Bravais Quasilattices of Icosahedral Quasicrystals

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A classification of icosahedral quasicrystals based the mutual-local-derivability (MLD) concept is performed. There are *eighteen MLD classes* within the reservation that the faces of the hyperatoms (windows) are perpendicular to the two-, three-, or fivefold axes. Each MLD class has a representative member to be called the *Bravais quasilattice* from which the structure of each member of the class is derived by decorating it according to a local rule depending on the member.

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The discovery of a quasicrystal in 1984 has introduced a new era in the study of crystallography [1]. It was found soon that quasicrystals as well as the Penrose patterns can be represented as sections of "higher-dimensional crystals" [2–4]. Later, Baake and his collaborators [5,6] proposed a classification scheme of quasicrystals by means of a new concept, namely, mutual local derivability (MLD). The present author proposed in a previous paper [7] an MLD classification of two-dimensional (2D) quasicrystals. However, the theory is incomplete for octagonal quasicrystals on account of a special property of the relevant 4D Bravais lattice. This prevents us from applying the theory to icosahedral quasicrystals of P or F type. The method is improved in this Letter, and applied to an MLD classification of icosahedral quasicrystals. This provides us with a firm basis for modeling structures of quasicrystals.

The quasicrystal has a long-range positional order with a noncrystallographic point symmetry (for a review, see Ref. [8]). The positions of atoms in it form a quasilattice (QL), which is a quasiperiodic set of points. Generally, a QL is given as a section of a *hypercrystal* through the physical space, $E_{\rm phys}$, as illustrated in Fig. 1 for the case of a 1D QL, namely, the Fibonacci lattice. The hypercrystal is a periodic structure in a *hyperspace*, $E_{\rm hyper}$, whose dimension, D, is twice the dimension d of $E_{\rm phys}$: $D = 2d$. Specifically, $d = 3$ and $D = 6$ for icosahedral QLs. The hyperspace is divided into the parallel space $E_\parallel$ and its orthogonal complement, $E_\perp$, the *perp space* with equal dimension, i.e., d. $E_\parallel$ is a simple translate of the physical space, and the translation vector combining $E_\parallel$ to $E_{\rm phys}$ is called the *phase*. The hypercrystal is composed of *hyperatoms* (or "atomic surfaces") which only extend along $E_\perp$. More precisely, the extension of the hyperatom in $E_\perp$ is given by an interval, a polygon or a polyhedron if $d = 1$, 2, or 3, respectively. QLs with different phases are not always congruent geometrically although they are indistinguishable macroscopically. They form a so-called locally isomorphic (LI) class [2]. Thus, every LI class of QLs is specified by the relevant hypercrystal. Remember that a phason shift, i.e., a small change of the phase, gives rise to disappearance of a part of the lattice points of a QL and appearance of new lattice points.

The translational symmetry of a hypercrystal is specified by a Bravais hyperlattice $\mathcal{L}$. A simple hypercrystal has only one hyperatom per one unit cell of $\mathcal{L}$. There exist three types of Bravais hyperlattices with the icosahedral symmetry, namely, primitive ($\mathcal{L}_P$), face-centered ($\mathcal{L}_F$), and body-centered types ($\mathcal{L}_I$) [9], whose properties are summarized in Ref. [10] and reproduced partially below; relations among them are similar to those among the three cubic Bravais lattices in 3D. We can assume $\mathcal{L}_P$ to be a 6D simple hypercubic lattice, whose lattice vectors are indexed by the standard basis vectors, ε_i, $i = 1-6$. $\mathcal{L}_P$ is divided into two equivalent sublattices being nested with each other: $\mathcal{L}_P = \mathcal{L}_F \cup (\mathbf{x}_1 + \mathcal{L}_F)$ with $\mathbf{x}_1 := [100000] (= \varepsilon_1)$ [11]. Similarly, $\mathcal{L}_{\rm I}$ is divided as $\mathcal{L}_{\rm I} = \mathcal{L}_P \cup (\mathbf{x}_2 + \mathcal{L}_P)$ with $\mathbf{x}_2 := \frac{1}{2}[111111]$ pointing a body-centered site of $\mathcal{L}_P$. Consequently, we may write

$$\mathcal{L}_I = \mathcal{L}_F \cup (\mathbf{x}_1 + \mathcal{L}_F) \cup (\mathbf{x}_2 + \mathcal{L}_F) \cup (\mathbf{x}_3 + \mathcal{L}_F), \quad (1)$$

with $\mathbf{x}_3 := \frac{1}{2}[\bar{1}11111]$. That is, $\mathcal{L}_I$ is the *double* (respectively *quadruple*) *lattice* of $\mathcal{L}_P$ (respectively $\mathcal{L}_F$). The common 6D point group, $\tilde{Y}_H$, of the three icosahedral hyperlattices acts separately onto the two subspaces, $E_\parallel$

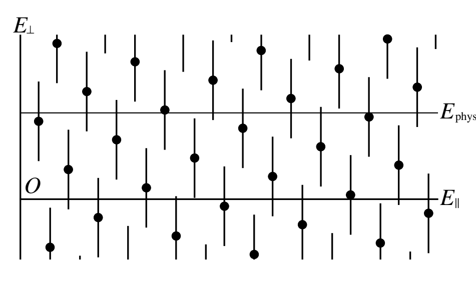

FIG. 1. The Fibonacci lattice is obtained as a section of a 2D hypercrystal but is displaced at the margin. The relevant 2D "hyperlattice," $\mathcal{L}_2$, is generated by the basis vectors, $\varepsilon_1 = a(1, -\tau)$ and $\varepsilon_2 = a(\tau, 1)$ with $\tau := (1 + \sqrt{5})/2$ being the golden ratio. The hyperatoms are vertical bars, whose lengths are equal to $a(1 + \tau)$.

and $E_\perp$, as 3D point groups which are isomorphic with the icosahedral point group, Y_h. Y_h has three types of symmetry axes, Δ, Λ, and Σ, which refer, respectively, to the five-, three- and twofold axes of an icosahedron. The projections of $\pm\varepsilon_i$ onto $E_\parallel$ (respectively $E_\perp$) form a full set of the 12 vertex vectors of a regular icosahedron in $E_\parallel$ (respectively $E_\perp$). It follows that $E_\parallel$ (respectively $E_\perp$) is maximally incommensurate with every icosahedral hyperlattice, $\mathcal{L}$, and the projection, $\mathcal{L}_\parallel$ (respectively $\mathcal{L}_\perp$), of $\mathcal{L}$ onto $E_\parallel$ (respectively $E_\perp$) is a 6D $\mathbf{Z}$ module (an additive group). The two modules, $\mathcal{L}_\parallel$ and $\mathcal{L}_\perp$, has a scaling symmetry as $\tau\mathcal{L}_\parallel = \mathcal{L}_\parallel$ and $\bar{\tau}\mathcal{L}_\perp = \mathcal{L}_\perp$ provided that $\mathcal{L}$ is $\mathcal{L}_F$ or $\mathcal{L}_I$, where $\tau := (1+\sqrt{5})/2$ is the golden ratio and $\bar{\tau}\,[= (1-\sqrt{5})/2 = -1/\tau]$ is its algebraic conjugate. Therefore, the two hyperlattices, $\mathcal{L}_F$ and $\mathcal{L}_I$, are left invariant against a *hyperscaling transformation*, T, which scales $E_\parallel$ and $E_\perp$ by τ and $\bar{\tau}$, respectively. Of the four equivalent sublattices to which $\mathcal{L}_I$ is divided as given by Eq. (1), only the sublattice $\mathcal{L}_F$ is left invariant against T but other three are permuted cyclically by T. $\mathcal{L}_P$ has also a hyperscaling symmetry but T (or τ) above must be replaced by T^3 (or τ^3). Incidentally, the 2D version of T applies to the 2D hyperlattice, $\mathcal{L}_2$, in Fig. 1 because $T\varepsilon_1 = \varepsilon_2$ and $T\varepsilon_2 = \varepsilon_1 + \varepsilon_2$. The space group (exactly, superspace group) of $\mathcal{L}$ acts onto E_{hyper}, and every lattice point of $\mathcal{L}$ is a full symmetry point with the point symmetry $\tilde{Y}_h$. For the case of the two hyperlattices, $\mathcal{L}_P$ and $\mathcal{L}_F$, however, there are other types of full symmetry points than their lattice points: a body-centered site of $\mathcal{L}_P$, for example, is so. The *augmented lattice* of $\mathcal{L}$ is defined by the set, $\hat{\mathcal{L}}$, of all the full symmetry points in E_{hyper}. It can be shown that $\hat{\mathcal{L}} = \mathcal{L}_I$ for all the three cases, $\mathcal{L} = \mathcal{L}_P$, $\mathcal{L}_F$ and $\mathcal{L}_I$. It is essential in our theory to distinguish the two lattices $\mathcal{L}$ and $\hat{\mathcal{L}}$, which are identical only for $\mathcal{L}_I$ [12].

For the 2D hyperlattice, $\mathcal{L}_2$, we obtain $\mathcal{L}_\perp = a\mathbf{Z}[\tau]$ with $\mathbf{Z}[\tau] := \{p + q\tau \mid p,\ q \in \mathbf{Z}\}$ being a 2D $\mathbf{Z}$ module. The 6D $\mathbf{Z}$ module $\mathcal{L}_\perp$ of an icosahedral hyperlattice $\mathcal{L}$ yields a similar 2D module, $\mathcal{M}$, if it is projected onto a symmetry axis of Y_h in $E_\perp$ [4]. We shall call $\mathcal{M}$ the *projection module*, which plays an important role in a later argument. The three types of icosahedral hyperlattices and the three types of the symmetry axes yield nine types of projection modules, which are denoted as P_Δ, F_Δ, F_Λ, etc. Investigating the nine cases separately, we can conclude that $\mathcal{M}$ assumes $a\mathbf{Z}[\tau^3]$ for P_Δ and P_Λ but $a\mathbf{Z}[\tau]$ otherwise, where a is a constant depending on the type of the projection module [13]. $\mathcal{M}$ is a submodule of the *extended module*, $\hat{\mathcal{M}}$, which is the relevant projection module of the augmented lattice $\hat{\mathcal{L}}$ $(= \mathcal{L}_I)$. We may write $\hat{\mathcal{M}} = \hat{a}\mathbf{Z}[\tau]$, where $\hat{a} = a/2$ for F_Δ and F_Λ but $\hat{a} = a$ for the remaining seven cases.

There are three types of symmetry-adapted polyhedrons as shown in Fig. 2, namely, a regular dodecahedron, a regular icosahedron and a rhombic triacontahedron. The faces of them are normal to the symmetry axes of the types, Δ, Λ, and Σ, respectively, so that faces of different polyhedrons are *never parallel*. The size parameter ξ of such a polyhedron is defined by the distance between a pair of parallel faces. If hyperatoms with the shape of such a polyhedron are located on the lattice points of an icosahedral Bravais hyperlattice, we obtain an important icosahedral hypercrystal (or the relevant QL), whose space group is symmorphic and its point group is $\tilde{Y}_h$. Varying ξ, we obtain a continuous series of hypercrystals (or QLs), which form a *species*. There are nine species corresponding to the nine types of projection modules, and we may denote the former nine by the same symbols as those for the latter. We shall restrict the present MLD classification to hypercrystals belonging to these species. An icosahedral QL has a set of parallel *quasilattice planes* [4] (QLPs) so that all its lattice points are located dividedly on them, the 2D versions of which are quasilattice lines as shown in Fig. 3. The arrangement of the QLPs defines a 1D QL, the projection QL [4]. A QLP is called *proper* if it is

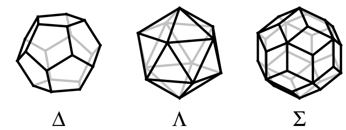

FIG. 2. Three types of symmetry-adapted polyhedrons.

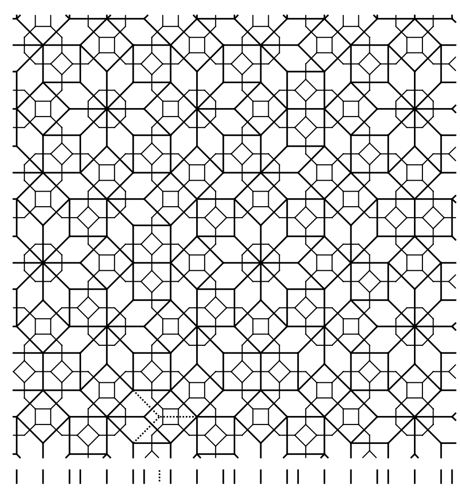

FIG. 3. The two 2D octagonal QLs superimposed in this figure are derived from a 4D hypercubic lattice. The lattice points of each QL are located on the vertices of the network distinguished by the line thickness. They are located dividedly on vertical quasilattice lines: the arrangement of the quasilattice lines of the thick QL produces a 1D QL shown as the array of bars at the bottom. A phason shift easily makes the seventh quasilattice line jump to the right as indicated by the dotted lines. This figure mimics well various things realized in icosahedral QLs.

normal to a relevant symmetry axis to the species of the QL. Also, a projection QL is called *proper* if so are the relevant QLPs. From a thermodynamical reason, we can restrict our consideration to the QLs (or hypercrystals) satisfying the so-called the *gluing condition* (or, equivalently, the closeness condition) [14], which demands that lattice points (atoms) must not disappear under a phason shift but only jump a finite distance. In fact, all the lattice points on a proper QLP jump simultaneously to form a new QLP (see Fig. 3). That is, a 2D or 3D QL satisfies the gluing condition if and only if its proper projection QL satisfies the gluing condition as a 1D QL. A hyperatom of a 1D QL (or the relevant 2D hypercrystal), for example, can be "glued" with another if the top end of the former is on the same level as the bottom end of the latter. Inspecting Fig. 1 we see that the Fibonacci lattice satisfies the gluing condition. Generally, the gluing condition is satisfied by a 2D or 3D QL if and only if the size parameter ξ of the hyperatom belongs to the relevant projection module $\mathcal{M}$. We will represent hereafter ξ in unit of the "lattice constant" a of $\mathcal{M}$, so that $\xi \in \mathbf{Z}[\tau]$ or $\mathbf{Z}[\tau^3]$. Each hypercrystal in a single species is specified by a positive number in the countable set $\mathbf{Z}[\tau]$ or $\mathbf{Z}[\tau^3]$.

Two QLs are MLD (mutually locally derivable) [5,6] if and only if there exists a local rule such that the position of each lattice point of one of them is determined by the relevant local structure of the other and vice versa. For example, the two 2D octagonal QLs in Fig. 3 are MLD, and we can easily identify a local rule by which one of the two is derived from the other. Exactly speaking, the MLD relationship is a relationship between two LI classes rather than two QLs, so that it is a relationship between the relevant two hypercrystals. The set of all the hypercrystals with a common hyperlattice is divided into MLD classes. MLD classifications were made quite recently for low-dimensional QLs in Refs. [7,15]. We assume naturally that two QLs being MLD have common local centers of symmetries [5–7] as is the case for the two QLs in Fig. 3. Then, the hyperlattices of the two hypercrystals coincide or assume two sublattices of the relevant augmented lattice as illustrated in Fig. 4. That is, two hypercrystals can be MLD with each other in the coincident configuration or the nesting configuration; the latter configuration is possible only when $\mathcal{L} \neq \hat{\mathcal{L}}$. Since two hypercrystals belonging to different species are never MLD [7], the problem is reduced to the MLD classification of hypercrystals belonging to each of the nine species.

A necessary and sufficient condition for two QLs (or hypercrystals) to be MLD is that they satisfy the *intergluing condition*: a jump, originating from a phason shift, of a proper QLP of one QL always accompanies a similar jump in the other (cf. Figs. 3 and 4). The marker in dashed line in Fig. 4 shows that the 2D hypercrystals (a) and (b) are glued with each other in the coincident configuration, while they are glued with (c) in the nesting configuration.

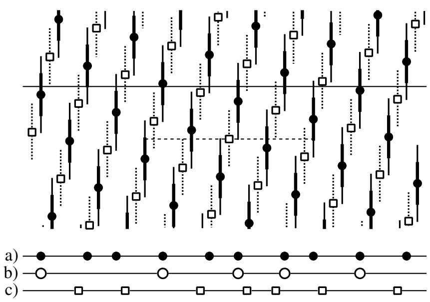

FIG. 4. In this figure are superimposed three 2D hypercrystals on the same 2D "hyperlattice," $\mathcal{L}_2$, as in Fig. 1. The three types of hyperatoms are vertical lines, whose lengths are (a) $1 + \tau$ (thin); (b) $3 - \tau$ (thick); and (c) two (dotted) in unit of $a = 1$. The hyperatoms are located on the lattice points of $\mathcal{L}_2$ for the hypercrystals (a) and (b) but on the centers of square unit cells for (c). The former two of the three hypercrystals are in the coincident configuration, while they are in the nesting configuration with the last.

The intergluing condition for two hypercrystals is formulated generally as $\frac{1}{2}\xi + \frac{1}{2}\xi' \in \hat{\mathcal{M}}$, where ξ and ξ' are the size parameters of the two hyperatoms. Hereafter, we need to discuss separately the two cases: $\hat{a} = 1/2$ and $\hat{a} = 1$ (with $a = 1$), the former of which applies to F_Δ and F_Λ but the latter to the remaining seven cases. For $\hat{a} = 1/2$ we obtain $\hat{\mathcal{M}} = \mathbf{Z}[\tau]/2$, and $\xi + \xi' \in \mathbf{Z}[\tau]$. This condition is trivially satisfied, so that all the hypercrystals of each of the two species form a single MLD class. For this case, we can choose $1 \in \mathcal{M}$ as the representative member of $\mathcal{M}$. For $\hat{a} = 1$, however, the intergluing condition is written as $\xi + \xi' \in 2\mathbf{Z}[\tau]$, so that ξ and ξ' need to have a common "parity" with respect to $\mathbf{Z}[\tau]$. $\mathcal{M}$ can be divided into several *residue classes* with respect to parities [15]; each residue class is an infinite set of numbers of the form $\xi + 2\nu$ with ξ being a representative of the class and $\nu \in \mathbf{Z}[\tau]$. The number of the residue classes is four (respectively two) if $\mathcal{M} = \mathbf{Z}[\tau]$ (respectively $\mathcal{M} = \mathbf{Z}[\tau^3]$), and the representatives of the four (respectively two) can be chosen to be 2, 1, τ, and $\tau^2\,(= 1 + \tau)$ (respectively two and one) [16]. Each residue class yields one MLD class for each of the three species, P_Δ, P_Λ, and

TABLE I. The 18 MLD classes are grouped into four. The number of MLD classes in each group is equal to the product of the number of species listed in the fourth column and that of the residue classes whose representatives, ξ, are listed in the fifth column. However, the three odd residue classes being braced must be counted once in total.

Case	$\mathcal{M}$	$\hat{\mathcal{M}}$	Species	Odd ξ	Even ξ	Number
I	$\mathbf{Z}[\tau]$	$\frac{1}{2}\mathbf{Z}[\tau]$	F_Δ, F_Λ	1		$2 \times 1 = 2$
II	$\mathbf{Z}[\tau]$	$\mathbf{Z}[\tau]$	F_Σ, I_Δ, I_Λ, I_Σ	$\{1, \tau, \tau^2\}$	2	$4 \times 2 = 8$
III	$\mathbf{Z}[\tau]$	$\mathbf{Z}[\tau]$	P_Σ	$1, \tau, \tau^2$	2	$1 \times 4 = 4$
IV	$\mathbf{Z}[\tau^3]$	$\mathbf{Z}[\tau]$	P_Δ, P_Λ	1	2	$2 \times 2 = 4$

P_Σ, and the number of the MLD classes derived from $\mathcal{L}_P$ is eight in total. However, the situation is different for the four species, F_Σ, I_Δ, I_Λ, and I_Σ, because the two hyperlattices, $\mathcal{L}_F$ and $\mathcal{L}_I$, have a hyperscaling symmetry with the transformation, T [16]. As a consequence, the relevant three MLD classes for the odd residue classes are merged into a single scaling MLD class [7,15], and the number of the MLD classes derived from $\mathcal{L}_F$ (respectively $\mathcal{L}_I$) is four (respectively six) in total. Thus, there are altogether 18 MLD classes of icosahedral QLs. This completes an MLD classification of icosahedral QLs, which is summarized in Table I. A key point of the present formalism is that two hypercrystals can be MLD with each other in the nesting configuration if $\mathcal{L} \neq \hat{\mathcal{L}}$.

A representative member of each MLD class of icosahedral QLs is chosen to be the one with hyperatoms whose size parameter ξ is equal to a number listed in Table I. We may call it a *Bravais quasilattice* because the structure of every quasicrystal being MLD with it is, by the very definition of the MLD relationship, represented as its decoration with *a local rule*. For example, the union of the two QLs in Fig. 3 can be regarded as a 2D "quasicrystal" derived from the Bravais quasilattice (the thick one). Each type of the decorated atoms of icosahedral quasicrystals considered here has its own hyperatom, whose faces are *parallel* to those of the relevant symmetry-adapted polyhedron [8]. This together with the self-guing condition are restrictions, though not serious, of the present theory. From the group-theoretical point of view, it is the Bravais hyperlattice that is the counterpart of the Bravais QL in the classical crystallography, and *the Bravais QL is a new concept with no classical counterparts.* It has been shown by this Letter that the three icosahedral Bravais hyperlattices listed in Ref. [9] are divided into 18 MLD classes. Thus, the MLD classification of quasicrystals is more refined than the conventional classification based on the Bravais hyperlattices. We expect that the present work will contribute greatly to building new or better models for known quasicrystals and new quasicrystals to be found in the future.

Finally, we add MLD classifications of several icosahedral tilings among those listed in Ref. [17]. The tilings $\mathcal{T}^{(P)}$, $\mathcal{T}^{*(2F)}$, and $\mathcal{T}^{*(I)}$ in the notation of this reference belong to $P_\Sigma(2)$, $F_\Sigma(2)$, and $I_\Delta(1)$, respectively, while $\mathcal{T}^{(D)}$ and $\mathcal{T}^{(SS)}$ belong both to $F_\Delta(1)$. However, $\mathcal{T}^{(2F)}$ is out of our classification scheme because it is composed of subquasilattices belonging to different species; more precisely, one subquasilattice belongs to $F_\Delta(1)$ but the remaining two to $F_\Sigma(1)$. On the other hand, the two famous models of icosahedral quasicrystals, namely, Yamomoto and Katz-Gratias models, belong both to $F_\Sigma(2)$.

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[12] Of the 4D hyperlattices of the octagonal, decagonal and dodecagonal QLs in 2D, only the octagonal case satisfies $\mathcal{L} \neq \hat{\mathcal{L}}$. Specifically, $\hat{\mathcal{L}} = \mathcal{L} \cup (\mathbf{x} + \mathcal{L})$ with $\mathbf{x}$ being a 4D vector pointing a body-centered site of $\mathcal{L}$, which is a hypercubic lattice in 4D. For this point, see K. Niizeki, J. Phys. A **22**, 4281 (1989).
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$$\mathbf{Z}[\tau] = (2\mathbf{Z}[\tau]) \cup (1 + 2\mathbf{Z}[\tau]) \cup (\tau + 2\mathbf{Z}[\tau]) \cup (\tau^2 + 2\mathbf{Z}[\tau]), \mathbf{Z}[\tau^3] = (2\mathbf{Z}[\tau]) \cup (1 + 2\mathbf{Z}[\tau]).$$

The first equality is equivalent to a relationship which is derived from the equality

$$\mathcal{L}_\mathrm{I} = \mathcal{L}_\mathrm{F} \cup (\mathbf{x}_1 + \mathcal{L}_\mathrm{F}) \cup (\mathbf{x}_2 + \mathcal{L}_\mathrm{F}) \cup (\mathbf{x}_3 + \mathcal{L}_\mathrm{F})$$

by projecting it onto a symmetry axis Δ in $E_\perp$ or $E_\parallel$, while the second equality is derived from the equality $\tau^3 = 1 + 2\tau$. The module, $\mathbf{Z}[\tau]$, has the scaling symmetry, $\tau\mathbf{Z}[\tau] = \mathbf{Z}[\tau]$ but the three odd residue classes of $\mathbf{Z}[\tau]$ are permuted cyclically on the scaling.
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