Reflection quasilattices and the maximal quasilattice

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We introduce the concept of a *reflection quasilattice*, the quasiperiodic generalization of a Bravais lattice with irreducible reflection symmetry. Among their applications, reflection quasilattices are the reciprocal (i.e., Bragg diffraction) lattices for quasicrystals and quasicrystal tilings, such as Penrose tilings, with irreducible reflection symmetry and discrete scale invariance. In a follow-up paper, we will show that reflection quasilattices can be used to generate tilings in real space with properties analogous to those in Penrose tilings, but with different symmetries and in various dimensions. Here we explain that reflection quasilattices only exist in dimensions two, three, and four, and we prove that there is a unique reflection quasilattice in dimension four: the "maximal reflection quasilattice" in terms of dimensionality and symmetry. Unlike crystallographic Bravais lattices, all reflection quasilattices are invariant under rescaling by certain discrete scale factors. We tabulate the complete set of scale factors for all reflection quasilattices in dimension $d > 2$, and for all those with quadratic irrational scale factors in $d = 2$.

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I. INTRODUCTION

Our starting point is Coxeter's celebrated classification of the finite reflection groups in terms of irreducible root systems and Coxeter-Dynkin diagrams [1–5]. These come in two flavors: crystallographic and noncrystallographic (see Refs. [6,7]). We introduce two simple definitions: if Φ is an irreducible (crystallographic or noncrystallographic) root system, and $G(\Phi)$ is the corresponding reflection group, the Φ root (quasi)lattice Λ_Φ is the set of all integer linear combinations of the Φ roots; and a Φ reflection (quasi)lattice is any $G(\Phi)$-invariant subset of Λ_Φ that is closed under addition and subtraction. (The prefix "quasi," referring to quasiperiodic, is used when Φ is noncrystallographic.) Thus, Λ_Φ is always one of the Φ reflection (quasi)lattices.

In this paper, we explain why the reflection quasilattices ("reflection QLs") are of particular interest, and why the above definitions are particularly apt. We show that the d-dimensional reflection QLs are the noncrystallographic generalization of the special class of d-dimensional Bravais lattices whose point symmetry is an irreducible reflection group $G(\Phi)$ of full rank d. They play a fundamental physical role: first, as the reciprocal (i.e., Bragg diffraction) lattices for quasicrystals [8–13] and quasicrystal patterns/tilings [14] with point symmetry $G(\Phi)$; and second, as the basis for classifying the space groups corresponding to $G(\Phi)$ [15–17]. Reflection QLs have two other key properties of physical interest. (i) First, their discrete point symmetry $G(\Phi)$ is sufficient to rigidly fix their shape (with no continuously tunable parameters, apart from overall rescaling); and, consequently, the associated quasicrystals and tilings are governed by certain irrational ratios that are "locked in" by symmetry, so that they do not require any fine tuning and are intrinsically robust (e.g., against fluctuations of temperature and pressure in the laboratory). (ii) Second, in contrast to any ordinary lattice, and in contrast to the broader class of quasilattices defined in previous work [18,19], every reflection QL is precisely invariant under rescaling by a special set of characteristic *scale factors*, and thus exhibits a discrete scale invariance which suggests interesting connections to other instances of scale invariance in physics. Reflection QLs are the reciprocal lattices for many of the most experimentally and/or mathematically interesting and widely studied quasicrystals and tilings, including (i) the Penrose tiling [20–22]; (ii) natural generalizations of it that share its key properties (including its Ammann-grid decoration [17,23–25]); and (iii) a variety of other quasicrystals obtained from higher-dimensional root lattices by the cut-and-project method [13,26–31]. In fact, in a forthcoming paper [17], we show how reflection QLs can be used to systematically generate tilings with matching rules, inflation rules, and Ammann-grid decorations analogous to those in Penrose tilings (but with different symmetries, and in various dimensions), in a way that illuminates the deep web of connections between aperiodic translational order, noncrystallographic orientational order, and discrete scale invariance that these tilings embody.

In this paper, we explain that reflection QLs only occur in two, three, and four dimensions, and prove that there is a unique reflection QL in four dimensions (4D), which we present explicitly. This is the final and maximal reflection QL—the reflection QL of highest dimension and highest symmetry. We discuss the relation of these results to earlier work [18,19] on a related class of quasilattices in two dimensions (2D) and three dimensions (3D), and to number theoretic results about the quaternions [13,32–35].

For all the reflection QLs in dimension $d > 2$, and all the *quadratic* reflection QLs (i.e., reflection QLs with quadratic irrational scale factors) in dimension $d = 2$, we tabulate the corresponding scale factors, and prove that we have the complete set.

II. NONCRYSTALLOGRAPHIC ROOT SYSTEMS

For an introduction to finite reflection groups (finite Coxeter groups), roots systems, and Coxeter-Dynkin diagrams, see Chap. 4, Sec. 2 in [6] (for a brief introduction) and Part 1 (i.e., Chaps. 1–4) in [7] (for more detail). For an introduction to a wide range of relevant mathematics underlying our study, see [13].

The irreducible finite reflection groups and their corresponding root systems may be neatly described by Coxeter-Dynkin diagrams (see [6,7]). These come in two varieties: crystallographic and noncrystallographic. The crystallographic cases are familiar from the theory of Lie groups and Lie algebras: they come in four infinite families (A_n, B_n, C_n, and D_n) and five exceptional cases (G_2, F_4, E_6, E_7, and E_8). The remaining root systems are noncrystallographic: almost all of these are in 2D (I_2^n, $n = 5,7,8,9,\ldots$), with just one in 3D (H_3), one in 4D (H_4), and none in higher dimensions.

Let us describe the noncrystallographic roots systems:

First consider I_2^n. In geometric terms, the $2n$ roots of I_2^n are perpendicular to the n mirror planes of an equilateral n-sided polygon; note that when n is odd, these mirror planes are all equivalent (each intersects a vertex and its opposite edge), but when n is even the mirror planes split into two inequivalent sets (those that intersect two opposite vertices, and those that intersect two opposite edges). In algebraic terms, we can think of the $2n$ roots as $2n$ complex numbers. When n is odd, these are the $(2n)$th roots of unity: ζ_{2n}^k $(k = 1,\ldots,2n)$, where $\zeta_n \equiv \exp(2\pi i/n)$. When n is even, the $2n$ roots break into two rings: (i) a first ring ζ_n^k $(k = 1,\ldots,n)$; and (ii) a second ring which we can think of as $\zeta_n^k + \zeta_n^{k+1}$ $(k = 1,\ldots,n)$. The I_2^n reflections generate the symmetry group of the regular n-gon, of order $2n$.

Next consider H_3. If we let τ denote the golden ratio $\frac{1}{2}(1+\sqrt{5})$, the H_3 roots are the 30 vectors obtained from

$$\{\pm 1,0,0\} \qquad \text{and} \qquad \tfrac{1}{2}\{\pm\tau,\pm 1,\pm 1/\tau\} \tag{1}$$

by taking all combinations of $\pm$ signs, and all even permutations of the three coordinates. These point to the 30 edge midpoints of a regular icosahedron, and the corresponding reflections generate the full symmetry group of the icosahedron (of order 120).

Finally consider H_4. From a geometric standpoint, the H_4 roots are the 120 vectors obtained from

$$\begin{array}{c}\{\pm 1,0,0,0\},\\ (1/2)\{\pm 1,\pm 1,\pm 1,\pm 1\},\\ (1/2)\{0,\pm\tau,\pm 1,\pm 1/\tau\}\end{array} \tag{2}$$

by taking all combinations of $\pm$ signs, and all even permutations of the four coordinates: these are the 120 vertices of a 4D regular polytope called the 600 cell [4]. From the algebraic standpoint, they are the set of 120 "unit icosians" [6] within the skew field of quaternions $\mathbb{H}$ (see [36] for an introduction). The H_4 reflections generate the symmetry group of the 600 cell: this group has $120^2 = 14\,400$ elements, corresponding to all maps from $\mathbb{H} \to \mathbb{H}$ of the form $Q \to \bar{q}_1 Q q_2$ or $Q \to \bar{q}_1 \bar{Q} q_2$, where q_1 and q_2 are any two unit icosians [27,36].

III. ROOT AND REFLECTION LATTICES AND QUASILATTICES: DEFINITIONS

Let Φ be a finite irreducible (crystallographic or noncrystallographic) root system, with $G(\Phi)$ the corresponding reflection group. We introduce two definitions:

Definition 1. The Φ "root (quasi)lattice" Λ_Φ is the set of all integer linear combinations of the Φ roots.

Definition 2. A Φ "reflection (quasi)lattice" is any subset of Λ_Φ (including Λ_Φ itself) that is (i) $G(\Phi)$ invariant and (ii) closed under addition and subtraction.

Here "quasi" is used when Φ is noncrystallographic, and we abbreviate quasilattice as QL. The term "lattice" without any prefix refers to crystallographic only.

Let Φ have rank d: if Φ is crystallographic, a Φ root (or reflection) lattice is an ordinary lattice in $\mathbb{R}^d$ (with some finite minimum separation between nearest neighbors); while if Φ is noncrystallographic, then a Φ root (or reflection) QL is a *dense* set of points in $\mathbb{R}^d$ (with points arbitrarily close to every point in $\mathbb{R}^d$).

IV. REMARKS ON THESE DEFINITIONS

Definition 1 is clear: it is the noncrystallographic generalization of a (crystallographic) root lattice. But to fully appreciate Definition 2, it is helpful to review the definition of a "G lattice" proposed by Rokhsar, Mermin and Wright [19]:

Let G be a point group in $\mathbb{R}^d$, and let Λ be a rank-d set of vectors in $\mathbb{R}^d$. Λ is a d-dimensional G lattice if it (i) is G invariant; (ii) is closed under addition and subtraction; and (iii) is of the minimal integer rank compatible with G invariance. This is the noncrystallographic generalization of the idea of a Bravais lattice with point group G (since, when G is crystallographic, the G lattices are precisely the Bravais lattices with point group G).

Remark 1. The reflection (quasi)lattices are a natural subclass of Bravais (quasi)lattices: those whose point group is an irreducible reflection group of full rank. That is, the reflection (quasi)lattices are the d-dimensional G lattices for which $G = G(\Phi)$ is an irreducible rank d reflection group. This can be proved as follows. First of all, one can check that any set of vectors that is $G(\Phi)$ invariant and closed under addition and subtraction must contain a copy of the Φ root system itself. [Let us check the H_4 case to illustrate: if Λ is H_4 symmetric and $\lambda = \{w,x,y,z\}$ is any element in Λ with $w \neq 0$, then by an H_4 transformation, $\lambda' = \{w,-x,-y,-z\}$ is also in Λ, and hence so is $\lambda + \lambda' = \{2w,0,0,0\}$, which is $2w$ times the H_4 root $\{1,0,0,0\}$. Thus, by H_4 symmetry, Λ must contain the whole H_4 root system (times $2w$).] We draw two implications from this. First, a Φ reflection (quasi)lattice has the minimal integer rank compatible with $G(\Phi)$ invariance, and is hence a $G(\Phi)$ lattice. Second, by the "geometric lemma" in [19] (which says that, if Λ has integer rank n, then any n integrally independent vectors in Λ integrally span Λ, after a suitable rescaling) it follows that any $G(\Phi)$ lattice is integrally spanned by the Φ roots, and is hence a Φ reflection (quasi)lattice.

Remark 2. Compared to the earlier approach of defining and studying the class of G lattices, our approach of defining and studying the class of reflection lattices and quasilattices has key advantages. (i) Speaking first in general terms, Definition 2 is a more elegant starting point than the definition of a G lattice, and more connected to the heart of mathematics via root lattices. (ii) In particular, the G-lattice definition relies on the awkward minimal-integer-rank condition, which is needed to exclude a host of other, less interesting, "non-minimal" or "incommensurately modulated" crystals and quasicrystals [16]. By contrast, Definition 2 has the conceptual advantage that, since it is fundamentally based on the notion of a root system, the minimal-integer-rank property is achieved *automatically*, with no need to impose this as a separate condition. (iii) Similarly, the most interesting quasicrystals and aperiodic tilings (such as the Penrose tiling) exhibit discrete scale invariance: reflection quasilattices have this property automatically, whereas G quasilattices do not. (iv) From Definition 2 and Remark 1, we infer another feature that is interesting, both mathematically and physically: a reflection (quasi)lattice is a special type of Bravais (quasi)lattice whose shape is completely "locked in" by its point group (with no tunable shape parameters, apart from overall rescaling).

V. THE REFLECTION QUASILATTICES

Reflection QLs in two dimensions. For each integer $n = 5,7,8,9\ldots$, the I_2^n root QL is the ring of cyclotomic integers $\mathbb{Z}(\zeta_n)$—i.e., the set of all integer linear combinations of the nth roots of unity ζ_n^k. (Note: when n is odd, the I_2^n and I_2^{2n} root QLs are redundant.) By the logic in [19] (see also [37,38]), all *other* I_2^n reflection QLs correspond to nontrivial ideals within $\mathbb{Z}(\zeta_n)$: finding all such ideals is an important unsolved problem in algebraic number theory, so we cannot enumerate all the I_2^n reflection QLs for general n; but for all $n < 23$, and all even $n < 46$, the only I_2^n reflection QL is the I_2^n root QL.

Reflection QLs in three dimensions. The argument in Sec. 3 of [19] implies that there are precisely three reflection QLs in 3D (all of type H_3). To describe them, first recall that the H_3 roots (1) point to the edge midpoints of a regular icosahedron. The 12 vertices of this icosahedron are then the 12 vectors obtained from $\{\pm 1, \pm\tau, 0\}$ by taking all combinations of $\pm$ signs and all even permutations of the coordinates. Now choose $v_1,\ldots,v_6$ to be six of these vectors that are integrally independent (e.g., the six vectors obtained from $\{1,\pm\tau,0\}$ by including both $\pm$ options, and all even permutations of the coordinates). The three reflection QLs (H_3^1, H_3^2, and H_3^3) consist of all linear combinations $m_1 v_1 + \cdots + m_6 v_6$, where the coefficients satisfy an appropriate restriction: for H_3^1, the coefficients m_i must be integers; for H_3^2, the coefficients m_i must be integers whose sum $m_1 + \cdots + m_6$ is even; and for H_3^3, the coefficients m_i must either be all integers ($m_i \in \mathbb{Z}$) or all half-integers ($m_i \in \mathbb{Z} + \frac{1}{2}$). We refer to these three H_3 reflection QLs as "primitive," "fcc," and "bcc," respectively, since they arise by orthogonally projecting the six-dimensional primitive cubic, fcc, or bcc lattices, respectively, on a maximally symmetric 3D subspace.

The maximal reflection QL. We next prove that there is a unique reflection QL in 4D. This is the "maximal reflection QL," maximal in terms of both dimensionality and symmetry.

First note that the only available root system for a reflection QL Λ in 4D is H_4. Every vector $\lambda \in \Lambda$ can then be written as an integer linear combination of the 120 H_4 roots, which can, in turn, be written as an integer linear combination of the eight vectors

$$\begin{array}{cccc} \{\frac{1}{2},0,0,0\}, & \{0,\frac{1}{2},0,0\}, & \{0,0,\frac{1}{2},0\}, & \{0,0,0,\frac{1}{2}\}, \\ \{\frac{\tau}{2},0,0,0\}, & \{0,\frac{\tau}{2},0,0\}, & \{0,0,\frac{\tau}{2},0\}, & \{0,0,0,\frac{\tau}{2}\}. \end{array} \quad (3)$$

So the subset of vectors in Λ that are proportional to $\{1,0,0,0\}$ can all be written in the form $(1/2)\{m + n\tau,0,0,0\}$ (with $m,n \in \mathbb{Z}$)—i.e., they are a subset of (a scaled copy of) the "golden integers" (the set of numbers $m + n\tau$ with $m,n \in \mathbb{Z}$). Now consider any such vector $\{w,0,0,0\}$. By H_4 symmetry, Λ must also also contain w times every H_4 root and, in particular, it must contain $(w/2)\{\tau,1/\tau,1,0\}$ and $(w/2)\{\tau,-1/\tau,-1,0\}$ as well as their sum $\tau\{w,0,0,0\}$. Hence we can apply the "algebraic lemma" proved in [18] (which says that any subset of the golden integers that is closed under addition and subtraction and scaling by τ must be a scaled copy of the golden integers) to infer that the subset of vectors in Λ that are proportional to $\{1,0,0,0\}$ are a scaled copy of the golden integers. Let us rescale the QL so that the vectors proportional to $\{1,0,0,0\}$ are precisely the set of all golden integers times $\{1,0,0,0\}$ (and, by symmetry, the vectors proportional to any root are precisely the set of all golden integers times that root). So Λ *must* contain all the golden integers times each H_4 root, and all integer linear combinations of such vectors. We will next show that it cannot contain anything else.

To see this, first recall that if Λ contains a vector $\lambda = \{w,x,y,z\}$, it also contains the vector $\{2w,0,0,0\}$; and, by a similar argument, it also contains the vectors $\{0,2x,0,0\}$, $\{0,0,2y,0\}$, and $\{0,0,0,2z\}$. Since $2w$, $2x$, $2y$, and $2z$ must all be golden integers, it follows that any vector $\lambda \in \Lambda$ must have the form

$$\lambda = (1/2)\{m_0 + n_0\tau, m_1 + n_1\tau, m_2 + n_2\tau, m_3 + n_3\tau\} \quad (4)$$

(with $m_i,n_i \in \mathbb{Z}$). But if we apply any H_4 transformation to λ, the requirement that the new vector λ' must also have this form (with new integers m_i',n_i') restricts the possible values of the integers m_i and n_i. It is enough to consider the transformation $\lambda' = \lambda q$ where q is any unit icosian (2); in this way we obtain the constraints

$$\begin{aligned} m_\alpha + m_\beta + m_\gamma + m_\delta &= \text{even}, \\ n_\alpha + n_\beta + n_\gamma + n_\delta &= \text{even}, \\ m_\alpha + n_\alpha + m_\beta + n_\gamma &= \text{even}, \end{aligned} \quad (5)$$

where the indices $\{\alpha,\beta,\gamma,\delta\}$ are any even permutation of $\{0,1,2,3\}$. In considering which combinations of m_i and n_i are allowed, it is also enough to consider m_i and n_i to be valued mod 2, since we already know that Λ contains all golden integers times the four Cartesian unit vectors, so if it contains the combination $\{m_0,m_1,m_2,m_3,n_0,n_1,n_2,n_3\}$, it also contains the combination where one or more of these integers is shifted by ± 2. Thus, we can simply enumerate all 16 allowed vectors (4) satisfying the constraints (5): namely, $\{0,0,0,0\}$, $\frac{1}{2}\{1,1,1,1\}$, $\frac{1}{2}\{\tau,\tau,\tau,\tau\}$, $\frac{1}{2}\{1+\tau,1+\tau,1+\tau,1+\tau\}$, and all even permutations of $\frac{1}{2}\{0,1+\tau,\tau,1\}$. But each of these vectors is a golden integer times a root, which we already proved *had* to be in Λ.

Thus, an H_4 reflection QL must contain all integer linear combinations of the H_4 roots, and nothing else—this completes the proof that it is unique (and is none other than the H_4 root QL). This corresponds to the ring of quaternions known as the icosians, which may be obtained by orthogonally projecting the E_8 root lattice on a maximally symmetric 4D subspace [6,27]. In fact, our geometric proof turns out to be ultimately equivalent to the number-theoretic result that every left ideal in the icosians is principal [13,32–35].

TABLE I. All reflection quasilattices ("reflection QLs") in dimension $d > 2$, and all *quadratic* reflection QLs (i.e., reflection QLs with scale factor given by a quadratic irrational) in $d = 2$. Here $\tau \equiv \frac{1}{2}(1+\sqrt{5})$ is the golden ratio. The reflection QLs that are also root quasilattices are labeled "root," while the descriptions "primitive/fcc/bcc" are explained in the text.

Reflection quasilattice	Description	Scale factor
I_2^5/I_2^{10}	root	τ
I_2^8	root	$1+\sqrt{2}$
I_2^{12}	root	$2+\sqrt{3}$
H_3^1	primitive	τ^3
H_3^2	fcc (root)	τ
H_3^3	bcc	τ
H_4	root	τ

VI. DISCRETE SCALE INVARIANCE

Unlike an ordinary lattice, which has no scale invariance, each reflection QL has discrete scale invariance—it is exactly invariant under rescaling by any integer power of one or more "scale factors." Just as we cannot enumerate all the reflection QLs in 2D, we cannot enumerate all of their scale factors in 2D—but we *can* say that the scale factors for the I_2^n reflection QLs will be irrationals of order $\phi(n)/2$ [37], where Euler's totient function $\phi(n)$ is the number of positive integers less than n (including 1) that share no common factor with n; and also that a *subset* of the scale factors for the I_2^n *root* QL will be given by elementary expressions called the real cyclotomic units [37].

An important set of 2D reflection QLs are the three cases with $\phi(n)/2 = 2$: I_2^5/I_2^{10}, I_2^8, and I_2^{12}. For these three 2D reflection QLs, and for the 3D H_3 and 4D H_4 reflection QLs, the scale factors are quadratic irrationals. Following similar reasoning to that in [13,15,16], the complete set of possible scale factors can be derived explicitly by the following argument. If a QL is invariant under rescaling by η, then any 1D sublattice must also be invariant under the same rescaling. In other words, the scaling group of the QL must be a subgroup of the scaling group of its 1D sublattice. Each of the I_2^5/I_2^{10}, I_2^8, I_2^{12}, H_3, and H_4 reflection QLs contain a 1D sublattice corresponding to a ring of real quadratic integers $\mathbb{Z}(\sqrt{\kappa})$: I_2^5/I_2^{10}, H_3, and H_4 contain $\mathbb{Z}(\sqrt{5})$, I_2^8 contains $\mathbb{Z}(\sqrt{2})$, and I_2^{12} contains $\mathbb{Z}(\sqrt{3})$. But the scale factors of $\mathbb{Z}(\sqrt{\kappa})$ (where κ is a positive square-free integer) are precisely $\pm u^k$ where k is any integer and the "fundamental unit" u is given by $(a+b\sqrt{\Delta})/2$ where a and b are the smallest positive integer solutions of $a^2 - \Delta b^2 = \pm 4$ and Δ is the discriminant of $\mathbb{Q}(\kappa)$ ($\Delta = \kappa$ if $\kappa = 1 \bmod 4$, and $\Delta = 4\kappa$ if $\kappa = 2$ or $3 \bmod 4$) [39]. So, for $\mathbb{Z}(\sqrt{5})$, $\mathbb{Z}(\sqrt{2})$, and $\mathbb{Z}(\sqrt{3})$, the fundamental units are $\tau = \frac{1}{2}(1+\sqrt{5})$ (the golden ratio), $1+\sqrt{2}$ (the silver ratio), and $2+\sqrt{3}$, respectively. We then check that the reflection QL is symmetric under the full scaling group $\pm u^k$ of its 1D sublattice, except for H_3^1 which is invariant under the subgroup $\pm(u^3)^k$.

Table I summarizes our results.

VII. DISCUSSION

We conclude by mentioning a few directions for future work. First, we note that the crystallographic root lattices are among the most important lattices in mathematics, playing a key role in the study of Lie algebras, Lie groups, representation theory, quivers, catastrophes, singularity theory, and other contexts [6,40–43]. As generalizations, the root QLs and reflection QLs may lead to some extensions of these applications. Second, as will be detailed in a forthcoming paper [17], there is a direct relationship between reflection QLs and tessellations that have the matching-rule, inflation-rule, and Ammann-grid properties of Penrose tilings. Given our proof here that there are only a handful of reflection QLs in dimension $d > 2$, we can determine the complete set of irreducible Penrose-like tilings in $d > 2$. Finally, on a more speculative level, it is natural to notice that the maximal reflection QL—a very distinctive and beautiful object—exists in 4D, which is also the apparent dimension of space-time: it is interesting to consider the connections to fundamental physics, or to novel discretization schemes for Euclideanized 4D field theory.

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