

Coincidences, Colourings and Similarities

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Abstract

This contribution is based on a talk given by the second author in Kyoto at RIMS, June 2010. It gives an overview of some recent developments in the theory of coincidence site lattices (CSLs). In particular, the connections between similar sublattices and CSLs, coincidences of lattice colourings, and coincidences of shifted lattices are discussed.

1 Coincidence Site Lattices (CSLs)

1.1 Brief historical overview

1911: first ideas by Friedel [1]

mid sixties, seventies: CSLs are investigated to describe grain boundaries in crystals

Ranganathan, Bollmann, Grimmer, ... [2, 3, 4]...

mid ninties: generalization for quasicrystals: Coincidence Site Modules (CSMs)
Baake, Pleasants, Warrington, ... [5, 6]...

2002: Quantizing Using Lattice Intersections
Sloane, Beferull-Lozano [7]

20xy: Baake, Grimm, Heuer, Moody, Pleasants, Scharlau, Loquias, Glied, Huck, PZ, Zou, ...

1.2 Commensurate Lattices

A key notion is the concept of commensurability. We call two lattices Γ_1 and Γ_2 commensurate, if one of the following properties is satisfied.

Lemma 1.1. *The following are equivalent:*

- $\Gamma_1 \cap \Gamma_2$ is a sublattice of both Γ_1 and Γ_2 .
- $\Gamma_1 \cap \Gamma_2$ is a sublattice of Γ_1 or Γ_2 .
- There exists an $m \in \mathbb{N}$ such that $m\Gamma_1 \subseteq \Gamma_2$ and $m\Gamma_2 \subseteq \Gamma_1$.
- There exists an $m \in \mathbb{N}$ such that $m\Gamma_1 \subseteq \Gamma_2$ or $m\Gamma_2 \subseteq \Gamma_1$.

1.3 Ordinary CSLs

Definition 1.1. Let $\Gamma \subset \mathbb{R}^d$ be a lattice, $R \in O(d)$. Then

$$\Gamma(R) := \Gamma \cap R\Gamma$$

is called a (simple,ordinary) coincidence site lattice (CSL), if Γ and $R\Gamma$ are commensurate. The index

$$\Sigma(R) := [\Gamma : \Gamma(R)] < \infty$$

is called coincidence index.

For a concise introduction we refer to [8].

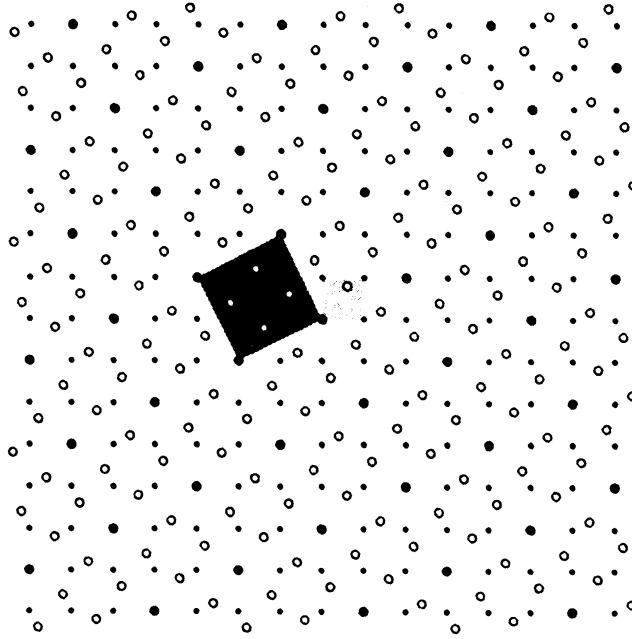


Figure 1: The figure shows a square lattice (black dots) and a copy (red circles) rotated by $e^{i\varphi} = \frac{2+i}{2-i}$ (corresponding to a rotation through an angle $\varphi = \arctan 4/3$). One clearly sees the CSL formed by the coinciding dots and circles. The shaded areas indicate a fundamental domain for each of the lattices.

1.4 Coincidence isometries

Lemma 1.2. The set of all coincidence isometries

$$OC(\Gamma) := \{R \in O(d) \mid \Sigma(R) < \infty\}$$

forms a group, a subgroup of $O(d)$. Likewise

$$SOC(\Gamma) := OC(\Gamma) \cap SO(d)$$

is a group.

The group of coincidence isometries is never empty. In particular, if $P(\Gamma)$ denotes the point group of Γ , we have

Lemma 1.3. *The following are equivalent:*

1. $R \in P(\Gamma)$
2. $\Sigma(R) = 1$

Corollary 1.4. $P(\Gamma) = \{R \in OC(\Gamma) \mid \Sigma(R) = 1\} \subseteq OC(\Gamma)$

1.5 Some Properties of the Coincidence Index

Lemma 1.5. *For any coincidence isometry R*

$$\Sigma(R) = \Sigma(R^{-1}).$$

1.6 Coincidences of the dual lattice

Lemma 1.6. *Γ and its dual lattice Γ^* have the same coincidence isometries, i.e.*

$$\begin{aligned} OC(\Gamma^*) &= OC(\Gamma). \\ SOC(\Gamma^*) &= SOC(\Gamma). \end{aligned}$$

The coincidence index is the same for both lattices:

$$\Sigma(R)^* = \Sigma(R).$$

1.7 Coincidences of Sublattices

Lemma 1.7. *Let $\Gamma_1 \subseteq \Gamma$ with index $m := [\Gamma : \Gamma_1]$. Then*

$$OC(\Gamma_1) = OC(\Gamma).$$

Let $\Sigma_1(R)$ be the coincidence index with respect to Γ_1 . Then

$$\begin{aligned} \Sigma(R) &\mid m\Sigma_1(R) \\ \Sigma_1(R) &\mid m\Sigma(R). \end{aligned}$$

Compare [8, 9].

1.8 Example $\mathbb{Z}^2 \simeq \mathbb{Z}[i]$

For more details on this example, see [8].

1.8.1 Coincidence rotations

Let $\varepsilon \in \{\pm 1, \pm i\}$ be a unit of $\mathbb{Z}[i]$, and write any splitting prime $p \equiv 1 \pmod{4}$ as $p = \omega_p \bar{\omega}_p$. Then the coincidence rotations are all of the form

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

where only finitely many $n_p \neq 0$.

1.8.2 Coincidence index

$$\Sigma(e^{i\varphi}) = \prod_{p \equiv 1(4)} p^{|n_p|}$$

1.8.3 Spectrum

set of all integers that contain only prime factors $p \equiv 1 \pmod{4}$.

1.8.4 CSLs of $\mathbb{Z}[i]$

Let

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

Then the CSL corresponding to the rotation $e^{i\varphi}$ is given by

$$\mathbb{Z}[i] \cap e^{i\varphi} \mathbb{Z}[i] = \omega(\varphi) \mathbb{Z}[i]$$

1.8.5 Generating functions

The number $f(m)$ of different CSLs can be nicely expressed in terms of the Dirichlet series

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

1.9 Example: Ammann-Beenker tiling

Coincidences of aperiodic tilings can be described via their underlying limit translation module, giving rise to CSMs (coincidence site modules). For the application to tilings an additional so-called acceptance factor has to be taken into account. [6, 8]

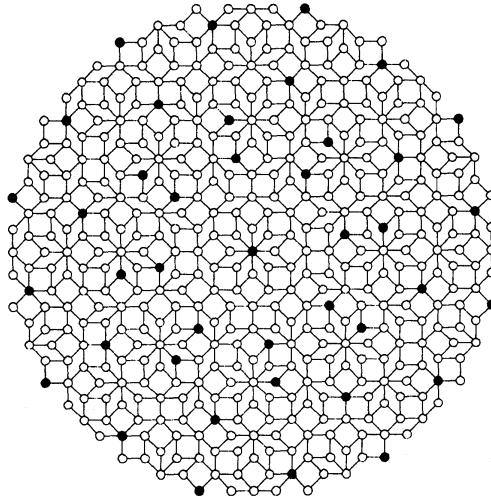


Figure 2: Amman Beenker tiling. The black dots indicate the coincidences for a rotation R about the center by $\theta = \tan^{-1}(-2\sqrt{2}) \approx 109.5^\circ$, $\Sigma(R) = 9$ acceptance factor = 0.980572924... [9, 10]

1.10 Equal CSLs

Lemma 1.8. $S \in P(\Gamma) \implies \Gamma(R) = \Gamma(RS)$

Though the converse is true for several lattices, like the square and triangle lattice in $d = 2$ and the cubic lattices in $d = 3$, it does not hold in general.

In particular, there are rotations $S \notin P(\Gamma)$ such that $\Gamma(R) = \Gamma(RS)$ for the following lattices: $\Gamma = (2\mathbb{Z})^2 \times \mathbb{Z}$, $\mathbb{Z}^4$, D_4 , A_4

Open question: When does $\Gamma(R) = \Gamma(RS)$ imply $S \in P(\Gamma)$?

1.10.1 Example: Root lattice A_4

Let $f(m)$ be the number of CSLs and $|P(A_4)|f^{rot}(m)$ the number of coincidence isometries of the root lattice A_4 of index m , where $|P(A_4)|$ denotes the order of the point group $P(A_4)$. Clearly $f^{rot}(m) \geq f(m)$. The following generating functions show that they are not equal in general.

$$\begin{aligned}
 \Phi_{A_4}^{rot}(s) &= \sum_{m=1}^{\infty} \frac{f^{rot}(m)}{m^s} \\
 &= \frac{1 + 5^{1-s}}{1 - 5^{2-s}} \prod_{p \equiv \pm 1(5)} \frac{(1 + p^{-s})(1 + p^{1-s})}{(1 - p^{1-s})(1 - p^{2-s})} \prod_{p \equiv \pm 2(5)} \frac{1 + p^{-s}}{1 - p^{2-s}} \\
 &= 1 + \frac{5}{2^s} + \frac{10}{3^s} + \frac{20}{4^s} + \frac{30}{5^s} + \frac{50}{6^s} + \frac{50}{7^s} + \frac{80}{8^s} + \frac{90}{9^s} + \frac{150}{10^s} + \frac{144}{11^s} + \dots
 \end{aligned}$$

$$\begin{aligned}
\Phi_{A_1}(s) &= \sum_{m=1}^{\infty} \frac{f(m)}{m^s} \\
&= \left(1 + 6 \frac{5^{-s}}{1 \cdot 5^{2-s}}\right) \prod_{p \equiv \pm 2(5)} \frac{1+p^{-s}}{1-p^{2-s}} \prod_{p \equiv \pm 1(5)} \frac{1+p^{-s}+2p^{1-s}+2p^{-2s}+p^{1-2s}+p^{1-3s}}{(1-p^{2-s})(1-p^{1-2s})} \\
&= 1 + \frac{5}{2^s} + \frac{10}{3^s} + \frac{20}{4^s} + \frac{6}{5^s} + \frac{50}{6^s} + \frac{50}{7^s} + \frac{80}{8^s} + \frac{90}{9^s} + \frac{30}{10^s} + \frac{144}{11^s} + \dots
\end{aligned}$$

For more details, see [11, 12, 13]

1.11 Multiple CSLs

Definition 1.2. Let $\Gamma \subset \mathbb{R}^d$ be a lattice, $R_i \in OC(\Gamma)$. Then

$$\Gamma(R_1, \dots, R_n) := \Gamma \cap R_1\Gamma \cap \dots \cap R_n\Gamma = \Gamma(R_1) \cap \dots \cap \Gamma(R_n)$$

is called a multiple coincidence site lattice (MCSL).

The index

$$\Sigma(R_1, \dots, R_n) := [\Gamma : \Gamma(R_1, \dots, R_n)] < \infty$$

is called coincidence index.

For more information, see [14, 15, 16].

1.12 Known CSLs (and similar sublattices)

- Square lattice, hexagonal lattice [8, 17]
- certain planar modules with N -fold symmetry [6, 17]
- cubic lattices and related modules [4, 18, 8, 19, 20]
- hypercubic lattices [8, 21]
- A_4 -lattice, ring of icosians [11, 12, 13]

2 Similar Sublattices

For more details see [22, 23, 24, 25].

2.1 Similarity Transformations

Definition 2.1. Let $\alpha \in \mathbb{R}^+$ and $R \in O(d)$. Then

$$\begin{aligned}
A: \mathbb{R}^d &\rightarrow \mathbb{R}^d \\
x &\rightarrow \alpha Rx
\end{aligned}$$

is called a linear similarity transformation.

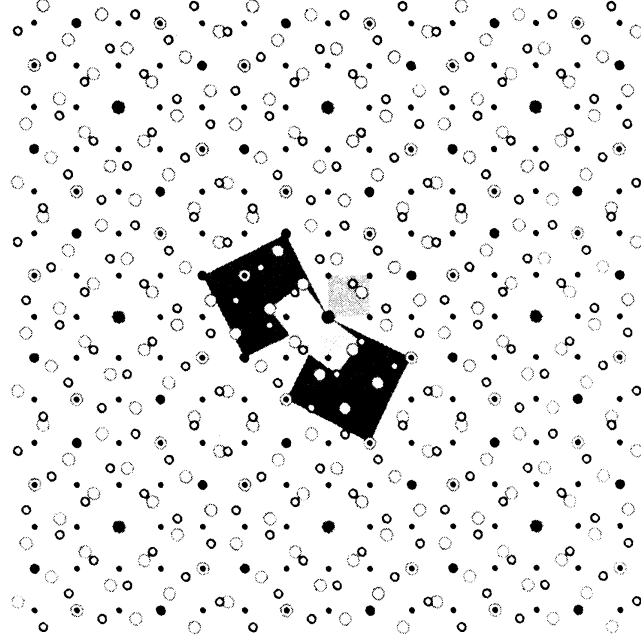


Figure 3: A square lattice and two copies of it rotated by $e^{i\varphi} = \frac{2+i}{2-i}$ (red circles) and $e^{-i\varphi} = \frac{2-i}{2+i}$ (green circles), respectively. The MCSL $\Gamma(e^{i\varphi}, e^{-i\varphi})$ consists of all points where the black dots and the red and green circles coincide, a fundamental domain of it is given by the yellow area.

2.2 Similar Sublattice

Definition 2.2. Let $A = \alpha R$ be a linear similarity transformation and $\Gamma \subseteq \mathbb{R}^d$ a lattice. Then A is called a similarity transformation of Γ if

$$A\Gamma = \alpha R\Gamma \subseteq \Gamma.$$

In this case $A\Gamma = \alpha R\Gamma$ is called a similar sublattice (similarity sublattice).

2.3 Index of a Similar Sublattice

Lemma 2.1. For any similar sublattice of the lattice $\Gamma \subseteq \mathbb{R}^d$:

$$[\Gamma : \alpha R\Gamma] = \alpha^d \in \mathbb{N}.$$

2.4 Similarity Isometries

Definition 2.3. An isometry $R \in O(d)$ is called a similarity isometry of Γ , if there exists an $\alpha \in \mathbb{R}^+$ such that αR is a similarity transformation of Γ .

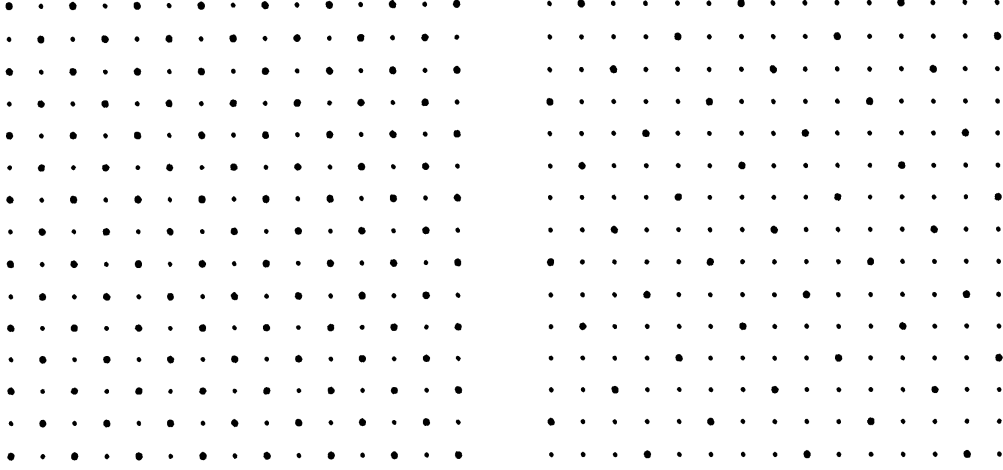


Figure 4: Similar sublattices of a square lattice of index 2 and 5, the latter also occurring as CSL, see above.

Lemma 2.2. *The set of all similarity isometries of Γ forms a group, called $OS(\Gamma)$. In particular $OS(\Gamma)$ is a countable subgroup of $O(d)$. Likewise $SOS(\Gamma) := OS(\Gamma) \cap SO(d)$ is a countable subgroup of $SO(d)$.*

3 Coincidence Isometries versus Similarity Isometries

Theorem 3.1. *For any d -dimensional lattice Γ we have*

- $OC(\Gamma) \subseteq OS(\Gamma)$
- $OS(\Gamma)/OC(\Gamma)$ is abelian.
- Moreover $g^d = e$ for any $g \in OS(\Gamma)/OC(\Gamma)$.
- In particular, if $d = p$ for some prime p , then $OS(\Gamma)/OC(\Gamma)$ is a p -group.

See [26, 27].

3.1 Coincidence Isometries versus Similarity Isometries

Lemma 3.2.

$$OC(\Gamma) = \{R \in OS(\Gamma) \mid \text{den}(R) \in \mathbb{N}\} \subseteq OS(\Gamma) \subset O(d)$$

3.2 Denominator (“Minimal Blow-up factor”)

Definition 3.1. *Let $R \in OS(\Gamma)$. Then*

$$\text{den}_\Gamma(R) := \min\{\alpha \in \mathbb{R}^+ \mid \alpha R\Gamma \subseteq \Gamma\}.$$

Lemma 3.3. *Let $R \in OS(\Gamma)$. Then*

$$\{\alpha \in \mathbb{R} \mid \alpha R\Gamma \subseteq \Gamma\} = \text{den}_\Gamma(R)\mathbb{Z}.$$

Lemma 3.4. $\text{den}_\Gamma(R) = 1$ *if and only if* $R \in P(\Gamma)$.

Lemma 3.5. *Let $R \in OS(\Gamma)$. Then*

$$\text{den}_\Gamma(R)^d \in \mathbb{N}$$

3.3 Coincidence Index and Denominator

Lemma 3.6. *Let $m := \text{lcm}(\text{den}_\Gamma(R), \text{den}_\Gamma(R^{-1}))$ and $n := \text{gcd}(\text{den}_\Gamma(R), \text{den}_\Gamma(R^{-1}))$. Then*

$$m \mid \Sigma(R) \mid n^d \quad \text{and} \quad \Sigma(R)^2 \mid m^d$$

Remark 3.1. *If $d = 2$ then*

$$\Sigma(R) = \text{den}_{\Gamma'}(R) = \text{den}_{\Gamma'}(R^{-1}).$$

3.4 Primitive Similar Sublattices

Definition 3.2. *A similar sublattice Γ_1 of Γ is called primitive, if $\frac{1}{n}\Gamma_1 \not\subseteq \Gamma$ for all $n > 1$.*

Lemma 3.7. *A similar sublattice Γ_1 of Γ is primitive if and only if there exists an $R \in OS(\Gamma)$ such that*

$$\Gamma_1 = \text{den}_\Gamma(R)R\Gamma.$$

3.5 Example: square lattice

Let $a(m)$ and $a^{pr}(m)$ denote the number of similar and primitive similar sublattices of the square lattice. These functions are multiplicative and have the following generating function. See [23].

$$\begin{aligned} D_{\mathbb{Z}^2}(s) &= \sum_{m=1}^{\infty} \frac{a(m)}{m^s} = \zeta_{\mathbb{Q}(i)}(s) = \frac{1}{1-2^{-s}} \prod_{p \equiv 1(4)} \frac{1}{(1-p^{-s})^2} \\ &= 1 + \frac{1}{2^s} + \frac{1}{4^s} + \frac{2}{5^s} + \frac{1}{8^s} + \frac{1}{9^s} + \frac{2}{10^s} + \frac{2}{13^s} + \frac{1}{16^s} + \dots \\ D_{\mathbb{Z}^2}^{pr}(s) &= \sum_{m=1}^{\infty} \frac{a^{pr}(m)}{m^s} = \frac{1}{\zeta(2s)} D_{\mathbb{Z}^2}(s) \\ &= (1+2^{-s}) \prod_{p \equiv 1(4)} \frac{1+p^{-s}}{1-p^{-s}} \\ &= 1 + \frac{1}{2^s} + \frac{2}{5^s} + \frac{2}{10^s} + \frac{2}{13^s} + \frac{2}{17^s} + \frac{2}{25^s} + \frac{2}{26^s} + \dots \end{aligned}$$

4 Colourings

Here we consider special colourings of lattices. For a fixed sublattice Γ_2 of Γ_1 we assign all points of a coset the same colour, with different colours for different cosets. [28, 29, 30, 9]

4.1 Colour symmetries

symmetry operation leaves lattice and colours fixed

colour symmetry leaves lattice fixed but permutes colors

In our case:

- all lattice translations are colour symmetries
- there is a bijection between colours and cosets
- to each colouring (up to colour permutations) there corresponds a unique coset decomposition $\Gamma_1 = \bigcup_{\ell} (c_{\ell} + \Gamma_2)$ and vice versa

4.2 Coincidences and colourings

Idea: use colourings of lattices to find out more about coincidence indices of sublattices [10, 9]

Let Γ_2 a sublattice of Γ_1 of index m , and let $\Sigma_i(R)$ be the coincidence index of R with respect to Γ_i for $i \in \{1, 2\}$.

Theorem 4.1.

$$\Sigma_2(R) = \frac{t \cdot u \cdot \Sigma_1(R)}{m} = \frac{s \cdot v \cdot \Sigma_1(R)}{m}$$

and $s, t, u, v \mid m$. Here s and t are the number of colours in the induced colouring of $\Gamma_1(R^{-1})$ and $\Gamma_1(R)$, respectively. u is the number of colours c_j with the property that some point of $\Gamma_1(R^{-1})$ coloured c_j is mapped under R onto a point coloured $c_0 = 0$ in $\Gamma_1(R)$; v is the number of colours in the colouring of $\Gamma_1(R)$ that are intersected by the images under R of those points of $\Gamma_1(R^{-1})$ coloured c_0 .

4.3 Colour coincidences

Definition 4.1. We call R a colour coincidence, if one of the following two equivalent conditions is satisfied

1. colouring of $\Gamma_1(R)$ is a rotated copy of the colouring of $\Gamma_1(R^{-1})$ (up to colour permutations)
2. R leaves colour c_0 fixed

Theorem 4.2. *If R is a colour coincidence, then $\Sigma_2(R)$ divides $\Sigma_1(R)$.*

Open question: Do colour coincidences form a group?

What is known:

- R colour coincidence $\iff R^{-1}$ colour coincidence
- R, S colour coincidences and $\Sigma_1(R), \Sigma_1(S)$ coprime $\iff RS$ colour coincidence

5 Shifted lattices

5.1 Coincidence isometries

Here we consider linear isometries of lattices shifted by some vector $x \in \mathbb{R}^d$, i.e. sets $x + \Gamma$. One extends all the definitions in the natural way. One gets

Theorem 5.1. $OC(x + \Gamma) = \{R \in OC(\Gamma) : Rx - x \in \Gamma + R\Gamma\}$

- In general, $OC(x + \Gamma)$ is not a group.

For further details and applications to multilattices and sublattices see [31, 9].

5.2 Coincidence isometries of $\mathbb{Z}[i]$

Theorem 5.2. *Let $\Gamma = \mathbb{Z}[i]$ and $x \in \mathbb{C}$.*

1. $SOC(x + \Gamma)$ is a subgroup of $SOC(\Gamma)$
2. $OC(x + \Gamma)$ is a subgroup of $OC(\Gamma)$ if and only if $T_1 T_2 \in SOC(x + \Gamma)$ for any $T_1, T_2 \in OC(x + \Gamma) \setminus SOC(x + \Gamma)$.

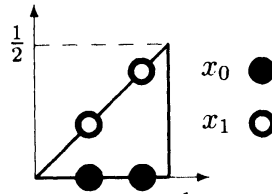
Lemma 5.3. *Let $x = \frac{p}{q}$ where $p, q \in \mathbb{Z}[i]$, p and q relatively prime. Then*

$$SOC(x + \Gamma) = SOC\left(\frac{1}{q} + \Gamma\right)$$

Lemma 5.4. *If p and q are relatively prime, then*

$$SOC\left(\frac{1}{pq} + \Gamma\right) = SOC\left(\frac{1}{p} + \Gamma\right) \cap SOC\left(\frac{1}{q} + \Gamma\right)$$

5.3 Example $\mathbb{Z}[i]$: specific shift vectors (1)



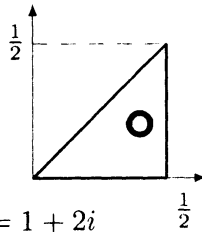
- $x_0 = \frac{1}{5}, \frac{2}{5}$ and $x_1 = \frac{1}{5} + \frac{1}{5}i, \frac{2}{5} + \frac{2}{5}i \Rightarrow \frac{1}{q} = 5$
- $SOC(x_0 + \Gamma) = SOC(x_1 + \Gamma)$
- $OC(x_0 + \Gamma)$ and $OC(x_1 + \Gamma)$ are groups

The generating function $\Phi_x(s)$ of the shifted CSLs reads as follows (the generating function $\Phi(s)$ of the CSLs of $\mathbb{Z}[i]$ is repeated for easier comparison)

$$\begin{aligned}\Phi_x(s) &= 1 + \frac{2}{13^s} + \frac{2}{17^s} + \frac{2}{29^s} + \frac{2}{37^s} + \frac{2}{41^s} + \frac{2}{53^s} + \frac{2}{61^s} + \frac{2}{73^s} + \dots \\ \Phi(s) &= 1 + \frac{2}{5^s} + \frac{2}{13^s} + \frac{2}{17^s} + \frac{2}{25^s} + \frac{2}{29^s} + \frac{2}{37^s} + \frac{2}{41^s} + \frac{2}{53^s} \\ &\quad + \frac{2}{61^s} + \frac{4}{65^s} + \frac{2}{73^s} + \dots\end{aligned}$$

The rotations and the orientation reversing isometries both generate the same CSLs.

5.4 Example: $\mathbb{Z}[i]$: specific shift vectors (2)



- $x = \frac{2}{5} + \frac{1}{5}i = \frac{i}{1+2i} \Rightarrow q = 1 + 2i$
- $SOC(x + \Gamma) = SOC(\frac{1}{5} + \Gamma)$
- $OC(x + \Gamma)$ is **NOT** a group!

Here rotations and orientation reversing isometries generate different CSLs. $\Phi_x(s)$ generates the counting function of shifted CSLs that are generated by rotations only, whereas $\Psi_x(s)$ generates the counting function of all shifted CSLs. Again, $\Phi(s)$ of the unshifted $\mathbb{Z}[i]$ is included for comparison.

$$\begin{aligned}\Phi_x(s) &= 1 + \frac{2}{13^s} + \frac{2}{17^s} + \frac{2}{29^s} + \frac{2}{37^s} + \frac{2}{41^s} + \frac{2}{53^s} + \frac{2}{61^s} + \frac{2}{73^s} + \dots \\ \Phi(s) &= 1 + \frac{2}{5^s} + \frac{2}{13^s} + \frac{2}{17^s} + \frac{2}{25^s} + \frac{2}{29^s} + \frac{2}{37^s} + \frac{2}{41^s} + \frac{2}{53^s} \\ &\quad + \frac{2}{61^s} + \frac{4}{65^s} + \frac{2}{73^s} + \dots \\ \Psi_x(s) &= 1 + \frac{4}{5^s} + \frac{2}{13^s} + \frac{2}{17^s} + \frac{4}{25^s} + \frac{2}{29^s} + \frac{2}{37^s} + \frac{2}{41^s} + \frac{2}{53^s} \\ &\quad + \frac{2}{61^s} + \frac{8}{65^s} + \frac{2}{73^s} + \dots\end{aligned}$$

For further examples see [9].

6 Conclusions

There are a lot of connections ...

- colourings $\leftrightarrow$ similar sublattices
- similar sublattices $\leftrightarrow$ CSLs
- CSLs $\leftrightarrow$ colourings

Acknowledgements

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