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Multiple coincidences for dimensions $d \leq 3$

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Ordinary coincidence site lattices (CSLs) are very well understood for a large class of lattices in dimensions $d \leq 4$, as well as its generalisation for various highly symmetric modules. Here we consider multiple coincidence site lattices, i.e. intersections of several ordinary CSLs, which appear in connection with triple and multiple junctions. We restrict our considerations to the most prominent lattices in dimensions $d \leq 3$ and present an outlook for further lattices and modules.

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1 Introduction

Ordinary coincidence site lattices (CSLs) have proved useful in connection with grain boundaries in crystals (see e.g. [1, 2] and references therein) and are thus well understood for lattices in dimensions $d \leq 3$, for the cubic lattices in particular see e.g. [3–8]. This concept allows several generalisations. On the one hand, one can extend it to modules, where first steps have been made more than a decade ago to meet the needs of aperiodic structures, see e.g. [7, 9, 10]. On the other hand, one can consider the intersection of more than two lattices, so-called multiple coincidence site lattices. This is of interest in connection with triple and multiple junctions [11, 12] in solid state physics and in connection with quantising procedures [13, 14] in information theory. So far, multiple coincidences are well understood only for some highly symmetric lattices and modules in the plane, see [15]. Since so far only some preliminary results on the cubic case have been published [16], we here present the main results for the cubic case, whose details will be published elsewhere [17].

We recall some definitions first [7]. Let $\Gamma \subseteq \mathbb{R}^d$ be a d-dimensional lattice and $R \in \mathrm{SO}(d)$ a rotation (we restrict our considerations here to proper rotations for simplicity). Then R is called an (ordinary) *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 (CSL)*. The *coincidence index* $\Sigma(R)$ is defined as the index of $\Gamma(R)$ in Γ, and $\sigma = \{\Sigma(R) \mid R \in SOC(\Gamma)\}$, the set of all possible coincidence indices, is called the (ordinary) coincidence spectrum. Note in passing that the set of coincidence rotations forms a group under matrix multiplication, called $\mathrm{SOC}(\Gamma)$. An immediate extension of these notions is the following [15, 17]:

Definition 1.1 Let Γ be a d-dimensional lattice and R_i, $i \in \{1, \ldots n\}$ coincidence rotations of Γ. Then the lattice

$$\Gamma(R_1, \ldots, R_n) := \Gamma \cap R_1\Gamma \cap \ldots \cap R_n\Gamma = \Gamma(R_1) \cap \ldots \cap \Gamma(R_n) \tag{1}$$

is called a multiple CSL (MCSL). Its index in Γ is denoted by $\Sigma(R_1, \ldots, R_n)$. The corresponding spectra are $\sigma_n := \{\Sigma(R_1, \ldots, R_n) \mid R_i \in SOC(\Gamma)\}$ for n fixed and $\sigma_\infty = \bigcup_{n\in\mathbb{N}} \sigma_n$, the latter one called full coincidence spectrum.

Note that the requirement that the R_i are all coincidence rotations is necessary and sufficient for $\Sigma(R_1, \ldots, R_m)$ to be finite. In fact, this is a simple consequence of the second homomorphism theorem for

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groups. Another consequence is the following lemma [17], which puts restrictions on the possible values of coincidence indices:

LEMMA 1.2 *$\Sigma(R_1, \ldots, R_n)$ divides $\Sigma(R_1) \cdot \ldots \cdot \Sigma(R_n)$.*

On the other hand, it is obvious that $\sigma \subseteq \sigma_m \subseteq \sigma_n \subseteq \sigma_\infty$ for $m \leq n$, since $\sigma_n = \bigcup_{m \leq n} \sigma_m$. These two facts often guarantee that the spectrum stays the same for multiple CSLs, i.e. $\sigma = \sigma_\infty$. This holds true, among others, for the 2–dimensional square lattice, the 3–dimensional cubic lattices and the 4–dimensional centred hypercubic lattice. It also holds true for the 4–dimensional primitive hypercubic lattice. However, the argumentation is more subtle in this case and makes use of

LEMMA 1.3 *Let $\Gamma_1 \subseteq \Gamma_2$ have index m in Γ_2. Then, the indices Σ_i of the MCSLs $\Gamma_i(R_1, \ldots, R_n)$ in Γ_i satisfy $\Sigma_2 | m\Sigma_1$.*

2 2-dimensional lattices and modules

An instructive example is the 2-dimensional square lattice. We identify it with the Gaussian integers $\mathbb{Z}[i] = \{m + ni \mid m, n \in \mathbb{Z}\}$, which enables us to make use of number theory. Rotations can then be represented by unimodular complex numbers $e^{i\phi}$ and it turns out that ω corresponds to a coincidence rotation if and only if $e^{i\phi} \in \mathbb{Q}(i)$ (for details, see [7,15]). Hence, we may write $e^{i\phi} = \frac{\alpha}{\beta}$ with $\beta = \bar{\alpha} \in \mathbb{Z}[i]$, where we may assume that α and its complex conjugate $\bar{\alpha}$ are coprime, since we may cancel common factors. Decomposing α into prime factors we see that $e^{i\phi}$ may be written as [7]

$$e^{i\phi} = \varepsilon \prod_{p \equiv 1\,(4)} \left(\frac{\omega_p}{\bar{\omega}_p} \right)^{n_p}, \tag{2}$$

where ε is a unit, i.e. one of the numbers $\pm 1, \pm i$, and ω_p are the prime factors of the complex splitting primes $p = \omega_p \bar{\omega}_p = 1 \pmod 4$. The ω_p are not defined uniquely, since the roles of ω_p and $\bar{\omega}_p$ may be interchanged and ω_p may be multiplied by a unit. However, there are no further ambiguities and a different choice of the prime factors ω_p can only affect ε and the sign of $n_p \in \mathbb{Z}$. No other real primes p can contribute, since $p = 3 \pmod 4$ is a prime also in $\mathbb{Z}[i]$ (these are the so-called inert primes) and $2 = (1+i)(1-i) = -i(1+i)$ is a ramified prime, i.e. the prime factors $1+i$ and $1-i$ are associated, i.e. $(1+i)/(1-i) = i$ is a unit [18]. Clearly, only a finite number of n_p may be non-zero.

The coincidence index $\Sigma(e^{i\phi})$ is given by [7]

$$\Sigma(e^{i\phi}) = \prod_{p \equiv 1\,(4)} p^{|n_p|}, \tag{3}$$

which is independent of the particular choice of the ω_p. The spectrum of possible coincidence indices is the set of all integers whose prime factorisation consists of primes $p = 1 \pmod 4$ only. Note that $\Sigma(e^{i\phi}) = |\omega(\phi)|^2$, where we have defined

$$\omega(\phi) := \prod_{\substack{p \equiv 1\,(4) \\ n_p > 0}} \omega_p^{n_p} \prod_{\substack{p \equiv 1\,(4) \\ n_p < 0}} \bar{\omega}_p^{n_p}. \tag{4}$$

This definition enables us to state the corresponding coincidence lattice explicitly [15]

$$\Gamma \cap R(\phi)\Gamma = \mathbb{Z}[i] \cap e^{i\phi}\mathbb{Z}[i] = \omega(\phi)\mathbb{Z}[i]. \tag{5}$$

In terms of algebraic number theory this means that every CSL is a principal ideal of $\mathbb{Z}[i]$, thus reducing the problem of counting the CSLs to the analogous problem for ideals of $\mathbb{Z}[i]$, which is well studied. Moreover

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this fact enables us to find the MCSLs very elegantly, see below. Another consequence is the fact that any CSL is again a square lattice, which is easily seen from [12] or [13].

Let $f(m)$ denote the number of different CSLs of index m. It is clear from the above considerations that $f(m)$ vanishes unless all prime factors are congruent to 1 (mod 4), in this case $f(m) = 2^n$, where n is the number of distinct prime divisors of m. In particular, $f(m)$ is a multiplicative function, which suggests to use a Dirichlet series as generating function. It reads [7]

$$\begin{aligned}\Phi(s) &= \sum_{m=1}^{\infty} \frac{f(m)}{m^s} = \prod_{p=1(4)} \frac{1+p^{-s}}{1-p^{-s}} \qquad (6)\\ &= 1 + \frac{2}{5^s} + \frac{2}{13^s} + \frac{2}{17^s} + \frac{2}{25^s} + \frac{2}{29^s} + \frac{2}{37^s} + \frac{2}{41^s} + \frac{2}{53^s} + \frac{2}{61^s} + \frac{4}{65^s} + \frac{2}{73^s} + \frac{4}{85^s} + \frac{2}{89^s} + \cdots\end{aligned}$$

Since any MCSL can be viewed as the intersection of ordinary CSLs, we need to consider only finite intersections of ideals $\omega(\phi)\mathbb{Z}[i]$ due to Eq. (5). But any intersection of ideals is again an ideal, and since any ideal of $\mathbb{Z}[i]$ is a principal ideal, we end up with

$$\Gamma \cap R(\phi_1)\Gamma \cap \ldots \cap R(\phi_k)\Gamma = \omega(\phi_1)\mathbb{Z}[i] \cap \ldots \cap \omega(\phi_k)\mathbb{Z}[i] = \omega\mathbb{Z}[i], \qquad (7)$$

where ω is the least common multiple (lcm) of $\omega(\phi_1), \ldots, \omega(\phi_k)$. Again, its index is just the number theoretic norm of $\omega = \prod_{p\equiv 1\,(4)} \omega_p^{n_p^+} \bar{\omega}_p^{n_p^-}$, i.e.

$$\Sigma(e^{i\phi_1}, \ldots, e^{i\phi_k}) = |\omega|^2 = \prod_{p=1(4)} p^{n_p^+ + n_p^-}, \qquad (8)$$

where $n_p^+ = \max(0, n_p^{(1)}, \ldots, n_p^{(k)})$ and $n_p^- = \max(0, -n_p^{(1)}, \ldots, -n_p^{(k)})$, see [15] for details. This implies that the spectrum stays the same, a fact that one can alternatively deduce from our general considerations in Sec. 1. However, new lattices emerge, since ω may contain both ω_p and $\bar{\omega}_p$, which is not possible in the case of ordinary CSLs. In fact, all new MCSLs are just an integer multiple of an ordinary CSL and any MCSL can be written as the intersection of at most two ordinary CSLs [15].

Thus the total number $f_\infty(m)$ of MCSLs of a given index m is again a multiplicative function [15]

$$\begin{aligned}\Phi_\infty(s) &= \sum_{m=1}^{\infty} \frac{f_\infty(m)}{m^s} = \Phi_(s)\zeta(s) = \prod_{p=1(4)} \frac{1}{(1-p^{-s})^2} \qquad (9)\\ &= 1 + \frac{2}{5^s} + \frac{2}{13^s} + \frac{2}{17^s} + \frac{3}{25^s} + \frac{2}{29^s} + \frac{2}{37^s} + \frac{2}{41^s} + \frac{2}{53^s} + \frac{2}{61^s} + \frac{4}{65^s} + \frac{2}{73^s} + \frac{4}{85^s} + \cdots\end{aligned}$$

$$\Phi_\infty(s) - \Phi(s) = \Phi(s)(\zeta(s) - 1) = \frac{1}{25^s} + \frac{2}{125^s} + \frac{1}{169^s} + \frac{1}{289^s} + \frac{1}{325^s} + \frac{1}{425^s} + \frac{3}{625^s} + \frac{2}{725^s} + \ldots \qquad (10)$$

In a similar way, one can treat the hexagonal lattice. Moreover, these results can be generalised for several modules related to N–fold symmetry, as long as the corresponding number field has class number one, which comprises the cases of 5–, 8–, 10–, and 12–fold symmetry [9, 15].

3 Cubic lattices

It is well known that $R \in \mathrm{SO}(3)$ is a coincidence rotation of a cubic lattice if and only if R is a matrix with rational entries, i.e., if $R \in \mathrm{SO}(3, \mathbb{Q})$ (see [3–8]). These coincidence rotations can be parameterised

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by quaternions $\boldsymbol{q} = (\kappa, \lambda, \mu, \nu)$ with integral coefficients $\kappa, \lambda, \mu, \nu$ in the following way [7, 8, 20–22]:

$$R(\boldsymbol{q}) = \frac{1}{|\boldsymbol{q}|^2} \begin{pmatrix} \kappa^2 + \lambda^2 - \mu^2 - \nu^2 & -2\kappa\nu + 2\lambda\mu & 2\kappa\mu + 2\lambda\nu \\ 2\kappa\nu + 2\lambda\mu & \kappa^2 - \lambda^2 + \mu^2 - \nu^2 & -2\kappa\lambda + 2\mu\nu \\ -2\kappa\mu + 2\lambda\nu & 2\kappa\lambda + 2\mu\nu & \kappa^2 - \lambda^2 - \mu^2 + \nu^2 \end{pmatrix}, \tag{11}$$

where $|\boldsymbol{q}|^2 = \kappa^2 + \lambda^2 + \mu^2 + \nu^2$ is called the (reduced number theoretic) norm of $\boldsymbol{q}$. Note that we will call a quaternion an *integer quaternion* if it is a quaternion $(\kappa, \lambda, \mu, \nu)$ with integral entries $\kappa, \lambda, \mu, \nu$ or the sum of such a quaternion with the quaternion $(1, 1, 1, 1)/2$. The set of all integer quaternions forms a ring under quaternion addition and multiplication and is usually referred to as the Hurwitz ring, denoted by $\boldsymbol{H}$. We call a quaternion $\boldsymbol{r} = (\kappa, \lambda, \mu, \nu)$ with integral entries *primitive* if $\gcd(\kappa, \lambda, \mu, \nu) = 1$. In fact, we can parameterise every coincidence rotation by a primitive quaternion, and we will always do so in the following. Finally note that $\bar{\boldsymbol{q}} = (\kappa, -\lambda, -\mu, -\nu)$ is the conjugate of $\boldsymbol{q}$.

One can show that the coincidence index is given by $\Sigma(R(\boldsymbol{q})) = |\boldsymbol{q}|^2/2^\ell$ (if $\boldsymbol{q}$ is primitive), 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 σ 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 $R' = RQ$ generate the same CSL. For any $R(\boldsymbol{q})$, we can find an $R' = R(\boldsymbol{q}') = RQ$ such that $|\boldsymbol{q}'|^2$ is odd, i.e. $\Sigma(R') = |\boldsymbol{q}'|^2$. We will call such a quaternion, i.e. a primitive quaternion with $|\boldsymbol{q}|^2$ odd, a reduced quaternion.

The quaternions cannot only be used to parameterise the rotations but there is also a close connection of the integer quaternions with the cubic lattices, in particular with the body centred cubic lattice, on which we concentrate in the following. To see this, let $\boldsymbol{Q}$ be the algebra of real quaternions and 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 $\Gamma_B = P\boldsymbol{H}$, i.e. the body centred cubic lattice is obtained by a projection of $\boldsymbol{H}$ onto $\mathbb{R}^3$. Moreover Lemma 5.1 of [8] tells us that $\Gamma_B(R(\boldsymbol{q})) = P(\boldsymbol{qH})$ (if $\boldsymbol{q}$ is reduced), where $\boldsymbol{qH}$ is a right ideal of $\boldsymbol{H}$. In fact, this establishes a one to one correspondence of CSLs and right ideals $\boldsymbol{qH}$ generated by a reduced $\boldsymbol{q}$, which is a key in the discussion of the body centred CSLs. In particular, finding the number $f(m)$ of different CSLs of given index m is equivalent to counting the corresponding right ideals of $\boldsymbol{H}$ according to the square root of their usual ideal index. One can show that $f(m)$ 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]. These findings are generalised to other cases in 3–space in [10].

Turning to the MCSLs, we first observe that the spectrum does not change, i.e. $\sigma_\infty = \sigma$, since σ already consists of all odd positive integers, and even integers are not allowed due to Lemma 1.2. But of course new lattices emerge. To quantify this let $f_n(m)$ be the number of distinct MCSLs of index m which are intersections of at most n distinct ordinary CSLs, and let $f_\infty(m)$ be the total number of MCSLs of index m. In fact we can explicitly calculate all $f_n(m)$ and it turns out that $f_3(m) = f_n(m) = f_\infty(m)$ for all $n \geq 3$. Moreover, all f_n are multiplicative functions, so we can again use the Dirichlet series approach.

THEOREM 3.1 *$f_2(m)$ is a multiplicative arithmetic function. For any odd prime p and any integer $r > 0$, we have*

$$\begin{aligned} f_2(p^r) =& (r/2 + 1/2)\,(p + 1)p^{r-1} + (r/2 - 1)p^{r-2} - (r/2 - [r/2])p^{r-4} \\ &+ \frac{p^{r-1} - p^{r-2[r/3]-1}}{p^2 - 1} + \frac{p^{4[r/3]-r+2} - p^{4[r/2]-r-2}}{2(p^2 - 1)}, \end{aligned} \tag{12}$$

where the Gauß bracket $[x]$ denotes the largest integer n with $n \leq x$. The corresponding Dirichlet series

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$$\Phi_2(s) := \sum_{n=1}^{\infty} \frac{f_2(n)}{n^s} = \prod_{p\in\mathbb{P}\setminus\{2\}} \phi_2(p,s) \tag{13}$$

$$= 1 + \frac{4}{3^s} + \frac{6}{5^s} + \frac{8}{7^s} + \frac{18}{9^s} + \frac{12}{11^s} + \frac{14}{13^s} + \frac{24}{15^s} + \frac{18}{17^s} + \frac{20}{19^s} + \frac{32}{21^s} + \frac{24}{23^s} + \frac{45}{25^s} + \frac{75}{27^s} + \cdots$$

$$\phi_2(p,s) := \sum_{r=1}^{\infty} \frac{f_2(p^r)}{p^{rs}} = 1 + \frac{(p+1)}{2p}\left(\frac{1}{(1-p^{1-s})^2} - 1\right) + \frac{(p+1)p^{-3s}}{2\,(1-p^{1-3s})}\left(\frac{1-p^{1-2s}}{(1-p^{1-s})^2} + 1\right). \tag{14}$$

To appreciate the number of new MCSLs we also state the difference $\Phi_2(s) - \Phi(s)$. Note that $f_2(m) = f(m)$ for square–free indices Σ, thus all terms n^{-s} with n square–free are missing in the expansion

$$\Phi_2(s) - \Phi(s) = \frac{6}{9^s} + \frac{15}{25^s} + \frac{39}{27^s} + \frac{36}{45^s} + \frac{28}{49^s} + \frac{48}{63^s} + \frac{60}{75^s} + \frac{174}{81^s} + \frac{72}{99^s} + \frac{84}{117^s} + \cdots \tag{15}$$

In contrast to the square lattice, the intersection of two ordinary MCSLs does not give us all possible MCSLs. However, the next theorem tells us implicitly that every MCSL can be written as the intersection of at most three ordinary CSLs, thus $f_3(\Sigma)$ is already the total number of MCSLs.

THEOREM 3.2 *$f_3(m) = f_\infty(m)$ is multiplicative and vanishes at all even integers. For any odd prime p and any integer $r > 0$ it reads*

$$f_3(p^r) = \sum_{0\le n\le r/3} f_2(p^{r-3n}). \tag{16}$$

The corresponding Dirichlet series is given by

$$\Phi_3(s) := \sum_{n=1}^{\infty} \frac{f_3(n)}{n^s} = (1-2^{-3s})\zeta(3s)\Phi_2(s) \tag{17}$$

$$= 1 + \frac{4}{3^s} + \frac{6}{5^s} + \frac{8}{7^s} + \frac{18}{9^s} + \frac{12}{11^s} + \frac{14}{13^s} + \frac{24}{15^s} + \frac{18}{17^s} + \frac{20}{19^s} + \frac{32}{21^s} + \frac{24}{23^s} + \frac{45}{25^s} + \frac{76}{27^s} + \cdots,$$

where $\Phi_2(s)$ is given by Eq. (13).

It is remarkable that $\Phi_3(s)$ is just a product of $\Phi_2(s)$ with a ζ-function (and a factor involving the prime number 2). This is a consequence of the fact that every MCSL is just an integer multiple of an intersection of two ordinary CSLs. In fact, most new MCSLs emerge from the intersection of two ordinary MCSLs, which can be easily seen if we compare $\Phi_2(s) - \Phi(s)$ with

$$\Phi_3(s) - \Phi_2(s) = \frac{1}{27^s} + \frac{4}{81^s} + \frac{1}{125^s} + \frac{6}{135^s} + \frac{8}{189^s} + \frac{18}{243^s} + \frac{12}{297^s} + \frac{1}{343^s} + \frac{14}{351^s} + \frac{4}{375^s} + \cdots. \tag{18}$$

Note that these results are valid for all three types of cubic lattices, in particular the multiplicity functions are the same for all cubic lattices. This is well known for the ordinary CSLs and extends to MCSLs due to Lemma 1.3. It is thus sufficient to prove these results for the body centred cubic lattice, where one has explicit expressions for the MCSLs [17]. For instance, given two reduced quaternions $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$, with least right common multiple $\boldsymbol{q}$, we have $\Gamma_B(R(\boldsymbol{q}_1), R(\boldsymbol{q}_2)) = P(\boldsymbol{q}\boldsymbol{H} + \boldsymbol{q}_1\boldsymbol{H}\bar{\boldsymbol{q}}_2) = P(\boldsymbol{q}\boldsymbol{H} + \boldsymbol{q}_2\boldsymbol{H}\bar{\boldsymbol{q}}_1)$.

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4 Conclusions and Outlook

We have seen that the coincidence spectrum does not change for a large class of lattices and modules, similarly the set of MCSLs stabilises after a few steps. However, all cases so far concern problems in low dimensions with high symmetry, so we cannot draw any conclusions for the general case yet. Further investigations are necessary, in particular some highly symmetric modules in 3-space and the hypercubic lattices in 4 dimensions seem to be the most natural (and fruitful) next candidates to attack and in fact work on these topics is in progress.

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