

Well-rounded sublattices and coincidence site lattices

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Abstract A lattice is called well-rounded, if its lattice vectors of minimal length span the ambient space. We show that there are interesting connections between the existence of well-rounded sublattices and coincidence site lattices (CSLs). Furthermore, we count the number of well-rounded sublattices for several planar lattices and give their asymptotic behaviour.

1 Introduction

A lattice in \mathbb{R}^d is called well-rounded, if its (non-zero) lattice vectors of minimal length span \mathbb{R}^d . This means that there exist at least $2d$ lattice vectors of minimal positive length, and \mathbb{R}^d has a basis consisting of lattice vectors of minimal length. However, such a basis need not be a primitive lattice basis in dimensions $d \geq 4$.

Well-rounded lattices are important for several reasons. Many important lattices occurring in mathematics and physics are well-rounded. For instance, the hexagonal lattice and the square lattice in \mathbb{R}^2 and the cubic lattices in \mathbb{R}^3 are well-rounded, as are the hypercubic lattices and the A_4 -lattice in \mathbb{R}^4 , which play an important role in quasicrystallography. Examples in higher dimensions are the Leech lattice, the Barnes-Wall lattices, and the Coxeter-Todd lattice; see [6] for background.

Let us briefly mention two problems of mathematical crystallography where well-rounded lattices occur. They are connected to the question of densest lattice sphere packings, as all extreme lattices (those lattices corresponding to densest lattice sphere packings) are perfect (i.e. the lattice vectors of minimal length determine the Gram matrix uniquely) and are thus well-rounded. They also play an important role in reduction theory, as they are exactly those lattices for which all the successive minima are equal [9].

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Here, we want to deal with two specific questions: Has a given lattice well-rounded sublattices, and if so, what are the well-rounded sublattices and how many are there. The first question is answered in Sec. 2 for planar lattices and a partial answer is given for $d > 2$. The second question is much more difficult in general. Thus we restrict the discussion to 2 dimensions, and present some results in Sec. 3.

2 Well-rounded lattices and CSLs

Here, we want to deal with the question whether a lattice has a well-rounded sublattice. It turns out that this question is related to the theory of coincidence site lattices (CSLs), so let us review the notion of CSL first. Let Λ be a lattice in \mathbb{R}^d and let $R \in O(d)$ be an isometry. Then $\Lambda(R) = \Lambda \cap R\Lambda$ is called a *coincidence site lattice (CSL)* if $\Lambda(R)$ is a sublattice of full rank in Λ ; the corresponding R is called coincidence isometry. The corresponding index of $\Lambda(R)$ in Λ is called coincidence index $\Sigma_\Lambda(R)$, or $\Sigma(R)$ for short. The set of all coincidence isometries forms a group, which we call $OC(\Lambda)$, see [2] for details.

Let us look at the planar case first. Here, any two linearly independent lattice vectors of minimal (non-zero) length form a basis of Λ . Let γ be the angle between them. Now a well-rounded lattice is necessarily a rhombic (centred rectangular) lattice such that $\frac{\pi}{3} < \gamma < \frac{2\pi}{3}$, $\gamma \neq \frac{\pi}{2}$ or a square (corresponding to $\gamma = \frac{\pi}{2}$) or a hexagonal lattice (corresponding to $\gamma = \frac{\pi}{3}$ or $\gamma = \frac{2\pi}{3}$). Thus, its symmetry group is at least $D_2 = 2mm$, or in other words, there is at least one reflection symmetry present. As Λ and all of its sublattices have the same group of coincidence isometries [2], we can infer that a lattice possesses a well-rounded sublattice only if it has a coincidence reflection. As the converse holds as well, we have (compare [5])

Theorem 1. *A planar lattice $\Lambda \in \mathbb{R}^2$ has a well-rounded sublattice if and only if it has a coincidence reflection.*

An alternative criterion tells us that a planar lattice has a well-rounded sublattice if and only if it has a rhombic or rectangular sublattice [8]. The existence of well-rounded sublattices can also be characterised by the entries of the Gram matrices of Λ , see [8] and [5] for various criteria.

One is tempted to generalise these criteria to d dimensions, by using orthogonal lattices, the d -dimensional analogue of rectangular lattices and orthorhombic lattices in 3 dimensions. However, this does not work since a lattice may be well-rounded without having an orthogonal sublattice. As an example, consider a rhombohedral lattice in \mathbb{R}^3 , which in general does not have an orthorhombic sublattice. Nevertheless, an orthogonal lattice has well-rounded sublattices, and one even has

Theorem 2. *Let G be the symmetry group of an orthogonal lattice, i.e. a lattice that is spanned by an orthogonal basis. Then Λ has a well-rounded sublattice if $G \subseteq OC(\Lambda)$.*

This theorem can be proved by induction. The idea is to show that $G \subseteq OC(\Lambda)$ implies the existence of an orthogonal sublattice, which in turn implies the existence of well-rounded sublattices.

However, note that the intuitive idea of choosing a “body-centred orthogonal” lattice fails in dimensions $d > 4$. For if we construct a lattice as the linear span of the 2^d vectors $\sum_{i=1}^d s_i^{(j)} b_i$, where the b_i form an orthogonal basis of \mathbb{R}^d and $s_i^{(j)} \in \{1, -1\}$, then these vectors do not have minimal lengths as at least one of the vectors $2b_i$ is shorter. Nevertheless, a modification of this idea works where we choose a suitable subset of the vectors $\sum_{i=1}^d s_i^{(j)} b_i$. In particular, if the basis vectors b_i all have approximately the same length and d is even, we can construct a well-rounded sublattice as the linear span of $\sum_{i=1}^d s_i^{(j)} b_i$, where j runs over all possible solutions of $\sum_{i=1}^d s_i^{(j)} \equiv 0 \pmod{d}$.

An immediate consequence of Theorem 2 is that every rational lattice has well-rounded sublattices, as $OC(\Lambda)$ contains all reflections generated by a lattice vector [10].

3 Well-rounded sublattices of planar lattices

We now turn to our second question, i.e., we want to find all well-rounded sublattices of a given lattice. We concentrate on some planar lattices here. To begin with, we want to find all well-rounded sublattices of the square lattice. W.l.o.g we may identify it with $\mathbb{Z}^2 \simeq \mathbb{Z}[i]$. The idea now is the following. From the previous section, we know that a planar lattice is well-rounded if and only if it is a rhombic lattice with $\frac{\pi}{3} < \gamma < \frac{2\pi}{3}$, a square or a hexagonal lattice. Now a sublattice of a square lattice cannot be hexagonal, so that we can exclude the latter case, i.e. we only have to find all rhombic and square well-rounded sublattices. The latter are just the similar sublattices of the square lattice, which are well known [3, 5]. The Dirichlet series generating function of their counting function reads

$$\Phi_{\square}(s) = \sum_{n \in \mathbb{N}} \frac{s_{\square}(n)}{n^s} = \zeta(2s) \Phi_{\square}^{\text{pr}}(s) = \zeta_{\mathbb{Q}(i)}(s) = L(s, \chi_{-4}) \zeta(s) \quad (1)$$

where $s_{\square}(n)$ is the number of similar sublattices of the square lattice with index n . Here, $\Phi_{\square}^{\text{pr}}(s)$ is the generating function of the primitive similar sublattices, $\zeta(s)$ is the Riemann zeta function and $\zeta_{\mathbb{Q}(i)}(s)$ is the Dedekind zeta function of the complex number field $\mathbb{Q}(i)$.

Hence it remains to find all rhombic well-rounded sublattices. Now each rhombic sublattice has a rectangular sublattice of index 2, and it is well-rounded if and only if $\frac{a}{\sqrt{3}} \leq b \leq a\sqrt{3}$ holds, where a and b are the lengths of the orthogonal basis vectors of the corresponding rectangular sublattice. Thus we only need to find all rectangular sublattices satisfying the condition above. In fact, as all square lattices are similar, it is sufficient to find all rectangular sublattices whose symmetry axes are parallel to

those of the square lattice, and we finally get [5]

$$\Phi_{\text{wr},\text{even}}(s) = \frac{2}{2^s} \Phi_{\square}^{\text{pr}}(s) \sum_{p \in \mathbb{N}} \sum_{p < q < \sqrt{3}p} \frac{1}{p^s q^s} \quad (2)$$

$$\Phi_{\text{wr},\text{odd}}(s) = \frac{2}{1+2^{-s}} \Phi_{\square}^{\text{pr}}(s) \sum_{k \in \mathbb{N}} \sum_{k < \ell < \sqrt{3}k + \frac{\sqrt{3}-1}{2}} \frac{1}{(2k+1)^s (2\ell+1)^s} \quad (3)$$

where $\Phi_{\text{wr},\text{even}}(s)$ and $\Phi_{\text{wr},\text{odd}}(s)$ are the generating functions counting the rhombic well-rounded sublattices of even and odd indices, respectively. Putting everything together we arrive at the following result [5]

Theorem 3. *Let $a_{\square}(n)$ be the number of well-rounded sublattices of the square lattice with index n , and $\Phi_{\square,\text{wr}}(s) = \sum_{n=1}^{\infty} a_{\square}(n)n^{-s}$ the corresponding Dirichlet series generating function. It is given by $\Phi_{\square,\text{wr}}(s) = \Phi_{\square}(s) + \Phi_{\text{wr},\text{even}}(s) + \Phi_{\text{wr},\text{odd}}(s)$ with the functions from Eqs (1), (2) and (3).*

If $s > 1$, we have the inequality

$$D_{\square}(s) - \Phi_{\square}(s) < \Phi_{\square,\text{wr}}(s) < D_{\square}(s) + \Phi_{\square}(s).$$

with $\Phi_{\square}(s)$ from Eq. (1) and the function

$$D_{\square}(s) = \frac{2+2^s}{1+2^s} \frac{1-\sqrt{3}^{1-s}}{s-1} \frac{L(s, \chi_{-4})}{\zeta(2s)} \zeta(s) \zeta(2s-1),$$

As a consequence, the summatory function $A_{\square}(x) = \sum_{n \leq x} a_{\square}(n)$ possesses the asymptotic growth behaviour

$$A_{\square}(x) = \frac{\log(3)}{2\pi} x \log(x) + \mathcal{O}(x \log(x))$$

as $x \rightarrow \infty$.

The lower and upper bounds are obtained by approximating the sums in Eqs. (2) and (3) by integrals via the Euler summation formula, whereas the statement about the asymptotic behaviour of $A_{\square}(x)$ follows from Delange's theorem, which relates the asymptotic behaviour of $A_{\square}(x)$ with the analytic properties of $\Phi_{\square,\text{wr}}(s)$, in particular with its pole at $s = 1$.

In fact, we can get additional information about the asymptotic behaviour of $A_{\square}(x)$ by applying some methods of analytic number theory, including Dirichlet's hyperbola method and the above mentioned Euler summation formula (see e.g. [1]).

Theorem 4. *Let $a_{\square}(n)$ be the number of well-rounded sublattices of the square lattice with index n . Then, the summatory function $A_{\square}(x) = \sum_{n \leq x} a_{\square}(n)$ possesses the asymptotic growth behaviour*

$$A_{\square}(x) = \frac{\log(3)}{3} \frac{L(1, \chi_{-4})}{\zeta(2)} x (\log(x) - 1) + c_{\square} x + \mathcal{O}(x^{3/4} \log(x))$$

$$= \frac{\log(3)}{2\pi} x \log(x) + \left(c_{\square} - \frac{\log(3)}{2\pi} \right) x + \mathcal{O}(x^{3/4} \log(x))$$

where

$$\begin{aligned} c_{\square} &:= \frac{L(1, \chi_{-4})}{\zeta(2)} \left(\zeta(2) + \frac{\log(3)}{3} \left(\frac{L'(1, \chi_{-4})}{L(1, \chi_{-4})} + \gamma - 2 \frac{\zeta'(2)}{\zeta(2)} \right) \right) \\ &\quad + \frac{\log(3)}{3} \left(2\gamma - \frac{\log(3)}{4} - \frac{\log(2)}{6} \right) - \sum_{p=1}^{\infty} \frac{1}{p} \left(\frac{\log(3)}{2} - \sum_{p < q < p\sqrt{3}} \frac{1}{q} \right) \\ &\quad - \frac{4}{3} \sum_{k=0}^{\infty} \frac{1}{2k+1} \left(\frac{1}{4} \log(3) - \sum_{k < \ell < k\sqrt{3} + (\sqrt{3}-1)/2} \frac{1}{2\ell+1} \right) \\ &\approx 0.6272237 \end{aligned}$$

is the coefficient of $(s-1)^{-1}$ in the Laurent series of $\sum_n \frac{a_{\square}(n)}{n^s}$ around $s=1$. Here, γ is the Euler-Mascheroni constant.

Similar calculations are also possible for the hexagonal lattice. If $a_{\Delta}(n)$ is the number of well-rounded sublattices of the triangular lattice with index n , then the corresponding Dirichlet series generating function $\Phi_{\Delta, \text{wr}}(s) = \sum_{n=1}^{\infty} a_{\Delta}(n) n^{-s}$ is given by

$$\Phi_{\Delta, \text{wr}}(s) = \Phi_{\Delta}(s) + \Phi_{\Delta, \text{wr}, \text{even}}(s) + \Phi_{\Delta, \text{wr}, \text{odd}}(s),$$

where

$$\Phi_{\Delta}(s) = \zeta_{\mathbb{Q}(\rho)}(s) = L(s, \chi_{-3}) \zeta(s), \quad (4)$$

is the generating function for the similar sublattices of the hexagonal lattice and

$$\Phi_{\Delta, \text{wr}, \text{even}}(s) = \frac{3}{4^s (1+3^{-s})} \sum_{p \in \mathbb{N}} \sum_{p < q < 3p} \frac{1}{p^s q^s} \Phi_{\Delta}^{\text{pr}}(s), \quad (5)$$

$$\Phi_{\Delta, \text{wr}, \text{odd}}(s) = \frac{3}{1+3^{-s}} \sum_{k \in \mathbb{N}} \sum_{k < \ell < 3k+1} \frac{1}{(2k+1)^s (2\ell+1)^s} \Phi_{\Delta}^{\text{pr}}(s) \quad (6)$$

are the corresponding Dirichlet series for the number of rhombic well-rounded sublattices with even and odd indices, respectively. For the asymptotic behaviour we get [5]

Theorem 5. *The summatory function $A_{\Delta}(x) = \sum_{n \leq x} a_{\Delta}(n)$ possesses the asymptotic growth behaviour*

$$\begin{aligned} A_{\Delta}(x) &= \frac{9 \log(3)}{16} \frac{L(1, \chi_{-3})}{\zeta(2)} x (\log(x) - 1) + c_{\Delta} x + \mathcal{O}(x^{3/4} \log(x)) \\ &= \frac{3\sqrt{3} \log(3)}{8\pi} x (\log(x) - 1) + c_{\Delta} x + \mathcal{O}(x^{3/4} \log(x)) \end{aligned}$$

where $c_\Delta \approx 0.4915036$ is the coefficient of $(s-1)^{-1}$ in the Laurent series of $\sum_n \frac{a_\Delta(n)}{n^s}$ around $s = 1$. \square

In both examples, we have infinitely many coincidence reflections, which results in a large number of well-rounded sublattices and in an asymptotic growth behaviour of $x \log(x)$. A similar behaviour is to be expected for all rational lattices, but so far only weaker results have been obtained [7].

However, in general we have less coincidence reflections, and we want to conclude with this case. In fact, if the lattice is not rational, there are either no or exactly two coincidence reflections [10, 5], and both of them have the same coincidence index. It is remarkable that in the latter case the asymptotic behaviour does not depend on the details of the lattice but only on the coincidence index of its two coincidence reflections. In particular we have [5]

Theorem 6. *Let Λ be a planar lattice that has exactly two coincidence reflections. Let Σ be their common coincidence index and let $a_\Lambda(n)$ denote the number of well-rounded sublattices of Λ with index n . Then, the summatory function $A_\Lambda(x) = \sum_{m \leq x} a_\Lambda(m)$ possesses the asymptotic growth behaviour $A_\Lambda(x) = \frac{\log 3}{4\Sigma} x + \mathcal{O}(\sqrt{x})$.*

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