [6]. Thus the results of the hypercubic case are quite similar to the three–dimensional results, although proofs are a bit more lengthy and the resulting formulas are a bit more complex. However, there is one big difference between three and four dimensions: Whereas all important quantities like Σ, number of CSLs etc. are equal for all three kinds of cubic lattices, this is no longer true for four dimensions. For a given coincidence rotation R, the coincidence indices for the primitive and the face centered hypercubic lattice are in general not the same, which is not surprising since the point groups are different, too. Thus we must deal with both cases separately. However, one can derive the results of the primitive lattice from the corresponding results of the face centered lattice. Thus we concentrate on the latter and sketch how these results can then be used for the primitive hypercubic lattice.

Now let us recall some basic facts and fix the notation. Let $\boldsymbol{L} \subseteq \mathbb{R}^n$ be an n-dimensional lattice and R a rotation. Then $\boldsymbol{L}(R) = \boldsymbol{L} \cap R\boldsymbol{L}$ is called a *coincidence site lattice* (CSL) if it is a sublattice of finite index of $\boldsymbol{L}$, the corresponding rotation is called a coincidence rotation [5]. The coincidence index $\Sigma(R)$ is defined as the index of $\boldsymbol{L}(R)$ in $\boldsymbol{L}$. By index we mean the group theoretical index of $\boldsymbol{L}(R)$ in $\boldsymbol{L}$, where we view $\boldsymbol{L}(R)$ and $\boldsymbol{L}$ as additive groups.

Any rotation in 4 dimensions can be parameterized by two quaternions $\boldsymbol{p} = (k, \ell, m, n)$ and $\boldsymbol{q} = (a, b, c, d)$ in the following way [7, 8, 9]:

$$R(\boldsymbol{p}, \boldsymbol{q}) = \frac{1}{|\boldsymbol{p}\boldsymbol{q}|} M(\boldsymbol{p}, \boldsymbol{q}) \tag{1}$$

$$M(\boldsymbol{p}, \boldsymbol{q}) = \begin{pmatrix} \langle \boldsymbol{p}|\boldsymbol{q}\rangle & \langle \boldsymbol{p}\boldsymbol{u}_1|\boldsymbol{q}\rangle & \langle \boldsymbol{p}\boldsymbol{u}_2|\boldsymbol{q}\rangle & \langle \boldsymbol{p}\boldsymbol{u}_3|\boldsymbol{q}\rangle \\ \langle \boldsymbol{p}|\boldsymbol{u}_1\boldsymbol{q}\rangle & \langle \boldsymbol{p}\boldsymbol{u}_1|\boldsymbol{u}_1\boldsymbol{q}\rangle & \langle \boldsymbol{p}\boldsymbol{u}_2|\boldsymbol{u}_1\boldsymbol{q}\rangle & \langle \boldsymbol{p}\boldsymbol{u}_3|\boldsymbol{u}_1\boldsymbol{q}\rangle \\ \langle \boldsymbol{p}|\boldsymbol{u}_2\boldsymbol{q}\rangle & \langle \boldsymbol{p}\boldsymbol{u}_1|\boldsymbol{u}_2\boldsymbol{q}\rangle & \langle \boldsymbol{p}\boldsymbol{u}_2|\boldsymbol{u}_2\boldsymbol{q}\rangle & \langle \boldsymbol{p}\boldsymbol{u}_3|\boldsymbol{u}_2\boldsymbol{q}\rangle \\ \langle \boldsymbol{p}|\boldsymbol{u}_3\boldsymbol{q}\rangle & \langle \boldsymbol{p}\boldsymbol{u}_1|\boldsymbol{u}_3\boldsymbol{q}\rangle & \langle \boldsymbol{p}\boldsymbol{u}_2|\boldsymbol{u}_3\boldsymbol{q}\rangle & \langle \boldsymbol{p}\boldsymbol{u}_3|\boldsymbol{u}_3\boldsymbol{q}\rangle \end{pmatrix} \tag{2}$$

$$= \begin{pmatrix} ak+b\ell+cm+dn & -a\ell+bk+cn-dm & -am-bn+ck+d\ell & -an+bm-c\ell+dk \\ a\ell-bk+cn-dm & ak+b\ell-cm-dn & -an+bm+c\ell-dk & am+bn+ck+d\ell \\ am-bn-ck+d\ell & an+bm+c\ell+dk & ak-b\ell+cm-dn & -a\ell-bk+cn+dm \\ an+bm-c\ell-dk & -am+bn-ck+d\ell & a\ell+bk+cn+dm & ak-b\ell-cm+dn \end{pmatrix} \tag{3}$$

Here, $\boldsymbol{u}_i$ are the unit quaternions $\boldsymbol{u}_0 = (1,0,0,0)$, $\boldsymbol{u}_1 = (0,1,0,0)$, $\boldsymbol{u}_2 = (0,0,1,0)$ and $\boldsymbol{u}_3 = (0,0,0,1)$ and $|\boldsymbol{p}|^2 = k^2+\ell^2+m^2+n^2$ is the norm of $\boldsymbol{p}$. Furthermore we have made use of the inner product $\langle \boldsymbol{p}|\boldsymbol{q}\rangle := ak+b\ell+cm+dn$. If we identify the quaternions with the elements of $\mathbb{Z}^4$ (or $\mathbb{R}^4$) in the obvious way, then the action of $M(\boldsymbol{p},\boldsymbol{q})$ on a vector $\boldsymbol{x} \in \mathbb{Z}^4$ can be written as $M(\boldsymbol{p},\boldsymbol{q})\boldsymbol{x} = \boldsymbol{p}\boldsymbol{x}\bar{\boldsymbol{q}}$. Here $\bar{\boldsymbol{q}} = (a,-b,-c,-d)$ denotes the conjugate of $\boldsymbol{q}$. By an *integral* quaternion we mean a quaternion with integral coefficients. If the greatest common divisor of all coefficients is 1, we call the quaternion *primitive*. In the following, all quaternions will be either primitive or normalized to unity. It will always be clear from the context which convention has been chosen. Obviously $R(\boldsymbol{p},\boldsymbol{q})$ is a rational matrix if $\boldsymbol{p}$ and $\boldsymbol{q}$ are integral quaternions such that $|\boldsymbol{p}\boldsymbol{q}|$ is an integer. In this case we call the pair $(\boldsymbol{p},\boldsymbol{q})$ *admissible* [5]. On the other hand any rational orthogonal matrix R can be parameterized by an admissible pair of integral quaternions. Furthermore recall $\boldsymbol{p}^{-1} = \frac{1}{|\boldsymbol{p}|^2}\bar{\boldsymbol{p}}$.

2 The CSLs and their Σ–values

In 4 dimensions there are only two different hypercubic lattices, namely the primitive and the centered hypercubic lattices. They are equivalent to $\boldsymbol{L}_P = \mathbb{Z}^4$ and $\boldsymbol{L}_F = D_4$, respectively. $D_4 \subset \mathbb{Z}^4$ is of index 2 and consists of all integer vectors $\boldsymbol{n}$ with $|\boldsymbol{n}|^2$ even. It is known that R is a coincidence rotation of $\mathbb{Z}^4$ or D_4, if and only if all its entries are rational [5], i.e. $R = R(\boldsymbol{p},\boldsymbol{q})$ for some admissible pair of primitive quaternions $(\boldsymbol{p},\boldsymbol{q})$. In order to analyze the CSLs it is often convenient to find some appropriate sublattices of the CSLs. To this end we define the *denominator*

$$\mathrm{den}(R) = \gcd\{k \in \mathbb{N} | kR\boldsymbol{L} \subseteq \boldsymbol{L}(R)\}, \tag{4}$$

where gcd denotes the greatest common divisor. Since $\mathrm{den}(R)\cdot \boldsymbol{L}$ is a sublattice of $\boldsymbol{L}(R)$ it follows that

$$\mathrm{den}(R) \le \Sigma(R) \le \mathrm{den}(R)^n, \tag{5}$$

where $n=4$ is the dimension of $\boldsymbol{L}$. In case of the primitive cubic lattice this definition coincides with [5]

$$\mathrm{den}_P(R) = \gcd\{k \in \mathbb{N} | kR \text{ integer matrix}\}, \tag{6}$$

whereas for the centered lattice we find

$$\mathrm{den}_F(R) = 2^{-\ell}\,\mathrm{den}_P(R), \tag{7}$$

where $\ell = 0,1$ is the maximal power such that 2^ℓ divides $\mathrm{den}_P(R)$. In particular we find for any admissible pair $\boldsymbol{p},\boldsymbol{q}$

$$\mathrm{den}_F(R(\boldsymbol{p},\boldsymbol{q})) = 2^{-\ell}|\boldsymbol{p}\boldsymbol{q}|, \tag{8}$$

where $\ell = 0,1,2$ is the maximal power such that 2^ℓ divides $|\boldsymbol{p}\boldsymbol{q}|$.

It follows from Eq. (5) that R is a symmetry operation of $\boldsymbol{L}$ if and only if $\mathrm{den}(R) = 1$. Thus $R(\boldsymbol{p},\boldsymbol{q})$ is a symmetry operation of the centered lattice D_4 if and only if $|\boldsymbol{p}|^2 = 1,4$ and $|\boldsymbol{q}|^2 = 1,4$ or $|\boldsymbol{p}|^2 = |\boldsymbol{q}|^2 = 2$. This gives the well known 576 pure symmetry rotations of D_4. Note that not all of them are integer matrices, which reflects the fact that the symmetry group of D_4 is larger than those of $\mathbb{Z}^4$. In fact only 192 rotations are integer matrices, namely the pure symmetry rotations of $\mathbb{Z}^4$. These are the rotations corresponding to the pairs $(\boldsymbol{p},\boldsymbol{q})$ such that $|\boldsymbol{p}|^2 = |\boldsymbol{q}|^2 = 1$ or $|\boldsymbol{p}|^2 = |\boldsymbol{q}|^2 = 2$ with $\langle \boldsymbol{p}|\boldsymbol{q}\rangle$ even or $|\boldsymbol{p}|^2 = |\boldsymbol{q}|^2 = 4$ with $\langle \boldsymbol{p}|\boldsymbol{q}\rangle$ divisible by 4.

We consider the face centered lattice first, formulating and proving a result that was first stated (without proof) in [5], Eq. (3.21).

Theorem 2.1 *Let $\boldsymbol{p},\boldsymbol{q}$ be an admissible pair of primitive integer quaternions and let $\Sigma(\boldsymbol{p}) = 2^{-\ell}|\boldsymbol{p}|^2$, where $\ell = 0,1,2$ is the maximal power such that 2^ℓ divides $|\boldsymbol{p}|^2$. Then, for the fcc–lattice, the rotation $R(\boldsymbol{p},\boldsymbol{q})$ has coincidence index*

$$\Sigma_F(\boldsymbol{p},\boldsymbol{q}) := \Sigma_F(R(\boldsymbol{p},\boldsymbol{q})) = \mathrm{lcm}(\Sigma(\boldsymbol{p}),\Sigma(\boldsymbol{q})). \tag{9}$$

Proof: Let us write $|\boldsymbol{p}|^2 = \alpha^2\gamma$, $|\boldsymbol{q}|^2 = \beta^2\gamma$, where $\gamma = \gcd(|\boldsymbol{p}|^2, |\boldsymbol{q}|^2)$. Further let $\boldsymbol{p}^{(i)} = \boldsymbol{p}\boldsymbol{u}_i$ and $\bar{\boldsymbol{q}}^{(i)} = \bar{\boldsymbol{u}}_i\bar{\boldsymbol{q}}$. Then $\beta\boldsymbol{p}^{(i)}$ and $\alpha\bar{\boldsymbol{q}}^{(j)}$ are integer vectors with integer pre-images. Thus they are in $\boldsymbol{L}_P(R)$ and hence certainly $2\beta\boldsymbol{p}^{(i)}$ and $2\alpha\bar{\boldsymbol{q}}^{(j)}$ are in $\boldsymbol{L}_F(R)$.[1] Thus if $i \neq j$ and $k \neq \ell$ the four vectors $2\beta\boldsymbol{p}^{(i)}, 2\beta\boldsymbol{p}^{(j)}, 2\alpha\bar{\boldsymbol{q}}^{(k)}, 2\alpha\bar{\boldsymbol{q}}^{(\ell)}$ span a sublattice of $\boldsymbol{L}_F(R)$. Now

$$\det\left(\beta\boldsymbol{p}^{(i)}, \beta\boldsymbol{p}^{(j)}, \alpha\bar{\boldsymbol{q}}^{(k)}, \alpha\bar{\boldsymbol{q}}^{(\ell)}\right) = \alpha^2\beta^2(\langle\boldsymbol{p}^{(i)}|\bar{\boldsymbol{q}}^{(k')}\rangle\langle\boldsymbol{p}^{(j)}|\bar{\boldsymbol{q}}^{(\ell')}\rangle - \langle\boldsymbol{p}^{(i)}|\bar{\boldsymbol{q}}^{(\ell')}\rangle\langle\boldsymbol{p}^{(j)}|\bar{\boldsymbol{q}}^{(k')}\rangle, \tag{10}$$

[1] Unless $|\boldsymbol{p}|^2$ and $|\boldsymbol{q}|^2$ are both odd, even $\beta\boldsymbol{p}^{(i)}$ and $\alpha\bar{\boldsymbol{q}}^{(j)}$ are elements of $\boldsymbol{L}_F(R)$. In any case $\beta(\boldsymbol{p}^{(i)}+\boldsymbol{p}^{(j)}) \in \boldsymbol{L}_F(R)$ and $\alpha(\bar{\boldsymbol{q}}^{(k)}+\bar{\boldsymbol{q}}^{(\ell)}) \in \boldsymbol{L}_F(R)$.

where k', ℓ' are chosen such that (k', ℓ', k, ℓ) is an even permutation of $(0,1,2,3)$. Hence we conclude that $\Sigma_F(R)$ divides $8\alpha^2\beta^2 c$, where c is the greatest common divisor of $c^{ijk\ell} = \langle \boldsymbol{p}^{(i)}|\bar{\boldsymbol{q}}^{(k)}\rangle\langle \boldsymbol{p}^{(j)}|\bar{\boldsymbol{q}}^{(\ell)}\rangle - \langle \boldsymbol{p}^{(i)}|\bar{\boldsymbol{q}}^{(\ell)}\rangle\langle \boldsymbol{p}^{(j)}|\bar{\boldsymbol{q}}^{(k)}\rangle)$. Using the expansion

$$|\boldsymbol{p}|^2\boldsymbol{a} = \sum_{i=0}^{3}\langle \boldsymbol{p}^{(i)}|\boldsymbol{a}\rangle \boldsymbol{p}^{(i)} \tag{11}$$

we see that c divides

$$\sum_{i=0}^{3} c^{ijk\ell}\langle \boldsymbol{p}^{(i)}|\boldsymbol{a}\rangle = |\boldsymbol{p}|^2(\langle \boldsymbol{a}|\bar{\boldsymbol{q}}^{(k)}\rangle\langle \boldsymbol{p}^{(j)}|\bar{\boldsymbol{q}}^{(\ell)}\rangle - \langle \boldsymbol{a}|\bar{\boldsymbol{q}}^{(\ell)}\rangle\langle \boldsymbol{p}^{(j)}|\bar{\boldsymbol{q}}^{(k)}\rangle) \tag{12}$$

for any integer quaternion $\boldsymbol{a}$. We now choose $\boldsymbol{a}$ such that $\langle \boldsymbol{a}|\bar{\boldsymbol{q}}^{(k)}\rangle = 0$, in particular if $k=0$ we choose $\boldsymbol{a} = q_\ell \boldsymbol{u}_0 + q_0\boldsymbol{u}_\ell$ and $\boldsymbol{a} = \bar{\boldsymbol{q}}^{(\ell)} - q_\ell\boldsymbol{u}_0 - q_0\boldsymbol{u}_\ell$. Hence c must divide $|\boldsymbol{p}|^2(q_m^2+q_n^2)\langle \boldsymbol{p}^{(j)}|\bar{\boldsymbol{q}}\rangle$. Now $\bar{\boldsymbol{q}}$ is primitive so that the greatest common divisor of all combinations $q_m^2+q_n^2$ is at most 2. Thus c divides $2|\boldsymbol{p}|^2\langle \boldsymbol{p}^{(j)}|\bar{\boldsymbol{q}}\rangle$. Similarly one proofs that c divides $2|\boldsymbol{p}|^2\langle \boldsymbol{p}^{(j)}|\bar{\boldsymbol{q}}^{(k)}\rangle$ for arbitrary k, and hence c must divide $8|\boldsymbol{p}|^2$ because $\boldsymbol{q}$ and $\boldsymbol{p}$ are both primitive. In the same way one shows that c divides $8|\boldsymbol{q}|^2$. Thus c divides 8γ and $\Sigma_F(R)$ divides $64\alpha^2\beta^2\gamma$. But $\Sigma_F(R)$ divides $\mathrm{den}_F(R)^4$, which is odd. So $\Sigma_F(R)$ divides $\mathrm{lcm}(\Sigma(\boldsymbol{p}), \Sigma(\boldsymbol{q}))$.

It remains to show the converse statement, $\mathrm{lcm}(\Sigma(\boldsymbol{p}), \Sigma(\boldsymbol{q})) \le \Sigma_F(R)$. To this end, we count the vectors $\boldsymbol{y} \in \boldsymbol{L}_F(R)$ contained in the hypercube $H(2\beta\boldsymbol{p}^{(i)})$ spanned by $2\beta\boldsymbol{p}^{(i)}$. If there are n_F of them then $\Sigma_F(R) = 8\beta^4|\boldsymbol{p}|^4/n_F = 8\alpha^4|\boldsymbol{q}|^4/n_F$. Now $\boldsymbol{L}_F(R)$ is a sublattice of $\boldsymbol{L}_P(R)$, so that $\Sigma_F(R)$ is a multiple of $8\beta^4|\boldsymbol{p}|^4/n_P$ if n_P denotes the number of vectors $\boldsymbol{y} \in \boldsymbol{L}_P(R)$ contained in the hypercube $H(2\beta\boldsymbol{p}^{(i)})$. Now $n_P = 16n'_P$, where n'_P is the number of the vectors $\boldsymbol{y} \in \boldsymbol{L}_P(R)$ contained in the smaller hypercube $H(\beta\boldsymbol{p}^{(i)})$ spanned by $\beta\boldsymbol{p}^{(i)}$. Equivalently we can count their pre-images $\boldsymbol{x} = R^{-1}\boldsymbol{y}$ lying inside the hypercube $H(\alpha\boldsymbol{u}_i\boldsymbol{q})$. In the following we identify $H(\alpha\boldsymbol{u}_i\boldsymbol{q})$ with the factor group $\boldsymbol{L}_P/\boldsymbol{L}_{\boldsymbol{q}}$, where $\boldsymbol{L}_{\boldsymbol{q}}$ denotes the $\mathbb{Z}$–span of the vectors $\alpha\boldsymbol{u}_i\boldsymbol{q}$.

Observe that any vector $\boldsymbol{x}$ of $H(\alpha\boldsymbol{u}_i\boldsymbol{q})$ can be expressed as

$$\boldsymbol{x} = \frac{1}{|\boldsymbol{q}|^2}\sum_{i=0}^{3}\langle \boldsymbol{x}|\boldsymbol{u}_i\boldsymbol{q}\rangle \boldsymbol{u}_i\boldsymbol{q}, \tag{13}$$

such that $0 \le \langle \boldsymbol{x}|\boldsymbol{u}_i\boldsymbol{q}\rangle < \alpha|\boldsymbol{q}|^2$. Now $\boldsymbol{x}$ is in $\boldsymbol{L}_P(R)$ if its image

$$R(\boldsymbol{p},\boldsymbol{q})\boldsymbol{x} = \frac{1}{|\boldsymbol{p}\boldsymbol{q}|}\sum_{i=0}^{3}\boldsymbol{p}^{(i)}\langle \boldsymbol{x}|\boldsymbol{u}_i\boldsymbol{q}\rangle \tag{14}$$

is an integral vector. Since

$$\langle \boldsymbol{p}^{(i)}|R\boldsymbol{x}\rangle = \frac{|\boldsymbol{p}|}{|\boldsymbol{q}|}\langle \boldsymbol{x}|\boldsymbol{u}_i\boldsymbol{q}\rangle = \frac{\alpha}{\beta}\langle \boldsymbol{x}|\boldsymbol{u}_i\boldsymbol{q}\rangle \tag{15}$$

all coefficients $\langle \boldsymbol{x}|\boldsymbol{u}_i\boldsymbol{q}\rangle$ must be divisible by β. In order to determine the vectors that satisfy this condition we first observe that there exists a vector $\boldsymbol{x}$ such that $\langle \boldsymbol{x}|\boldsymbol{q}\rangle = 1$ since $\boldsymbol{q}$ is primitive. Regarding $\boldsymbol{x}$ as an element of the abelian group $\boldsymbol{L}_P/\boldsymbol{L}_{\boldsymbol{q}}$ we see that it has order $\alpha|\boldsymbol{q}|^2$. Among all vectors $\boldsymbol{x}'$ with $\langle \boldsymbol{x}'|\boldsymbol{q}\rangle = 0$ there exists one of order $\alpha|\boldsymbol{q}|^2/2$ or $\alpha|\boldsymbol{q}|^2$, depending on whether $|\boldsymbol{q}|^2$ is divisible by 4 or not.[2] Hence $\boldsymbol{x}$ and $\boldsymbol{x}'$ generate a subgroup of order $\alpha^2|\boldsymbol{q}|^4$ or $\alpha^2|\boldsymbol{q}|^4/2$ of $\boldsymbol{L}_P/\boldsymbol{L}_{\boldsymbol{q}}$. Condition (15) is satisfied by $\alpha^2|\boldsymbol{q}|^4/\beta^2$ or $\alpha^2|\boldsymbol{q}|^4/(2\beta^2)$ of them, respectively. Thus $\boldsymbol{L}_P/\boldsymbol{L}_{\boldsymbol{q}}$ contains at most $\alpha^4|\boldsymbol{q}|^4/\beta^2$ vectors satisfying condition (15) and hence n'_P is a divisor of $\alpha^4|\boldsymbol{q}|^4/\beta^2$. Let $\boldsymbol{L}_P^\beta$ denote the subgroup of $\boldsymbol{L}_P/\boldsymbol{L}_{\boldsymbol{q}}$ that is formed by the vectors satisfying cond. (15) and assume $\boldsymbol{x} \in \boldsymbol{L}_P^\beta$ in the following. We can rewrite Eq. (14) as

$$R(\boldsymbol{p},\boldsymbol{q})\boldsymbol{x} = \frac{1}{|\boldsymbol{p}\boldsymbol{q}|}\sum_{i=0}^{3}\boldsymbol{u}_i\langle \boldsymbol{x}|\bar{\boldsymbol{p}}\boldsymbol{u}_i\boldsymbol{q}\rangle = \sum_{i=0}^{3}\boldsymbol{u}_i\frac{\langle \boldsymbol{x}|\bar{\boldsymbol{p}}\boldsymbol{u}_i\boldsymbol{q}\rangle}{\alpha\beta\gamma}, \tag{16}$$

i.e. $|\boldsymbol{p}\boldsymbol{q}|$ must divide $\langle \boldsymbol{x}|\bar{\boldsymbol{p}}\boldsymbol{u}_i\boldsymbol{q}\rangle$ By assumption, β divides $\langle \boldsymbol{x}|\bar{\boldsymbol{p}}\boldsymbol{u}_i\boldsymbol{q}\rangle$. On the other hand, since $\mathrm{den}(R) = |\boldsymbol{p}\boldsymbol{q}|/2^\ell$, there exists an element $\boldsymbol{x}$ of order $\alpha\gamma/2^\ell$ or higher. Thus at most $2^\ell|\boldsymbol{L}_P^\beta|/(\alpha\gamma)$ vectors $\boldsymbol{x} \in \boldsymbol{L}_P/\boldsymbol{L}_{\boldsymbol{q}}$ satisfy condition (14) and hence n'_P divides $2^{\ell+1}\alpha^3|\boldsymbol{q}|^4/(\beta^2\gamma) = 2^{\ell+1}\alpha^3|\boldsymbol{q}|^2$. From this we infer that $\Sigma_F(R)$ is a multiple of $\alpha|\boldsymbol{q}|^2/2^{\ell+2}$ and hence a multiple of $\Sigma(\boldsymbol{q})$. Analogously we prove that $\Sigma_F(R)$ is a multiple of $\Sigma(\boldsymbol{p})$. Thus $\mathrm{lcm}(\Sigma(\boldsymbol{p}), \Sigma(\boldsymbol{q})) \le \Sigma_F(R)$ and the claim follows. □

[2] Consider the vectors $q_\ell\boldsymbol{u}_0 - q_0\boldsymbol{u}_\ell$ and $\boldsymbol{u}_\ell\boldsymbol{q} + q_\ell\boldsymbol{u}_0 - q_0\boldsymbol{u}_\ell$. Their orders are multiples of $\alpha|\boldsymbol{q}|^2/\gcd(\alpha|\boldsymbol{q}|^2, q_\ell^2+q_m^2)$ and an appropriate combination thereof gives the desired vector $\boldsymbol{x}'$.

From this result we can easily infer the coincidence index $\Sigma_P(R)$ for the primitive lattice. Since $\boldsymbol{L}_F$ is a sublattice of index 2 of $\boldsymbol{L}_P$, $\Sigma_P(R)$ must divide $2\Sigma_F(R)$ and $\Sigma_F(R)$ must divide $2\Sigma_P(R)$.[5] Since $\Sigma_F(R)$ is odd we have $\Sigma_P(R)=\Sigma_F(R)$ or $\Sigma_P(R)=2\Sigma_F(R)$. Due to Eq. (5) the index $\Sigma_P(R)$ is odd if $\mathrm{den}(R)$ is odd and even if $\mathrm{den}(R)$ is even. Hence we have proved

Theorem 2.2 *Let $\boldsymbol{p},\boldsymbol{q}$ be an admissible pair of primitive integer quaternions and let $\Sigma(\boldsymbol{q})=2^{-\ell}|\boldsymbol{q}|^2$, where $\ell=0,1,2$ is the maximal power such that 2^ℓ divides $|\boldsymbol{q}|^2$. Then, for the primitive lattice, the rotation $R(\boldsymbol{p},\boldsymbol{q})$ has coincidence index*

$$\Sigma_P(\boldsymbol{p},\boldsymbol{q}) := \Sigma_P(R(\boldsymbol{p},\boldsymbol{q})) = \mathrm{lcm}[\Sigma(\boldsymbol{p}),\Sigma(\boldsymbol{q}),\mathrm{den}(R(\boldsymbol{p},\boldsymbol{q}))]. \tag{17}$$

This was first stated, without proof, in [5].

3 Equivalent CSLs

Different coincidence rotations may generate the same CSL or rotated copies of each other. It is natural to group these rotations and CSLs in appropriately chosen equivalence classes. The natural way is to call two coincidence rotations *equivalent* if they are in the same double coset of the symmetry group of the lattice [6, 10, 11]. To be precise, let G_P and G_F denote the symmetry groups of the primitive and the face–centered hypercubic lattice. Then we call two coincidence rotations R, R' *P–equivalent* (*F–equivalent*) if there exist two rotations $Q,Q'\in G_P$ ($Q,Q'\in G_F$) such that $R=QR'Q'$. Accordingly, we call two CSLs P–equivalent (F–equivalent) if the corresponding coincidence rotations are P–equivalent (F–equivalent). In particular, R and RQ, $Q\in G_{P,F}$ give rise to the same CSL.

Hence two coincidence rotations are equivalent if they belong to the same double coset G_PRG_P or G_FRG_F. These double cosets can be calculated if one knows the subgroups $H_i(R):=G_i\cap RG_iR^{-1}$, $i=P,F$. In order to determine these groups we make use of the fact that $SU(2)\times SU(2)$ is a double cover of the 4–dimensional rotation group $SO(4)$, which is reflected in the parameterization Eq. (2). Although the corresponding double cover of G_F and G_P is not a direct product but a subdirect product, we can make use of this special property and reduce the 4–dimensional case to the 3–dimensional one.

In order to do this we recall that the 3–dimensional rotations can be parameterized by quaternions as well [7, 8, 9]. The group $\mathcal{G}$ of order $|\mathcal{G}|=48$ generated by the quaternions $(\pm1,0,0,0)$, $\frac{1}{\sqrt{2}}(\pm1,\pm1,0,0)$, $\frac{1}{2}(\pm1,\pm1,\pm1,\pm1)$ and permutations thereof is a double cover of the cubic symmetry group O of order $|O|=24$. Based on the notion of equivalence of 3–dimensional coincidence rotations we introduce the following equivalence notion for quaternions: Two quaternions $\boldsymbol{q}$ and $\boldsymbol{q}'$ are *equivalent* ($\boldsymbol{q}\sim\boldsymbol{q}'$) if there exist quaternions $\boldsymbol{s},\boldsymbol{s}'\in\mathcal{G}$ such that $\boldsymbol{q}'=\boldsymbol{s}\boldsymbol{q}\boldsymbol{s}'$. Their equivalence classes are known [6] and the different types are summarized in Table 1. Here $\mathcal{H}(\boldsymbol{q}):=\mathcal{G}\cap\boldsymbol{q}\mathcal{G}\boldsymbol{q}^{-1}$. Furthermore the number of inequivalent CSLs for a given Σ is known [11, 6]. These numbers are summarized in Table 2 for all special quaternions $\boldsymbol{q}$. The number of inequivalent CSLs for a general $\boldsymbol{q}$ can be obtained by considering the total number of CSLs [6].

Let $\mathcal{G}'\subseteq\mathcal{G}$ be the group generated by the quaternions $(\pm1,0,0,0)$, $\frac{1}{2}(\pm1,\pm1,\pm1,\pm1)$ and permutations thereof. Now the group $\mathcal{G}_F=\mathcal{G}'\otimes\mathcal{G}'\cup(\frac{1}{\sqrt{2}}(1,1,0,0),\frac{1}{\sqrt{2}}(1,1,0,0))\mathcal{G}'\otimes\mathcal{G}'$ is a double cover of G_F. We call two pairs of quaternions $(\boldsymbol{p},\boldsymbol{q})$ and $(\boldsymbol{p}',\boldsymbol{q}')$ *F–equivalent* if the corresponding rotations $R(\boldsymbol{p},\boldsymbol{q})$ and $R(\boldsymbol{p}',\boldsymbol{q}')$ are F–equivalent. If $(\boldsymbol{p},\boldsymbol{q})$ and $(\boldsymbol{p}',\boldsymbol{q}')$ are F–equivalent then $\boldsymbol{p}\sim\boldsymbol{p}'$ and $\boldsymbol{q}\sim\boldsymbol{q}'$, but the converse is not true in general. Let us analyze the converse situation. Let $\boldsymbol{p}\sim\boldsymbol{p}'$ and $\boldsymbol{q}\sim\boldsymbol{q}'$, i.e. there exist $\boldsymbol{r},\boldsymbol{r}',\boldsymbol{s},\boldsymbol{s}'\in\mathcal{G}$ such that $\boldsymbol{p}'=\boldsymbol{r}\boldsymbol{p}\boldsymbol{r}'$ and $\boldsymbol{q}'=\boldsymbol{s}\boldsymbol{q}\boldsymbol{s}'$. If both pairs $(\boldsymbol{p},\boldsymbol{q})$ and $(\boldsymbol{p}',\boldsymbol{q}')$ are admissible, then $(\boldsymbol{r}\boldsymbol{r}',\boldsymbol{s}\boldsymbol{s}')$ must be admissible, too. If $(\boldsymbol{r},\boldsymbol{s})$ is admissible, then so is $(\boldsymbol{r}',\boldsymbol{s}')$, and $(\boldsymbol{p},\boldsymbol{q})$ and $(\boldsymbol{p}',\boldsymbol{q}')$ are F–equivalent. If $(\boldsymbol{r},\boldsymbol{s})$ is *not* admissible, then $(\boldsymbol{p},\boldsymbol{q})$ and $(\boldsymbol{p}',\boldsymbol{q}')$ are F–equivalent only if there exist admissible pairs $(\boldsymbol{r}_1,\boldsymbol{s}_1)$ and $(\boldsymbol{r}_1',\boldsymbol{s}_1')$ such that $\boldsymbol{r}\boldsymbol{p}\boldsymbol{r}'=\boldsymbol{r}_1\boldsymbol{p}\boldsymbol{r}_1'$ and $\boldsymbol{s}\boldsymbol{q}\boldsymbol{s}'=\boldsymbol{s}_1\boldsymbol{q}\boldsymbol{s}_1'$. This is possible if and only if $\mathcal{H}(\boldsymbol{p})$ or $\mathcal{H}(\boldsymbol{q})$ contains one of the quaternions $\frac{1}{\sqrt{2}}(\pm1,\pm1,0,0)$ or a permutation thereof. The latter statement is equivalent to the statement that $\boldsymbol{p}$ or $\boldsymbol{q}$ is equivalent to one of the following quaternions: $(1,0,0,0)$, $(0,1,1,1)$, $(m,n,0,0)$ or $(m,n,n,0)$. We can summarize these considerations as follows: If $(\boldsymbol{p},\boldsymbol{q})$ and $(\boldsymbol{p}',\boldsymbol{q}')$ are F–equivalent then $\boldsymbol{p}\sim\boldsymbol{p}'$ and $\boldsymbol{q}\sim\boldsymbol{q}'$. Conversely $\boldsymbol{p}\sim\boldsymbol{p}'$ and $\boldsymbol{q}\sim\boldsymbol{q}'$ implies that $(\boldsymbol{p},\boldsymbol{q})$ and $(\boldsymbol{p}',\boldsymbol{q}')$ are F–equivalent if $\boldsymbol{p}$ or $\boldsymbol{q}$ is equivalent to one of the following quaternions: $(1,0,0,0)$, $(0,1,1,1)$, $(m,n,0,0)$ or $(m,n,n,0)$.

Assume now that $\boldsymbol{p}\sim(m,n,n,n)$ and $\boldsymbol{q}\sim(m',n',n',n')$. Then we may not conclude that the admissible pair $(\boldsymbol{p},\boldsymbol{q})$ is F–equivalent to $((m,n,n,n),(m',n',n',n'))$. However, we may conclude that $(\boldsymbol{p},\boldsymbol{q})$ is F–equivalent either to $((m,n,n,n),(m',n',n',n'))$ or $((m,n,n,n),(m',-n',-n',-n'))$. Note that the latter pairs are not F–equivalent. Nevertheless, they are of the same type.

Having this in mind we can use Table 1 to calculate all types of possible F–equivalence classes. Instead of calculating the groups $H_F(R(\boldsymbol{p},\boldsymbol{q}))$ directly we compute their corresponding double covers $\mathcal{H}_F(\boldsymbol{p},\boldsymbol{q})$. It turns out that they are simply given by $\mathcal{H}_F(\boldsymbol{p},\boldsymbol{q})=(\mathcal{H}(\boldsymbol{p})\otimes\mathcal{H}(\boldsymbol{q}))\cap\mathcal{G}'$. The results are listed in Table 3. In order to save space we have omitted some pairs. These can be easily obtained by interchanging the role of $\boldsymbol{p}$ and $\boldsymbol{q}$ and adapting the corresponding subgroup $\mathcal{H}_F$. In addition, we have used the definition $\mathcal{H}_i':=\mathcal{H}_i\cap\mathcal{G}'$.

The fact that $\mathcal{G}_F$ is a special subgroup of $\mathcal{G} \times \mathcal{G}$ enables us to derive the number of different and inequivalent CSLs from the 3–dimensional case. First, we consider the total number of different CSLs $f_F(\Sigma)$. Recall that the total number of different CSLs $f(\Sigma)$ for a given Σ in the 3–dimensional case is given by [6, 5]

$$f(1) = 1 \tag{18}$$

$$f(2) = 0 \tag{19}$$

$$f(p^r) = (p+1)p^{r-1} \qquad \text{if } p \text{ is an odd prime, } r \geq 1 \tag{20}$$

$$f(mn) = f(m)f(n) \qquad \text{if } m, n \text{ are coprime.} \tag{21}$$

The multiplicativity of $f(\Sigma)$ is due to the uniqueness of the (left) prime factorization of the integer quaternions [8]. The same reasoning holds true in four dimensions, too, so we only need to calculate $f_F(p^r)$. To this end we note that there are precisely $f(\Sigma(\boldsymbol{p}))f(\Sigma(\boldsymbol{q}))$ different CSLs for given $\Sigma(\boldsymbol{p})$ and $\Sigma(\boldsymbol{q})$. Summing up all admissible combinations of $(\Sigma(\boldsymbol{p}), \Sigma(\boldsymbol{q}))$ that give a fixed p^r we obtain [5]

$$f_F(p^r) = \frac{p+1}{p-1} p^{r-1}(p^{r+1} + p^{r-1} - 2). \tag{22}$$

In a similar way we can calculate the number of inequivalent CSLs of a certain type, say $(\boldsymbol{p}, \boldsymbol{q}) \equiv ((0,1,1,1),(0,1,1,1))$ or $((m,n,n,n),(m',n',n',n'))$. These results are summarized in Tables 4 and 5.

Let us discuss some of them. Consider pairs of type $((1,0,0,0),(m,n,n,n))$ first. Then $\Sigma(\boldsymbol{p},\boldsymbol{q}) = \Sigma_F$ implies $\Sigma(\boldsymbol{q}) = \Sigma_F$. Hence the number of inequivalent CSLs is equal to the number of inequivalent quaternions $\boldsymbol{q} = (m,n,n,n)$, which can be read off directly from Table 2. Thus there are precisely 2^{k-1} inequivalent CSLs if $p = 1 \bmod 6$ for all the k different prime factors of Σ_F. Note that a prime factor 3 cannot exist, since Σ_F must be a square as $(\boldsymbol{p},\boldsymbol{q})$ must be an admissible pair.

Consider now pairs of type $((m,n,n,n),(m',n',n',n'))$. Such pairs can only exist if $\Sigma_F(\boldsymbol{p},\boldsymbol{q}) = 3^t \prod_i p_i^{2r_i} \prod_j q_j^{2s_j+1}$ where all prime factors $p_i, q_j = 1 \bmod 6$ and $t = 0,1$. This implies that $\Sigma(\boldsymbol{p}) = 3^t \prod_i p_i^{2r'_i} \prod_j q_j^{2s'_j+1}$ and $\Sigma(\boldsymbol{q}) = 3^t \prod_i p_i^{2r''_i} \prod_j q_j^{2s''_j+1}$ with $r_i = \max(r'_i, r''_i), s_j = \max(s'_j, s''_j)$. For a fixed combination of $\{r'_i, s'_j\}$, there are $2^{k'-1}$ inequivalent quaternions $\boldsymbol{p}$, where k' is the number of different prime factors $p_i, q_j \neq 3$ contained in $\Sigma(\boldsymbol{p})$. If we use the notation $\nu(a) = 0,1$ for $a = 0$, $a \geq 1$, respectively, we can write $2^{m'-1} = 1/2 \prod_i 2^{\nu(2r'_i)} \prod_j 2^{\nu(2s'_j+1)}$. In order to get the number of inequivalent admissible pairs $(\boldsymbol{p},\boldsymbol{q})$ we have to take the sum over all possible combinations of r'_i, r''_i, s'_j, s''_j. Note that r'_i runs through $0, \ldots, r_i$ if $r''_i = r_i$ and vice versa. Hence the number of inequivalent admissible pairs reads

$$\frac{1}{2} \sum_{(r'_i, r''_i, s'_j, s''_j)} \prod_i 2^{\nu(2r'_i)+\nu(2r''_i)} \prod_j 2^{\nu(2s'_j+1)+\nu(2s''_j+1)} \tag{23}$$

$$= \frac{1}{2} \prod_i \left(\sum_{r'_i=0}^{r_i-1} 2^{\nu(2r'_i)+\nu(2r_i)} + \sum_{r''_i=0}^{r_i-1} 2^{\nu(2r_i)+\nu(2r''_i)} + 2^{\nu(2r_i)+\nu(2r_i)} \right) \tag{24}$$

$$\cdot \prod_j \left(\sum_{s'_j=0}^{s_j-1} 2^{\nu(2s'_j+1)+\nu(2s_j+1)} + \sum_{s''_j=0}^{s_j-1} 2^{\nu(2s_j+1)+\nu(2s''_j+1)} + 2^{\nu(2s_j+1)+\nu(2s''_j+1)} \right) \tag{25}$$

$$= \frac{1}{2} \prod_i (8r_i) \prod_j [4(2s_j+1)] = 2 \cdot 4^{k-1} \prod_i (2r_i) \prod_j (2s_j+1), \tag{26}$$

where k is the number of different prime factors $p_i, q_j \neq 3$. If $\Sigma_F(\boldsymbol{p},\boldsymbol{q})$ contains at least one odd prime power $q_j^{2s_j+1}$, we have finished. Otherwise we have to take into account that the sum above includes 2^{k-1} pairs of the form $((m,n,n,n),(1,0,0,0))$ or $((m,n,n,n),(0,1,1,1))$. Hence a term 2^k must be subtracted from the sum above. Thus there exist

$$n_{F22} = 2 \cdot 4^{k-1} \prod_\ell t_\ell - \delta\, 2^k \tag{27}$$

inequivalent admissible pairs $((m,n,n,n),(m',n',n',n'))$ for a fixed $\Sigma_F(\boldsymbol{p},\boldsymbol{q}) = 3^t \prod_\ell p_\ell^{t_\ell}$ with $p_\ell = 1 \bmod 6$ and $t = 0,1$. Here $\delta = 1$ if all t_ℓ are even and $\delta = 0$ otherwise.

Next we consider the case $((m,n,n,n),(m',n',0,0))$, which is an example where $\boldsymbol{p}$ and $\boldsymbol{q}$ are of different type. First observe that $\Sigma(\boldsymbol{q})$ may only contain prime factors $p = 1 \bmod 4$, whereas $\Sigma(\boldsymbol{p})$ may only contain prime factors $p = 1 \bmod 6$ and $p = 3$, for the latter only the powers 3^0 and 3^1 are allowed. Since the pair must be admissible, the factor $p = 3$ is ruled out and the coincidence index takes the form $\Sigma_F(\boldsymbol{p},\boldsymbol{q}) = \prod_i p_i^{2r_i} \prod_j p_j'^{2r'_j} \prod_\ell q_\ell^{s_\ell}$ where

$p_i = 1 \bmod 4, p_i \neq 1 \bmod 6$, $p'_j = 1 \bmod 6, p'_j \neq 1 \bmod 4$, $q_\ell = 1 \bmod 4, q_\ell = 1 \bmod 6$. Hence $\Sigma(\boldsymbol{q}) = \prod_i p_i^{2r_i} \prod_\ell q_\ell^{s'_\ell}$, $\Sigma(\boldsymbol{p}) = \prod_j {p'_j}^{2r'_j} \prod_\ell q_\ell^{s''_\ell}$ where $s_\ell = \max(s'_\ell, s''_\ell)$. Again we have to sum over all possible combinations s'_ℓ, s''_ℓ and finally obtain the number n_{F23} of F–inequivalent admissible pairs

$$n_{F23} = 2^{k_1+k_2} 4^{k_3-1} \prod_\ell s_\ell, \tag{28}$$

if $k_1 \geq 1$ and $k_2 \geq 1$. Here k_1, k_2, k_3 are the number of different prime factors p_i, p'_j, q_ℓ. If $k_1 = 0, k_2 \neq 0$ this expression includes the pairs of type $((m,n,n,n),(1,0,0,0))$, so that a term $2^{k_2+k_3-1}$ must be subtracted. Thus

$$n_{F23} = 2^{k_2}(4^{k_3-1} \prod_\ell s_\ell - 2^{k_3-2}). \tag{29}$$

A similar expression is obtained for $k_2 = 0$. Finally, if $k_1 = k_2 = 0$, we get

$$n_{F23} = 4^{k_3-1} \prod_\ell s_\ell - 2^{k_3-1}. \tag{30}$$

At last, let us consider pairs where at least one quaternion is completely general. As an example, we use $((m,n,n,n),\boldsymbol{q})$. In this case, the approach is slightly different from the previous cases, since we lack a nice formula for the three–dimensional case. But we can proceed as follows: We first calculate the number of different admissible pairs $((m,n,n,n),\boldsymbol{q})$, where $\boldsymbol{q}$ is a general or a special quaternion. We then subtract the number of all special combinations $((m,n,n,n),\boldsymbol{q})$ and finally divide by the number of equivalent pairs. We first note that $\Sigma((m,n,n,n),\boldsymbol{q})$ must be of the form $\Sigma = 3^r \prod_i p_i^{s_i} \prod_j q_j^{2t_j}$, where $p_i = 1 \pmod 6$ and $q_j \neq 1 \pmod 6$ and $r \geq 0$ and at least one $s_i \geq 1$. We have to sum over all pairs with $\Sigma(m,n,n,n) = 3^{r'} \prod_i p_i^{s'_i}$, $\Sigma(\boldsymbol{q}) = 3^r \prod_i p_i^{s''_i} \prod_j q_j^{2t_j}$ such that $r' \leq 1, r' = r \pmod 2), s_i = \max(s'_i, s''_i)$. For fixed $\Sigma(m,n,n,n)$ and $\Sigma(\boldsymbol{q})$ we have the following situation: There are $2^{k-1} = 1/2 \prod_i 2^{1-\delta_{0,s'_i}}$ inequivalent quaternions of type (m,n,n,n) (if at least one $s'_i > 0$, k is the number of different prime factors > 3) and there are $48 \cdot (4 \cdot 3^{r-1})^{1-\delta_{0,r}} \prod_i (p_i+1) p_i^{s''_i-1} \prod_j (q_j+1) q_j^{2t_j-1}$ different (in general *not* inequivalent) quaternions $\boldsymbol{q}$. Note that the product ranges only over those i for which $s''_i > 0$. If we use Gauss' symbol $[x]$ in order to denote the largest integer $n \leq x$ we may rewrite this as $48 \cdot [4 \cdot 3^{r-1}] \prod_i [(p_i+1) p_i^{s''_i-1}] \prod_j (q_j+1) q_j^{2t_j-1}$ and take the product over all i. Hence for fixed $\Sigma(m,n,n,n)$ and $\Sigma(\boldsymbol{q})$ we have

$$1/2 \cdot 8 \cdot 48 \cdot 1/2 \prod_i 2^{1-\delta_{0,s'_i}} \cdot 48 \cdot [4 \cdot 3^{r-1}] \prod_i [(p_i+1) p_i^{s''_i-1}] \prod_j (q_j+1) q_j^{2t_j-1} \tag{31}$$

different (in general *not* inequivalent admissible pairs). Note that we have added a factor 1/2 taking into account that only half of the pairs are admissible. Summing over all possible combinations of $\Sigma(m,n,n,n)$ and $\Sigma(\boldsymbol{q})$ we get

$$1152 m_{F2} = 4 \cdot 1152 \cdot [4 \cdot 3^{r-1}] \prod_i \left(\sum_{\ell_i=1}^{[s_i/2]} 2^{1-\delta_{0,s_i-2\ell_i}} (p_i+1) p_i^{s_i-1} + \sum_{\ell_i=0}^{[s_i/2]} 2[(p_i+1) p_i^{s_i-2\ell_i-1}] \right) \prod_j (q_j+1) q_j^{2t_j-1} \tag{32}$$

$$= 4 \cdot 1152 \cdot [4 \cdot 3^{r-1}] \prod_i \left((s_i+1)(p_i+1) p_i^{s_i-1} + 2 \frac{p_i^{s_i-1} - 1}{p_i - 1} \right) \prod_j (q_j+1) q_j^{2t_j-1} \tag{33}$$

different admissible pairs if there is at least one s_i is odd. Otherwise we must exclude the term with $\ell_i = s_i/2$ for all i in the first sum, i.e.

$$m_{F2} = 4 \cdot [4 \cdot 3^{r-1}] \left(\prod_i \left((s_i+1)(p_i+1) p_i^{s_i-1} + 2 \frac{p_i^{s_i-1} - 1}{p_i - 1} \right) - \delta_{F2} \prod_i (p_i+1) p_i^{s_i-1} \right) \prod_j (q_j+1) q_j^{2t_j-1}, \tag{34}$$

where $\delta_{F2} = 0, 1$ according to whether there exists an odd s_i or not. From this expression we subtract all admissible pairs with special $\boldsymbol{q}$, divide by the number of equivalent pairs and obtain the following expression for the number of inequivalent admissible quaternions of type $((m,n,n,n),\boldsymbol{q})$:

$$n_{F25} = \frac{1}{96} \left(m_{F2} - \sum_{i=0}^{4} g_{F2i} n_{F2i} \right). \tag{35}$$

Similar expression are obtained for n_{F35} and n_{F45}. And finally we can compute n_{F55} by recalling the total number of different quaternions f_F given in Eq. (22):

$$f_F = \sum_{i,j=0}^{5} g_{Fij} n_{Fij}. \tag{36}$$

Finally let us have a short look on the primitive hypercubic lattice. Similar results can be proved for this case. The best way to obtain them is to derive them directly from the previous results. We just have to keep in mind that the symmetry group G_P is a subgroup of index 3 of G_F. In particular, the coset decomposition for the corresponding groups of quaternions reads

$$\mathcal{G}_F = \mathcal{G}_P \cup \big((1,0,0,0), \tfrac{1}{2}(1,1,1,1)\big)\, \mathcal{G}_P \cup \big((1,0,0,0), \tfrac{1}{2}(1,-1,-1,-1)\big)\, \mathcal{G}_P. \tag{37}$$

If we apply this decomposition to the double cosets $\mathcal{G}_F(\boldsymbol{p},\boldsymbol{q})\mathcal{G}_F$, we get the double cosets of $\mathcal{G}_P$, which are just the P–equivalence classes of admissible pairs, see Tab. 6. The corresponding groups $\mathcal{H}_P(\boldsymbol{p},\boldsymbol{q})$ can now be inferred from the corresponding groups $\mathcal{H}_F(\boldsymbol{p},\boldsymbol{q})$. In particular, we have $\mathcal{H}_P(\boldsymbol{p},\boldsymbol{q}) \subseteq \mathcal{H}_F(\boldsymbol{p},\boldsymbol{q}) \cap \mathcal{G}_P$, which simplifies the determination of $\mathcal{H}_P(\boldsymbol{p},\boldsymbol{q})$ considerably. The results are shown in Tab. 7. Combining these results with the numbers n_{Fij} of F–inequivalent admissible pairs, we get the number of P–inequivalent admissible pairs, which are listed in Tab. 8.

4 Conclusions and Outlook

We have calculated the coincidence index Σ for both kinds of four–dimensional hypercubic lattices. Moreover, we have determined all CSLs and their equivalence classes as well as the total number of different and inequivalent CSLs for fixed Σ. Here, equivalence always means equivalence up to proper rotations. But of course there exist reflections that leave the hypercubic lattices invariant and one can be interested in extending the notion of equivalence to the full symmetry group. We briefly sketch how one can include the improper rotations. First note that the special reflection $m : \boldsymbol{q} \to (q_0, -q_1, -q_2, -q_3)$ just corresponds to quaternion conjugation. Now any symmetry operation is a product of this reflection and a rotation, and it is sufficient to consider this reflection in detail. Since $mR(\boldsymbol{p},\boldsymbol{q}) = R(\boldsymbol{q},\boldsymbol{p})m$, it follows that the admissible pairs $(\boldsymbol{p},\boldsymbol{q})$ and $(\boldsymbol{q},\boldsymbol{p})$ are equivalent. Thus we have two situations: If $(\boldsymbol{p},\boldsymbol{q})$ and $(\boldsymbol{q},\boldsymbol{p})$ are not equivalent under proper rotations, than their equivalence classes merge to form a single equivalence class. If $(\boldsymbol{p},\boldsymbol{q})$ and $(\boldsymbol{q},\boldsymbol{p})$ are already equivalent under proper rotations, than the equivalence class stays the same and the corresponding symmetry group $H(\boldsymbol{p},\boldsymbol{q})$ contains a symmetry operation which is a conjugate of m. Thus we know all equivalence classes and their symmetry groups $H(\boldsymbol{p},\boldsymbol{q})$. It is then straightforward to calculate the number of inequivalent CSLs.

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References

[1] Bollmann, W.: Crystal Defects and Crystalline Interfaces. Springer, Berlin, 1970.

[2] Bollmann, W.: Crystal lattices, interfaces, matrices. published by the author, Geneva, 1982.

[3] Duneau, M.; Katz, A.: Quasiperiodic patterns. Phys. Rev. Lett. **54** (1985) 2688–2691.

[4] Baake, M.: A Guide to Mathematical Quasicrystals In: *Quasicrystals*, (Eds. J.-B. Suck, M. Schreiber, P. Häußler), p. 17–48, Springer, Berlin, 2002.

[5] Baake, M.: Solution of the coincidence problem in dimensions $d \leq 4$. In: *The Mathematics of Long-Range Aperiodic Order* (Ed. R. V. Moody), p. 9–44, Kluwer, Dordrecht, 1997.

[6] Zeiner, P.: Symmetries of coincidence site lattices of cubic lattices. Z. Kristallogr. **220** (2005) 915–925.

[7] Koecher, M.; Remmert, R.: Hamilton's Quaternions. In: *Numbers* (Eds. H.-D. Ebbinghaus et. al.), p. 189–220. Springer, 1991.

[8] Hurwitz, A.: Vorlesungen über die Zahlentheorie der Quaternionen. Springer, Berlin 1919.

[9] du Val, P Homographies, Quaternions and rotations. Clarendon Press, Oxford, 1964.

[10] Grimmer, H.: Disorientations and coincidence rotations for cubic lattices. Acta Cryst. A **30** (1974) 685–688.

[11] Grimmer, H: Coincidence site lattices: New results and comments on papers by Fortnow and Woirgard-de Fouquet. Scripta Met. **10** (1976) 387–391.

$\boldsymbol{q}$	$\mathcal{H}(\boldsymbol{q})$	$\lvert\mathcal{H}(\boldsymbol{q})\rvert$	$\lvert\mathcal{G}\boldsymbol{q}\mathcal{G}\rvert$
$(1,0,0,0)$	$\mathcal{G}$	48	48
$(0,1,1,1)\sim(3,1,1,1)$	$\mathcal{H}_1=[(-1,0,0,0),(1,1,1,1),(0,1,-1,0)]$	12	$4\cdot 48=192$
(m,n,n,n)	$\mathcal{H}_2=[(-1,0,0,0),(1,1,1,1)]$	6	$8\cdot 48=384$
$(m,n,0,0)$	$\mathcal{H}_3=[(-1,0,0,0),(1,1,0,0)]$	8	$6\cdot 48=288$
$(m,n,n,0)$	$\mathcal{H}_4=[(-1,0,0,0),(0,1,1,0)]$	4	$12\cdot 48=576$
otherwise	$\mathcal{H}_5=[(-1,0,0,0)]$	2	$24\cdot 48=1152$

Table 1: Equivalence classes of quaternions: Any primitive quaternion is equivalent to one of the quaternions in the first column. The second column gives a set of generators of $\mathcal{H}(\boldsymbol{q})$. The third column gives the order of $|\mathcal{H}(\boldsymbol{q})|$ and the forth column states the number of equivalent $\boldsymbol{q}$, which is 48 times the number of equivalent 3–dimensional CSLs.

$\boldsymbol{q}$	inequiv. CSLs	condition
$(1,0,0,0)$	1	$\Sigma=1$
$(0,1,1,1)$	1	$\Sigma=3$
(m,n,n,n)	2^{k-1}	$p=1 \bmod 6$ for all prime factors $p\neq 3$ of $\Sigma>3$, the factor $p=3$ occurs at most once and k is the number of different prime factors $p=1 \bmod 6$ of Σ.
$(m,n,0,0)$	2^{k-1}	$p=1 \bmod 4$ for all prime factors p of Σ and k is the number of different prime factors of Σ.
$(m,n,n,0)$	2^{k-1}	$p=1$ or $3 \bmod 8$ for all prime factors p of Σ, where k is the number of different prime factors of $\Sigma>3$.

Table 2: Number of inequivalent cubic CSLs/coincidence rotations for a fixed value Σ. The last column gives the condition under which these values hold. If this condition is not satisfied, the corresponding number of inequivalent CSLs is 0 for the particular type of $\boldsymbol{q}$.

$\boldsymbol{p}$	$\boldsymbol{q}$	$\mathcal{H}_F(\boldsymbol{p},\boldsymbol{q})$	$\lvert\mathcal{H}_F(\boldsymbol{p},\boldsymbol{q})\rvert$	$\lvert G_F R(\boldsymbol{p},\boldsymbol{q}) G_F\rvert$
$(1,0,0,0)$	$(1,0,0,0)$	$\mathcal{G}_F$	1152	$576 g_{F00}=576$
$(1,0,0,0)$	(m,n,n,n)	$\mathcal{G}'\otimes\mathcal{H}'_2$	144	$576 g_{F02}=8\cdot 576$
$(1,0,0,0)$	$(m,n,0,0)$	$\mathcal{G}'\otimes\mathcal{H}'_3\cup(\frac{1}{\sqrt{2}}(1,1,0,0),\frac{1}{\sqrt{2}}(1,1,0,0))\mathcal{G}'\otimes\mathcal{H}'_3$	192	$576 g_{F03}=6\cdot 576$
$(1,0,0,0)$	$(m,n,n,0)$	$\mathcal{G}'\otimes\mathcal{H}'_4\cup(\frac{1}{\sqrt{2}}(1,1,0,0),\frac{1}{\sqrt{2}}(0,1,1,0))\mathcal{G}'\otimes\mathcal{H}'_4$	96	$576 g_{F04}=12\cdot 576$
$(1,0,0,0)$	general	$\mathcal{G}'\otimes\mathcal{H}'_5$	48	$576 g_{F05}=24\cdot 576$
$(0,1,1,1)$	$(0,1,1,1)$	$\mathcal{H}'_1\otimes\mathcal{H}'_1\cup(\frac{1}{\sqrt{2}}(0,1,-1,0),\frac{1}{\sqrt{2}}(0,1,-1,0))\mathcal{H}'_1\otimes\mathcal{H}'_1$	72	$576 g_{F11}=16\cdot 576$
$(0,1,1,1)$	(m,n,n,n)	$\mathcal{H}'_1\otimes\mathcal{H}'_2$	36	$576 g_{F12}=32\cdot 576$
$(0,1,1,1)$	$(m,n,0,0)$	$\mathcal{H}'_1\otimes\mathcal{H}'_3\cup(\frac{1}{\sqrt{2}}(0,1,-1,0),\frac{1}{\sqrt{2}}(1,1,0,0))\mathcal{H}'_1\otimes\mathcal{H}'_3$	48	$576 g_{F13}=24\cdot 576$
$(0,1,1,1)$	$(m,n,n,0)$	$\mathcal{H}'_1\otimes\mathcal{H}'_4\cup(\frac{1}{\sqrt{2}}(0,1,-1,0),\frac{1}{\sqrt{2}}(0,1,1,0))\mathcal{H}'_1\otimes\mathcal{H}'_4$	24	$576 g_{F14}=48\cdot 576$
$(0,1,1,1)$	general	$\mathcal{H}'_1\otimes\mathcal{H}'_5$	12	$576 g_{F15}=96\cdot 576$
(m,n,n,n)	(m',n',n',n')	$\mathcal{H}'_2\otimes\mathcal{H}'_2$	36	$576 g_{F22}=32\cdot 576$
(m,n,n,n)	$(m',n',0,0)$	$\mathcal{H}'_2\otimes\mathcal{H}'_3$	24	$576 g_{F23}=48\cdot 576$
(m,n,n,n)	$(m',n',n',0)$	$\mathcal{H}'_2\otimes\mathcal{H}'_4$	12	$576 g_{F24}=96\cdot 576$
(m,n,n,n)	general	$\mathcal{H}'_2\otimes\mathcal{H}'_5$	12	$576 g_{F25}=96\cdot 576$
$(m,n,0,0)$	$(m',n',0,0)$	$\mathcal{H}'_3\otimes\mathcal{H}'_3\cup(\frac{1}{\sqrt{2}}(1,1,0,0),\frac{1}{\sqrt{2}}(1,1,0,0))\mathcal{H}'_3\otimes\mathcal{H}'_3$	32	$576 g_{F33}=36\cdot 576$
$(m,n,0,0)$	$(m',n',n',0)$	$\mathcal{H}'_3\otimes\mathcal{H}'_4\cup(\frac{1}{\sqrt{2}}(1,1,0,0),\frac{1}{\sqrt{2}}(0,1,1,0))\mathcal{H}'_3\otimes\mathcal{H}'_4$	16	$576 g_{F34}=72\cdot 576$
$(m,n,0,0)$	general	$\mathcal{H}'_3\otimes\mathcal{H}'_5$	8	$576 g_{F35}=144\cdot 576$
$(m,n,n,0)$	$(m',n',n',0)$	$\mathcal{H}'_4\otimes\mathcal{H}'_4\cup(\frac{1}{\sqrt{2}}(0,1,1,0),\frac{1}{\sqrt{2}}(0,1,1,0))\mathcal{H}'_4\otimes\mathcal{H}'_4$	8	$576 g_{F44}=144\cdot 576$
$(m,n,n,0)$	general	$\mathcal{H}'_4\otimes\mathcal{H}'_5$	4	$576 g_{F45}=288\cdot 576$
general	general	$\mathcal{H}'_5\otimes\mathcal{H}'_5$	4	$576 g_{F55}=288\cdot 576$

Table 3: F–Equivalence classes of admissible pairs. For each admissible pair the corresponding group $\mathcal{H}_F(\boldsymbol{p},\boldsymbol{q})$ and its order is listed. The last column gives the number of equivalent coincidence rotations $R(\boldsymbol{p},\boldsymbol{q})$. By dividing these numbers by 576 we obtain the number of equivalent CSLs. In order to save space we have omitted some pairs. These can be easily obtained by interchanging the role of $\boldsymbol{p}$ and $\boldsymbol{q}$ and by adapting the subgroup $\mathcal{H}_F$ correspondingly.

$\boldsymbol{p}$	$\boldsymbol{q}$	inequivalent CSLs	condition
$(1,0,0,0)$	$(1,0,0,0)$	$n_{F00}=1$	$\Sigma_F=1$
$(1,0,0,0)$	(m,n,n,n)	$n_{F02}=2^{k-1}$	k is the number of different prime factors, all prime factors $p=1$ mod 6, Σ_F is a square
$(1,0,0,0)$	$(m,n,0,0)$	$n_{F03}=2^{k-1}$	k is the number of different prime factors, all prime factors $p=1$ mod 4, Σ_F is a square
$(1,0,0,0)$	$(m,n,n,0)$	$n_{F04}=2^{k-1}$	k is the number of different prime factors, all prime factors $p=1$ or 3 mod 8, Σ_F is a square
$(1,0,0,0)$	general	n_{F05}	Σ_F is a square
$(0,1,1,1)$	$(0,1,1,1)$	$n_{F11}=1$	$\Sigma_F=3$
$(0,1,1,1)$	(m,n,n,n)	$n_{F12}=2^{k-1}$	$\Sigma_F=3a^2$, k is the number of different prime factors of a, all prime factors $p=1$ mod 6
$(0,1,1,1)$	$(m,n,n,0)$	$n_{F14}=2^{k-1}$	$\Sigma_F=3a^2$, k is the number of different prime factors of Σ_F, all prime factors $p=1$ or 3 mod 8
$(0,1,1,1)$	general	n_{F15}	$\Sigma_F=3a^2$
(m,n,n,n)	(m',n',n',n')	$n_{F22}=2\cdot 4^{k-1}\prod_\ell t_\ell-\delta\,2^k$	$\Sigma_F=3^r a$, $r=0,1$, k is the number of different prime factors of a, which is not divisible by 3, all prime factors $p=1$ mod 6, $\delta=1$ if a is a square and $\delta=0$ otherwise
(m,n,n,n)	$(m',n',0,0)$	$n_{F23}=2^{k_1+k_2}4^{k_3-1}\prod_\ell t_\ell-\delta_1 2^{k_2+k_3-2}-\delta_2 2^{k_1+k_3-2}$	$\Sigma_F=\prod_i p_i^{2r_i}\prod_j {p'_j}^{2r'_j}\prod_\ell q_\ell^{t_\ell}$, $p_i=1\pmod 4\neq 1\pmod 6$, $p'_j=1\pmod 6\neq 1\pmod 4$, $q_\ell=1\pmod 4=1\pmod 6$, k_1,k_2,k_3 denote the number of different prime factors of type p_i, p'_j and q_ℓ, respectively. $\delta_1=0$ unless all t_ℓ are even and $k_1=0$, where $\delta_1=1$. An analogous definition applies for δ_2 with $k_1=0$ replaced by $k_2=0$.
(m,n,n,n)	general	n_{F25}	

Table 4: Number of F–inequivalent CSLs (Part 1). The last column gives the condition under which these values hold. If this condition is not satisfied, the corresponding number of inequivalent CSLs is 0 for the particular type of $(\boldsymbol{p},\boldsymbol{q})$. In order to save space we have omitted some pairs. These can be easily obtained by interchanging $\boldsymbol{p}$ and $\boldsymbol{q}$ and reading of the corresponding value $n_{Fij}=n_{Fji}$.

$\boldsymbol{p}$	$\boldsymbol{q}$	inequivalent CSLs	condition
(m,n,n,n)	$(m',n',n',0)$	$n_{F24} = 2^{k_1+k_2}4^{k_3-1}\prod_\ell t_\ell - 1/2(n_{F02}+n_{F12}+n_{F04}+n_{F14})$	$\Sigma_F = 3^s \prod_i p_i^{2r_i} \prod_j p_j'^{2r_j'} \prod_\ell q_\ell^{t_\ell}$, $p_i = 1 \pmod 6 \neq 1$ or $3 \pmod 8$, $p_j' = 1$ or $3 \pmod 8 \neq 1 \pmod 6$, $q_\ell = 1 \pmod 6 = 1$ or $3 \pmod 8$, there must be at least one prime factor $= 1 \pmod 6$ and one $= 1$ or $3 \pmod 8$. k_1, k_2 denote the number of different prime factors of type p_i and p_j', respectively. k_3 is the number of prime factors of type q_ℓ if $s = 0$ and the number of prime factors of type q_ℓ plus 1 if $s > 1$.
$(m,n,0,0)$	$(m',n',0,0)$	$n_{F33} = 4^{k-1}\prod_\ell t_\ell - \delta\, 2^{k-1}$	k is the number of different prime factors of Σ_F, all prime factors $p = 1 \bmod 4$, $\delta = 1$ if Σ_F is a square and $\delta = 0$ otherwise
$(m,n,0,0)$	$(m',n',n',0)$	$n_{F24} = 2^{k_1+k_2}4^{k_3-1}\prod_\ell t_\ell - 1/2(n_{F02}+n_{F12}+n_{F04}+n_{F14})$	$\Sigma_F = \prod_i p_i^{2r_i} \prod_j p_j'^{2r_j'} \prod_\ell q_\ell^{t_\ell}$, $p_i = 1 \pmod 4 \neq 1$ or $3 \pmod 8$, $p_j' = 3 \pmod 8$, $q_\ell = 1 \pmod 8$, there must be at least one prime factor $= 1 \pmod 4$ and one $= 1$ or $3 \pmod 8$. k_1, k_2, k_3 denote the number of different prime factors of type p_i, p_j', and q_ℓ, respectively.
$(m,n,0,0)$	general	n_{F35}	
$(m,n,n,0)$	$(m',n',n',0)$	$n_{F44} = 4^{k-1}\prod_\ell t_\ell - \delta\, 2^{k-1}$	k is the number of different prime factors of Σ_F, all prime factors $p = 1, 3 \bmod 8$, $\delta = 1$ if $\Sigma_F = a^2, 3a^2$ and $\delta = 0$ otherwise
$(m,n,n,0)$	general	n_{F45}	
general	general	n_{F55}	

Table 5: Number of F–inequivalent CSLs (Part 2)

$\boldsymbol{g} = (\boldsymbol{p}, \boldsymbol{q})$	double coset decomposition of $\mathcal{G}_F \boldsymbol{g} \mathcal{G}_F$
$((1,0,0,0),(1,0,0,0))$	$\mathcal{G}_P \cup \boldsymbol{s_1}\mathcal{G}_P$
$((1,0,0,0),(m,n,n,n))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P$
$((1,0,0,0),(m,n,0,0))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P$
$((1,0,0,0),(m,n,n,0))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P$
$((1,0,0,0),(m,n,p,q))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P$
$((0,1,1,1),(0,1,1,1))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P$
$((0,1,1,1),(m,n,n,n))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P$
$((0,1,1,1),(m,n,0,0))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P$
$((0,1,1,1),(m,n,n,0))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P$
$((0,1,1,1),(m,n,p,q))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P$
$((m,n,n,n),(m',n',n',n'))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P$
$((m,n,n,n),(m',n',0,0))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P$
$((m,n,n,n),(m',n',n',0))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P$
$((m,n,n,n),(m',n',p',q'))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P$
$((m,n,0,0),(m',n',0,0))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P$
$((m,n,0,0),(m',n',n',0))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P$
$((m,n,0,0),(m',n',p',q'))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_2}\boldsymbol{g}\mathcal{G}_P \cup$ $\mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_2}\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_2}\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P$
$((m,n,n,0),(m',n',n',0))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P$
$((m,n,n,0),(m',n',p',q'))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_2}\boldsymbol{g}\mathcal{G}_P \cup$ $\mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_2}\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_2}\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P$
$((m,n,p,q),(m',n',p',q'))$	$\mathcal{G}_P\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_2}\boldsymbol{g}\mathcal{G}_P \cup$ $\mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_1}\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_2}\boldsymbol{g}\boldsymbol{s_1}\mathcal{G}_P \cup \mathcal{G}_P\boldsymbol{s_2}\boldsymbol{g}\boldsymbol{s_2}\mathcal{G}_P$

Table 6: Splitting of F–equivalence classes into P–equivalence classes. The last column gives the decomposition of the F–equivalence class $\mathcal{G}_F(\boldsymbol{p},\boldsymbol{q})\mathcal{G}_F$ into double cosets of $\mathcal{G}_P$. Here, $\boldsymbol{s_1} = (\boldsymbol{u_0}, \frac{1}{2}(1,1,1,1)), \boldsymbol{s_2} = (\boldsymbol{u_0}, \frac{1}{2}(-1,1,1,1))$. In order to save space we have omitted some pairs. These can be easily obtained by interchanging $\boldsymbol{p}$ and $\boldsymbol{q}$ and adapting the decomposition correspondingly, i.e. we have to interchange the corresponding quaternions of the pairs $\boldsymbol{g}\boldsymbol{s_1}$, $\boldsymbol{s_1}\boldsymbol{g}$, ... as well.

$\boldsymbol{p}$	$\boldsymbol{q}$	non–trivial generators of $\mathcal{H}_P(\boldsymbol{p},\boldsymbol{q})$	$\lvert\mathcal{H}_P(\boldsymbol{p},\boldsymbol{q})\rvert$	$\lvert G_P R(\boldsymbol{p},\boldsymbol{q}) G_P\rvert$
$(1,0,0,0)$	$(1,0,0,0)$	$\mathcal{G}_P$	384	192
$(1,0,0,0)$	$(1,1,1,1)$	$(\boldsymbol{u}_1,\boldsymbol{u}_0),(\boldsymbol{u}_2,\boldsymbol{u}_0),(\boldsymbol{u}_0,\boldsymbol{u}_1),(\boldsymbol{u}_0,\boldsymbol{u}_2),(\frac{1}{2}(1,1,1,1),\frac{1}{2}(1,1,1,1))$	192	$2\cdot 192$
$(1,0,0,0)$	(m,n,n,n)	$(\boldsymbol{u}_1,\boldsymbol{u}_0),(\boldsymbol{u}_2,\boldsymbol{u}_0),(\frac{1}{2}(1,1,1,1),\frac{1}{2}(1,1,1,1))$	48	$8\cdot 192$
$(1,0,0,0)$	$(m,n,0,0)$	$(\boldsymbol{u}_1,\boldsymbol{u}_0),(\boldsymbol{u}_2,\boldsymbol{u}_0),(\frac{1}{\sqrt{2}}(1,1,0,0),\frac{1}{\sqrt{2}}(1,1,0,0))$	64	$6\cdot 192$
$(1,0,0,0)$	$(\frac{m-n}{2},\frac{m+n}{2},\frac{m-n}{2},\frac{m+n}{2})$	$(\boldsymbol{u}_1,\boldsymbol{u}_0),(\boldsymbol{u}_2,\boldsymbol{u}_0),(\boldsymbol{u}_0,\boldsymbol{u}_1)$	32	$12\cdot 192$
$(1,0,0,0)$	$(m,n,n,0)$	$(\boldsymbol{u}_1,\boldsymbol{u}_0),(\boldsymbol{u}_2,\boldsymbol{u}_0),(\frac{1}{\sqrt{2}}(0,1,1,0),\frac{1}{\sqrt{2}}(0,1,1,0))$	32	$12\cdot 192$
$(1,0,0,0)$	$(\frac{m}{2}-n,\frac{m}{2}+n,\frac{m}{2},\frac{m}{2})$	$(\boldsymbol{u}_1,\boldsymbol{u}_0),(\boldsymbol{u}_2,\boldsymbol{u}_0)$	16	$24\cdot 192$
$(1,0,0,0)$	general	$(\boldsymbol{u}_1,\boldsymbol{u}_0),(\boldsymbol{u}_2,\boldsymbol{u}_0)$	16	$24\cdot 192$
$(0,1,1,1)$	$(0,1,1,1)$	$(\frac{1}{2}(1,1,1,1),\frac{1}{2}(1,1,1,1)),(\frac{1}{\sqrt{2}}(0,1,-1,0),\frac{1}{\sqrt{2}}(0,1,-1,0))$	24	$16\cdot 192$
$(0,1,1,1)$	$(3,1,1,1)$	$(\frac{1}{2}(1,1,1,1),\frac{1}{2}(1,1,1,1))$	12	$32\cdot 192$
$(0,1,1,1)$	(m,n,n,n)	$(\frac{1}{2}(1,1,1,1),\frac{1}{2}(1,1,1,1))$	12	$32\cdot 192$
$(0,1,1,1)$	$(m,n,0,0)$	$(\frac{1}{\sqrt{2}}(0,0,1,-1),\frac{1}{\sqrt{2}}(1,1,0,0))$	16	$24\cdot 192$
$(0,1,1,1)$	$(\frac{m-n}{2},\frac{m+n}{2},\frac{m-n}{2},\frac{m+n}{2})$	$(\boldsymbol{u}_0,\boldsymbol{u}_1)$	8	$48\cdot 192$
$(0,1,1,1)$	$(m,n,n,0)$	$(\frac{1}{\sqrt{2}}(0,1,-1,0),\frac{1}{\sqrt{2}}(0,1,1,0))$	8	$48\cdot 192$
$(0,1,1,1)$	$(\frac{m}{2}-n,\frac{m}{2}+n,\frac{m}{2},\frac{m}{2})$	—	4	$96\cdot 192$
$(0,1,1,1)$	general	—	4	$96\cdot 192$
(m,n,n,n)	(m',n',n',n')	$(\frac{1}{2}(1,1,1,1),\frac{1}{2}(1,1,1,1))$	12	$32\cdot 192$
(m,n,n,n)	$(m',n',0,0)$	$(\boldsymbol{u}_0,\boldsymbol{u}_1)$	8	$48\cdot 192$
(m,n,n,n)	$(m',n',n',0)$	—	4	$96\cdot 192$
(m,n,n,n)	general	—	4	$96\cdot 192$
$(m,n,0,0)$	$(m',n',0,0)$	$(\frac{1}{\sqrt{2}}(1,1,0,0),\frac{1}{\sqrt{2}}(1,1,0,0)),(\frac{1}{\sqrt{2}}(1,1,0,0),\frac{1}{\sqrt{2}}(1,-1,0,0))$	32	$12\cdot 192$
$(m,n,0,0)$	$(m',0,n',0)$	$(\boldsymbol{u}_1,\boldsymbol{u}_0),(\boldsymbol{u}_0,\boldsymbol{u}_2)$	16	$24\cdot 192$
$(m,n,0,0)$	$(\frac{m'-n'}{2},\frac{m'+n'}{2},\frac{m'-n'}{2},\frac{m'+n'}{2})$	$(\boldsymbol{u}_1,\boldsymbol{u}_0),(\boldsymbol{u}_0,\boldsymbol{u}_1)$	16	$24\cdot 192$
$(m,n,0,0)$	$(\frac{m'-n'}{2},\frac{m'+n'}{2},\frac{m'+n'}{2},\frac{m'-n'}{2})$	$(\boldsymbol{u}_1,\boldsymbol{u}_0),(\boldsymbol{u}_0,\boldsymbol{u}_2)$	16	$24\cdot 192$
$(m,n,0,0)$	$(\frac{m'-n'}{2},\frac{m'-n'}{2},\frac{m'+n'}{2},\frac{m'+n'}{2})$	$(\boldsymbol{u}_1,\boldsymbol{u}_0),(\boldsymbol{u}_0,\boldsymbol{u}_3)$	16	$24\cdot 192$
$(m,n,0,0)$	$(m',n',n',0)$	$(\boldsymbol{u}_1,\boldsymbol{u}_0)$	8	$48\cdot 192$
$(m,n,0,0)$	$(m',0,n',n')$	$(\frac{1}{\sqrt{2}}(1,1,0,0),\frac{1}{\sqrt{2}}(0,0,1,1))$	16	$24\cdot 192$
$(m,n,0,0)$	$(\frac{m'}{2}-n',\frac{m'}{2}+n',\frac{m'}{2},\frac{m'}{2})$	$(\boldsymbol{u}_1,\boldsymbol{u}_0)$	8	$48\cdot 192$
$(m,n,0,0)$	$(-\frac{m'}{2}-n',\frac{m'}{2},\frac{m'}{2}-n',\frac{m'}{2})$	$(\boldsymbol{u}_1,\boldsymbol{u}_0)$	8	$48\cdot 192$
$(m,n,0,0)$	$(\frac{m'}{2}-n',\frac{m'}{2},\frac{m'}{2}+n',\frac{m'}{2})$	$(\boldsymbol{u}_1,\boldsymbol{u}_0)$	8	$48\cdot 192$
$(m,n,0,0)$	general	$(\boldsymbol{u}_1,\boldsymbol{u}_0)$	8	$48\cdot 192$
$(m,n,n,0)$	$(m',n',n',0)$	$(\frac{1}{\sqrt{2}}(0,1,1,0),\frac{1}{\sqrt{2}}(0,1,1,0))$	8	$48\cdot 192$
$(m,n,n,0)$	$(m',0,n',n')$	—	4	$96\cdot 192$
$(m,n,n,0)$	$(\frac{m'}{2}-n',\frac{m'}{2}+n',\frac{m'}{2},\frac{m'}{2})$	—	4	$96\cdot 192$
$(m,n,n,0)$	$(-\frac{m'}{2}-n',\frac{m'}{2},\frac{m'}{2}-n',\frac{m'}{2})$	—	4	$96\cdot 192$
$(m,n,n,0)$	$(\frac{m'}{2}-n',\frac{m'}{2},\frac{m'}{2}+n',\frac{m'}{2})$	—	4	$96\cdot 192$
$(m,n,n,0)$	general	—	4	$96\cdot 192$
general	general	—	4	$96\cdot 192$

Table 7: P–Equivalence classes of admissible pairs. The groups $\mathcal{H}_P(\boldsymbol{p},\boldsymbol{q})$ are given in terms of their generators listed in the third column, where we always have to add the trivial generators $((-1,0,0,0),(1,0,0,0))$ and $((1,0,0,0),(-1,0,0,0))$. The last column gives the number of P–equivalent coincidence rotations $R(\boldsymbol{p},\boldsymbol{q})$. By dividing these numbers by 192 we obtain the number of P–equivalent CSLs. In order to save space we have omitted some pairs. These can be easily obtained by interchanging $\boldsymbol{p}$ and $\boldsymbol{q}$ and adapting the generators correspondingly.

$(\boldsymbol{p}, \boldsymbol{q})$	# inequiv. pairs $\Sigma_P = \Sigma_F$	# inequiv. pairs $\Sigma_P = 2\Sigma_F$
$((1,0,0,0),(1,0,0,0))$	1	—
$(1,0,0,0),(1,1,1,1)$	—	1
$((1,0,0,0),(m,n,n,n))$	n_{F02}	$2n_{F02}$
$((1,0,0,0),(m,n,0,0))$	n_{F03}	—
$((1,0,0,0),(m-n,m+n,m-n,m+n))$	—	n_{F03}
$((1,0,0,0),(m,n,n,0))$	n_{F04}	—
$((1,0,0,0),(m-2n,m+2n,m,m))$	—	n_{F04}
$((1,0,0,0),(m,n,p,q))$	n_{F05}	$2n_{F05}$
$((0,1,1,1),(0,1,1,1))$	1	—
$((0,1,1,1),(3,1,1,1))$	—	1
$((0,1,1,1),(m,n,n,n))$	n_{F12}	$2n_{F12}$
$((0,1,1,1),(m,n,n,0))$	n_{F14}	—
$((0,1,1,1),(m-2n,m+2n,m,m))$	—	n_{F14}
$((0,1,1,1),(m,n,p,q))$	n_{F15}	$2n_{F15}$
$((m,n,n,n),(m',n',n',n'))$	n_{F22}	$2n_{F22}$
$((m,n,n,n),(m',n',0,0))$	n_{F23}	$2n_{F23}$
$((m,n,n,n),(m',n',n',0))$	n_{F24}	$2n_{F24}$
$((m,n,n,n),(m',n',p',q'))$	n_{F25}	$2n_{F25}$
$((m,n,0,0),(m',n',0,0))$	n_{F33}	—
$((m,n,0,0),(m',0,n',0))$	n_{F33}	—
$((m,n,0,0),(m'-n',m'+n',m'-n',m'+n'))$	—	n_{F33}
$((m,n,0,0),(m'-n',m'+n',m'+n',m'-n'))$	—	n_{F33}
$((m,n,0,0),(m'-n',m'-n',m'+n',m'+n'))$	—	n_{F33}
$((m,n,0,0),(m',n',n',0))$	n_{F34}	—
$((m,n,0,0),(m',0,n',n'))$	n_{F34}	—
$((m,n,0,0),(m'-2n',m'+2n',m',m'))$	—	n_{F34}
$((m,n,0,0),(-m'-2n',m',m'-2n',m'))$	—	n_{F34}
$((m,n,0,0),(m'-2n',m',m'+2n',m'))$	—	n_{F34}
$((m,n,0,0),(m',n',p',q'))$	$3n_{F35}$	$6n_{F35}$
$((m,n,n,0),(m',n',n',0))$	n_{F44}	—
$((m,n,n,0),(m',0,n',n'))$	n_{F44}	—
$((m,n,n,0),(m'-2n',m'+2n',2,m'))$	—	n_{F44}
$((m,n,n,0),(-m'-2n',m',m'-2n',m'))$	—	n_{F44}
$((m,n,n,0),(m'-2n',m',m'+2n',m'))$	—	n_{F44}
$((m,n,n,0),(m',n',p',q'))$	$3n_{F45}$	$6n_{F45}$
$((m,n,p,q),(m',n',p',q'))$	$3n_{F55}$	$6n_{F55}$

Table 8: Number of P–inequivalent admissible pairs. The second column gives the number of inequivalent pairs for odd values of Σ whereas the third column gives the same information for even values of Σ. In order to save space we have omitted some pairs. These can be easily obtained by interchanging $\boldsymbol{p}$ and $\boldsymbol{q}$.