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A classification of the space groups of approximant lattices to a decagonal quasilattice

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Abstract. A periodic approximant to a two-dimensional (2D) decagonal quasilattice is obtained by the projection method from a 4D periodic lattice, \tilde{L} , which is a commensurate deformation of the 4D decagonal lattice. The Bravais lattice of the approximant is given by the restriction of \tilde{L} onto the physical space, while its space group by the symmetry of the phase vector with respect to the 2D lattice, L_s , which is the projection of \tilde{L} onto the internal space. There exist 12 space groups of the rectangular approximants, pmm, pmg, pgm, pgg, pml, p1m, pgl, p1g, cmm(Γ), cmm(Υ), cm1 and c1m, which are derived from the special points or special lines of L_s .

1. Introduction

Approximant crystals to a quasicrystal are of current interest (see, for example, Spaepen *et al* 1990, Zhang and Kuo 1990). The structure of a quasicrystal is described with a quasilattice, which is obtained by the cut-and-projection method from a periodic lattice L in higher dimensions (Janssen 1988). Similarly, the structure of an approximant crystal is described with an approximant lattice (AL), which is obtained by the same method from a deformed lattice \tilde{L} of L ; the deformation is made so that \tilde{L} is fully commensurate with the physical space (Elser and Henley 1985, Henley 1985, Ishii 1989, Niizeki 1991b, c).

The quasicrystal and the relevant quasilattice have a non-crystallographic point symmetry and their approximants have crystallographic ones, which are subgroups of the former (Ishii 1989). The Bravais class to which an AL belongs is determined by \tilde{L} (Niizeki 1991b). A classification of Bravais classes of ALs to the icosahedral quasilattice has been completed (Niizeki 1991b, c). A similar classification for the case of the two-dimensional (2D) decagonal quasilattice is given by Zhang and Kuo (1990).

We shall develop in this paper a theory of the space groups of the ALs. Our theory is applicable to the case of any quasilattice. However, we present it by applying it to the case of the decagonal quasilattice because an abstract theory would burden the readers.

In section 2, we shall summarize the properties of the 2D decagonal quasilattice and the 4D decagonal lattice which yields that quasilattice. We apply in section 3 a rectangular deformation on the decagonal lattice and investigate 2D lattices which are obtained as a section and a projection of the deformed lattice. Special points and other special manifolds of the 2D lattices and the 4D ones are investigated in section 4. The space group of a shifted physical space relative to \tilde{L} is investigated in section 5 and the special manifolds associated with the space group are in section 6. The space

groups of the ALs to the decagonal quasilattice are classified completely in section 7. We discuss in section 8 several other subjects concerning the approximants to a quasilattice. The subject of section 6 precedes that of section 7 from the logical point of view but one may understand more easily the former if it is read after the latter.

In this paper, a vector is always treated as a column vector but its components are shown as a row vector.

2. The 2D decagonal quasilattice and the 4D decagonal lattice

The 4D Euclidean space E_4 into which the 4D decagonal lattice L is embedded is divided into the physical space E_2 and the internal space E'_2 ; $E_4 = E_2 \oplus E'_2$. Five 4D vectors ε_i , $i = 0-4$, are defined by $\varepsilon_i = (e_i, e'_i)$, where $e_i = [\cos(i\theta), \sin(i\theta)] \in E_2$ and $e'_i = [\cos(2i\theta), \sin(2i\theta)] \in E'_2$ with $\theta = 2\pi/5$. They satisfy $\varepsilon_0 + \varepsilon_1 + \dots + \varepsilon_4 = 0$. ε_i fix Cartesian coordinate systems of E_2 , E'_2 and E_4 . Only four of the ε_i are linearly independent and generate L . We take ε_i , $i = 1-4$, as the basis vectors of L ; $L = \{\Sigma_i n_i \varepsilon_i | n_i \in \mathbb{Z}\}$ (cf Niizeki 1989a). The volume of a unit cell of L is given by $\det(\varepsilon_1 \varepsilon_2 \varepsilon_3 \varepsilon_4) = 5\sqrt{5}/4$. Since L is a Bravais lattice, it forms an additive group (\mathbb{Z} -module), which represents the translational symmetry of L . We shall identify L with the additive group.

Let L_p (or L'_p) be the projection of L onto E_2 (or E'_2). Then it is a \mathbb{Z} -module generated by e_i (or e'_i), $i = 1-4$, which are linearly independent over \mathbb{Z} , the integral domain of integers. L_p (or L'_p) is a dense set and called a pre-quasilattice. There exists a natural bijection between any pair of L , L_p and L'_p (Katz and Duneau 1986). A lattice vector l of L_p and its associate l' of L'_p form a lattice vector (l, l') of L .

The ten vectors, $\pm e_i$, $i = 0-4$, are the vertex vectors of the unit regular decagon in E_2 and are permuted among themselves by $10\text{ mm } (D_{10})$, the point group of the decagon. Therefore, L_p is invariant against $G = 10\text{ mm}$. In fact, L_p is invariant against the quasi-space group (Niizeki 1991a), $g_p = \{\{\sigma | l\} | \sigma \in G, l \in L_p\} \cong G * L_p$, where $*$ stands for the semi-direct product and the Seitz notation has been used. G can be lifted to a 4D point group which represents the point symmetry of L . G and its lifted version are isomorphic to each other and are identified. Then G acts also on E'_2 . Note, however, that the rotation through $2\pi/5$ of E_2 , for example, is changed to the rotation through $4\pi/5$ of E'_2 .

A decagonal quasilattice is the set of points as given by

$$Q = \{l | l \in L_p, l' \in \phi + W\} \quad (1)$$

where ϕ ($\in E'_2$) is the phase vector, l' the associate of l and W ($\subset E'_2$) the window. We assume that W is a polygonal domain which is invariant against G . Then, Q has G as its macroscopic point group. The local isomorphism class of $Q = Q(\phi, W)$ is determined by W but independent of ϕ .

Let $\Pi(\phi) \equiv \phi + E_2$ ($= \{\phi + x | x \in E_2\}$) be a shifted physical space and $\Sigma(\phi, W) \equiv \Pi(\phi) + W$ be a strip. Then Q is formed of the projections onto E_2 of the lattice points of L in $\Sigma(\phi, W)$.

A representative choice for W is the unit decagon in E'_2 , whose vertex vectors are given by $\pm e'_i$, $i = 0-4$. Then Q is given by the set of the vertex vectors of the Penrose tiling with pentagonal tiles, which is shown in figure 1 (Niizeki 1989a, b).

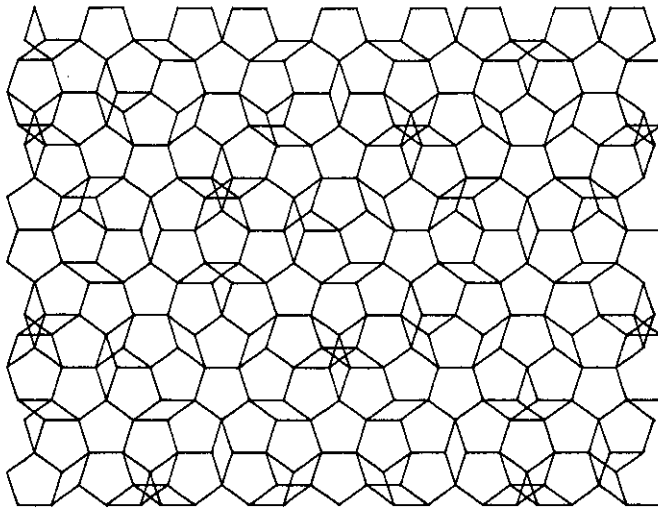


Figure 1. The decagonal quasilattice obtained from the 4D decagonal lattice L by using a window of the unit decagon. The lattice points are given by the positions of the vertices of the decagonal Penrose tiling with the pentagonal tiles. The centres of stars (or pentagons) are derived from the special points of type P' (or P) of L , while the middle points of the bonds (or the centres of the skinny rhombi) from those of type X (or C) of L .

3. Approximant lattices to the 4D decagonal lattice

$D_{10}(10\text{ mm})$ has two kinds of mirrors, representatives of which are the horizontal and the vertical mirrors. Two lattice vectors e_0 and $e_1 + e_4$ are parallel to the horizontal axis and are related by $e_0 - \tau(e_1 + e_4) = 0$ with $\tau = (1 + \sqrt{5})/2$. This linear relationship (LR) is equivalent to $-\tau(e_1 + e_4) - (e_2 + e_3)/\tau = 0$ because $e_0 + e_1 + \dots + e_4 = 0$. Similarly, an LR along the vertical direction is given by $(e_1 - e_4) - \tau(e_2 - e_3) = 0$. e'_i satisfy similar LRs to those for e_i but τ is replaced by its algebraic conjugate $\tau' = (1 - \sqrt{5})/2$ ($= -1/\tau$).

We shall deform the internal components e'_i of e_i so that the resulting deformed lattice \tilde{L} is fully commensurate with E_2 (Niizeki 1991b). This is performed by changing e'_i into \tilde{e}'_i so that they satisfy similar LRs to those of e'_i but τ' (or, equivalently, τ) in the LRs is replaced by its rational approximants. To be more specific, the LRs among \tilde{e}'_i are $p\tilde{e}'_0 + q(\tilde{e}'_1 + \tilde{e}'_4) = 0$ and $r(\tilde{e}'_1 - \tilde{e}'_4) + s(\tilde{e}'_2 - \tilde{e}'_3) = 0$, where p/q and r/s are rational approximants to τ . Using those LRs together with $\tilde{e}'_0 + \tilde{e}'_1 + \dots + \tilde{e}'_4 = 0$, we may write the 2×4 matrix formed by \tilde{e}'_i , $i = 1-4$, as

$$(\tilde{e}'_1 \tilde{e}'_2 \tilde{e}'_3 \tilde{e}'_4) = \begin{pmatrix} b_1 & 0 \\ 0 & b_2 \end{pmatrix} \begin{pmatrix} -p & t & t & -p \\ s & -r & r & -s \end{pmatrix} \quad (2)$$

with $t = p - q$. Note that $\tilde{e}'_0 = (2qb_1, 0)$. The values of b_1 and b_2 have no effects in our theory because the internal space is ultimately crushed by the projection.

The deformed lattice \tilde{L} generated by $\tilde{e}_i = (e_i, \tilde{e}'_i)$ is designated by $\langle p/q, r/s \rangle$. \tilde{L} is considered to be an approximant to L . Note that p/q (or r/s) is a simple fraction, so that either p or q is odd.

A rational approximant to τ is given usually by the ratio of two consecutive Fibonacci numbers; the Fibonacci series $\{F_i\} = \{0, 1, 1, 2, 3, 5, 8, \dots\}$ is generated by the recursion relation $F_{k+1} = F_k + F_{k-1}$ with $F_0 = 0$ and $F_1 = 1$.

$\pm \tilde{e}'_i$, $i=0-4$, form a deformed decagon whose point group is $mm (D_2)$, so that the point group \tilde{G} of \tilde{L} is mm ; \tilde{L} is a rectangular approximant to L . \tilde{G} is a maximal subgroup of $G=10mm$. The space group of \tilde{L} is given by $\tilde{g} = \tilde{G} * \tilde{L}$.

Any position vector in E_4 can be indexed with ϵ_i as $[x_1x_2x_3x_4] \equiv \sum_i x_i \epsilon_i$. When ϵ_i is deformed into \tilde{e}'_i the position vector is transformed to $[x_1x_2x_3x_4] \sim \sum_i x_i \tilde{e}'_i$. This is a homogeneous affine transformation of E_4 , which represents the phason strain (Ishii 1989). It leaves E_2 invariant and commutable with \tilde{G} . The details of the phason strain are summarized in appendix 1. We shall abbreviate from now on the superscript "'" of the second index scheme because the first index scheme is not used.

The projection of \tilde{L} onto E_2 is identical to L_p but the one onto E'_2 is different from L'_p . We shall denote the latter by L_s ; $L_s = \{\sum_i n_i \tilde{e}'_i | n_i \in \mathbf{Z}\}$, which is, obviously, a Bravais lattice. It is equal to the primitive rectangular lattice $L_s^{(0)} = \{m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 | m_1, m_2 \in \mathbf{Z}\}$ or its sublattice, where $\mathbf{b}_1 = (b_1, 0)$ and $\mathbf{b}_2 = (0, b_2)$. From equation (2), $m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 \in L_s$ with

$$m_1 = -p(n_1 + n_4) + t(n_2 + n_3) \quad (3a)$$

$$m_2 = s(n_1 - n_4) - r(n_2 - n_3). \quad (3b)$$

Therefore, $m_1 + m_2$ is even, if the following condition is satisfied:

$$p \equiv s \pmod{2} \quad t \equiv r \pmod{2}. \quad (4)$$

It can be proved that L_s is equal to $\{m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 | m_1, m_2 \in \mathbf{Z}, m_1 + m_2 = \text{even}\}$ if this condition is satisfied but, otherwise, to $L_s^{(0)}$. A proof is given in appendix 2. Thus, the space group of L_s is pmm or cmm . It is given by $g_s = \tilde{G} * L_s$. We shall call L_s the shadow lattice of \tilde{L} . g_p is redefined here as $g_p = \tilde{G} * L_p$.

A surjection (an onto-mapping) φ from L_p onto L_s is defined naturally as $l = \sum_i n_i \epsilon_i \in L_p \xrightarrow{\varphi} \sum_i n_i \tilde{e}'_i \in L_s$. φ is not a bijection. It can be extended to a surjection from g_p onto g_s : $\{\sigma | \mathbf{u}\} \in g_p \xrightarrow{\varphi} \{\sigma | \mathbf{v}\} \in g_s$ with $\mathbf{v} = \varphi(\mathbf{u})$. Note that $\{\sigma | \xi\} \in \tilde{g}$ with $\xi = (\mathbf{u}, \mathbf{v})$.

Let $L_0 = \{l | l \in L_p, \varphi(l) = 0\}$ ($= \varphi^{-1}(0)$, the kernel of φ). Then, it is written as $L_0 = \tilde{L} \cap E_2$. L_0 is the maximal subgroup (submodule) of \tilde{L} among those which leave E_2 invariant. The LRS among \tilde{e}'_i result in

$$\mathbf{a}_1 = p\mathbf{e}_0 + q(\mathbf{e}_1 + \mathbf{e}_4) \quad (= -t(\mathbf{e}_1 + \mathbf{e}_4) - p(\mathbf{e}_2 + \mathbf{e}_3)) \quad (5a)$$

$$\mathbf{a}_2 = r(\mathbf{e}_1 - \mathbf{e}_4) + s(\mathbf{e}_2 - \mathbf{e}_3) \quad (5b)$$

belonging to L_0 ; \mathbf{a}_1 is horizontal and \mathbf{a}_2 vertical. It follows from these arguments that L_0 is a 2D Bravais lattice whose point group is mm . Note that E_2 is a lattice plane of \tilde{L} and L_0 is the 2D lattice given as the 2D section of \tilde{L} ; our deformation of L into \tilde{L} is made so that the relevant 2D lattice plane of L overlaps perfectly with E_2 .

Using the homomorphism theorem: $L_s \simeq L_p/L_0$ ($\simeq \tilde{L}/L_0$), we can prove that $\tilde{\Omega} = \Omega_0 \Omega_s$, where $\tilde{\Omega}$, Ω_0 and Ω_s are the volumes of the unit cells of \tilde{L} , L_0 and L_s , respectively.

\mathbf{a}_1 (or \mathbf{a}_2) is the shortest lattice vector of L_0 among those parallel to the horizontal (or vertical) axis. If $(\mathbf{a}_1 + \mathbf{a}_2)/2 \notin L_0$, then \mathbf{a}_1 and \mathbf{a}_2 are the basis vectors of L_0 and L_0 belongs to the Bravais class pmm but, otherwise, $\mathbf{a}'_1 = (\mathbf{a}_1 - \mathbf{a}_2)/2$ and $\mathbf{a}'_2 = (\mathbf{a}_1 + \mathbf{a}_2)/2$ are the basis vectors of L_0 and L_0 belongs to cmm . It follows from equations (5) that a necessary and sufficient condition for $(\mathbf{a}_1 + \mathbf{a}_2)/2$ to belong to L_0 coincides with condition (4) above. That is, L_0 belongs to a common Bravais class as that of L_s . The space group of L_0 is $g_0 = \tilde{G} * L_0$.

We proceed to the case $\langle p/q, r/s \rangle = \langle F_{k+1}/F_k, F_{k+1}/F_k \rangle$. Then, we obtain $\mathbf{a}_1 = \tau^k \mathbf{e}_0$ and $\mathbf{a}_2 = \tau^{k'}(\mathbf{e}_1 - \mathbf{e}_4)$, so that $a_1 = |\mathbf{a}_1| = \tau^k$ and $a_2 = |\mathbf{a}_2| = \tau^{k'} 2 \sin(2\pi/5)$, where use has been made of the equality, $F_k + \tau F_{k+1} = \tau^{k+1}$. Using the recursion relation of the

Fibonacci numbers, we can prove that L_0 for $\langle F_{k+1}/F_k, F_{k+1}/F_k \rangle$ belongs to pmm if $k'=k$ or $k'=k-1$. On the other hand, there exist two important cases where the centring occurs in L_0 (Zhang and Kuo 1990), namely, $\langle F_{k+2}/F_{k+1}, F_k/F_{k-1} \rangle$ and $\langle F_k/F_{k-1}, F_{k+1}/F_k \rangle$, which satisfy condition (4) because $r=p-q$ and $s=2q-p$ for the former and $r=p+q$ and $s=p$ for the latter. We obtain $\mathbf{a}'_1 = \tau^k(-\mathbf{e}_2)$ and $\mathbf{a}'_2 = \tau^k(-\mathbf{e}_3)$ for the former, so that the unit cell of L_0 is similar to the fat tile in the Penrose tiling with rhombic tiles. Similarly, $\mathbf{a}'_1 = \tau^k \mathbf{e}_4$ and $\mathbf{a}'_2 = \tau^k \mathbf{e}_1$ for the latter and the unit cell of L_0 is similar to the skinny tile. The case where p and q are Lucas numbers is discussed in appendix 3.

4. Special points and other special manifolds of 2D lattices and 4D ones

An extensive discussion on the subject in this section is given in Niizeki (1989b, 1991a).

A point group is called a centring group if the origin is its sole fixed point. For example, a point group including the inversion operation is a centring group. A point of a periodic pattern is called a special point (SP) if its point symmetry with respect to the relevant space group g is represented by a centring group, which is a subgroup of the point group of g . Equivalent SPs of g are grouped into a class. g has a centre of inversion symmetry if and only if its point group includes the inversion. g is symmorphic if it has an SP with the full point symmetry of g .

In this section, we confine our considerations only to the case of a Bravais lattice, which has a symmorphic space group. Then every SP is classified into type I or II according to whether it has the inversion symmetry or not, respectively. A necessary and sufficient condition for an SP to be of type I is that its position vector is a half of a lattice vector. For example, the centring subgroups of the 2D point group mm are mm or 2, so that the 2D Bravais lattice pmm (or cmm) has type I SPs only; pmm (or cmm) has four (or three) inequivalent SPs as shown in figure 2, where each SP is represented by a symbol following the convention in solid state physics (Bradley and Cracknell 1972). The point groups of these SPs are mm except that S of cmm has 2.

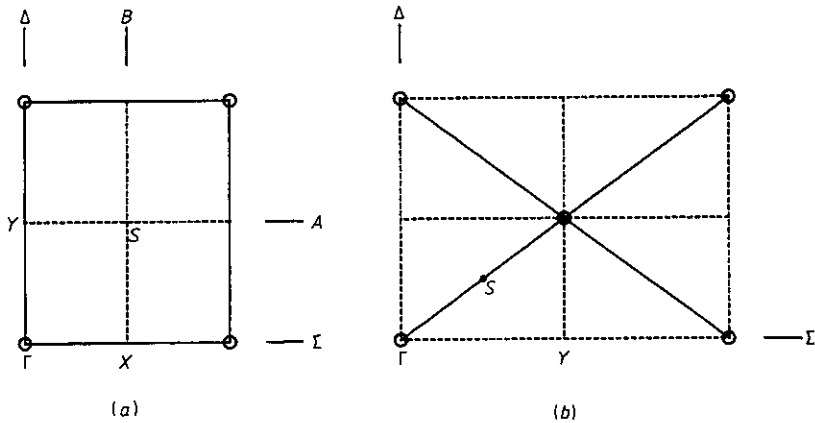


Figure 2. The SPs and special lines of (a) the primitive rectangular lattice and (b) those of the centred one. The point groups of the SPs are given by mm except the case of S of cmm, where it is given by 2. Type I (or II) special lines represented by Greek (or Roman) letters pass (or do not pass) lattice points. The special line Σ in (a), for example, is compatible with SPs Γ and X but not with Y and S . Conversely, the SP Γ in (a), for example, is compatible with special lines Σ and Δ but not with A and B .

The special manifolds associated with the subgroups $m1$ and $1\ m$ of mm are special lines, which represent the axes of the horizontal and vertical mirrors. Every mirror of a 2D lattice is classified into type I or II according to whether its mirror axis passes a lattice point or not, respectively. A type I (or II) mirror is denoted by a Greek (or Roman) letter as shown in figure 2. Note that cmm has no type II mirrors.

The 4D decagonal lattice L has six classes of SP_s : Γ, X, C, M, P and P' (Niizeki 1989b). The point group of Γ is $10\ mm$, those of X, C and M are mm and those of P and P' $5m$; Γ, X, C and M are of type I while P and P' of type II. SP_s with point group mm (or $5\ m$) can assume five (or two) orientations in L .

When L is deformed into \tilde{L} , the point group degrades from $10\ mm$ to mm . Correspondingly, the point groups of the SP_s of L degrade into their subgroups. Since the point group of \tilde{L} is equal (exactly, isomorphic) to mm , \tilde{L} has type I SP_s only. The type I SP_s of L change to SP_s of \tilde{L} because the inversion symmetry is retained on the deformation but the type II ones do not. The point group of Γ degrades from $10\ mm$ to mm . That of X remains unchanged or degrades into 2 depending on the orientation of X with respect to the point group \tilde{G} ($=mm$) of \tilde{L} . More precisely, X can assume three inequivalent orientations with respect to \tilde{G} and the point group is unchanged only when the axes of the mirrors of X are common to those of \tilde{G} . We shall distinguish the three SP_s of \tilde{L} using the symbols X, X' and X'' ; the point group of X is mm . The same is true for the case of C or M of L . In summary, \tilde{L} has ten kinds of SP_s . It is important in a later argument that any SP of \tilde{L} is indexed as $[h_1h_2h_3h_4]$ with $2h_i \in Z$ because it is of type I.

It can be shown easily from $L_0 = \tilde{L} \cap E_2$ that SP_s of L_0 are given by those of \tilde{L} but located on E_2 . Every SP of L_0 has the same point group as that of the SP in \tilde{L} . On the other hand, there exists a surjection from the set of all the SP_s of \tilde{L} onto those of L_s , because the SP_s of either lattice are indexed by integers and half integers.

Special lines of a 2D lattice, e.g. L_0 , are the mirror axes. A mirror of \tilde{L} has a fixed plane in E_4 and the plane is called a special plane of \tilde{L} . Special planes of \tilde{L} are classified into type I or II in a similar way as in the case of the 2D lattice. The crossing line between E_2 (or E'_2) and a special plane of \tilde{L} is the axis of a mirror in g_p (or g_s).

5. The space group of a shifted physical space

An element of \tilde{g} acts on $\Pi(\phi)$ ($=\phi + E_2$), the shifted physical space, as a 2D congruent transformation if it leaves $\Pi(\phi)$ invariant. Let us denote by $\tilde{g}(\phi)$ the set of all such elements of \tilde{g} . Then it is a subgroup of \tilde{g} ; its translational part is given by L_0 . It acts on $\Pi(\phi)$ as a 2D space group, which we shall denote as $g_p(\phi)$. An element of $g_p(\phi)$ is written as $\{\sigma|l\}$ with $\sigma \in \tilde{G}$ and $l \in L_p$, so that $g_p(\phi)$ is considered to be a subgroup of g_p ($=\tilde{G} * L_p$).

Let $\{\sigma|u\} \in g_p(\phi)$ and $v = \varphi(u)$. Then $\{\sigma|v\} \in g_s$ and $\{\sigma|\xi\} \in \tilde{g}(\phi)$ with $\xi = (u, v) \in \tilde{L}$. Moreover, $\{\sigma|v\}\phi = \phi$. Therefore, $g_s(\phi) = \varphi(g_p(\phi))$ ($=\{\{\sigma|\varphi(u)\}|\{\sigma|u\} \in g_p(\phi)\}$) is nothing but the point group of ϕ with respect to L . Conversely, $g_p(\phi)$ is obtained from $g_s(\phi)$ by $g_p(\phi) = \varphi^{-1}(g_s(\phi))$. It follows that the point group of $g_p(\phi)$ is equal (exactly, isomorphic) to $g_s(\phi)$.

We proceed to theorem 1.

Theorem 1. If $v = \phi' - \phi \in L_s$, then $g_p(\phi)$ and $g_p(\phi')$ are translationally isomorphic.

Proof. $g_s(\phi') = \{E|v\}g_s(\phi)\{E|v\}^{-1}$ with $\{E|v\} \in g_s$, so that $g_p(\phi') = \{E|u\}g_p(\phi)\{E|u\}^{-1}$ with $u \in \varphi^{-1}(v)$. □

Theorem 2. Let $\{\sigma|v\} \in g_s(\phi)$ be a mirror. Then a necessary and sufficient condition for existence of $u \in \varphi^{-1}(v)$ such that $\{\sigma|u\} (\in g_p(\phi))$ is a mirror is that $\{\sigma|v\}$ is of type I.

Proof. We first show the necessity. If $\{\sigma|u\}$ is a mirror, then u must be perpendicular to the axis of σ . If σ is horizontal (or vertical), we may write $u = k_1(e_1 - e_4) + k_2(e_2 - e_3)$ (or $u = k_1(e_1 + e_4) + k_2(e_2 + e_3)$) with $k_1, k_2 \in \mathbb{Z}$. It follows from equation 2 that $v (= \varphi(u)) = 2v_0$ with $v_0 = (sk_1 - rk_2)b_2$ (or $v_0 = (-pk_1 + tk_2)b_1$) $\in L_s$. Consequently, the axis of $\{\sigma|v\}$ passes lattice point v_0 of L_s .

We show next the sufficiency. Let $\{\sigma|v\}$ be a type I mirror of L_s and assume that $v_0 \in L_s$ is located on the axis of the mirror. Then $\{\sigma|0\} \in g_s(\phi')$ with $\phi' = \phi - v_0$. By theorem 1, we may assume from the outset that $v = 0$. Then $0 \in \varphi^{-1}(0)$, so that $\{\sigma|0\}$ is a mirror of $g_p(\phi)$. □

Theorem 2 shows that a mirror of $g_s(\phi)$ yields mirrors or glides of $g_p(\phi)$ if it is of type I or II, respectively.

We may draw the following conclusions from the above considerations. Firstly, if ϕ is generic, then $g_p(\phi) = L_0$, the translational part of g_0 , so that its point group is trivial. Secondly, if $g_s(\phi)$ is a non-trivial point group, $g_p(\phi)$ is determined by the special manifold (an SP or a special line) of L_s on which ϕ is located. In particular, the point group of $g_p(\phi)$ is equal to that of ϕ in L_s . We consider from now on only the non-trivial cases. Then ϕ in $g_p(\phi)$ may be denoted by the symbol which represents the class of the relevant special manifold, e.g. $g_p(\Gamma)$ and $g_p(A)$.

If L_0 (or L_s) belongs to pmm, there exist eight space groups, pmm, pmg, pgm, pgg, pm1, p1m, pg1, p1g, which are derived from four classes of SPs of L_s and another four of special lines. On the other hand, if L_0 belongs to cmm, there exist five space groups, cmm(Γ), cmm(Y), cm1, c1m and 'c2'. The first two are isomorphic and are distinguished by the relevant SPs of L_s . The space group of the last one, 'c2', is actually p2 because point group 2 does not conform to a rectangular Bravais class. Note here that two space groups pm1 and p1m, for example, are distinguished because the horizontal mirror in pm1 and the vertical one in p1m are inequivalent.

6. The special points and special lines $g_p(\phi)$

6.1. The case of special points

We consider in this subsection only the case where L_0 (and L_s) belongs to pmm; the results are easily generalized to the case of cmm. Moreover, we assume that $g_p(\phi)$ has SPs , i.e. centres of symmetries. An SP of $g_p(\phi)$ is that of \tilde{L} but located on $\Pi(\phi)$. Therefore, an SP of $g_p(\phi)$ is represented by, say, X if it belongs to class X of SPs of \tilde{L} . ϕ is the projection of (the position vector of) the SP of \tilde{L} onto E'_2 , so that it must coincide with an SP of L_s . Conversely, if ϕ is an SP of L_s , $g_p(\phi)$ has SPs . The point groups of the SPs are mm or 2 and all the SPs have inversion symmetry.

Let $[h_1h_2h_3h_4]$ be an SP of \tilde{L} . Then it is located on $\Pi(\phi)$ with $\phi = \sum_i h_i \tilde{e}'_i$. Another SP , $[h'_1h'_2h'_3h'_4]$, is on the same plane if and only if $\sum_i n_i e_i \in L_0$ with $n_i = 2(h_i - h'_i) \in \mathbb{Z}$. It follows that ten classes of SPs of \tilde{L} are divided into several disjoint groups (sets) as follows: if $\Pi(\phi)$ includes an SP belonging to a class in a group, it includes SPs belonging to all classes in the group.

We can conclude from the above considerations that there exist only four SPs of $g_p(\phi)$ per unit cell; they are at x , $x + a_1/2$, $x + a_2/2$ and $x + (a_1 + a_2)/2$ with x being a representative of the four SPs. These four must be translationally inequivalent. Since \tilde{L} has four classes, Γ , X , C and M , of SPs with point group mm, SPs belonging to the four classes are located on $E_2 (= \Pi(0))$. These four classes yield Γ , X , Y and S of $g_p(\Gamma)$, which belongs to pmm.

On the other hand, an SP of class X' can assume two different orientations so that two X' 's with different orientations can be located on a single $\Pi(\phi)$. The same is true for the remaining five classes of SPs with point group 2. These six classes of SPs are paired into three which are associated with three space groups, $g_p(X)$ (=pmg), $g_p(Y)$ (=pgm) and $g_p(S)$ (=pgg). These three space groups have no centres with the full point symmetry (mm) because they are non-symmorphic.

6.2. The case of special lines

Many rectangular approximants to the decagonal quasilattice have mirrors. It can be shown easily that $g_p(\phi)$ has a mirror if and only if $\Pi(\phi)$ has a crossing line with a mirror plane (a special plane) of \tilde{L} ; the crossing line is nothing but the axis of the mirror. Theorem 2 in section 5 shows that only type I special planes can have crossing lines with $\Pi(\phi)$.

7. The space group of an approximant lattice

An AL to the decagonal quasilattice (see equation (1)) is obtained from \tilde{L} by the cut-and-project method as

$$\tilde{Q} = \{l | l \in L_p, \varphi(l) \in \phi + \tilde{W}\} \quad (6)$$

where \tilde{W} is the distorted window due to the phason strain. We shall call \tilde{L} the mother lattice of \tilde{Q} . If W is the unit decagon, \tilde{W} is a decagon whose vertex vectors are given by $\pm \tilde{e}_i'$. The point group of \tilde{W} is given by \tilde{G} (=mm).

Let $S \equiv \varphi(\tilde{Q})$. Then we obtain $S = S(\phi, \tilde{W}) \equiv L_s \cap (\phi + W)$, i.e. a cut of L_s by the shifted window. We may write $\tilde{Q} = \varphi^{-1}(S)$ or, equivalently, $\tilde{Q} = \{l | l \in L_p, \varphi(l) \in S\}$. That is, \tilde{Q} is a set of the projections onto E_2 of the lattice points of \tilde{L} projecting onto S in E_2' .

Since L_0 is the kernel of $\varphi: L_p \rightarrow L_s$, \tilde{Q} is a periodic lattice whose Bravais lattice is given by L_0 . Moreover, the number of the lattice points of \tilde{Q} in a unit cell is given by $N = |S|$, the number of the points in S . We shall call S the shadow of \tilde{Q} . We consider hereafter only the non-trivial case where $N \geq 2$. Two ALs \tilde{Q} and \tilde{Q}' are translationally congruent if and only if their shadows S and S' are translationally equivalent with respect to L_s .

We consider the space group of \tilde{Q} . The point group of S , $G(S)$, is of fundamental importance. $G(S)$ is a subgroup of g_s because S is a non-trivial subset of L_s . Since \tilde{W} has the full symmetry of \tilde{G} , $G(S)$ with $S = S(\phi, \tilde{W})$ is dependent on ϕ but not on \tilde{W} . It is important to notice here the following fact: $S(\phi, \tilde{W}) = S(\phi', \tilde{W})$ if ϕ' is in a neighbourhood of ϕ because L_s is discrete. We can redefine ϕ without changing S in such a way that $G(S)$ coincides with $g_s(\phi)$, the point group of ϕ with respect to L_s . We assume hereafter that ϕ is always chosen in this way. Then ϕ represents the centre of symmetry of $G(S)$ provided that it exists. It follows that the space group of \tilde{Q} is given by $g_p(\phi) (= \varphi^{-1}(g_s(\phi)))$. Thus, the classification in section 5 of the space groups

of the shifted physical spaces is considered to be a classification of the space groups of AL_s .

Once the mother lattice, $L (= \langle p/q, r/s \rangle)$, is fixed, the AL_s associated with SP_s of L_s are uniquely determined. The situation is different in the case of AL_s associated with special lines of L_s . Let us consider, for example, the case of class Σ of special lines. Then there exist several AL_s associated with Σ because ϕ can take any value on Σ . They have a common space group $pm1$ (or $cm1$). The number is finite on account of the finiteness of \tilde{W} . It increases as the order of the approximant \tilde{L} is increased because the unit cell of L_s becomes very small compared to \tilde{W} . The same is true for AL_s associated with other special lines of L_s . Therefore we may call the series of AL_s associated with a special line of L_s a quasi-continuous series.

We show in figure 3 several AL_s to the decagonal quasilattice.

8. Discussions

The space group of $\tilde{Q}(\phi, \tilde{W})$ is $p1$ for a generic ϕ . We shall call such an AL an irregular AL because its point symmetry does not conform to the Bravais lattice L_0 . Also, 'c2' is an irregular AL . The situation when AL_s with different structures have a common Bravais lattice will be called a polymorphism. On the other hand, two or more AL_s will be called isomers if their space groups are identical. For example, $cmm(\Gamma)$ and $cmm(Y)$ are isomers and so are AL_s in every quasi-continuous series.

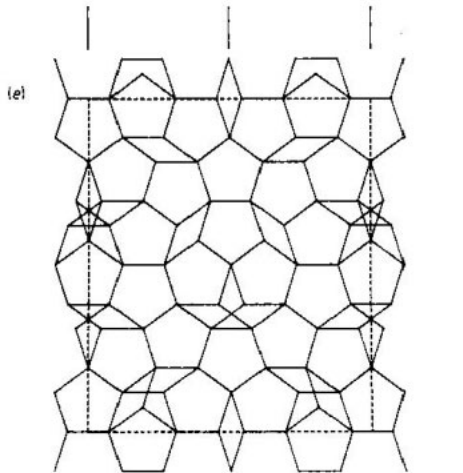
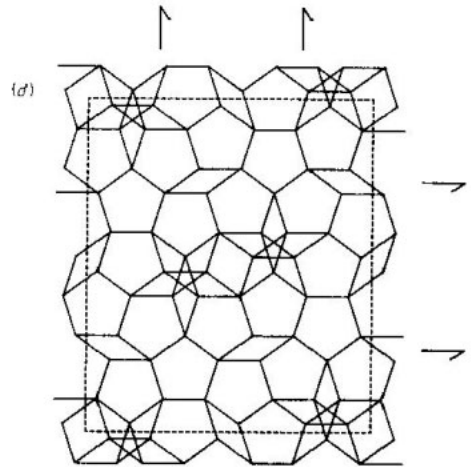
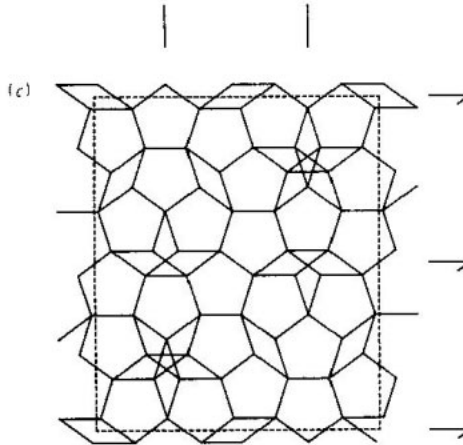
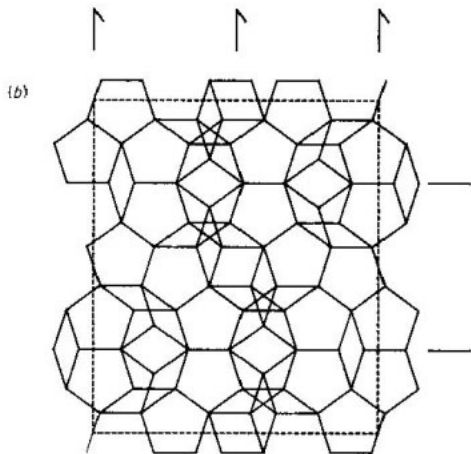
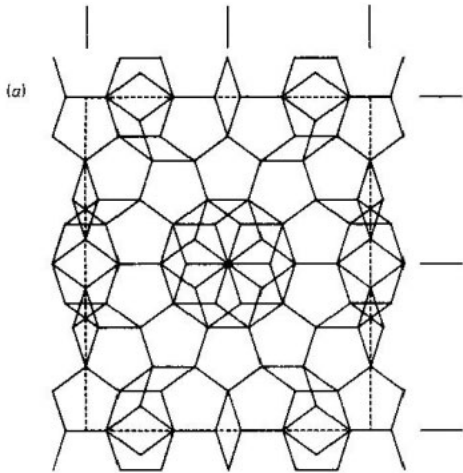
If ϕ is located on an SP or a special line of L_s , it may occur that two or more lattice points of L_s are located on the boundary of the domain $\phi + \tilde{W}$. Then, a difficulty occurs: if one of these points is included in $S (= L_s \cap (\phi + \tilde{W}))$, another one on the opposite boundary must be discarded and vice versa (Niizeki 1989b). This is resolved by shifting ϕ infinitesimally in an appropriate direction. Then the symmetry of the AL is broken (Niizeki 1989b) and the space group degrades into one of its subgroups.

On the other hand, if the lattice points on the boundary are all included, the point symmetry of ϕ is succeeded by $\tilde{Q}(\phi, \tilde{W})$. This treatment of the problem is equivalent to a restoration of the broken symmetry by a symmetrization.

The problem occurs in the case where ϕ is located on a special line of type Σ ; lattice points of L_s are located on the top edge and the bottom one of $\phi + \tilde{W}$, the shifted decagon. Therefore, AL of type pmm and pmg , for example, incur such difficulties. If ϕ is shifted vertically by an infinitesimal amount, they degrade to $p1m$ and $p1g$, respectively, because the horizontal mirror is broken. Another type of problem occurs in the case of pmm , where $\phi = 0$, because the vertices of \tilde{W} are the lattice points of L_s . Note, however, that the difficulties discussed here are due to our choice of the window and it may not occur for a different choice.

The decagonal quasilattice has a selfsimilarity whose scale is given by τ (Niizeki 1989a). This is because $TL = L$ or, equivalently, $T(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4) = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4)M$, where T is a linear transformation given by $T = (\tau, \tau, \tau', \tau')^{diag} (\tau' = -1/\tau)$ and M is a unimodular matrix; T scales E_2 and E'_2 differently. However, $T\tilde{L} \neq \tilde{L}$. We can show, instead, that $T\langle p/q, r/s \rangle = \langle p'/q', r'/s' \rangle$ with $p' = p + q, q' = p, r' = r + s$ and $s' = r$. That is, T changes \tilde{L} into the next generation of \tilde{L} . Using this result, we can show that there exists a deflation procedure which changes an AL into another AL whose lattice constants are τ -times the original ones. This subject will be fully discussed elsewhere.

An AL has only a few centres of global point symmetries per unit cell. A higher-order AL has, however, many centres of local point symmetries. They are derived from similar



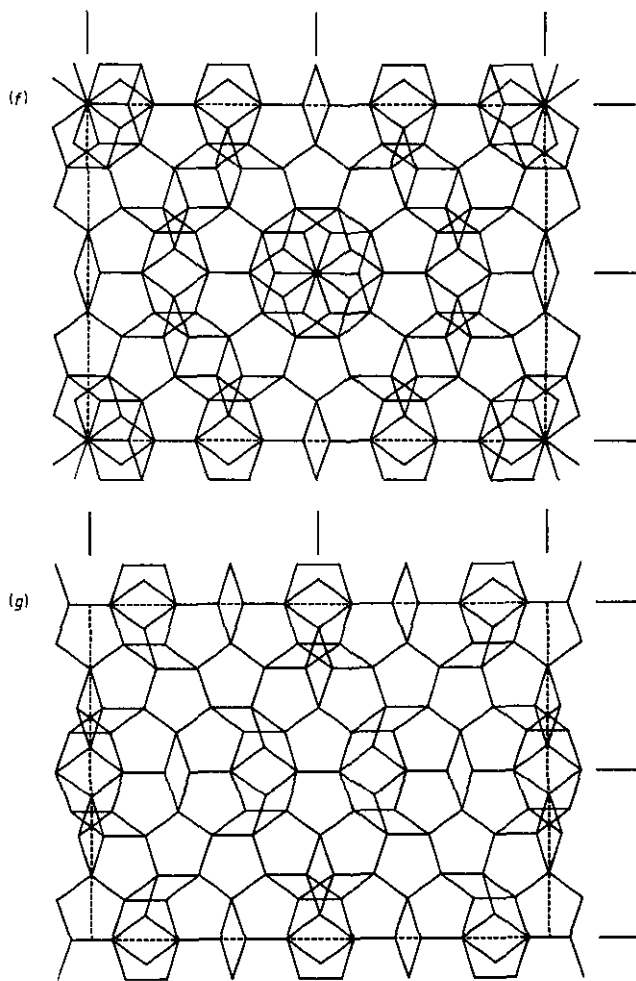


Figure 3. Periodic approximants to the decagonal quasilattice in figure 1. A bar shows a mirror and an arrow a glide. An approximant is characterized by the mother lattice, $\langle p/q, r/s \rangle$, and the SP (or the special line) on which the phase vector is located. The attributes of the approximants (a)–(g) are listed in the following table. The last row shows the space groups.

(a)	(b)	(c)	(d)	(e)	(f)	(g)
$\langle \frac{5}{3}, \frac{3}{2} \rangle$	$\langle \frac{5}{3}, \frac{3}{2} \rangle$	$\langle \frac{5}{3}, \frac{3}{2} \rangle$	$\langle \frac{5}{3}, \frac{3}{2} \rangle$	$\langle \frac{5}{3}, \frac{3}{2} \rangle$	$\langle \frac{5}{3}, \frac{3}{2} \rangle$	$\langle \frac{5}{3}, \frac{3}{2} \rangle$
Γ	X	Y	S	Σ	Γ'	Y
pmm	pmg	pgm	pgg	p1m	cmm	cmm

The frustrations derived from horizontal mirrors or some other reasons are treated by symmetrization in (a), (b), (d), (f) and (g). The tiles of fat rhombi in these approximants are caused by the symmetrization; such tiles are absent in the ideal quasilattice (see figure 1). The centre of a fat rhombus is derived from an SP of type M of the mother lattice. The centres of local decagonal symmetries in (a) and (f) are also due to the symmetrization.

The vertices and the centres of the unit cell of each approximant (except (e)) are SPs of the lattice, as are the middle points of the edges. The SPs of (a), for example, are derived from SPs of type Γ , X, C and M of the mother lattice, while the ones of (b), (c) and (d) (the centres of inversion symmetry) from those of X' , X'' , C' , C'' , M' and M'' . The approximant (e) is derived from (a) as a result of the symmetry breaking due to the frustration.

centres of \tilde{L} ; the latter centres are derived from SPs of L . For example, the centre of a star (or a pentagon enclosed by five pentagons) in figure 3(c) (pgm) is derived from an SP of type P' (or P) of L .

TWO ALs with a common window but different phase vectors are not necessarily locally isomorphic in contrast to the case of quasilattices. We consider here the physics behind this result. The translational symmetry of g_p is 4D-like but that of g_0 is just 2D. This means that not only the point symmetry but also the translational symmetry is broken partially on a phase transition from a quasicrystal to its periodic approximant. This symmetry breaking yields a periodic 'field' (in the internal space) which couples with ϕ and, consequently, ϕ is locked to a particular value which minimizes the free energy. The 'field' will depend on the chemical potentials of the components of the quasicrystal, so that the location of the minimum can change depending on the concentrations of the components. Therefore a quasicrystal can have two or more approximants which belong to a single group of polymorphs. Note that occurrence of an approximant crystal described by an irregular AL is not excluded *a priori* though it will be rare that the free energy has a minimum at a low symmetry point in E_2^2 . However, an irregular approximant may be realized on account of the symmetry breaking due to the frustration.

We may say that a class of SPs of a space group is compatible with that of special lines if an SP belonging to the former is located on a special line to the latter (Niizeki 1991a); in the compatible case, the point group of the special line is a subgroup of that of the SP. For example, Σ and Δ of pmm are compatible with Γ but A and B are not. Correspondingly, $g_p(\Sigma)$ and $g_p(\Delta)$ are subgroups of $g_p(\Gamma)$ but $g_p(A)$ and $g_p(B)$ are not. The space group of an AL associated with a special line is derived from that associated with an SP on the special line.

The theory developed in this paper is basically applicable to the classification of the space groups of ALs to any quasilattice. The remark presented in the last paragraph considerably simplifies the problem. Applying the present theory to the case of the 3D icosahedral quasilattice, a complete classification of the space groups of the cubic, the orthorhombic and the rhombohedral approximants has been established. The results will be published elsewhere (Niizeki 1991d).

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Appendix 1

The phason strain is represented by the 4D matrix H satisfying $(\tilde{e}_1 \tilde{e}_2 \tilde{e}_3 \tilde{e}_4) = H(\epsilon_1 \epsilon_2 \epsilon_3 \epsilon_4)$. We may choose H so that $H = I + H'$ where I is the unit matrix and H' has non-vanishing matrix elements only in the bottom-left 2×2 block, which is denoted by Δ . Then $(\tilde{e}'_1 \tilde{e}'_2 \tilde{e}'_3 \tilde{e}'_4) = (e'_1 e'_2 e'_3 e'_4) + \Delta(e_1 e_2 e_3 e_4)$. Since $\det H = 1$, the transformation is volume-conserving. Δ is a diagonal matrix because H is commutable with \tilde{G} (mm). To be more specific, we obtain $\Delta = (\delta_1, \delta_2)^{\text{diag}}$ with $\delta_1 = \tau(q\tau - p)/(q + p\tau)$ and $\delta_2 = (s\tau - r)/(s + r\tau)$. In the case of $\langle F_{k+1}/F_k, F_{k'+1}/F_{k'} \rangle$, we obtain $\delta_1 = -(-1/\tau^2)^k$

and $\delta_2 = -1/\tau \cdot (-1/\tau^2)^k$ (Zhang and Kuo 1990). Note that the values of b_1 and b_2 are fixed as $b_1 = (\sqrt{5} \cos(\pi/5))/(q + p\tau)$ and $b_2 = (\sqrt{5}\tau \sin(\pi/5))/(s + r\tau)$.

Appendix 2

If $n_1 = n_4$ and $n_2 = n_3$, then $m_1 = 2(-pn_1 + tn_2)$ and $m_2 = 0$. There exist n_1 and n_2 such that $-pn_1 + tn_2 = 1$ because p and $t (= p - q)$ are relative primes by the assumption that p/q is a simple fraction. It follows that $2b_1 \in L_s$. Similarly, $2b_2 \in L_s$. Since L_s is a Bravais lattice, the set $\{2(k_1b_1 + k_2b_2) | k_1, k_2 \in \mathbf{Z}\}$ must be a superlattice (a sublattice) of L_s .

The next problem is to search the lattice points of L_s in a unit cell of the superlattice. Such lattice points are written as $m_1b_1 + m_2b_2$ in which m_1 and m_2 as given by equation (3) are considered in mod 2. Since the sign may be changed arbitrarily without changing the parity, we may write $m_1 \equiv pk_1 + tk_2$ and $m_2 \equiv sk_1 + rk_2 \pmod{2}$ with $k_1 = n_1 + n_4$ and $k_2 = n_2 + n_3$. There exist two cases depending on whether $\Delta = pr - ts$ vanishes or not in mod 2. If the condition (4) is satisfied, then $\Delta \equiv 0 \pmod{2}$. On the other hand, if it is not, then $\Delta \equiv 1 \pmod{2}$, which is easily proved by using the fact that p and t (or s and r) cannot be even together.

If $\Delta \equiv 1 \pmod{2}$, the linear transformation from (k_1, k_2) to (m_1, m_2) is inverted in $\text{GF}(2)$ ($= \mathbf{Z}/2\mathbf{Z}$) as $k_1 \equiv rm_1 + tm_2$ and $k_2 \equiv sm_1 + pm_2 \pmod{2}$, so that the pair (m_1, m_2) can assume any of the four combinations $(0, 0)$, $(0, 1)$, $(1, 0)$ and $(1, 1)$ in mod 2. It follows that $L_s = L_s^{(0)}$ in this case. On the other hand, if $\Delta \equiv 0 \pmod{2}$, then $m_1 + m_2 \equiv 0 \pmod{2}$ as shown in the text. Moreover, m_1 can assume both the parities because s and r are not even together. This completes the proof.

Appendix 3

It is well known that Lucas numbers $L_k = F_{k+1} + F_{k-1}$ yield the second series of rational approximants to τ , though these approximants are less accurate than those by the Fibonacci numbers. $\langle L_k/L_{k-1}, F_{k+1}/F_k \rangle$ (or $\langle L_{k+2}/L_{k+1}, F_k/F_{k-1} \rangle$) belongs to cmm because $p = 2r - s$ and $q = 3s - r$ (or $p = 4r + 3s$ and $q = 3r + s$). The basis vectors are $a'_1 = \tau^k(e_0 - e_1)$ and $a'_2 = \tau^k(e_0 - e_2)$ (or $a'_1 = \tau^k(e_0 - e_2)$ and $a'_2 = \tau^k(e_0 - e_3)$); the rhombic unit cell is similar to the fat (or skinny) tile. The unit cell is, however, different in size and orientation from $\langle F_{k+2}/F_{k+1}, F_k/F_{k-1} \rangle$ (or $\langle F_k/F_{k-1}, F_{k+1}/F_k \rangle$), though both are similar.

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