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A classification of special points of icosahedral quasilattices

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Abstract. We investigate special points of icosahedral quasilattices in three dimensions (3D). They are given as the projections onto the real space of the special points of icosahedral lattices which are periodic lattices in 6D. There exist three Bravais classes of 6D icosahedral lattices and we present a complete classification of their special points.

1. Introduction

We have investigated in the preceding paper (Niizeki 1989b) special points of quasilattices in two dimensions (2D). The quasilattices are obtained by the cut-and-projection method (Janssen 1986, Niizeki 1988a) from 4D periodic lattices, i.e. octagonal, decagonal and dodecagonal lattices, and the special points of the quasilattices are obtained with the same method from those of the starting periodic lattices. We have presented a complete classification of the special points of these periodic lattices. The results are applied to classifications of local and global point symmetries of the relevant 2D quasilattices.

On the other hand, we have shown in Niizeki and Akamatsu (1989) (to be referred to as I) that the special points in the reciprocal space of a 3D icosahedral quasilattice (IQL) are useful in understanding the properties of the electronic wavefunctions in the 'plane-wave representation'; the quasi-dispersion relation of electron in the IQL is stationary at the special points as in the case of a periodic lattice.

IQL are obtained generally with the cut-and-projection method from 6D periodic lattices whose point symmetries are isomorphic to Y_h ($\bar{5}\bar{3}m$), the full icosahedral point group in 3D (Elser 1986, Janssen 1986, Katz and Duneau 1986). There exist three 6D icosahedral lattices, $P\bar{5}\bar{3}m$, $F\bar{5}\bar{3}m$ and $I\bar{5}\bar{3}m$, and they give rise to three Bravais classes of IQL (Janssen 1986, Rokhsar *et al* 1987, Levitov and Rhyner 1988).

The special points of IQL are obtained with the cut-and-projection method from those of the starting lattices in 6D. We have treated only $P\bar{5}\bar{3}m$ in I. We shall restrict our arguments to the cases where the space groups of the 6D lattices are symmorphic and their point groups are isomorphic to Y_h.

In § 2, we introduce the three 6D icosahedral lattices and present their relationships to IQL. In § 3, we present a general theory of the special points of a (periodic) Bravais lattice with a symmorphic space group. In § 4, we shall classify the special points of the 6D lattices and, in § 5, discuss related subjects.

2. The 6D icosahedral lattices and 3D icosahedral quasilattices derived from them

A regular icosahedron $\mathcal{Y}$ in E_3 ($\simeq\mathbb{R}^3$), the 3D Euclidean space, has six fivefold axes, ten threefold axes and fifteen twofold ones, which pass through the vertices, the face

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centres and the middle points of the edges, respectively. $\mathscr{Y}$ has inversion symmetry and the full point group of $\mathscr{Y}$ is Y_h, whose order is 120; $|\mathrm{Y}_h| = 120$.

The twelve vertices of $\mathscr{Y}$ are grouped into six pairs by the inversion symmetry and six of the twelve vertex vectors of $\mathscr{Y}$ centred at the origin of E_3 are linearly independent over $\mathbb{Q}$, the rational field. We choose the cartesian coordinate system so that the three axes are parallel to three twofold axes which are orthogonal to each other. By choosing the size of $\mathscr{Y}$ appropriately, we can assume that the six independent vertex vectors are given by $\boldsymbol{a}_1 = (\tau, 1, 0)$, $\boldsymbol{a}_2 = (0, \tau, 1)$, $\boldsymbol{a}_3 = (1, 0, \tau)$, $\boldsymbol{a}_4 = (\tau, -1, 0)$, $\boldsymbol{a}_5 = (0, \tau, -1)$ and $\boldsymbol{a}_6 = (-1, 0, \tau)$, where $\tau = (1+\sqrt{5})/2$ is the golden ratio. The two vectors, $\boldsymbol{a}_1 + \boldsymbol{a}_2 + \boldsymbol{a}_3$ and $\boldsymbol{a}_4 + \boldsymbol{a}_5 + \boldsymbol{a}_6$, are parallel to the threefold axis along $(1, 1, 1) \equiv [111]$. Note that $|\boldsymbol{a}_i| = \sqrt{\tau+2}$ for all i and $\boldsymbol{a}_i \cdot \boldsymbol{a}_j/(|\boldsymbol{a}_i||\boldsymbol{a}_j|)$ $(i \neq j)$ takes $1/\sqrt{5}$ or $-1/\sqrt{5}$. An element of Y_h permutes the $\boldsymbol{a}_i$ among themselves and, subsequently, inverts some of them.

The algebraic conjugate of τ is given by $\tilde{\tau} = (1-\sqrt{5})/2$ $(= -1/\tau)$. Let us define the conjugate vectors to $\boldsymbol{a}_i$ by $\tilde{\boldsymbol{a}}_i = -\tau \boldsymbol{a}_i|_{\tau \to \tilde{\tau}}$. Then, $\tilde{\boldsymbol{a}}_i$ are vertex vectors of another icosahedron, $\tilde{\mathscr{Y}}$, which differs from $\mathscr{Y}$ only in its orientation in E_3; $\tilde{\boldsymbol{a}}_i \cdot \tilde{\boldsymbol{a}}_j = -\boldsymbol{a}_i \cdot \boldsymbol{a}_j$ $(i \neq j)$. We shall call $\tilde{\mathscr{Y}}$ the conjugate of $\mathscr{Y}$.

We can consider, alternatively, that $\tilde{\mathscr{Y}}$ is contained in the conjugate space $\tilde{E}_3$ which is another 3D Euclidean space, orthogonal to E_3. Let $E_6 = E_3 \oplus \tilde{E}_3$ and $\boldsymbol{\varepsilon}_i = (\boldsymbol{a}_i, \tilde{\boldsymbol{a}}_i)$, $i = 1$-6. Then, we obtain $\boldsymbol{\varepsilon}_i \cdot \boldsymbol{\varepsilon}_j = a^2 \delta_{ij}$ with $a = \sqrt{2\tau+4}$. Therefore, $L_{\mathrm{P}} = \{n_1\boldsymbol{\varepsilon}_1 + n_2\boldsymbol{\varepsilon}_2 + \ldots + n_6\boldsymbol{\varepsilon}_6 | n_i \in \boldsymbol{Z}\}$ is a simple hypercubic lattice in 6D. We shall sometimes denote $\boldsymbol{l} = n_1\boldsymbol{\varepsilon}_1 + \ldots + n_6\boldsymbol{\varepsilon}_6 \in L_{\mathrm{P}}$ as $\boldsymbol{l} = [n_1 n_2 \ldots n_6]$ with the n_i being the indices of $\boldsymbol{l}$.

The point group of L_{P} is $\Omega(6)$, the 6D hyperoctahedral point group. $\Omega(6)$ is given by a semidirect product of the symmetric group $\mathrm{S}(6)$ consisting of all the permutations among the $\boldsymbol{\varepsilon}_i$ and an Abelian mirror group generated by the six mirrors, each of which inverts one of the $\boldsymbol{\varepsilon}_i$. It follows that $|\Omega(6)| = 6!2^6 = 46\,080$. The maximal subgroup of $\Omega(6)$ among those which leave E_3 $(\subset E_6)$ invariant is Y'_h, the 6D icosahedral group, which is isomorphic to Y_h; Y_h is the restriction of Y'_h onto E_3 and the action of $\sigma' \in \mathrm{Y}'_h$ on $\boldsymbol{\varepsilon}_i$ is the same as the action of the corresponding element $\sigma \in \mathrm{Y}_h$ on $\boldsymbol{a}_i$. The $\boldsymbol{\varepsilon}_i$ are basis vectors of a 6D unimodular representation of Y_h $(\simeq \mathrm{Y}'_h)$. $\tilde{E}_3$ is also an invariant subspace against Y'_h. $\tilde{\mathrm{Y}}_h$, the restriction of Y'_h onto $\tilde{E}_3$, is isomorphic to Y_h. We shall denote the projectors from E_6 onto E_3 (or $\tilde{E}_3$) by π (or $\tilde{\pi}$). Then, $\pi([n_1 \ldots n_6]) = n_1\boldsymbol{a}_1 + \ldots + n_6\boldsymbol{a}_6$ and $\tilde{\pi}([n_1 \ldots n_6]) = n_1\tilde{\boldsymbol{a}}_1 + \ldots + n_6\tilde{\boldsymbol{a}}_6$.

A 6D periodic lattice is called an icosahedral lattice if its point group is equal to Y'_h. Though L_{P} has a larger point symmetry than Y'_h, we can consider it to be a special icosahedral lattice. A more general icosahedral lattice is formed with basis vectors $(\boldsymbol{a}_i, c\tilde{\boldsymbol{a}}_i)$, $i = 1$-6, where $c(\neq 0)$ is an arbitary constant.

If $\boldsymbol{a}_i$ are scaled up through the ratio τ, the resulting vectors are rationally related to $\boldsymbol{a}_i$ as

$$\tau(\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_6) = (\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_6)\mathbf{M} \tag{1}$$

$$\mathbf{M} = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & -1 & 1 \end{pmatrix}. \tag{2}$$

Similarly, the $\tilde{\boldsymbol{a}}_i$ are transformed by $\tilde{\tau}$ among themselves with the same matrix $\mathbf{M}$. Accordingly, we obtain

$$\mathbf{T}(\boldsymbol{\varepsilon}_1, \boldsymbol{\varepsilon}_2, \ldots, \boldsymbol{\varepsilon}_6) = (\boldsymbol{\varepsilon}_1, \boldsymbol{\varepsilon}_2, \ldots, \boldsymbol{\varepsilon}_6)\mathbf{M} \tag{3}$$

where $\mathbf{T} = \mathrm{diag}(\tau, \tau, \tau, \tilde{\tau}, \tilde{\tau}, \tilde{\tau})$ is a diagonal matrix in 6D. Since $\det \mathbf{T} = -1$, $\mathbf{T}$ represents a volume-conserving linear transformation of E_6. $\mathbf{T}$ leaves E_3 and $\tilde{E}_3$ invariant. It acts as similarity transformations onto the two subspaces and, therefore, commutes with all the elements of Y'_h. τ satisfies $\tau^3 = 2\tau + 1$, so that we obtain $\mathbf{T}^3 = 2\mathbf{T} + \mathbf{E}$ and $\mathbf{M}^3 = 2\mathbf{M} + \mathbf{E}$ with $\mathbf{E}$ being the 6D unit matrix. It follows that $\mathbf{M}^3$ is a unimodular matrix and $\mathbf{T}^3$ induces an automorphism of L_P; $\mathbf{T}^3 L_P = L_P$ (Elser 1985, Katz and Duneau 1986).

L_P has two sublattices with the hyperoctahedral point symmetry, namely, the face centred hypercubic lattice L_F and the body-centred lattice L_I; $L_F = \{[n_1 \ldots n_6] \mid n_i \in \boldsymbol{Z}$ and $n_1 + \ldots n_6 \equiv 0 \bmod 2\}$ and $L_I = \{[n_1 \ldots n_6] \mid n_i \in \boldsymbol{Z}$ and n_i are either all even or all odd$\}$. Note that L_F (or L_I) is a superlattice of L_P such that the unit cell is doubled (or 32pled). Note also that L_I is a superlattice of L_F. The three 6D lattices belong to different Bravais classes not only as hyperoctahedral lattices but also as 6D icosahedral lattices (Janssen 1986, Rokhsar *et al* 1987, Levitov and Rhyner 1988). The space groups of the three icosahedral lattices are $P\bar{5}\bar{3}m$, $F\bar{5}\bar{3}m$ and $I\bar{5}\bar{3}m$.

It is a matter of simple algebra to show the following. If $\boldsymbol{l} = [n_1 \ldots n_6] \in L_F$ or L_I then $\boldsymbol{l}' = \mathbf{T}\boldsymbol{l} = [n'_1 \ldots n'_6] \in L_F$ or L_I, respectively, so that $\mathbf{T}$ is an automorphism of L_F and L_I (Rokhsar *et al* 1987, Levitov and Rhyner 1988).

We can now construct 3D icosahedral quasilattices from the 6D icosahedral lattices with the cut-and-projection method. A finite domain S in $\tilde{E}_3$ is called starlike if $tS \subset S$ for $\forall t \in (0, 1)$. A starlike domain is simply connected. Let W be a starlike domain in $\tilde{E}_3$ and assume that it is invariant under $\tilde{Y}_h$. Then the set of points in E_3 defined by

$$Q_P(\boldsymbol{\phi}, W) = \{\pi(\boldsymbol{l}) \mid \boldsymbol{l} \in L_P \text{ and } \tilde{\pi}(\boldsymbol{l}) \in \boldsymbol{\phi} + W\} \tag{4}$$

is an icosahedral quasilattice, where $\boldsymbol{\phi} \in \tilde{E}_3$ is an arbitrary vector, a so-called phase vector. W is called a window. The local isomorphism class to which $Q_P(\boldsymbol{\phi}, W)$ belongs is determined by W, but is independent of $\boldsymbol{\phi}$. Therefore, we shall sometimes denote $Q_P(\boldsymbol{\phi}, W)$ simply as $Q_P(W)$. $Q_P(W)$ has a macroscopic point symmetry represented by Y_h. It has a selfsimilarity with ratio τ^3; $Q_P(\tilde{\tau}^3 W)$ is a sublattice (subset) of $Q_P(W)$ (because $\tilde{\tau}^3 W \subset W$) and is locally isomorphic to $\tau^3 Q_P(W)$ (Katz and Duneau 1986).

The projection of the Voronoi cell of $0 \in L_P$ (the origin of E_6) onto $\tilde{E}_3$ is a rhombic triacontahedron $\mathcal{T}$. $Q_P(\mathcal{T})$ is a 3D Penrose tiling with two kinds of rhombohedrons (Elser 1986, Katz and Duneau 1986).

Different icosahedral quasilattices $Q_F(\boldsymbol{\phi}, W)$ and $Q_I(\boldsymbol{\phi}, W)$ are constructed from L_F and L_I by equations similar to (4). They are sublattices of $Q_P(\boldsymbol{\phi}, W)$. $Q_F(W')$ and $Q_I(W')$ are never locally isomorphic to $Q_P(W)$ however W' is chosen. $Q_F(W)$ and $Q_I(W)$ are selfsimilar with respect to scaling with τ.

3. A general theory of a classification of the special points of a Bravais lattice

Let $\mathcal{G}$ be a d-dimensional space group and assume that it is symmorphic. Then, it is constructed as a semidirect product of a point group G and a translational group, which is identified with a Bravais lattice (a d-dimensional Z-module) L. We shall denote this fact as $\mathcal{G} = \mathrm{G} * L$. We assume that G includes the inversion operation I: $I\boldsymbol{x} = -\boldsymbol{x}$ for $\forall \boldsymbol{x} \in E_d$.

Let H be a subgroup of G. Then, we shall call H a centring (sub-)group if the origin is the only fixed point of E_d with respect to the action of H. The inversion operation I has the origin as its only fixed point, so that a subgroup of G (including itself) is a centring group if it includes I. Let H and H′ be subgroups of G such that $\mathrm{H} \subset \mathrm{H}'$ and assume that H is a centring group. Then, so is H′.

The point group of $x \in E_d$ is defined by $G(x) = \{\sigma | \sigma \in G$ and $\sigma x \equiv x \bmod L\}$. Obviously, $G(x) = G(x+l)$ for $\forall l \in L$. $G(x)$ is nothing but the isotropy group of x with respect to the action of G onto the torus, $T^d = E_d/L$ ($\simeq \mathbb{R}^d/\mathbb{Z}^d$).

$x \in E_d$ is called a special point of L if $G(x)$ is a centring group. Let x_0 be a special point (of L). Then, the set of all the translationally equivalent special points to x_0 is given by $L(x_0) = x_0 + L$ $(= \{x_0 + l | l \in L\})$, so that special points can be considered in modulo L.

If $x_0 \in E_d$ is a special point of L, we obtain that $G(\sigma x_0) = \sigma G(x_0)\sigma^{-1} \simeq G(x_0)$. Therefore, σx_0 is an equivalent special point to x_0 with respect to the space group $\mathscr{G}$. The total number of equivalent special points (modulo L) to x_0 is given by $|G|/|G(x_0)|$, which we shall call the order of x_0. It is obvious that every special point of L is an isolated point, so that the set of all the special points of L is a discrete set in E_d and the number of different special points (modulo L) is finite.

A sublattice L' of L is called a G-superlattice of L if L' is a Bravais lattice and its point group includes G. For example, L_F is a Y'_h-superlattice of L_P. Let q be the number of lattice points of L in a unit cell of L'. Then, L is divided into q sublattices which are translationally equivalent to L'.

Let L' be a G-superlattice of L. Then, $G'(x) \equiv \{\sigma | \sigma \in G$ and $\sigma x \equiv x \bmod L'\} \subset G(x)$. Therefore, a special point of L' is always a special point of L but the converse is not necessarily true. If we know all the special points of L, all the special points of L' are obtained from those by examining whether they are actually so.

Let G' be a subgroup of G. Then, $G'(x) = \{\sigma | \sigma \in G'$ and $\sigma x \equiv x \bmod L\} \subset G(x)$, $\forall x \in E_d$. Therefore, a special point of L with respect to the space group $\mathscr{g}' = G' * L$ is also a special point of L with respect to $\mathscr{g}$, but the converse is not always true. All the special points of L with respect to $\mathscr{g}'$ are obtained from those with respect to $\mathscr{g}$ by examining them. Note, however, that two equivalent special points with respect to $\mathscr{g}$ are not necessarily equivalent with respect to $\mathscr{g}'$.

The special points of L are divided into type I or II according to whether the relevant point groups include the inversion operation or not, respectively. The condition that $Ix \equiv x \bmod L$ $x \in E_d$ is equivalent to $2x \equiv 0 \bmod L$. Therefore, the set of all the type-I special points of L coincides with the half lattice, $L^{(H)} = L/2$ $(= \{l/2 | l \in L\})$. The number of the lattice points of $L^{(H)}$ in a unit cell of L is equal to 2^d.

The origin of E_d is a type-I special point of L because $G(0) = G$. Therefore, L $(= L(0))$ is a trivial but important set of equivalent special points of L . We shall denote this class of special points by Γ, following the convention in the band-structure theory of solids.

We consider here a special case where there exists a special point x_0 such that $G(x_0) = G$ but $x_0 \notin L$ (for example, this is the case for the simple cubic lattice). Then, we can show easily that $G(x) = G(x_0 + x)$ $\forall x \in E_d$. Therefore, all the special points (modulo L) are grouped into pairs such that each pair of special points have a common point symmetry and their separation is equal to x_0 in modulo L. It is usual that $2x_0 \equiv 0 \bmod L$, so that the relationship between the members of each pair is symmetric.

All the lattice points of $L^{(H)}$ are special points of L as noted previously and, moreover, L is a G-superlattice of $L^{(H)}$. There can exist other Bravais lattices having similar properties. It can be shown generally that there exists a Bravais lattice K such that K includes all the special points of L and, moreover, L is a G-superlattice of K.

E_d is divided into Voronoi cells of the lattice points of L; the cells are translationally congruent with the one centred at the origin, which we shall denote as V_0. V_0 is a polytope whose point symmetry is equal to G. A member of a translationally equivalent set of special points is included in V_0. All the special points but the Γ point included in V_0 are located on the boundary. Some of them coincide with the vertices of V_0. Others may coincide with the middle points of the edges, the centres of the 2D surfaces etc. In particular, the centre of a $(d-1)$-dimensional surface of V_0 is a type-I special point, which is equal to half a lattice vector of L; the surface bisects the lattice vector perpendicularly.

4. The special points of icosahedral lattices in 6D

In this section we shall identify Y'_h with Y_h, so that we shall denote subgroups of Y'_h by the symbols, D_{5d}, D_{2h}, etc, which represent 3D point groups.

4.1. The case of $P\bar{5}\bar{3}m$

The type-I special points of L_P are the lattice points of its half lattice $L_P^{(H)}$ and there are 64 different points modulo L_P. They are classified in I as listed in part (a) of table 1. The representative $\boldsymbol{x}_0$ of each class of special points is so chosen that the projection of the main axis of $G(\boldsymbol{x}_0)$ onto E_3 is parallel to $[\tau 10](=\boldsymbol{a}_1)$, $[111]$ or $[100]$ according as $G(\boldsymbol{x}_0)$ is isomorphic to D_{5d}, D_{3d} or D_{2h}, respectively.

Since $G(\boldsymbol{x}(R)) = Y_h$ with $\boldsymbol{x}(R) = [111111]/2$, a pair of special points, $\boldsymbol{x}_0$ and $\boldsymbol{x}(R) - \boldsymbol{x}_0$, have a common point symmetry. X_3 and M_3 would be equivalent to each other if $\Omega(6)$ were taken to be the point group of L_P.

Table 1. The special points of the 6D icosahedral lattices. The first row in each table lists symbols assigned to different classes of special points. The number suffixed to a symbol represents the order of the rotation whose axis coincides with the main axis of the point symmetry. The third row lists the number of different special points belonging to each class in a unit cell of the relevant lattice. The fourth row lists a representative of each class of special points.

(a) $P\bar{5}\bar{3}m$

symbol	Γ	X_5	X_2	X_3	M_3	M_2	M_5	R
point symmetry	Y_h	D_{5d}	D_{2h}	D_{3d}	D_{3d}	D_{2h}	D_{5d}	Y_h
order	1	6	15	10	10	15	6	1
representative	$[000000]$	$[\frac{1}{2}00000]$	$[\frac{1}{2}00\frac{1}{2}00]$	$[\frac{1}{2}\frac{1}{2}\frac{1}{2}000]$	$[000\frac{1}{2}\frac{1}{2}\frac{1}{2}]$	$[0\frac{1}{2}\frac{1}{2}0\bar{\frac{1}{2}}\frac{1}{2}]$	$[0\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\bar{\frac{1}{2}}]$	$[\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\bar{\frac{1}{2}}]$

(b) $F\bar{5}\bar{3}m$

symbol	Γ	H	N	N'	M	M'	P	P'
point symmetry	Y_h	Y_h	D_{2h}	D_{2h}	D_{2h}	D_{2h}	Y_h	Y_h
order	1	1	15	15	15	15	1	1
representative	$[000000]$	$[100000]$	$[\frac{1}{2}00\bar{\frac{1}{2}}00]$	$[0\frac{1}{2}00\frac{1}{2}0]$	$[\frac{1}{2}\frac{1}{2}0\bar{\frac{1}{2}}\frac{1}{2}0]$	$[0\frac{1}{2}\frac{1}{2}0\bar{\frac{1}{2}}\frac{1}{2}]$	$[\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\bar{\frac{1}{2}}]$	$[\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}]$

(c) $I\bar{5}\bar{3}m$

symbol	Γ	X_5	X_2	X_3	L_3	L'_3	L_5	L'_5
point symmetry	Y_h	D_{5d}	D_{2h}	D_{3d}	D_{3d}	D_{3d}	D_{5d}	D_{5d}
order	1	6	15	10	10	10	6	6
representative	$[000000]$	$[1000000]$	$[100100]$	$[111000]$	$[\frac{1}{2}\frac{1}{2}\frac{1}{2}\bar{\frac{1}{2}}\bar{\frac{1}{2}}\bar{\frac{1}{2}}]$	$[\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}]$	$[\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\bar{\frac{1}{2}}]$	$[\bar{\frac{1}{2}}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\bar{\frac{1}{2}}]$

We have mentioned in I, without any proof, that L_P has no type-II special points. We present here a proof of it. Of the centring subgroups of Y_h, only T, D_5, D_3 and D_2 do not include the inversion operation. Since T includes D_2 as its subgroup, the proposition under consideration is true if we can prove the following lemma.

Lemma. Let x_0 be a special point of L and assume that $H \subset G(x_0)$ with $H = D_5$, D_3 or D_2. Then, $x_0 \in L_P^{(H)}$.

Proof. D_5, D_3 and D_2 have ten, six and three twofold rotations respectively. Let H be one of the three point groups and assume that one of the basis vectors of L_P, say ε_i, is given. Then, there exists a twofold rotation σ of H such that $\sigma\varepsilon_i = -\varepsilon_i$. This statement can be confirmed by examining each case separately. Now, let $x_0 = [h_1 h_2 \dots h_6]$ be a special point such that $G(x_0) \supset H$. Then, we can conclude that $2h_i \equiv 0 \bmod Z$ for all i and, consequently, $x_0 \in L_P^{(H)}$. □

$V_0^{(P)}$, the Voronoi cell of the origin of L_P, is a 6D hypercube whose 64 vertices are $[h_1 h_2 \dots h_6]$ where h_i takes the values $\pm\frac{1}{2}$. That is, the vertices belong to class R of the special points of L_P. More generally, a special point is located on the centre of a k-dimensional surface (a hypercube) of $V_0^{(P)}$ if the number of zeros in the indices of the point is k.

4.2. *The case of $F\bar{5}\bar{3}m$*

The 64 type-I special points of L_F are classified as listed in part (b) of table 1. The symbols denoting different special points are chosen in analogy to the case of the face centred cubic lattice. Γ and H form L_P; $L_P = L_F \cup (x(H) + L_F)$ with $x(H) = [100000]$. P and P' are located on the body centres of the lattice L_P, so that Γ, H, P and P' form a 6D body centred hypercubic lattice $L_P \cup (x(P) + L_P)$, which is nothing but $L_I^{(H)}$. This result is consistent with the general result on the relationship between the special points of two lattices L and L' satisfying $L \subset L'$.

$V_0^{(F)}$ is a 6D polytope with 76 vertices. Twelve of them belong to H and the remaining 64 to P and P'. A 5D surface of $V_0^{(F)}$ is a polytope with 18 vertices; two of them belong to H and the remaining sixteen to P and P'. $V_0^{(F)}$ has 60 equivalent 5D surfaces whose centres belong to N and N'.

We will consider here whether L_F has any type-II special point. Since $L_F \subset L_P$, special points of L_F are those of L_P. The type-I special points of L_F are, indeed, special points of L_P. The point symmetries of other special points of L_P are D_{5d} and D_{3d}, whose centring subgroups without the inversion operation are D_5 and D_3, respectively. Let x_0 be a special point of L_P and assume that it belongs to, say, X_5. Then, it is shown easily that $\sigma x_0 - x_0$ is indexed with six integers which sum to an odd integer, where σ is any twofold rotation in $G(x_0)$ ($\simeq D_5$). Therefore, x_0 cannot be a special point of L_F. By similar arguments, we can show that M_5, X_3 and M_3 of L_P cannot be type-II special points of L_F.

4.3. *The case of $I\bar{5}\bar{3}m$*

Since $L_I = (2L_P) \cup ([111111] + 2L_P)$, we obtain $L_I^{(H)} = L_P \cup L_P'$ with $L_P' = [111111]/2 + L_P$. Therefore, 32 type-I special points of L_I form L_P and have indices with integers only. On the other hand, the remaining 32 type-I special points have indices with half-integers only. The former (or latter) 32 special points are classified into four classes as presented in the first (or last) four columns in part (*c*) of table 1. The last four classes would be equivalent if $\Omega(6)$ were taken to be the point group of L_I.

Γ and fifteen X_2 of L_I form L_F, which is a Y_h-superlattice of L_P.

Since $L_I \subset L_F$, special points of L_I are obtained from those of L_F. The question here is whether the special points N, N', M and M' in part (*b*) of table 1 are type-II special points of L_I. If the answer is affirmative the relevant point symmetry is D_2 ($\subset D_{2h}$). Let us assume that $x_0 \in E_6$ belongs to, say, N in part (*b*) of table 1. Then, we can show easily that $\sigma x_0 - x_0$ with $\sigma \in D_2$ is indexed with integers including both even and odd ones. Therefore, x_0 is not a special point of L_I. By similar arguments, we can conclude that L_I have no type-II special points.

$V_0^{(I)}$ is a 6D polytope with 160 vertices and 76 5D surfaces. The vertices belong to X_3. The centres of twelve 5D hypersurfaces belong to X_5 and the remaining 64 to L_3, L_3', L_5 and L_5'.

5. Discussions

The 4D decagonal and dodecagonal lattices investigated in Niizeki (1989b) have type-II special points. Furthermore, the *P*- (or *W*-) point of the face- (or body-) centred cubic lattice is also a type-II special point. Therefore, the present results that the three icosahedral lattices have no type-II special points are by no means obvious *a priori*, and we have presented proofs of them.

Let L be one of the three icosahedral lattices L_P, L_F and L_I and let $Q(W)$ be the icosahedral quasilattice obtained from L with window W. Then, $Q(W)$ is a discrete subset of $\pi(L)$, which is a dense set in E_3. Let $L[X]$ be the set of all the special points of L belonging to class X. Then, $\pi(L[X])$ is also a dense set. If a discrete subset of $\pi(L[X])$ is chosen appropriately, each point of the set represents the centre of a common local structure of $Q(W)$ with point symmetry $G(X)$ (Niizeki 1989b).

For example, the body centre of a rhombohedron in 3D Penrose tiling $Q_P(\mathcal{T})$ belongs to $\pi(L_P[X_3])$ or $\pi(L_P[M_3])$ depending on whether the rhombohedral angle is acute or obtuse, respectively. Similarly, the centre of a face of a rhombohedron belongs to $\pi(L_P[X_2])$. $Q_P(\mathcal{T})$ has the local structures of a rhombic icosahedron composed of two prolate rhombohedra and two oblate ones (Elser and Henley 1985, Henley 1986). It can be shown that their body centres belong to $\pi(L_P[M_2])$. Note, however, that the configuration of the interior of every rhombic icosahedron breaks the point symmetry D_{2h} (Henley 1986). We may call it a spontaneous symmetry breaking (Niizeki 1989b). We will not mention here the local structures associated with other special points of L_P.

I have not investigated yet local structures of $Q_F(W)$ nor $Q_I(W)$ for any W. The case where $W = \tilde{\pi}(V_0)$ with V_0 being the Voronoi cell of the origin will be promising; $\tilde{\pi}(V_0^{(F)})$ as well as $\tilde{\pi}(V_0^{(P)})$ is a rhombic triacontahedron, while $\tilde{\pi}(V_0^{(I)})$ is a regular dodecahedron. This subject awaits our intensive investigation.

Every icosahedral quasilattice has a selfsimilarity with ratio τ or τ^3. The local structures may change on the selfsimilarity transformation though their point symmetries cannot (Niizeki 1989b). This is because different classes of special points of L form a multiplet such that its members are permuted cyclically among themselves by the automorphism induced by M (or M^3 for the case of L_P). It is a matter of elementary algebra to find such a multiplet, so we present only the results. Γ is always a singlet. Other singlets are X_2, M_2 and R of L_P, M' of L_F and X_2 of L_I. L_P has two doublets $\{X_5, M_5\}$ and $\{X_3, M_3\}$. L_F has two triplets $\{H, P, P'\}$ and $\{N, N', M\}$. L_I has also two triplets $\{X_5, L_5, L_5'\}$ and $\{X_3, L_3, L_3'\}$. L_P has no higher multiplets than the doublets because $(M^3)^2 = 8M + 5E \equiv E \bmod 2$. On the other hand, $M^3 = 2M + E \equiv J + E \bmod 2$, with $J = {}^t uu$ where $u = (1, 1, 1, 1, 1, 1)$ is a row vector. Therefore, L_F and L_I can have triplets because $n_1 + n_2 + \ldots + n_6 \equiv 0 \bmod 2$ for $[n_1 n_2 \ldots n_6] \in L_F$ (or L_I).

The reciprocal lattice of L_P is given by $L_P^* = L_P|_{a \to a^*}$ with $a^* = 2\pi/a$, while those of L_F and L_I are by $L_F^* = L_I|_{a \to a^*}$ and $L_I^* = L_F|_{a \to a^*}$ with $a^* = \pi/a$. The relevant Voronoi cell V_0^* of each reciprocal lattice is the first Brillouin zone and the special points are high-symmetry points in the zone. On the other hand, the special points (wavevectors) in the reciprocal space of an icosahedral quasilattice are given by the projections of the special points of L_X^* with $X = \mathrm{P}$, F or I onto the 3D reciprocal space E_3^*. They form a dense set in the reciprocal space. However, the set is practically discrete because special points belonging to a single class have different intensities which are determined by the Fourier components of the window function with respect to the conjugate wavevectors (see I). Further details of this subject will be discussed elsewhere.

Let the 6D space group $\mathscr{g}'$ be a subgroup of $\mathscr{g} = \mathrm{Y}_h * L_X$ with $X = \mathrm{P}$, F or I. Then, special points defined with respect to $\mathscr{g}'$ are always special points of L_X with respect to $\mathscr{g}$. Therefore, the former special points are all obtained from the latter by examining them. Accordingly, the present results will be the basis of the investigation of special points of other icosahedral lattices including the case of a non-symmorphic space group (Janssen 1986, Rokhsar *et al* 1988, Levitov and Rhyner 1988).

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Note added in proof. Let C be a class of special points of an icosahedral lattice L_X with $X = \mathrm{P}$, F or I. Then, the local structure associated with a special point of $Q_X(W)$ with $W = \tilde{\pi}(V_0^{(X)})$ is a translate of $\pi((x_0 + L_X) \cap V_0^{(X)})$ with $x_0 \in L_X[C]$.

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