(IR)RATIONALIZING QUASICRYSTAL STRUCTURE

JULIANNA LIAN

Abstract. In this expository paper, we examine the structure of quasicrystals using Diophantine approximation. Quasicrystals are solid-state materials with long-range order and no translational periodicity. We first construct nonperiodic tilings via the cut-and-project method, which serves to accustom the reader to seeing irrational quantities that naturally appear in quasicrystals. Using the Fibonacci and Penrose tilings as examples, we show how irrational parameters emerge and produce aperiodic order. The one-dimensional quasicrystal is used as an exercise in showing absent periodicity and present long-range order. We determine that the quality of rational approximation to relevant irrational parameters governs how closely periodic behavior can appear over large finite regions, and discuss the role of badly approximable numbers. We conclude by extending the same irrational mechanisms to higher dimensions.

Contents

1. An apparent impossibility

Quasiperiodic crystals, or *quasicrystals*, are nonperiodic solid-state materials with long-range order (i.e. they obey some global organizing rule). The first quasicrystal was characterized by Dan Shechtman in 1982. Alongside colleagues who helped validate the discovery, Shechtman published the structure two years later as [SBGC84]. At the time, the discovery represented a glaring contradiction to symmetry rules of bona fide crystals with periodic order, only resolved after Levine and Steinhardt [LS84] distinguished *order* from *periodicity*. In 2011, the Nobel Prize in Chemistry was awarded to Shechtman for the discovery of quasicrystals. For a

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fuller history of the discovery, elucidation, and ongoing hunt for quasicrystals, see [SB12] and [Har22].

Diophantine approximation is the study of how well irrational numbers can be rationally approximated. For quasiperiodic structures, constructed from irrational parameters as we will see, Diophantine approximation allows us to discuss why a quasicrystal is nonperiodic, and how strongly it can resemble a periodic structure on large finite scales.

We examine how irrationality prevents exact periodicity, while the quality of rational approximation controls finite-scale near-periodicity. To justify their impossible existence, a mathematical construction of quasicrystals using the cut-and-project method is provided in Section 2 alongside its application to the one-dimensional Fibonacci and two-dimensional Penrose tilings. These examples show how irrational slopes, the golden ratio, and self-similarity enter the construction of quasicrystals. The relevance of Diophantine approximation is then made explicit in Section 3, and we examine how quasiperiodicity emerges from irrational parameters used for construction with a one-dimensional cut-and-project set. We prove that rational internal slope gives periodicity, while irrational internal slope gives nonperiodicity. We then explain why the local gaps are constrained to at most three lengths, and use continued fractions to connect partial quotients with near-periodic behavior. The final section returns to remark on the original icosahedral quasicrystal.

1.1. Crystal symmetry rules.

Crystals are solid-state materials with a periodic order constructed from elementary repeating units, or unit cells. Periodicity imposes constraints on the permissible rotational symmetries of unit cells.

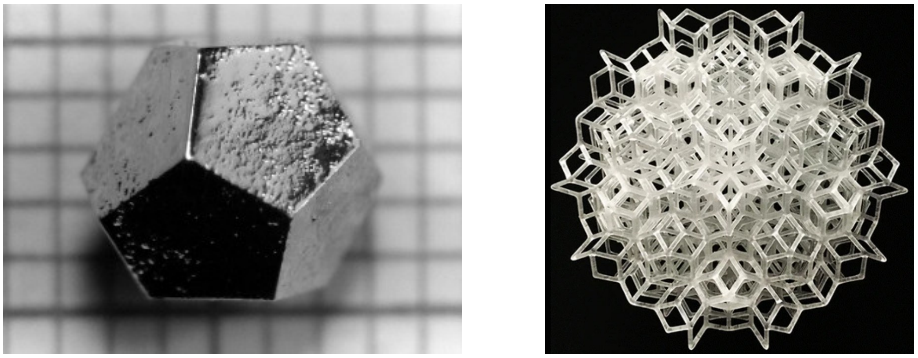
Theorem 1.1 (Crystallographic restriction theorem). *In a crystal lattice of two and three dimensions, only 1-, 2-, 3-, 4-, or 6-fold rotation axes are permissible.*

Theorem 1.1 identifies which rotational symmetries are compatible with translational symmetry. In a periodic lattice, allowed rotations must preserve a repeating lattice structure, disallowing certain rotation orders.

The icosahedral symmetry, composed of 5-, 3-, and 2-fold axes, of Shechtman's 1982 Al-Mn alloy therefore was in apparent violation! The rotational symmetry group of the regular icosahedron is the largest finite rotation group among polyhedral rotation groups, with six 5-fold, ten 3-fold, and fifteen 2-fold axes, and described by Steinhardt [Ste13] to be one of the *most* impossible natural crystal symmetries. Theorem 1.1, however, governs order only in periodic lattices and not in general. Structures lacking translational symmetry need not follow Theorem 1.1. Such is the response presented by Levine and Steinhardt [LS84], formally introducing the *quasicrystal* in 1984. Fig. 1 depicts a real macroscopic quasicrystal and a model of an icosahedral quasicrystalline structure.

2. Constructing quasicrystals

To realize the relevance of irrationality in quasicrystallinity, we first mathematically construct and justify for ourselves the existence of quasicrystals. We require a model that can encode a local arrangement of points, their relative spacing, and their symmetry properties. Tilings naturally capture rules that govern how these local arrangements must fit together. See [Gar89] for an instructive piece on tilings wherefrom a few key definitions we will use are summarized below.



(a) (b)

FIGURE 1. (a) A grain of icosahedral $Ho_9Mg_{14}Zn_{57}$ against a mm-grid lab-grown by [CF01], and (b) an illustrative wireframe 3D-printed model of an icosahedral quasicrystalline structure by [Ajl19].

DEFINITION 2.1 (Planar tiling). A collection of open and disjoint sets (tiles) whose closures cover a plane without any overlaps or gaps.

A tiling is termed *periodic* if a translation of the plane yields a picture indistinguishable from the original. For fun examples of periodic tilings, see the work of M. C. Escher (e.g. *Lizards*, 1942). In other words, a tiling is *periodic* if it is invariant under some nonzero translation. A tiling is *nonperiodic* if it has no nonzero translational period. A finite set of prototiles is called *aperiodic* if it admits at least one tiling of the plane, but every tiling it admits is nonperiodic. Nonperiodicity is a property of a particular tiling, while aperiodicity is better characterized as a property of a prototile set.

The cut-and-project method in Section 2.1 will allow us to generate nonperiodic tilings, which we will see applied to canonical quasiperiodic examples, the Fibonacci and Penrose tilings, in Section 2.2. Our strategy will be to use a periodic tiling in a higher-dimensional space from which a specific projection is selected and observed as a nonperiodic tiling in lower dimension.

2.1. **The cut-and-project method.** To identify the relevance of irrational parameters, we will use the following strategy for construction. Start with a periodic lattice in some higher-dimensional Euclidean space (ambient space), and recover from it a lower-dimensional (physical subspace) set by selecting and projecting specific lattice points. Often the higher-dimensional periodic lattice is defined in $\mathbb{Z}^n \subset \mathbb{R}^n$ to capture the discrete skeleton of a lattice within a continuous ambient space.

This *cut-and-project* method is an appropriate model for quasicrystal construction because it separates hidden periodicity and visible nonperiodicity. The ambient lattice supplies an underlying periodic structure which is *cut* into lower-dimensional subspaces. Select points are then *projected* from one subspace into another to generate the physical, nonperiodic structure with inherited geometric constraints from the hidden lattice. This order and absent translational periodicity are the exact quasicrystalline properties we are interested in recovering.

Construction 2.2. Cut-and-project method. Begin with a full-rank lattice $L \subset \mathbb{R}^n$, a direct-sum decomposition

$$\mathbb{R}^n = E_{\text{phys}} \oplus E_{\text{int}},$$

and the associated projections

$$\pi_{\text{phys}} : \mathbb{R}^n \to E_{\text{phys}} \qquad \pi_{\text{int}} : \mathbb{R}^n \to E_{\text{int}}.$$

We assume the following two conditions:

$$\pi_{\text{phys}}|_L \text{ is injective}$$

and

$$\pi_{\text{int}}(L) \text{ is dense in } E_{\text{int}}.$$

These are the precise irrationality conditions relative to L. The first says that no two distinct lattice points project to the same physical point. Equivalently, $L \cap E_{\text{int}} = \{0\}$. The second says that the internal coordinates of lattice points do not form a discrete lattice in E_{int}, but instead fill E_{int} densely.

A window is a bounded set

$$W \subset E_{\text{int}}$$

with nonempty interior. In the regular case, one also assumes that W is compact and that its boundary has measure zero; often one also chooses W so that

$$\partial W \cap \pi_{\text{int}}(L) = \varnothing,$$

which prevents ambiguity about lattice points lying exactly on the boundary.

The cut-and-project set determined by L and W is

$$\Gamma(L, W) = \{\pi_{\text{phys}}(x) : x \in L,\ \pi_{\text{int}}(x) \in W\}.$$

Thus W is an acceptance region in internal space. A lattice point x is retained when its internal projection $\pi_{\text{int}}(x)$ lies in W, and the retained point is then observed through its physical projection $\pi_{\text{phys}}(x)$.

2.2. **Quasiperiodic tilings.** We apply this versatile method for generating nonperiodic tilings to two quasiperiodic tiling examples. A *quasiperiodic* tiling is a nonperiodic tiling in which local finite patterns reappear throughout the tiling. For example, the frequency with which finite patches, or local configurations, recur can often be constrained by construction. Hence there is some organizing rule that governs the entire structure and imparts long-range order.

In these examples, we will illustrate three recurring features throughout this paper, nonperiodicity, self-similarity, and the appearance of the golden ratio, which will preface our discussion on Diophantine approximation in Section 3.1.

2.2.1. *Fibonacci tiling.* The Fibonacci tiling serves as an example of a nonperiodic tiling of the line whose finite patterns recur in an organized way. We will also see how ϕ arises from both tile frequencies and self-similar inflation. The simplest model of quasiperiodic order, the Fibonacci tiling, is the tiling of the line generated by the substitution rule below,

$$L \mapsto LS, \quad S \mapsto L$$

where L and S denote long and short intervals or tiles, respectively. Starting with L, we obtain the successive words

$$L, \quad LS, \quad LSL, \quad LSLLS, \quad LSLLSLSL, \ldots$$

whose word lengths are the Fibonacci numbers. We begin to see that in the limit this yields a tiling arranged in a pattern of intervals that is ordered but not periodic since no translation of the line leaves the arrangement invariant. Finite patches (i.e. LS, SL, LSL, etc.) recur throughout the tiling.

Remarkably, their relative frequencies converge! In particular, the ratio of the number of L-tiles to S-tiles is incommensurate (or irrational) and tends to $\phi = (1+\sqrt{5})/2$, the golden ratio. This can be explained by construction from the substitution rule.

Let L_n and S_n denote the numbers of L and S tiles after n substitution steps. Then

$$L_{n+1} = L_n + S_n, \quad S_{n+1} = L_n$$

The tile counts satisfy the Fibonacci recursion, and

$$\frac{L_{n+1}}{S_{n+1}} = \frac{L_n + S_n}{L_n} = 1 + \frac{S_n}{L_n}$$

So as n grows, this ratio approaches the positive solution of $x = 1 + 1/x$, namely $x = \phi$. The ratio is irrational, and thus the tiling cannot arise from periodic repetition of any finite patch.

Fibonacci tilings are also *self-similar*, which describes an invariance under scaling, inflation or deflation. When we *inflate* a tile, we enlarge it by a fixed scaling, and then reinterpret the enlarged tile as a disjoint union of the original set of tiles. *Deflation* is the analogous inverse operation.

Definition 2.3 (Self-similar polygonal tiling. Definition 2 from [BV21]). A tiling T of $\mathbb{R}^n$ is *self-similar* with map ψ if $\psi : \mathbb{R}^n \to \mathbb{R}^n$ is an expanding similarity,

$$\psi(x) = \lambda R x + t,$$

where $\lambda > 1$, R is an orthogonal transformation, and $t \in \mathbb{R}^n$, such that for every tile $t_0 \in T$, the image $\psi(t_0)$ is a finite union of tiles of T with disjoint interiors. The condition $\lambda > 1$ excludes constant maps and other degenerate transformations.

To illustrate this property, assign tile lengths $|L| = \phi$ and $|S| = 1$. The inflation map has scale factor ϕ. Therefore an S-tile is sent to an interval of length ϕ, which is exactly the length of one L-tile. An L-tile is sent to an interval of length $\phi^2 = \phi + 1$, which decomposes as one L-tile followed by one S-tile. Thus inflation by the single factor ϕ realizes the exact substitution rule that defines the Fibonacci tiling.

Now, let us generate a one-dimensional Fibonacci tiling by the cut-and-project method (Fig. 2). Start with a lattice in $\mathbb{Z}^2$, and choose a line of irrational slope for E_{phys} and the perpendicular internal subspace E_{int} which contains the bounded interval W. Project all lattice points lying within the window onto the physical line. Notice how the gaps between projected points take only two values, L and S. With an irrational slope, these appear in exactly the Fibonacci order.

2.2.2. *Penrose tilings.* Now let us examine the famous two-dimensional quasiperiodic tiling example discovered by Roger Penrose about a decade prior to Shechtman's discovery of the quasicrystal. We will again observe the appearance of irrational parameters, which begins to suggest how Diophantine approximation might be relevant to quasicrystalline structure.

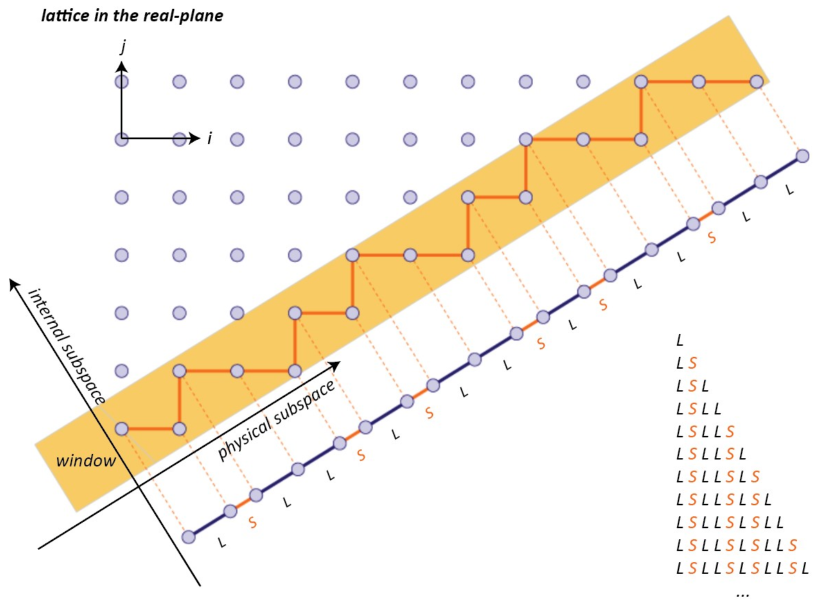


Figure 2. Cut-and-project construction of the one-dimensional Fibonacci tiling where the shaded orange region denotes the acceptance window oriented along the internal subspace. This figure was adapted from the Tilings Encyclopedia maintained online at [Til].

Definition 2.4 (Penrose tiling). A nonperiodic tiling of the plane by a finite set of prototiles (e.g. fat and skinny rhombuses) arranged according to matching rules that enforce global nonperiodicity.

Imagine we are tasked to tile an infinite plane in $\mathbb{R}^2$ with regular polygons. In the simplest case, we can envision a triangular tiling where triangles are fit together in an alternating up-and-down pattern. Squares can be tiled with each of their sides flush against one another, and a hexagonal tiling follows from our earlier triangular tiling. Now, attempt for yourself to construct a pentagonal tiling and notice how we arrive at unavoidable gaps or overlaps.

In the 1970s, Penrose realized a systematic pentagonal tiling supplemented with additional shapes to fill the unavoidable gaps. The original set of supplementary tiles are described in [Pen74]. The tiling has recurring local configurations across the entire plane, but with no repeating global order. This marked the beginning of the realization that there were several tilings (an uncountable number!) that could be constructed to have the same properties. The original Penrose tiling formulation was simplified to that of only two different rhombuses–the minimal set–and today, we recognize three main prototile sets by which an infinite number of Penrose tilings can be generated, summarized in [FN25]. The rhombic Penrose tiling, uses two rhombic prototiles, fat or skinny. See [FN25] Fig. 1 for visualization of the original prototile set, derivation of the tiling of fat and skinny rhombuses, and fivefold symmetry therein.

By the cut-and-project method, constructing the Penrose tiling classically in [Pen74] begins with a lattice in $\mathbb{R}^5$. We then choose a two-dimensional physical subspace E_{phys} and a complementary three-dimensional internal subspace E_{int}, both irrationally oriented relative to the lattice. We then retain only those lattice points whose internal projections lie within a suitable window W, which are then projected into E_{phys}.

Penrose tilings exhibit local 5-fold symmetry, and proved to be a fitting framework for understanding the unprecedented structure of quasicrystals. We note that Penrose tilings are also self-similar: fat and skinny rhombuses can be subdivided into rhombuses of the same two types or grouped into larger supertiles. Steinhardt [Ste96] demonstrates through repeated deflation operations that finite clusters (analogous to "finite patches" in 2.2.1) reproduce a larger fat rhombus by the irrational scaling factor ϕ.

It is perhaps interesting to mention that Penrose introduced these mathematical objects in the 1970s, from which crystallographer Alan Mackay [Mac81] was able to *hypothesize the existence of quasicrystals* in 1981, years before the publication of the first characterization. This raises a question about the geometric inevitability of quasiperiodic materials and whether we can gesture at their frequency of occurrence in nature. For a more comprehensive (and extraterrestrial) speculation, see [BDS20].

2.3. **Ascribing order to irrationality.** We have now seen that the relative frequency of long and short tiles in the Fibonacci tiling is characterized by the golden ratio ϕ, which reappears as a scaling in its self-similarity; in the cut-and-project construction of the tiling, selection of irrational physical and internal subspace slopes prevents translational periodicity while still producing a constrained arrangement of long and short intervals. In the Penrose tilings, self-similarity again appears under inflation by ϕ; in its cut-and-project construction, the subspace planes are chosen to be irrationally oriented with respect to the ambient lattice space to prevent rational alignment with any nonzero lattice direction.

By now, we can likely assign some responsibility to irrational quantities in determining quasiperiodic structure. Indeed, how strongly an arrangement can resemble a periodic one over finite scales depends on how well irrational parameters are rationally approximated. And here lies a natural entry for Diophantine approximation!

3. Diophantine approximation in quasicrystallinity

To explain the presence of irrational quantities seen in prior examples, we now examine an instructive one-dimensional quasiperiodic structure. We use this model to ascribe nonperiodicity to the choice of an irrationally oriented subspace in Section 3.1 and discuss the emergence of its long-range order in Section 3.2. We will apply this context to understanding the role of badly approximable numbers, like ϕ, in quasicrystal construction in Section 3.3. We conclude by returning to the original three-dimensional icosahedral quasicrystal in Section 3.4.

3.1. **Origin of nonperiodicity.** To identify irrationality as a source of nonperiodicity, we examine orientations of the internal subspace during cut-and-project construction of a one-dimensional quasicrystal. We assume that η is irrational so that the physical coordinate map

$$(a, b) \mapsto a + b\eta$$

is injective on $\mathbb{Z}^2$. Indeed, if $\eta = r/s \in \mathbb{Q}$, then distinct lattice points can have the same physical coordinate, for example,

$$(a, b) \quad \text{and} \quad (a + r, b - s)$$

project to the same value. Injectivity is part of the cut-and-project setup, so the physical slope must be irrational here. We will focus on the internal subspace, its slope ϵ, and its selection of points.

Let us claim that for a cut-and-project set from a two-dimensional lattice, rational orientation of the internal subspace (i.e. slope of the line) with respect to the ambient space yields a periodic projection. The claims we set out to prove are summarized in Proposition 3.1.

Recall that we let $\epsilon, \eta \in \mathbb{R}$ be distinct irrational numbers, and let window $W \subset \mathbb{R}$ be a bounded interval. Then define $\Gamma(L, W) = \{a + b\eta : a, b \in \mathbb{Z}, a + b\epsilon \in W\}$, where (a, b) is the integer coordinate of a lattice point. This is the standard cut-and-project set obtained from the lattice $\mathbb{Z}^2 \subset \mathbb{R}^2$ with a physical subspace (a line) determined by slope η, an internal subspace determined by slope ϵ, and an acceptance window W.

We can write a mapping of the lattice point $(a, b) \mapsto (a + b\eta, a + b\epsilon)$. Then

$$\pi_{\text{phys}}(a, b) = a + b\eta \qquad \pi_{\text{int}}(a, b) = a + b\epsilon$$

are the respective projections, and we have the cut-and-project set

$$\Gamma(L, W) = \{\pi_{\text{phys}}(a, b) : \pi_{\text{int}}(a, b) \in W\}$$

We now provide a proof for Proposition 3.1, which is adapted from ideas in [GMP03]. As a reminder, η denotes the physical slope and ϵ denotes the internal slope.

Proposition 3.1. *Let $\Gamma(L, W)$ be defined as above.*

1. *If $\epsilon = p/q \in \mathbb{Q}$ with $\gcd(p, q) = 1$, then $\Gamma(L, W)$ is periodic.*
2. *If $\epsilon \in \mathbb{R}/\mathbb{Q}$, then $\Gamma(L, W)$ has no nonzero translational period.*

Proof. For (1), if $\epsilon = p/q$ and $\gcd(p, q) = 1$, then the acceptance condition can be equivalently written

$$a + b\epsilon \in W \iff qa + bp \in qW$$

Now, we consider a translation of lattice coordinates, by $(p, -q)$. This is the smallest Euclidean distance we can move $(a, b) \mapsto (a + p, b - q)$ that will preserve the acceptance condition $qa + bp$, and indeed,

$$q(a + p) + p(b - q) = aq + qp + bp - pq = qa + bp$$

The quantity $qa + bp$ is invariant under this mapping of (a, b). So, if $a + b\epsilon \in W$, then

$$(a + p) + (b - q)\epsilon = a + b\epsilon \in W.$$

Equivalently, if the lattice point (a, b) is accepted by the window, then the translated lattice point $(a + p, b - q)$ is also accepted.

The physical coordinate of (a, b) is $a + b\eta$, and the physical coordinate of $(a + p, b - q)$ is

$$\pi_{\text{phys}}(a + p, b - q) = (a + p) + (b - q)\eta = a + b\eta + (p - q\eta)$$

Then the admissible lattice points come in pairs whose physical projections differ by a period $p - q\eta$. When $x = a + b\eta \in \Gamma(L, W)$, the translated point $x + (p - q\eta) \in$

$\Gamma(L,W)$. Applying the inverse lattice translation $(a,b)\mapsto(a-p,b+q)$ gives the reverse inclusion, so

$$\Gamma(L,W)+(p-q\eta)=\Gamma(L,W).$$

Then we have shown that $\Gamma(L,W)$ is invariant under translation by $p-q\eta$. Hence $\Gamma(L,W)$ is periodic.

For (2), assume $\epsilon\notin\mathbb{Q}$. Suppose that $\Gamma(L,W)$ has a nonzero period T. Choose any point $x_0\in\Gamma(L,W)$. Since T is a period, $x_0+T\in\Gamma(L,W)$. Both x_0 and x_0+T have physical coordinates of the form $a+b\eta$, so their difference lies in

$$\mathbb{Z}+\eta\mathbb{Z}.$$

Because η is irrational, this representation is unique. Hence there exist $u,v\in\mathbb{Z}$, not both zero, such that

$$T=u+v\eta.$$

Now let $(a,b)\in\mathbb{Z}^2$ be any accepted lattice point, so that

$$a+b\epsilon\in W.$$

Since T is a period,

$$(a+b\eta)+T=(a+u)+(b+v)\eta$$

must also be the physical coordinate of an accepted lattice point. Therefore

$$(a+u)+(b+v)\epsilon\in W.$$

Equivalently, $(a+b\epsilon)+(u+v\epsilon)\in W$. So translation by

$$s=u+v\epsilon$$

preserves the window condition on all accepted internal coordinates. Because ϵ is irrational, the additive group

$$\mathbb{Z}+\epsilon\mathbb{Z}=\{a+b\epsilon : a,b\in\mathbb{Z}\}$$

is dense in $\mathbb{R}$. Hence

$$W\cap(\mathbb{Z}+\epsilon\mathbb{Z})$$

is dense in W, since W is an interval. For every accepted internal coordinate $y\in W\cap(\mathbb{Z}+\epsilon\mathbb{Z})$, the period assumption implies

$$y+s\in W,\qquad s=u+v\epsilon.$$

Taking limits along accepted internal coordinates gives

$$\overline{W}+s\subseteq\overline{W},$$

where $\overline{W}$ is the closure of W. But $\overline{W}$ is a bounded interval, and no bounded interval contains a nonzero translate of itself. Therefore $s=0$. Since ϵ is irrational and $u,v\in\mathbb{Z}$, the equality $u+v\epsilon=0$ forces $u=v=0$. Hence $T=u+v\eta=0$, contradicting the assumption that T was nonzero! Hence no nonzero period exists for $\Gamma(L,W)$.

□

3.2. **Local configuration constrained to three gap lengths.** For a one-dimensional cut-and-project set $\Gamma(L, W)$ with interval window W, the distances between neighboring points are not arbitrary. When the points of $\Gamma(L, W)$ are ordered as

$$\cdots < x_n < x_{n+1} < \cdots ,$$

there are at most three possible values of the gap $x_{n+1} - x_n$. More precisely, there exist positive physical displacements

$$\Delta_1, \Delta_2 \in \mathbb{Z} + \eta\mathbb{Z}$$

such that

$$x_{n+1} - x_n \in \{\Delta_1, \Delta_2, \Delta_1 + \Delta_2\}$$

for every n. We remark on this result, and for the full proof see [GMP06].

Recall that each point $x_n \in \Gamma(L, W)$ comes from some lattice point $(a, b) \in \mathbb{Z}^2$ with the physical coordinate $x_n = a + b\eta$ and internal coordinate $x_n^* = a + b\epsilon \in W$.

Suppose we fix some x_n. We can represent the move to another lattice point as

$$(a, b) \mapsto (a + m, b + n), \qquad m, n \in \mathbb{Z}$$

so the new projected point is

$$(a + m) + (b + n)\eta = x_n + (m + n\eta)$$

Then every possible adjacent gap is of the form $m + n\eta$. Only displacements that yield an internal coordinate within W are allowed, that is,

$$(a + m) + (b + n)\epsilon = x_n^* + (m + n\epsilon) \in W$$

So the next point x_{n+1} following x_n is determined by the smallest positive physical displacement $m + n\eta$ whose corresponding internal displacement $m + n\epsilon$ keeps the internal coordinate inside W. This is because by definition, x_{n+1} is the first point lying to the right of x_n, so the gap length is exactly

$$x_{n+1} - x_n = \min\{m + n\eta > 0 : x_n + m + n\eta \in \Gamma(L, W)\}.$$

Then valid gap lengths are decided by the position of x_n^* within W.

For a physical displacement

$$\delta = m + n\eta,$$

write its internal displacement as

$$\delta^\star = m + n\epsilon.$$

For the bounded interval W, we can write $W = [c_1, c_1 + c_2)$ with $c_2 > 0$. Then for some fixed x, the above criteria for admissibility in W, $x^* + \delta^* \in W$, can be written

$$x^* \in [c_1 - \delta^*, c_1 + c_2 - \delta^*)$$

Each displacement then is an interval condition on x^*. Only when x^* crosses an endpoint do we exit W. The successor displacement changes when a shifted internal point reaches an endpoint of W. For two basic neighbor displacements Δ_1, Δ_2, we choose them so that

$$\Delta_1^* > 0, \quad \Delta_2^* < 0, \quad \Delta_1^* - \Delta_2^* \geq c_2$$

Then the move Δ_1 is admissible when $x^* \in [c_1, c_1 + c_2 - \Delta_1^*)$. And likewise, Δ_2 is admissible when $x^* \in [c_1 - \Delta_2^*, c_1 + c_2)$. The points $c_1 + c_2 - \Delta_1^*$ and $c_1 - \Delta_2^*$ partition the interval into at most three subintervals,

$$x_{n+1} - x_n = \begin{cases} \Delta_1, & x_n^\star \in [c_1,\ c_1 + c_2 - \Delta_1^\star), \\ \Delta_1 + \Delta_2, & x_n^\star \in [c_1 + c_2 - \Delta_1^\star,\ c_1 - \Delta_2^\star), \\ \Delta_2, & x_n^\star \in [c_1 - \Delta_2^\star,\ c_1 + c_2). \end{cases}$$

The proof idea following [GMP06] is to encode our admissibility criteria $x^* + \delta^* \in W$ by a stepping function. Once Δ_1, Δ_2 are identified, W is partitioned by two points into at most three subintervals. On each subinterval the successor displacement is constant, and yields the three possible gap lengths.

This result is a cut-and-project version of the classical *three gap theorem*, which states that for an irrational α the fractional parts

$$\{0, \alpha, 2\alpha, \ldots, N\alpha\}$$

partition the unit circle into intervals of at most three distinct lengths. In the present setting, the same mechanism appears through the internal coordinates of accepted lattice points. Ordering the projected physical points corresponds to an irrational rotation on the acceptance window W. The possible successor gaps are therefore constrained by the same *three gap principle*, but expressed in physical displacement lengths $m + n\eta$ rather than circle arc lengths.

Although the cut-and-project set $\Gamma(L, W)$ is nonperiodic, the local configuration of points is constrained to a finite gap structure. The structure is not random. There is a persistent ordering rule that constrains the entire structure, and so we say that long-range order is present. We have shown now another characteristic property of quasicrystalline structure.

3.3. **Badly approximable slopes and near-periodicity.** We now ask if we can gesture at the size and arrangement of gap lengths. In Section 3.1 we examined how an irrational slope determines the nonperiodic cut-and-project set $\Gamma(L, W)$ for a one-dimensional quasicrystal.

We now make precise what it means for a cut-and-project structure to look nearly periodic over large finite regions. The relevant quantity is how well an irrational α can be approximated by rationals. A rational slope gives an exact period, as in Proposition 3.1. An irrational slope gives no exact period, but a very accurate rational approximation $p/q \approx \alpha$ produces an approximate period. If this internal displacement is small compared with the distance to the boundary of W, the same acceptance decisions persist over a large finite region.

Thus Diophantine approximation controls finite-scale near-periodicity. Slopes with very large partial quotients have especially strong near-periods at selected scales. Slopes with bounded partial quotients are badly approximable, meaning that their rational approximations are never exceptionally accurate. They may still have approximate periods, but these approximate periods improve only at the controlled rate forced for every irrational number.

Let α be irrational. Its continued fraction is $\alpha = [a_0; a_1, a_2, a_3, ...]$, where $a_0 \in \mathbb{Z}$ and $a_n \in \mathbb{N}$ for $n \geq 1$ with convergents $p_n/q_n = [a_0; a_1, ..., a_n]$ (the rational approximants to α).

A standard bound of how well they rationally approximate α is

$$\left|\alpha - \frac{p_n}{q_n}\right| < \frac{1}{q_n^2}$$

so as the next partial quotient a_{n+1} increases, p_n/q_n becomes a more accurate rational approximation to α.

Let p_k/q_k be a convergent of an irrational slope α. Then

$$|q_k\alpha - p_k| < \frac{1}{q_{k+1}}.$$

In the one-dimensional cut-and-project model with internal coordinate $a + b\alpha$, the lattice translation

$$(a, b) \mapsto (a - p_k, b + q_k)$$

changes the internal coordinate by

$$(a - p_k) + (b + q_k)\alpha - (a + b\alpha) = q_k\alpha - p_k.$$

Thus the translation is an exact period when $\alpha = p_k/q_k$, and it is an approximate period when α is close to p_k/q_k. The smaller $|q_k\alpha - p_k|$ is, the farther an accepted internal coordinate can move before crossing the boundary of W. Therefore good rational approximations produce long finite regions that resemble periodic cut-and-project sets.

The next partial quotient controls this error because

$$q_{k+1} = a_{k+1}q_k + q_{k-1}.$$

A large a_{k+1} makes q_{k+1} large compared with q_k, forcing

$$|q_k\alpha - p_k|$$

to be unusually small. In geometric terms, a large partial quotient produces a strong near-period. By contrast, if the partial quotients of α are bounded, then α is badly approximable. Such slopes do not admit arbitrarily strong near-periods at unexpectedly large finite scales.

Definition 3.2 (Badly approximable numbers). An irrational number α is *badly approximable* if there exists a constant $c > 0$ such that for all integers p, q with $q > 0$,

$$\left|\alpha - \frac{p}{q}\right| > \frac{c}{q^2}$$

The size of the partial quotients governs the quality of approximation, where large partial quotients produce more accurate rational approximants, while bounded partial quotients prevent such well-approximation. In cut-and-project construction, more accurate rational approximants correspond to periodic models that approximate the nonperiodic behavior over longer finite scales. Bounded partial quotients have the characteristic that they cannot have this strong near-periodic behavior.

Theorem 3.3. *An irrational number α is badly approximable if and only if its continued fraction partial quotients (a_n) are bounded.*

When an irrational slope α is well-approximated by a rational, the cut-and-project construction over a large region would appear periodic with period q. By contrast, a badly approximable slope still has near-periods, but not anomalously strong ones relative to their scale. Such a result explains the role of badly approximable numbers in quasicrystal structure, numbers like ϕ and the silver mean $1 + \sqrt{2}$ in Cerovski et al. [CSG05] quasicrystals.

3.3.1. *Revisiting Fibonacci tilings.* Recall that the Fibonacci tiling from Section 2.2.1 is a one-dimensional cut-and-project set, generated by substitution, and is self-similar with a scaling factor ϕ. For the Fibonacci slope,

$$\phi = [1; 1, 1, 1, \dots],$$

all partial quotients are equal to 1. Hence ϕ is badly approximable. Notice how its convergents are ratios of consecutive Fibonacci numbers:

$$1,\ \frac{2}{1},\ \frac{3}{2},\ \frac{5}{3},\ \frac{8}{5}, \dots, \frac{F_{n+1}}{F_n}, \dots$$

The associated crystalline approximants are periodic cut-and-project sets obtained by replacing the irrational slope ϕ with F_{n+1}/F_n. Their periods grow with F_n, and the approximants converge to the nonperiodic Fibonacci tiling. Since the partial quotients remain bounded, these approximants improve at a controlled rate.

3.4. **Irrationality in higher dimensions.** We close by extending to higher-dimensional ambient space in order to construct three-dimensional quasicrystals. We return to the original motivating icosahedral quasicrystal for this exercise. The standard construction of the three-dimensional icosahedral starts with the decomposition of $\mathbb{R}^6$ ambient space into complementary physical and internal subspaces, $E_{\text{phys}} \oplus E_{\text{int}}$, where $E_{\text{phys}} \cong \mathbb{R}^3$ and $E_{\text{int}} \cong \mathbb{R}^3$.

Let $L \subset \mathbb{Z}^6$ be a lattice, and let

$$\pi_{\text{phys}} : \mathbb{R}^6 \to E_{\text{phys}}, \quad \pi_{\text{int}} : \mathbb{R}^6 \to E_{\text{int}}$$

denote the corresponding projections. Given a closed and bounded window $W \subset E_{\text{int}}$, we define the cut-and-project set

$$\Gamma(L, W) = \{\pi_{\text{phys}}(x) : x \in L, \pi_{\text{int}}(x) \in W\}$$

As before, we must select E_{phys} and E_{int} to be irrationally oriented relative to the periodic lattice L. Conveniently, the regular icosahedron can be realized with the coordinates

$$(0, \pm 1, \pm\phi), \quad (\pm 1, \pm\phi, 0), \quad (\pm\phi, 0, \pm 1)$$

Recall how both the Fibonacci tilings in Section 2.2.1 and the Penrose tilings in Section 2.2.2 are constructed using ϕ and such was the origin of their quasiperiodic properties. We observe that, of no surprise, the icosahedron is defined using ϕ as well!

Indeed, to generate the physical subspace, we choose the six vectors,

$$v_1 = (1, \phi, 0), \quad v_2 = (-1, \phi, 0), \quad v_3 = (0, 1, \phi)$$

$$v_4 = (0, -1, \phi), \quad v_5 = (\phi, 0, 1), \quad v_6 = (\phi, 0, -1)$$

whose negatives realize the twelve vertices of a regular icosahedron. For a full construction of the icosahedral quasicrystal see [CCAI25].

Irrational mechanisms in our simpler Fibonacci and Penrose examples apply to higher dimension. They reappear in the icosahedral and are key to quasicrystal structure.

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Massachusetts Institute of Technology
Email address: julilian@mit.edu