Multiple CSLs for the body centered cubic lattice

Peter Zeiner

Faculty of Mathematics, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany
and
Institute of Theoretical Physics & CMS, TU Wien, Wiedner Hauptstraße 8–10, 1040 Wien, Austria

E-mail: pzeiner@math.uni-bielefeld.de

Abstract. Ordinary Coincidence Site Lattices (CSLs) are defined as the intersection of a lattice Γ with a rotated copy $R\Gamma$ of itself. They are useful for classifying grain boundaries and have been studied extensively since the mid sixties. Recently the interests turned to so-called multiple CSLs, i.e. intersections of n rotated copies of a given lattice Γ, in particular in connection with lattice quantizers. Here we consider multiple CSLs for the 3-dimensional body centered cubic lattice, in particular we discuss the spectrum of coincidence indices and their multiplicity, in particular we show that the latter is a multiplicative function and give an explicit expression of it for some special cases.

1. Introduction

Ordinary coincidence site lattices (CSLs) have been studied intensively since the 1960s (see e.g. [1, 2] and references therein), because they are an important tool to characterize and analyze the structure of grain boundaries in crystals. Hence there is a vast literature on 3–dimensional CSLs, in particular on cubic lattices [3, 4, 5, 6, 7, 8]. CSLs in higher dimensions have been studied as well (see [7, 9] and references therein) with possible applications to quasiperiodic structures. In addition, the concept of CSLs has been generalized for modules, again to cover the needs of quasiperiodic structures [10, 7].

We want to discuss another generalization of CSLs here. Loosely speaking, CSLs are the intersection of two mutually rotated lattices. It is thus natural to consider the intersection of n mutually rotated lattices. This question has recently been raised in connection with quantizing procedures [11, 12], where it seems useful to represent a complex lattice as the intersection of simpler lattices. In the meantime this question has been answered in detail for several 2–dimensional lattices [13], so the next step is to consider a 3–dimensional example. We choose a cubic lattice here, namely the body–centered cubic lattice, since the cubic case is one of the best studied 3–dimensional cases. It might seem more natural to discuss the primitive cubic case first, but it turns out that the body centered case can be treated more elegantly. Moreover most results hold for all three cubic lattices. Details for the other cubic lattices shall be published elsewhere [14].

2. Ordinary CSLs

We recall some definitions first [7]. Let $\Gamma \subseteq \mathbb{R}^n$ be an n-dimensional lattice and $R \in SO(n)$ a rotation (we restrict our considerations here to proper rotations for simplicity). Then R is called a *coincidence rotation* if $\Gamma(R) := \Gamma \cap R\Gamma$ is a lattice of finite index in Γ. The corresponding lattice $\Gamma(R) = \Gamma \cap R\Gamma$ is called a *coincidence site lattice.* The *coincidence index* $\Sigma(R)$ is defined as the index of $\Gamma(R)$ in Γ. Note in passing that the set of coincidence rotations forms a group under matrix multiplication.

In the following let Γ be a body centered cubic lattice. Then $R \in SO(3)$ is a coincidence rotation if and only if R is a matrix with rational entries (see [3, 4, 5, 6, 7, 8]). They can be parameterized by integral quaternions $\boldsymbol{q} = (\kappa, \lambda, \mu, \nu)$, i.e., by quaternions with integral coefficients $\kappa, \lambda, \mu, \nu$ in the following way [15, 16, 17, 7, 8]:

$$R(\boldsymbol{q}) = \frac{1}{|\boldsymbol{q}|^2} \begin{pmatrix} \kappa^2+\lambda^2-\mu^2-\nu^2 & -2\kappa\nu+2\lambda\mu & 2\kappa\mu+2\lambda\nu \\ 2\kappa\nu+2\lambda\mu & \kappa^2-\lambda^2+\mu^2-\nu^2 & -2\kappa\lambda+2\mu\nu \\ -2\kappa\mu+2\lambda\nu & 2\kappa\lambda+2\mu\nu & \kappa^2-\lambda^2-\mu^2+\nu^2 \end{pmatrix}, \tag{1}$$

where $|\boldsymbol{q}|^2 = \kappa^2+\lambda^2+\mu^2+\nu^2$ is called the norm of $\boldsymbol{q}$. Note that we will call a quaternion an integer quaternion if it is an integral quaternion $(\kappa, \lambda, \mu, \nu)$ or the sum of an integral quaternion with the quaternion $(1,1,1,1)/2$. We call an integral quaternion $\boldsymbol{r} = (\kappa, \lambda, \mu, \nu)$ primitive if the greatest common divisor of $\kappa, \lambda, \mu, \nu$ equals 1. If not stated otherwise every (integral) quaternion will be assumed to be a primitive quaternion. Furthermore let $\boldsymbol{H} \subset \boldsymbol{Q}$ denote the ring of integer quaternions and the ring of real quaternions, respectively.

One can show that the coincidence index is given by $\Sigma(R(\boldsymbol{q})) = |\boldsymbol{q}|^2/2^\ell$, where ℓ is the maximal power such that 2^ℓ divides $|\boldsymbol{q}|^2$ (see e.g. [4, 6, 7]), i.e. $\Sigma(R)$ is always odd. On the other hand $\Sigma(R)$ runs over all positive odd integers if R runs over all coincidence rotations, i.e. the spectrum of coincidence rotations is the set of all positive odd integers. Let O denote the cubic symmetry group. Then $\Gamma(RQ) = \Gamma(R)$ if and only if $Q \in O$, i.e. R and RQ generate the same CSL, which motivates to call R and RQ *strongly equivalent.* In general one calls R and R' *equivalent* if there exist Q, Q' such that $R = QR'Q'$. For any $R(\boldsymbol{q})$ we can find a strongly equivalent $R' = R(\boldsymbol{q}')$ such that $|\boldsymbol{q}'|^2$ is odd, i.e. $\Sigma(R') = |\boldsymbol{q}'|^2$. Hence we will assume in the following that $|\boldsymbol{q}|^2$ is odd.

If we define the projection $P : \boldsymbol{Q} \to \mathbb{R}^3$ by $P(q_0, q_1, q_2, q_3) = (q_1, q_2, q_3)$ then $\Gamma = P\boldsymbol{H}$, i.e. the body centered cubic lattice is obtained by a projection of $\boldsymbol{H}$ onto $\mathbb{R}^3$. Moreover Lemma 5.1 of [8] tells us that $\Gamma(R(\boldsymbol{q})) = P(\boldsymbol{q}\boldsymbol{H})$, where $\boldsymbol{q}\boldsymbol{H}$ is a left ideal of $\boldsymbol{H}$. In fact this establishes a one to one correspondence of CSLs and left ideals of $\boldsymbol{H}$ (see [14]), which is a key in the discussion of the body centered CSLs. In particular, finding the number $f(\Sigma)$ of different CSLs of given index Σ is equivalent to counting the corresponding left ideals of $\boldsymbol{H}$. One can show that $f(\Sigma)$ is a multiplicative function, i.e. $f(mn) = f(m)f(n)$ if m and n are coprime, and in particular we have $f(1) = 1$, $f(2) = 0$ and $f(p^r) = (p+1)p^{r-1}$ for all odd primes p [7, 8].

3. Multiple CSLs

Now we turn to multiple CSLs, which we define as follows [13, 14]:

Definition 3.1 *Let Γ be an n-dimensional lattice and R_i, $i = 1, \ldots m$ coincidence rotations of Γ. Then the lattice*

$$\Gamma(R_1, \ldots, R_m) := \Gamma \cap R_1\Gamma \cap \ldots \cap R_m\Gamma = \Gamma(R_1) \cap \ldots \cap \Gamma(R_m) \tag{2}$$

is called a multiple CSL (MCSL). Its index in Γ is denoted by $\Sigma(R_1, \ldots, R_m)$.

Note that $\Sigma(R_1, \ldots, R_m)$ is finite since $\Gamma(R_1, \ldots, R_m)$ is a finite intersection of mutually commensurate lattices [7]. In particular, it follows from the second homomorphism theorem that

$$\Sigma(R_1, R_2) = \frac{\Sigma(R_1)\Sigma(R_2)}{\Sigma_+(R_1, R_2)}, \tag{3}$$

where $\Sigma_+(R_1,R_2)$ is the index of the direct sum $\Gamma_+(R_1,R_2)=\Gamma(R_1)+\Gamma(R_2)$ in Γ. In general one shows

$$\Sigma(R_1,\ldots,R_m)=\frac{\Sigma(R_1,\ldots,R_{m-1})\Sigma(R_m)}{\Sigma_+(R_1,\ldots,R_{m-1};R_m)}, \tag{4}$$

where $\Sigma_+(R_1,\ldots,R_{m-1};R_m)$ is the index of $\Gamma_+(R_1,\ldots,R_{m-1};R_m)=\Gamma(R_1,\ldots,R_{m-1})+\Gamma(R_m)$ in Γ. In particular, $\Sigma(R_1,\ldots,R_m)$ divides $\Sigma(R_1)\cdot\ldots\cdot\Sigma(R_m)$. In case of the 3–dimensional cubic lattices this implies immediately that the spectrum is the same for multiple and ordinary CSLs, i.e. $\Sigma(R_1,\ldots,R_m)$ runs over all odd positive integers, too. However, new lattices emerge and the multiplicity of a given index will increase. Note that the spectrum is preserved also for the square lattice and the 4–dimensional hypercubic lattices.

Having determined the spectrum we can attack the second main problem, the number $f_m(\Sigma)$ of different MCSLs. To this end we have to determine all possible MCSLs. We first note that $\Gamma_+(R_1,R_2)=P(\boldsymbol{q}_1\boldsymbol{H}+\boldsymbol{q}_2\boldsymbol{H})=P(\boldsymbol{q}\boldsymbol{H})$, where $\boldsymbol{q}$ is the greatest left common divisor (glcd) of $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$. Hence (recall that we may assume that $|\boldsymbol{q}_i|^2$ is odd)

$$\Sigma(R_1,R_2)=\frac{|\boldsymbol{q}_1|^2|\boldsymbol{q}_2|^2}{|\boldsymbol{q}|^2}\quad\text{with } \boldsymbol{q}=\mathrm{glcd}(\boldsymbol{q}_1,\boldsymbol{q}_2). \tag{5}$$

In case that $|\boldsymbol{q}_1|^2$ and $|\boldsymbol{q}_2|^2$ are relatively prime this reduces to $\Sigma(R_1,R_2)=|\boldsymbol{q}_1|^2|\boldsymbol{q}_2|^2$ which suggests the following lemma [14]:

Lemma 3.1 *Let $|\boldsymbol{q}_1|^2$ and $|\boldsymbol{q}_2|^2$ be relatively prime. Then there exists a quaternion $\boldsymbol{q}$, such that $\Gamma(R_1,R_2)=\Gamma(R(\boldsymbol{q}))$.*

The proof makes use of the fact there exists a right least common multiple $\boldsymbol{q}$ of $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$. Note that in this case the MCSL is equal to an ordinary CSL. This theorem can be immediately generalized for arbitrary m. Conversely we have [14]

Lemma 3.2 *Let $p_1^{\alpha_1}\cdots p_\ell^{\alpha_\ell}$ be the prime decomposition of $|\boldsymbol{q}|^2$. Then there exist quaternions $\boldsymbol{q}_i$ such that $|\boldsymbol{q}_i|^2=p_i^{\alpha_i}$ and $\Gamma(R(\boldsymbol{q}))=\Gamma(R(\boldsymbol{q}_1))\cap\ldots\cap\Gamma(R(\boldsymbol{q}_\ell))$.*

This decomposition is unique. More generally we have [14]

Lemma 3.3 *For any $\Gamma(R_1,\ldots,R_m)$ with $\Sigma(R_1,\ldots,R_m)=p_1^{\alpha_1}\cdots p_\ell^{\alpha_\ell}$ (all p_i distinct) there exists a unique decomposition $\Gamma(R_1,\ldots,R_m)=\Gamma_1\cap\ldots\cap\Gamma_\ell$ such that Γ_i is a MCSL with index $\Sigma_i=p_i^{\alpha_i}$.*

Thus the analysis of MCSLs can be reduced to the study of the MCSLs with prime power index. Another consequence is the multiplicity of f_m:

Theorem 3.4 *Let $f_m(\Sigma)$ be the number of different MCSLs for a given index Σ. Then $f_m(nn')=f_m(n)f_m(n')$ if n and n' are relatively prime.*

Since the analysis of general MCSLs with prime power index is rather cumbersome we confine our discussion to the intersection of two CSLs. The general discussion will be published elsewhere [14]. We may confine our discussion to the case that neither $\boldsymbol{q}_1$ nor $\boldsymbol{q}_2$ is a right multiple of the other, i.e. there does not exist an integer quaternion $\boldsymbol{r}$ such that $\boldsymbol{q}_1=\boldsymbol{q}_2\boldsymbol{r}$ or vice versa, since otherwise $\Gamma(R_1,R_2)$ reduces to $\Gamma(R_2)$ or $\Gamma(R_1)$, respectively. We first mention a representation of $\Gamma(R_1,R_2)$. Here $\bar{\boldsymbol{q}}=(\kappa,-\lambda,-\mu,-\nu)$ denotes the conjugate of $\boldsymbol{q}=(\kappa,\lambda,\mu,\nu)$.

Lemma 3.5 *Let $|\boldsymbol{q}_i|^2=p^{\alpha_i}$, $i=1,2$, p prime, none of the $\boldsymbol{q}_i$ a right multiple of the other one. Choose $\boldsymbol{r}$ such that $\boldsymbol{q}_1\boldsymbol{r}\bar{\boldsymbol{q}}_2$ is a primitive quaternion and let $\boldsymbol{q}$ be the least right common multiple of $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$. Then $\Gamma(R_1,R_2)=\Gamma(R(\boldsymbol{q}_1))\cap\Gamma(R(\boldsymbol{q}_2))=P(\boldsymbol{q}\boldsymbol{H}+\boldsymbol{q}_1\boldsymbol{r}\bar{\boldsymbol{q}}_2\mathbb{Z})$.*

Such an $\boldsymbol{r}$ is by no means unique. Its existence follows from the uniqueness of the left (or right) prime power decomposition of integer quaternions. Alternatively we may decompose $\Gamma(R_1, R_2)$ as follows:

Lemma 3.6 *Under the conditions of the previous lemma, we have* $\Gamma(R_1, R_2) = P(\boldsymbol{qH} + \boldsymbol{q}_1\boldsymbol{H}\bar{\boldsymbol{q}}_2) = P(\boldsymbol{qH} + \boldsymbol{q}_2\boldsymbol{H}\bar{\boldsymbol{q}}_1)$.

Note that $\boldsymbol{qH} + \boldsymbol{q}_2\boldsymbol{H}\bar{\boldsymbol{q}}_1$ is no ideal and hence $\Gamma(R_1, R_2)$ is neither an ordinary CSL nor a multiple of an ordinary CSL. Note further that $P(\boldsymbol{qH} + \boldsymbol{q}_1\boldsymbol{H}\bar{\boldsymbol{q}}_2)/P(\boldsymbol{qH})$ is a cyclic group of order $\frac{|\boldsymbol{q}|^2}{\max(|\boldsymbol{q}_1|^2, |\boldsymbol{q}_1|^2)}$ and that $P(\boldsymbol{qH})$ is a multiple of an ordinary CSL ($\boldsymbol{q}$ is not primitive here!). The next lemma tells us under which conditions different pairs of CSLs give rise to different MCSLs:

Lemma 3.7 *Let* $\boldsymbol{q}_i$ *be primitive quaternions with* $|\boldsymbol{q}_i|^2 = p^{\alpha_i}$*, where* p *is a prime and* $\alpha_1 \geq \alpha_2 \geq \alpha_4, \alpha_3 \geq \alpha_4$*. Let* $\boldsymbol{q}_{ij}$ *with* $|\boldsymbol{q}_{ij}|^2 = p^{\alpha_{ij}}$ *be the greatest left common divisor of* $\boldsymbol{q}_i$ *and* $\boldsymbol{q}_j$*. Then* $\Gamma(R_1) \cap \Gamma(R_2) = \Gamma(R_3) \cap \Gamma(R_4)$ *if and only if (in case of* $\alpha_1 = \alpha_2$ *possibly after interchanging* $\boldsymbol{q}_1$ *and* $\boldsymbol{q}_2$*)* $\alpha_1 = \alpha_3, \alpha_2 - \alpha_{12} = \alpha_4 - \alpha_{34}, \alpha_1 - \alpha_{13} \leq \min(\alpha_4 - \alpha_{34}, \alpha_{34})$ *and* $\alpha_2 - \alpha_{24} \leq \min(\alpha_4 - \alpha_{34}, \alpha_{34})$ *are satisfied.*

Thus we can calculate the number $f_2(\Sigma)$ of different MCSLs which are intersections of at most two ordinary CSLs:

Theorem 3.8 *Let* p *be an odd prime number. Then*

$$\begin{aligned} f_2(p^r) =& (r/2 + 1/2)\,(p+1)p^{r-1} + (r/2 - 1)p^{r-2} + (r/2 - [r/2])p^{r-4} \\ &+ \frac{p^{r-1} - p^{r-2[r/3]-1}}{p^2 - 1} + \frac{p^{4[r/3]-r+2} - p^{4[r/2]-r-2}}{2(p^2-1)}, \end{aligned} \tag{6}$$

where $[x]$ *is Gauss' symbol denoting the largest integer* n *such that* $n \leq x$*.*

Note that $f_2(p^r) = f_m(p^r)$ for $r = 1, 2$. Thus we know $f_m(\Sigma)$ for all Σ that are free from third powers. The more complex general case will be presented elsewhere [14].

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