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Minimal distances in quasicrystals

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Abstract. A general expression is derived for the minimal distance $\varepsilon(\Omega)$ between points of a cut and project quasicrystal $\Sigma(\Omega)$ in \mathbb{R}^n with a convex acceptance window Ω . The study of minimal distances amounts to the study of one-dimensional quasicrystals and their rescalings which occur in $\Sigma(\Omega)$. For an n -dimensional ball as Ω , the exact value of $\varepsilon(\Omega)$ is calculated for any radius; for Ω ‘close’ to a ball, a simple formula is given; for all Ω upper and lower bounds for $\varepsilon(\Omega)$ are found. The latter are easy to use even when Ω is of a complicated shape.

1. Introduction

Typical interatomic distances in solids are a few angstroms, varying only slightly from a solid to solid and/or between atoms of different types. In a quasicrystal the distances are around 2.5–3 Å [5]. Why should one study distances over a much wider range?

One can bring forward several reasons to study minimal distances in quasicrystal-like point sets.

Distances in a mathematical model of a quasicrystal must be scaled appropriately before they can be compared with absolute measures of a physical quasicrystal. In fact it is the physical quasicrystal which determines the scale of a model.

Quasicrystal point sets are of interest in physics and mathematics for reasons which go beyond applications in quasicrystal physics. They can be viewed as a generalization of lattices. Similarly as lattices are encountered outside crystallography, one may expect that their aperiodic generalizations will find a wider use.

Finally, knowledge of minimal distances in quasicrystals can point towards other properties of quasicrystals and methods of establishing them [7].

The aim of this paper is to describe the minimal distances in the cut and project quasicrystals. Therefore we adopt in this work a rather general form of the definition of such quasicrystals, following [2, 16]. Thus, a quasicrystal is a point set in \mathbb{R}^n and its coordinates relative to some basis are in the ring of integers, denoted $\mathbb{Z}[\tau]$, of the quadratic extension $\mathbb{Q}[\tau]$ of the rational numbers by $\tau = \frac{1}{2}(1 + \sqrt{5})$. The cut and project method implies the presence of a bounded acceptance window Ω and a mapping (star map) under which all points of the quasicrystal are mapped into Ω .

The size of the acceptance window of a given quasicrystal in \mathbb{R}^n determines the density of its points—atoms. It is generally understood and it is also an immediate consequence of the definition (1) below, that the larger the window volume, the higher the density of quasicrystal points. Apparently the only quantitative result in the literature about an explicit link between the linear dimensions of the acceptance window and the minimal distance in

the corresponding quasicrystal is found in [12] (see it also in [16]), and that is just for a single special case.

This paper is the second in a series of articles about rigorously established general algebraic properties of cut and project quasicrystals. The others are [6, 7]. In the first of them [6], we describe all scaling symmetries of a cut and project quasicrystal with convex Ω . More precisely, we show that the set of all scaling factors corresponding to any given point is a one-dimensional quasicrystal for the internal inflation centres (quasicrystal points). Similarly the scaling factors belonging to external inflation centres are given as subsets of points of certain one-dimensional quasicrystals. The content of this paper can be viewed as a general answer to the question raised in [12] about minimal distances in the cut and project quasicrystals.

Distances between points of one-dimensional quasicrystals are studied in section 3. The minimal distances in a general quasicrystal with connected acceptance-window interval is found as a function of the length of the interval. Any such quasicrystal is made of two or three distinct tiles. Subsequently [7] we will see that adjacent tiles, which are distinct, have lengths in the ratio τ (or τ^{-1}).

The knowledge of the structure of one-dimensional quasicrystals is crucial for the study of higher dimensional quasicrystals (section 4). The latter are collections of one-dimensional subquasicrystals intertwined and rescaled. In particular, any two points of a higher dimensional quasicrystal fix a straight line containing an infinite number of quasicrystal points. After an appropriate affine mapping they form a one-dimensional quasicrystal.

A general expression for the minimal distance of an n -dimensional cut and project quasicrystal is given in theorem 5.2 of section 5. It depends on the shape of the acceptance window Ω . For Ω satisfying a special property (27), the expression is essentially simplified (theorem 5.3). The lower and upper bounds for the minimal distance suitable for any Ω may also turn out to be practically useful.

Properties of quasicrystals shown in this paper can be seen on specific quasicrystals in literature (for example in [2–5, 11, 13–15]). Exceptions are the 2-tile quasicrystals of Penrose as we explain in the concluding example of this paper.

2. Mathematical preliminaries

Let us recall the basic algebraic structures used in the theory of cut and project quasicrystals.

Consider the algebraic number field $\mathbb{Q}[\sqrt{5}]$ and its nontrivial automorphism denoted by $'$ and defined by $a + b\sqrt{5} \rightarrow a - b\sqrt{5}$ with $a, b \in \mathbb{Z}$. In particular,

$$\tau = \frac{1}{2}(1 + \sqrt{5}) \longrightarrow \tau' = \frac{1}{2}(1 - \sqrt{5}).$$

Here τ and τ' are the roots of the algebraic equation $x^2 = x + 1$. The ring of integers of $\mathbb{Q}[\sqrt{5}]$ is denoted by $\mathbb{Z}[\tau] = \mathbb{Z} + \mathbb{Z}\tau$.

It is known that $\mathbb{Z}[\tau]$ is a Euclidean domain, in particular $\mathbb{Z}[\tau]$ is a unique factorization domain. For a set $F \subset \mathbb{Z}[\tau]$, one has $\gcd\{F'\} = (\gcd\{F})'$. The group of units of $\mathbb{Z}[\tau]$ consists of $\{\pm\tau^k | k \in \mathbb{Z}\}$. It is also known that each prime p of \mathbb{Z} of the form $p \equiv \pm 2 \pmod{5}$ remains prime in $\mathbb{Z}[\tau]$. Each prime p of \mathbb{Z} of the form $p \equiv \pm 1 \pmod{5}$ splits as a conjugated pair $p = qq'$ with $q \neq q'$.

Let M be a torsion free $\mathbb{Z}[\tau]$ -module of rank n with a basis $\{\alpha_1, \dots, \alpha_n\} \subset \mathbb{R}^n$, i.e. $M = \sum_{i=1}^n \mathbb{Z}[\tau]\alpha_i$. M is a $\mathbb{Z}[\tau]$ -lattice if it spans \mathbb{R}^n over \mathbb{R} . We will assume in the following that \mathbb{R}^n is equipped with a Euclidean norm.

Let $M \subset \mathbb{R}^n$ be a $\mathbb{Z}[\tau]$ -lattice for which the standard dot product is $\mathbb{Q}[\sqrt{5}]$ -valued on $M \times M$. A ‘star map’ is a mapping $f : M \rightarrow M^* \subset \mathbb{R}^n$ such that f is semilinear with respect to conjugation $'$ on $\mathbb{Z}[\tau]$ and M^* spans \mathbb{R}^n . Usually a star map is denoted by $x \rightarrow x^*$. In the one-dimensional case, we use $M = \mathbb{Z}[\tau]$ with star map $x \rightarrow x'$.

Definition 2.1. Let M be a $\mathbb{Z}[\tau]$ -lattice in \mathbb{R}^n with a star map $*$. Let $\Omega \subset \mathbb{R}^n$ be a bounded convex set with a non-empty interior called an acceptance window. The cut and project quasicrystal is the set

$$\Sigma(\Omega) = \{x \in M \mid x^* \in \Omega\}. \tag{1}$$

It is explained in [2, 16] and again in [6], why the quasicrystal $\Sigma(\Omega)$ is actually of the cut and project type. It is shown in [10] that $\Sigma(\Omega)$ is a ‘Delaunay set’, i.e.

- there is an $\varepsilon > 0$ such that $\|x - y\| \geq \varepsilon$ for all $x, y \in \Sigma(\Omega)$, $x \neq y$,
- there is an $R > 0$ such that any ball of radius R in \mathbb{R}^n intersects $\Sigma(\Omega)$ non-trivially.

The maximal possible ε in the Delone property is equal to the minimal distance between two points of the Delone set, or more formally

$$\varepsilon(\Sigma(\Omega)) = \inf\{\|x - y\| \mid x, y \in \Sigma(\Omega), x \neq y\}$$

is called the ‘minimal distance’ of the quasicrystal $\Sigma(\Omega)$. For simplicity of notation we often use $\varepsilon(\Omega)$ instead of $\varepsilon(\Sigma(\Omega))$.

Note, that $\Sigma(\Omega)$ is also almost a lattice [8, 10], i.e. there exists a finite set F such that

$$\Sigma(\Omega) - \Sigma(\Omega) \subset \Sigma(\Omega) + F. \tag{2}$$

This property assures that the minimal distance is achieved between two points of $\Sigma(\Omega)$ (and not as a limit of a sequence of differences of points).

3. One-dimensional quasicrystals

The main result of this section is a description of the structure of one-dimensional quasicrystals in general. In particular, we determine the minimal distance between quasicrystal points as an explicit function of the length of the acceptance interval. The result is an indispensable tool in the study of quasicrystals in higher dimensions.

On many occasions we make use of the step function $\chi : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ defined by

$$\chi(d) := \tau^{-k} \quad \text{for } d \in (\tau^k, \tau^{k+1}] \quad k \in \mathbb{Z} \tag{3}$$

and plotted on figure 1.

Since $\mathbb{R}_+ = \bigcup_{k \in \mathbb{Z}} (\tau^k, \tau^{k+1}]$, the step function χ is well defined. Note that for any $d > 0$,

$$\frac{1}{d} < \chi(d) \leq \frac{\tau}{d} \tag{4}$$

$$\chi\left(\frac{d}{\tau}\right) = \tau \chi(d). \tag{5}$$

The following theorem shows that the minimal distance depends on the length of the acceptance interval and not on its position in \mathbb{R} . The proposition states the result for an open interval only, but a slight modification of the proof yields the rest of the cases (see remark 3.3).

Theorem 3.1. Let $c, d \in \mathbb{R}$, $d > 0$. Then the minimal distance in one-dimensional quasicrystal with the acceptance interval $(c, c + d)$ is

$$\varepsilon(c, c + d) = \chi(d). \tag{6}$$

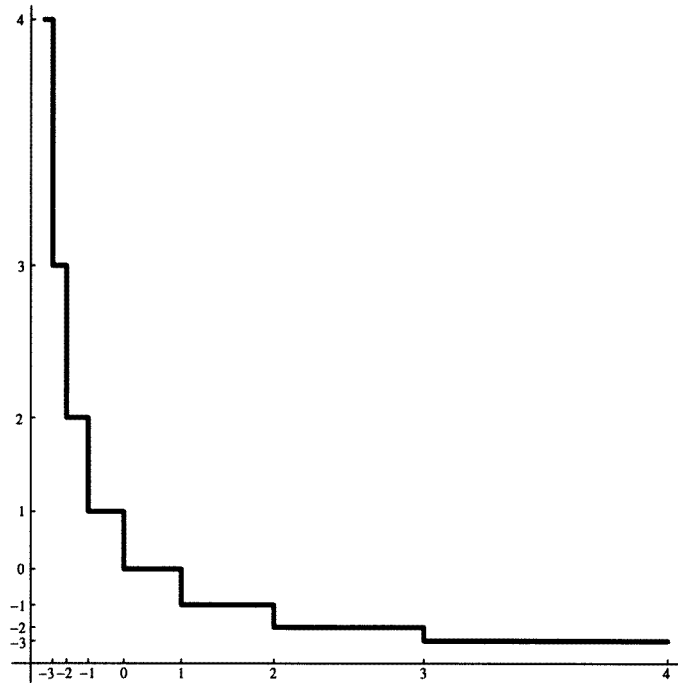


Figure 1. A fragment of the step function $\chi(d)$ of (3). The points marked on both axes correspond to τ^k , only the exponents k are shown.

Proof. If $x = a + b\tau \in \Sigma(c, c + d)$, then

$$c < x' = a + b\tau' = a - \frac{b}{\tau} < c + d \iff \frac{b}{\tau} + c < a < \frac{b}{\tau} + c + d. \quad (7)$$

For $d > 1$ we can always find an integer a , such that (7) holds. However, for $d < 1$ there are some $b \in \mathbb{Z}$ for which such an integer does not exist.

First, let us consider the case $d \in (\frac{1}{\tau}, 1]$. Put

$$B(d) := \{b \in \mathbb{Z} \mid \exists a \in \mathbb{Z}, (7) \text{ holds}\}. \quad (8)$$

For $d \leq 1$ and any $b \in \mathbb{Z}$ there exists at most one integer a such that (7) is fulfilled. The following holds

$$\Sigma(c, c + d) = \left\{ \left[\frac{b}{\tau} + c + d \right] + b\tau \mid b \in B(d) \right\}. \quad (9)$$

Let us define the sequence σ of elements p_b by

$$\sigma := \left\{ p_b \equiv \left[\frac{b}{\tau} + c + d \right] + b\tau \mid b \in \mathbb{Z} \right\}. \quad (10)$$

Obviously, $\Sigma(c, c + d) \subseteq \sigma$. Therefore the minimal distance in $\Sigma(c, c + d)$ is greater or equal to the minimal distance in σ . Since the points of σ form an increasing sequence, the minimal distance is recovered between two adjacent elements of the sequence

$$p_{b+1} - p_b = \left[\frac{b+1}{\tau} + c + d \right] + (b+1)\tau - \left[\frac{b}{\tau} + c + d \right] - b\tau \geq \tau. \quad (11)$$

Thus $\varepsilon(c, c + d) \geq \tau$. Next let us show that the equality is achieved.

Since $\mathbb{Z}[\tau]$ is dense in \mathbb{R} , we can find a point of the form $n\tau - m$ with $m, n \in \mathbb{Z}$ close enough to the point $\frac{1}{2}(d\tau + 1) + c\tau$. More precisely, for all $\delta > 0$ there exists $m, n \in \mathbb{Z}$ such that

$$\left| (\tau n - m) - \left(\frac{d\tau + 1}{2} + c\tau \right) \right| \leq \delta. \tag{12}$$

Take $\delta = \frac{1}{2}(\tau d - 1)$ and $b = m$. From (12) we have

$$-\frac{\tau d - 1}{2} + \frac{\tau d + 1}{2} + c\tau < \tau n - b < \frac{\tau d - 1}{2} + \frac{\tau d + 1}{2} + c\tau$$

or, equivalently,

$$\frac{b}{\tau} + c < \frac{b + 1}{\tau} + c < n < \frac{b}{\tau} + c + d < \frac{b + 1}{\tau} + c + d.$$

Since n is an integer, we have $b, b + 1 \in B(d)$ and

$$\left[\frac{b + 1}{\tau} + c + d \right] = \left[\frac{b}{\tau} + c + d \right].$$

This means that $p_b, p_{b+1} \in \Sigma(c, c + d)$ and $p_{b+1} - p_b = \tau$.

To prove the theorem for $d \in (\frac{1}{\tau^{k+1}}, \frac{1}{\tau^k}]$, we use the fact that $\varepsilon(\gamma\Sigma(\Omega)) = |\gamma|\varepsilon(\Sigma(\Omega))$ for any constant γ and any $\Sigma(\Omega)$. Also we use $\Sigma(\tau^k\Omega) = (\tau')^k\Sigma(\Omega)$ from [1], where Ω is a convex set. Thus we obtain

$$\begin{aligned} \varepsilon(c, c + d) &= \varepsilon(\Sigma(\tau^k(c\tau^{-k}, c\tau^{-k} + d\tau^{-k}))) = \varepsilon((\tau')^k\Sigma(c\tau^{-k}, c\tau^{-k} + d\tau^{-k})) \\ &= |\tau'|^k \varepsilon(\Sigma(c\tau^{-k}, c\tau^{-k} + d\tau^{-k})) = \frac{1}{\tau^k} \cdot \tau = \frac{1}{\tau^{k-1}} = \chi(d). \end{aligned} \tag{13}$$

□

Let us now observe that the proof provides an answer to the question; how many distinct tiles occur in a given $\Sigma(c, c + d)$? For $d \in (\frac{1}{\tau}, 1]$ and as $\Sigma(c, c + d)$ of (9) coincides with σ of (10), which is the case when $d = 1$, the distance between any two neighbouring quasicrystal points is simply given by the difference (11). Clearly, (11) admits only two values, τ and $\tau + 1$, depending on the integer parts of the expression.

Three distinct tiles occur precisely when $\Sigma(c, c + d) \neq \sigma$. In addition to the two tiles of the previous case, there is also $p_{b+2} - p_b$ for some $b \in \mathbb{Z}$, giving rise to the third tile of length $2\tau + 1$.

One arrives at the same conclusions when $d \in \tau^k(\frac{1}{\tau}, 1]$, arguing similarly as in (13). Thus for fixed c the 2-tile quasicrystals form a discrete set parametrized by $d = \tau^k$, $k = 0, 1, 2, \dots$

Denote the three distinct tiles by letters S (small), M (middle) and L (large). Some of the structural properties of one-dimensional quasicrystals can be relatively easily demonstrated using the above remarks and the τ -inflation invariance [1, 6]:

Proposition 3.2. Let $\Sigma(c, c + d)$ be a one-dimensional quasicrystal with $c, d \in \mathbb{R}$, and let k be an integer, such that $d \in (\tau^{k-1}, \tau^k]$. Then in $\Sigma(c, c + d)$

- there are never three tiles of the same length adjacent,
- the sequence SS never occurs,
- MM occurs if and only if $d \in (2\tau^{k-2}, \tau^k]$,
- LL occurs if and only if $d \in (\tau^{k-1}, 2\tau^{k-2})$,
- S is never adjacent to L,
- the sequence MML never occurs, i.e. MM is necessarily surrounded by S's.

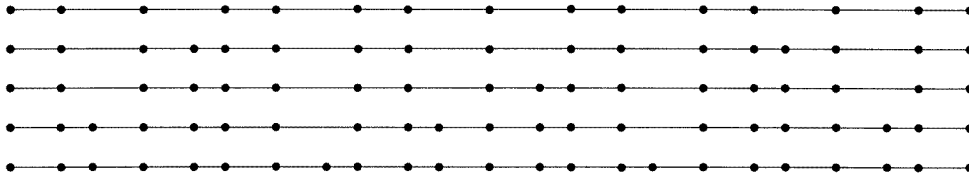


Figure 2. Vertically aligned fragments of five one-dimensional quasicrystals $\Sigma(-r, r)$ are shown for $2r = 1, \frac{1}{2}(1 + \frac{2}{\tau^2}), \frac{2}{\tau^2}, \frac{1}{2}(\frac{2}{\tau^2} + \frac{1}{\tau})$, and $\frac{1}{\tau}$, illustrating the points (i)–(iv).

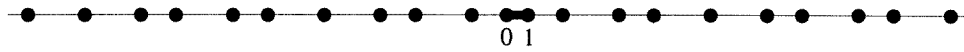


Figure 3. A fragment of the quasicrystal $\Sigma[0, 1]$. The thick line between quasicrystal points 0 and 1 marks the exceptional distance of the third type in an otherwise 2-tile quasicrystal.

The following five examples in figure 2 simultaneously illustrate several properties.

- (i) The existence of the 2- and 3- tile quasicrystals.
- (ii) The constancy of the minimal distance within each step of $\chi(d)$ of (3) and (6).
- (iii) The fact that the points added, when the acceptance interval increases, split the longest tiles into two.
- (iv) The tiling sequence is not arbitrary. See for example proposition 3.2.

The theorem was formulated for an open acceptance interval $(c, c + d)$. If a boundary point is not in $\mathbb{Z}[\tau]$, adding it to the window does not change the quasicrystal. However, if for example $c \in \mathbb{Z}[\tau]$, then $\Sigma[c, c + d) = \Sigma(c, c + d) \cup \{c'\}$. This fact has the following implications for the minimal distances.

Remark 3.3. If $d \neq \tau^k$ or $c \notin \mathbb{Z}[\tau]$, then

$$\varepsilon(c, c + d) = \varepsilon[c, c + d) = \varepsilon(c, c + d) = \varepsilon[c, c + d) = \chi(d). \quad (14)$$

If $d = \tau^k$ and $c \in \mathbb{Z}[\tau]$, then

$$\varepsilon(c, c + \tau^k) = \varepsilon[c, c + \tau^k) = \varepsilon(c, c + \tau^k) = \chi(d) \quad (15)$$

$$\varepsilon[c, c + \tau^k) = \tau^{-1}\chi(d). \quad (16)$$

In most cases addition of the boundary points to the acceptance interval does not change the minimal distance (equations (14), (15)). A special situation arises in the case (16): the minimal distance is smaller than $\chi(d)$ by τ^{-1} , but that happens in precisely one tile of the entire quasicrystal.

The quasicrystal $\Sigma[0, 1]$ is shown in figure 3. It is an important quasicrystal in its own right [6]. Here we use it to illustrate the case (16): the unique smallest tile occurs between 0 and 1.

Another example of a one-dimensional quasicrystal is the set

$$\mathbb{Z}_\tau = \left\{ x = \sum_{i=0}^k x_i \tau^i \mid k \in \mathbb{N}, x_i \in \{0, 1\}, x_i x_{i+1} = 0 \right\}$$

of all numbers integer in the τ -expansion [3, 4]. It can be identified with the positive part of the cut and project quasicrystal with the acceptance interval $(-1, \tau)$.

4. One-dimensional subquasicrystals in quasicrystals of higher dimension

Any straight line containing at least two points of M , contains infinitely many of them. Under the star map these points are transformed into points of M^* , forming a straight line there. The minimal distance in $\Sigma(\Omega) \subset \mathbb{R}^n$ is a distance between two quasicrystal points. Therefore the determination of the minimal distance in $\Sigma(\Omega)$ reduces to a choice of an appropriate one-dimensional problem, among the many, one finds in $\Sigma(\Omega)$. A description of subsets of $\Sigma(\Omega)$ found on straight lines is the aim of this section.

In general, distances between such points are not in $\mathbb{Z}[\tau]$. However, they can be linearly mapped into $\mathbb{Z}[\tau] \subset \mathbb{R}$. More precisely, one has the following lemma.

Lemma 4.1. Let $\Sigma(\Omega) \subset \mathbb{R}^n$ be a cut and project quasicrystal and P be a straight line in \mathbb{R}^n containing at least two points of $\Sigma(\Omega)$. Then there exists a linear mapping $\Phi : \mathbb{R} \rightarrow \mathbb{R}^n$ and a bounded interval $J \subset \mathbb{R}$, such that

$$P \cap \Sigma(\Omega) = \Phi \Sigma(J).$$

Proof. Let $x, y \in \Sigma(\Omega) \cap P$. Since $\Sigma(\Omega)$ is a subset of the $\mathbb{Z}[\tau]$ -module $M = \sum_{i=1}^n \mathbb{Z}[\tau]\alpha_i$, we can write $x = x_1\alpha_1 + \dots + x_n\alpha_n$ and $y - x = h_1\alpha_1 + \dots + h_n\alpha_n$, where $x_1, \dots, x_n, h_1, \dots, h_n \in \mathbb{Z}[\tau]$. Let us put $s = \gcd\{h_1, \dots, h_n\}$. The value of s is well defined because $\mathbb{Z}[\tau]$ is a Euclidean domain. Put $k_i := h_i/s$ for $i = 1, \dots, n$ and $k = k_1\alpha_1 + \dots + k_n\alpha_n$. Then $\gcd\{k_1, \dots, k_n\} = \gcd\{k'_1, \dots, k'_n\} = 1$.

First we prove that

$$P \cap M = \{x + tk \mid t \in \mathbb{Z}[\tau]\}. \tag{17}$$

Suppose $z \in P \cap M$, i.e. $z = (x_1 + tk_1)\alpha_1 + \dots + (x_n + tk_n)\alpha_n \in M$. Since $x_1 + tk_1 \in \mathbb{Z}[\tau]$, we have $t \in \mathbb{Q}[\tau]$ and thus t can be written in the form $t = \frac{p}{q}$, where $p, q \in \mathbb{Z}[\tau]$ and $\gcd\{p, q\} = 1$. The property $x_i + tk_i = x_i + \frac{p}{q}k_i \in \mathbb{Z}[\tau]$ implies that q divides pk_i . Together with the fact that $\gcd\{p, q\} = 1$, it shows that q divides k_i for all $i = 1, \dots, n$. Hence q divides $\gcd\{k_1, \dots, k_n\} = 1$. Consequently, q is a divisor of unity, i.e. $q = \tau^k$ for some $k \in \mathbb{Z}$, and $t = \frac{p}{q} \in \mathbb{Z}[\tau]$ as required.

Now, define the linear mapping $\Phi : \mathbb{R} \rightarrow \mathbb{R}^n$ by

$$\Phi(t) := x + tk. \tag{18}$$

From (17) we see that Φ , restricted to $\mathbb{Z}[\tau]$, is a bijection $\mathbb{Z}[\tau]$ onto $P \cap M$. Denoting by Q the straight line containing points x^* and y^* , by the same reason $Q \cap M = \{x^* + tk^* \mid t \in \mathbb{Z}[\tau]\}$ and the linear mapping

$$\Psi(t) := x^* + tk^* \tag{19}$$

restricted to $\mathbb{Z}[\tau]$, is a bijection $\mathbb{Z}[\tau]$ onto $Q \cap M$.

Note that

$$\Psi^{-1}(\Omega \cap Q \cap M) = \Psi^{-1}(\Omega \cap Q) \cap \Psi^{-1}(Q \cap M) = \Psi^{-1}(\Omega \cap Q) \cap \mathbb{Z}[\tau].$$

Since $\Omega \cap Q$ is an intersection of two convex sets and because Ψ is linear, we find that $\Psi^{-1}(\Omega \cap Q) = J$ is an interval in \mathbb{R} .

Define $\Sigma := \{t \in \mathbb{R} \mid \Phi(t) \in \Sigma(\Omega)\}$. Then

$$\begin{aligned} t \in \Sigma &\iff (t \in \mathbb{Z}[\tau] \text{ and } \Phi(t) \in \Sigma(\Omega)) \iff (t \in \mathbb{Z}[\tau] \text{ and } x + tk \in \Sigma(\Omega)) \\ &\iff (t \in \mathbb{Z}[\tau] \text{ and } x^* + t'k^* \in \Omega) \iff (t \in \mathbb{Z}[\tau] \text{ and } \Psi(t') \in \Omega) \\ &\iff \Psi(t') \in \Omega \cap Q \cap M \iff t' \in \Psi^{-1}(\Omega \cap Q \cap M) = J \cap \mathbb{Z}[\tau]. \end{aligned} \tag{20}$$

It means that Σ is a one-dimensional cut and project quasicrystal with acceptance window J . Moreover, from the definition of Σ , we have $\Sigma = \Phi^{-1}(P \cap \Sigma(\Omega))$ which completes the proof. \square

Let us point out that the proof enables us to determine the minimal distance in $P \cap \Sigma(\Omega)$. For that we map $P \cap \Sigma(\Omega) \subset \mathbb{R}^n$ into the one-dimensional quasicrystal $\Sigma(J) \subset \mathbb{Z}[\tau]$, according to lemma 4.1. Its acceptance interval $J \subset \mathbb{R}$ determines the minimal distance of $\Sigma(J)$. Since the map is linear, the minimal distance of $\Sigma(J)$ can be mapped back into $P \cap \Sigma(\Omega)$.

In order to get an explicit form for $\varepsilon(P \cap \Sigma(\Omega))$, we proceed as follows, using the notations from the proof of lemma 4.1.

Denote by d the lengths of the line segment $I = Q \cap \Omega$. From the definition (19) of Ψ we obtain, that the length of interval J is $d/\|k^*\|$, where k is a vector in the direction P with relatively prime coordinates in $\mathbb{Z}[\tau]$. Suppose that I is not closed with respect to the straight line Q , then $\varepsilon(J) = \chi(d/\|k^*\|)$, see proposition 3.1. Using the definition (18) of Φ , we have

$$\varepsilon(P \cap \Sigma(\Omega)) = \|k\| \chi \left(\frac{d}{\|k^*\|} \right). \quad (21)$$

This form of $\varepsilon(P \cap \Sigma(\Omega))$ will be essential for the proof of the main theorem of the next section. The minimal distances given by (21) are illustrated in figure 4.

We consider an example of a two-dimensional quasicrystal. As the corresponding $\mathbb{Z}[\tau]$ -module M we take the $\mathbb{Z}[\tau]$ -span of Δ_2 , the root system of the non-crystallographic Coxeter group H_2 . It consists of the ten points $\pm\zeta^j$ in \mathbb{C} , where $\zeta = e^{2i\pi/5}$ and $j = 0, \dots, 4$. The basis of $\mathbb{Z}[\tau]$ -module can be chosen as the vectors (simple roots)

$$\alpha_1 = 1 \quad \text{and} \quad \alpha_2 = \zeta^2 \quad (22)$$

with the star map defined by

$$\alpha_1^* = 1 \quad \text{and} \quad \alpha_2^* = \zeta^4. \quad (23)$$

The acceptance window Ω is the disk of radius 1, centred at the origin. In one of the examples in figure 4, the norm $\|k\| = 1$, while in the others it is not in $\mathbb{Z}[\tau]$.

5. Higher dimensional quasicrystals

The general formula for the minimal distance $\varepsilon(\Omega)$ in theorem 5.2 is not particularly practical to use. Therefore for special Ω 's which are not far from an n -dimensional ball (27), we provide a simpler expression for the minimal distance, which allows one to obtain specific value for various Ω (see for example corollary 5.5, 5.4).

In addition we provide lower and upper bounds for the minimal distance, which are easy to use even if the exact expressions are difficult to evaluate for Ω of complicated shapes. It is curious to note that the lower bound depends on a diameter of Ω , while the upper one is a function of the volume of Ω .

The quasicrystals we consider are found in a general $\mathbb{Z}[\tau]$ -lattice M , however for demonstrations in this section we need to use the following additional requirement.

$$\|k\|^2 \in \mathbb{Z}[\tau] \quad \text{for all } k = k_1\alpha_1 + \dots + k_n\alpha_n \quad \text{with } k_1, \dots, k_n \in \mathbb{Z}[\tau]. \quad (24)$$

This requirement is not particularly restrictive. In most cases one considers such M , where scalar products take values in $\mathbb{Z}[\tau]$. In those cases (24) holds automatically.

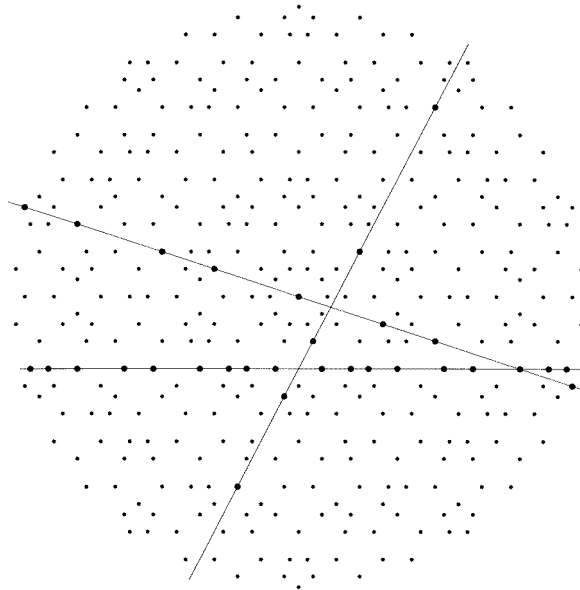


Figure 4. A selection of points of a two-dimensional quasicrystal belonging to different straight lines illustrate that any intersection of a line with an n -dimensional quasicrystal determines a one-dimensional quasicrystal, possibly up to rescaling by a factor generally not in $\mathbb{Z}[\tau]$. Only the horizontal example corresponds to the direction k with $\|k\| = 1$.

It was pointed out in connection with one-dimensional subquasicrystals that the question about the minimal distance is a one-dimensional problem (21). The following definition provides a suitable measure of linear sizes of Ω in different directions, which then is used in place of d in (21).

Definition 5.1. Let $\Omega \subset \mathbb{R}^n$ be a convex bounded set and let $k \in M$. The thickness $\text{th}(\Omega, k)$ of the set Ω in the direction k is

$$\text{th}(\Omega, k) := \sup\{\|y - x\| \mid x, y \in \Omega, y - x = tk \text{ for some } t \in \mathbb{R}\}. \quad (25)$$

The diameter $\text{diam}(\Omega)$ is given as the supremum of $\text{th}(\Omega, k)$ over all directions $k \in M$.

The minimal distance in $\Sigma(\Omega)$ is the smallest of the minimal distances (21) on all straight lines through $\Sigma(\Omega)$.

Theorem 5.2. Let $\Omega \subset \mathbb{R}^n$ be an open convex bounded set. Then

$$\varepsilon(\Omega) = \min \left\{ \|k\| \chi \left(\frac{\text{th}(\Omega, k^*)}{\|k^*\|} \right) \mid k \in M, k \neq 0 \right\}.$$

Proof. Since $\Sigma(\Omega)$ is almost a lattice (2), the value of $\inf\{\|x - y\| \mid x, y \in \Sigma(\Omega), x \neq y\}$ is achieved on some $x_0, y_0 \in \Sigma(\Omega)$. The distance between these points must be equal to the minimal distance in $P \cap \Sigma(\Omega)$, where P is a line containing x_0, y_0 . Thus we can use (21), which requires that the vector $k = k_1\alpha_1 + \dots + k_n\alpha_n$ is in the ‘normalized form’, i.e. $\text{gcd}\{k_1, \dots, k_n\} = 1$. Nevertheless, let $h = sk$, where $s \neq \tau^k$ is the greatest common divisor of coordinates of h , and where k is a ‘normalized’ vector. Then $\text{th}(\Omega, h) = \text{th}(\Omega, k)$ and

$$\|h\| \chi \left(\frac{\text{th}(\Omega, h)}{\|h^*\|} \right) \geq \frac{\|h\| \|h^*\|}{\text{th}(\Omega, h)} = |ss'| \frac{\|k\| \|k^*\|}{\text{th}(\Omega, k)} \geq \frac{|ss'|}{\tau} \|k\| \chi \left(\frac{\text{th}(\Omega, k)}{\|k^*\|} \right). \quad (26)$$

Here we have used (4).

Since ss' is a non-zero integer $\neq \pm 1$ (s is not a divisor of unity), we have $|ss'| \geq 2$. Therefore

$$\frac{|ss'|}{\tau} \|k\| \chi\left(\frac{\text{th}(\Omega, k)}{\|k^*\|}\right) > \|k\| \chi\left(\frac{\text{th}(\Omega, k)}{\|k^*\|}\right).$$

Thus ‘non-normalized’ vectors do not change the minimum distance. □

An Ω slightly different from a ball, admits a simpler expression for the minimal distance. More precisely, one has the following theorem.

Theorem 5.3. Let M be $\mathbb{Z}[\tau]$ -module satisfying (24) and let Ω be an open bounded convex set. Suppose that

$$\frac{\sup\{\text{th}(\Omega, k) | k \in M\}}{\inf\{\text{th}(\Omega, k) | k \in M\}} \leq \frac{2}{\tau} \tag{27}$$

then

$$\varepsilon(\Omega) = \min\{\chi(\text{th}(\Omega, k)) | k \in M, \|k\| \|k^*\| = 1\}.$$

Proof. Since $\|h^*\|^2 = (\|h\|^2)' \in \mathbb{Z}[\tau]$, we have $\|h^*\|^2 \|h\|^2 \in \mathbb{Z}$. Suppose that $\|h\|^2 \|h^*\|^2 > 1$. Then $\|h\|^2 \|h^*\|^2 \geq 4$ because 2 and 3 are prime in $\mathbb{Z}[\tau]$ and hence it is impossible to write them as a product of ss' . The theorem follows immediately from the inequalities

$$\|h\| \chi\left(\frac{\text{th}(\Omega, h^*)}{\|h^*\|}\right) \geq \frac{\|h\| \|h^*\|}{\text{th}(\Omega, h^*)} \geq \frac{2}{\text{th}(\Omega, h^*)} \geq \frac{\tau}{\text{th}(\Omega, k^*)} \geq \chi(\text{th}(\Omega, k^*))$$

which are valid for $h, k \in M$ such that $\|h\| \|h^*\| \neq 1$ and $\|k\| \|k^*\| = 1$. □

The equality $\|k\| \|k^*\| = 1$ with the assumption (24) implies $\|k\|^2 = \tau^j$ for some $j \in \mathbb{Z}$. This leads to a system of Diophantine equations for the coordinates $k_i \in \mathbb{Z}[\tau]$ of k . For example for M_2 , the $\mathbb{Z}[\tau]$ -module of H_2 described at the end of section 4, there is exactly 10 solutions (up to a τ^j multiple) to the system, each solution corresponding to one of the roots from Δ_2 .

Corollary 5.4. Let $M = \mathbb{Z}[\tau]\alpha_1 + \mathbb{Z}[\tau]\alpha_2$, where α_i is defined by (22) and star mapped by (23). Suppose that an open bounded convex set Ω satisfies (27) then

$$\varepsilon(\Omega) = \chi(\max\{\text{th}(\Omega, k) | k \in \Delta_2\}).$$

The exact value of the minimal distance is obtained for the most symmetric $\Omega \in \mathbb{R}^n$.

Corollary 5.5. Denote by $B(x, r)$ an open ball with centre x and radius r . Then the minimal distance in the quasicrystal $\Sigma(B(x, r))$ is given by

$$\varepsilon(B(x, r)) = \chi(2r). \tag{28}$$

Let us now find bounds for the minimal distance which could be used when the exact value cannot be simply calculated. A lower bound is found more easily.

Corollary 5.6. Let M be $\mathbb{Z}[\tau]$ -module satisfying (24) and let Ω be an open bounded convex set. Then

$$\varepsilon(\Omega) \geq \chi(\text{diam}(\Omega)). \tag{29}$$

The previous corollary contains proposition 3.1 in [12]. The proofs, however, are different.

Proof. Let us estimate from below the value of $\|k\| \chi(\text{th}(\Omega, k^*)/\|k^*\|)$. Recall relations (4)

and (5). If $\|k\|^2\|k^*\|^2 = 1$, then $\|k\| = \tau^k$, so that

$$\|k\| \chi\left(\frac{\text{th}(\Omega, k^*)}{\|k^*\|}\right) = \|k\| \|k^*\| \chi(\text{th}(\Omega, k^*)) = \chi(\text{th}(\Omega, k^*)) \geq \chi(\text{diam}(\Omega)).$$

If $\|k\|^2\|k^*\|^2 > 1$, one has

$$\|k\| \chi\left(\frac{\text{th}(\Omega, k^*)}{\|k^*\|}\right) \geq \frac{\|k\| \|k^*\|}{\text{th}(\Omega, k^*)} \geq \frac{2}{\text{diam}(\Omega)} > \frac{\tau}{\text{diam}(\Omega)} \geq \chi(\text{diam}(\Omega)).$$

□

The upper bound is given in the following theorem based on the theorem of Minkowski [9]. We need the following notation. Let e_1, \dots, e_n be the standard orthonormal basis of \mathbb{R}^n and $\alpha_1, \dots, \alpha_n$ a basis of \mathbb{R}^n . Denote

$$|\det \alpha| := |(\alpha_i | e_j)|.$$

Theorem 5.7. Let $\Omega \subset \mathbb{R}^n$ be a convex centrally symmetric set. Then

$$\varepsilon(\Omega) \leq \frac{4(2\tau - 1)}{\sqrt{\pi}} \cdot \sqrt[n]{\frac{\Gamma(\frac{n}{2} + 1) |\det \alpha| |\det \alpha^*|}{\text{vol}(\Omega)}}$$

where Γ is the gamma function.

Proof. For any $\delta > 0$ we can define a set $\tilde{\Omega} \subset \mathbb{R}^{2n}$ by

$$\tilde{\Omega} = \left\{ (x_1, \dots, x_n, y_1, \dots, y_n) \in \mathbb{R}^{2n} \mid \sum_{i=1}^n (x_i + \tau' y_i) \alpha_i^* \in \Omega, \left\| \sum_{i=1}^n (x_i + \tau y_i) \alpha_i \right\| \leq \delta \right\}.$$

Let us compute the volume of $\tilde{\Omega}$

$$\begin{aligned} \text{vol}(\tilde{\Omega}) &= \int_{\tilde{\Omega}} dx_1 \dots dx_n dy_1 \dots dy_n = (2\tau - 1)^{-n} \int_{u \in \Omega, v \in B(0, \delta)} du_1 \dots du_n dv_1 \dots dv_n \\ &= (2\tau - 1)^{-n} \frac{\text{vol}(\Omega)}{|\det \alpha^*|} \cdot \frac{\text{vol}(B(0, \delta))}{|\det \alpha|} \\ &= (2\tau - 1)^{-n} \frac{\text{vol}(\Omega)}{|\det \alpha^*| |\det \alpha|} \cdot \frac{\pi^{n/2} \delta^n}{\Gamma(n/2 + 1)}. \end{aligned}$$

Here we used the substitutions $u_i = x_i + \tau' y_i$ and $v_i = x_i + \tau y_i$ with the corresponding Jacobian $(\tau^2 + 1)/\tau = 2\tau - 1$. The vectors $\sum u_i \alpha_i^*$ and $\sum v_i \alpha_i$ are denoted respectively by u and v . The volume of a ball in \mathbb{R}^n , with radius δ , is $\pi^{n/2} \delta^n / \Gamma(n/2 + 1)$.

Next we choose δ such that $\text{vol}(\tilde{\Omega}) > 2^{2n} = 4^n$, i.e.

$$\delta > \frac{4(2\tau - 1)}{\sqrt{\pi}} \cdot \sqrt[n]{\frac{\Gamma(\frac{n}{2} + 1) |\det \alpha| |\det \alpha^*|}{\text{vol}(\Omega)}}. \tag{30}$$

Since $\tilde{\Omega}$ is a convex centrally symmetric set (because Ω and the ball are) with volume $> 2^{2n}$, we can use the Minkowski theorem, according to which there exists a non-zero point in $\tilde{\Omega}$ with integer coordinates. There exists $x = (x_1, \dots, x_n)$ and $y = (y_1, \dots, y_n)$, with $x_i, y_i \in \mathbb{Z}$, such that

$$\| \Sigma(x_i + \tau y_i) \alpha_i \| \leq \delta \text{ and } \Sigma(x_i + \tau' y_i) \alpha_i^* \in \Omega \iff \Sigma(x_i + \tau y_i) \alpha_i \in \Sigma(\Omega).$$

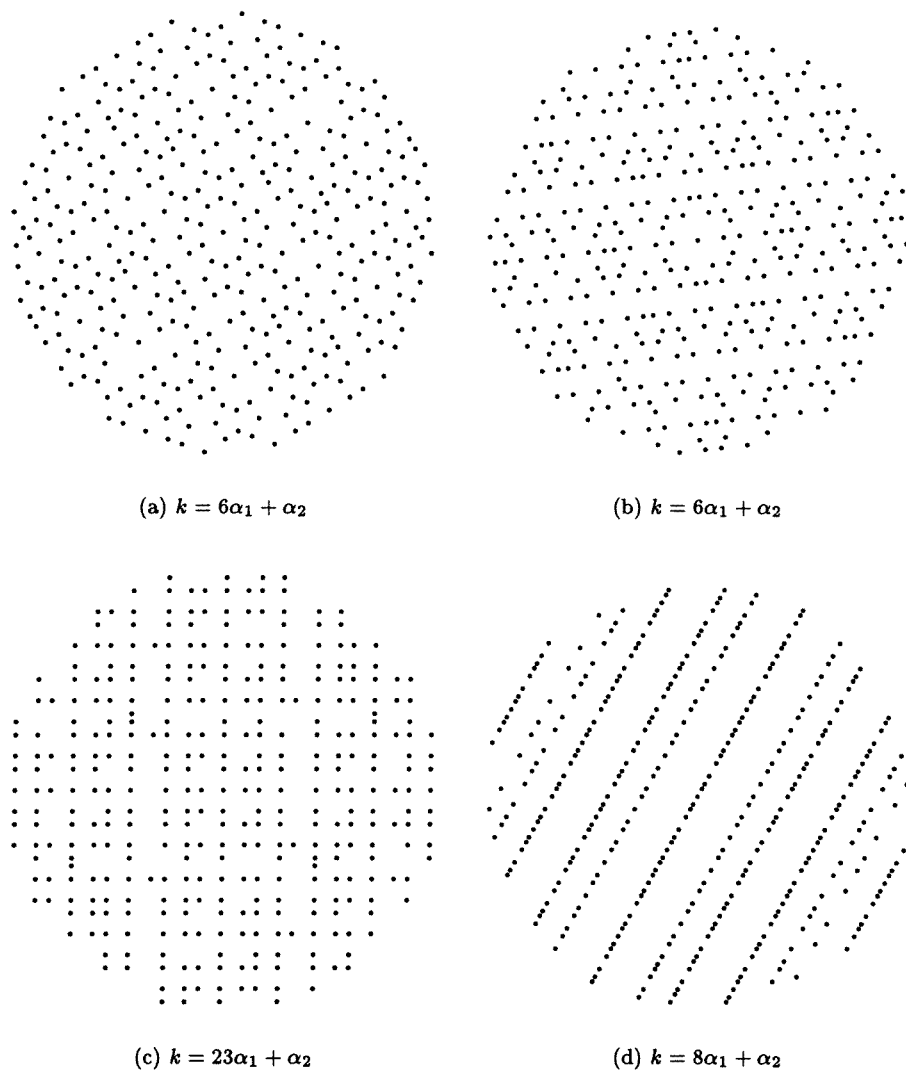


Figure 5. Examples of H_2 -quasicrystals, drawn in the same scale, with elliptic acceptance windows of volume π , centred at the origin. Directions k of the long elliptic axes are shown in each case; (a) and (b) differ by the length of the axes (20 and 50 respectively); (a), (c), and (d) differ only by orientation of the ellipse.

Since Ω is convex centrally symmetric, the zero vector $0 = 0^*$ lies in Ω and thus $0 \in \Sigma(\Omega)$.

Thus we have found two points of quasicrystal $\Sigma(\Omega)$ with distance $< \delta$. This means, that $\varepsilon(\Omega) \leq \delta$ for all δ satisfying (30). \square

In the examples in figure 5 we illustrate the variety of H_2 -quasicrystals, one obtains by changing the acceptance window, and the values of the upper and lower bounds for the minimal distance. In particular, $\Sigma(\Omega)$ with the same $\text{vol}(\Omega)$, have the same upper bound, given by the following corollary (cf proposition 4.1 of [12]).

Corollary 5.8. In the plane with $\mathbb{Z}[\tau]$ -module based on Δ_2 , we have $|\det \alpha| \cdot |\det \alpha^*| = \sqrt{5}/4$

and thus

$$\varepsilon(\Omega) \leq \frac{2(2\tau - 1)}{\sqrt{\pi}} \frac{\sqrt[4]{5}}{\sqrt{\text{vol}(\Omega)}}.$$

The lower bound is taken simply as (29) for any Ω . Its value depends on the $\text{diam}(\Omega)$. Note that the gap between $\varepsilon(\Omega)$ and $\chi(\text{diam}(\Omega))$ in (29) may be quite large. That is the case, for example, when the convex set Ω is cigar-like, long and narrow, oriented along the direction k , and with large $\|k\| \cdot \|k^*\|$. Therefore in figure 5 we show quasicrystals with long narrow elliptic Ω . However, in the case of circular Ω , one has $\varepsilon(\Omega) = \chi(\text{diam}(\Omega))$; such a quasicrystal can be seen in figure 4.

As the last example let us recall the well known rhombic Penrose tiling of the plane. The minimal distance between vertices of the tiles is clearly the short diagonal across the narrow tile. However, a more interesting problem is the rhombic Penrose quasicrystal, viewed as a union of four subquasicrystals each with its own convex Ω (for details see [11, section 4] and figure 2 of [6]). Then we can use our results to determine the minimal distance in each of them. There are two distinct minimal distances each occurring in two of the subquasicrystals. In the union of the four, they turn out to be the shorter diagonal of the thick Penrose rhomb and the longer diagonal of the thin one.

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