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Special lines of quasilattices: I. The case of irreducible quasilattices in two and three dimensions

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Abstract. A general theory for special lines in quasilattices is developed. Using the theory, we classify completely the special lines of the three Bravais classes of icosahedral quasilattices in three dimensions and another three of n-gonal quasilattices in two dimensions, where $n = 8$, 10 and 12. We establish compatibility relationships between the classes of special lines and those of special points for each of the six Bravais classes of quasilattices.

1. Introduction

In the one-electron theory of a periodic lattice, the energy band $E(k)$ is fundamentally important. It is usually displayed along high-symmetry directions in the reciprocal space (Koster 1957). It is stationary at high-symmetry points. We shall call these directions (or points) special lines (or points). They are generally called, together with mirror planes, special manifolds. The special manifolds of a periodic lattice in real space are called Wyckoff positions and are important in crystallography (Hahn 1987).

It has also been revealed that the electronic wavefunctions of a quasicrystal have rich structures in the reciprocal space, that is we have observed a quasi-dispersion relationship, whose change in the reciprocal space is well understood by introducing special points (Niizeki and Akamatsu 1990).

The real space structure of a quasicrystal is described by a quasilattice (QL), which is obtained by the cut-and-projection method from a periodic lattice in higher dimensions (Katz and Duneau 1986, Janssen 1988). The special points of a QL in the real space are useful in the investigation of the local structures of the QL (Niizeki 1989a).

In the case of a periodic lattice, special points or lines are located on special positions of the Wigner–Seitz cell (or the Brillouin zone in the reciprocal space (Koster 1957)). Therefore, enumeration of them and determination of their point groups are not so difficult. This, however, is not the case for QLs because their special manifolds are related to those of a periodic lattice with dimensions higher than three; we cannot visualize a higher-dimensional lattice. More precisely, it is not too difficult to determine the point group of a given special manifold but without a systematic method it is difficult to enumerate them without omission.

The special points of important QLs in two and three dimensions have been completely classified and listed (Niizeki 1989a, b, 1990a); the classification of special points in a QL is reduced to that of a higher-dimensional lattice. The situation is more

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complicated in the case of special lines as will be shown later. The purpose of the present paper is to establish a systematic method for enumerating them and to present a complete list of them for important QLs in two and three dimensions.

In section 2, we summarize the properties of irreducible QLs in two and three dimensions (see, for example, Janssen 1988). In section 3, the special lines and planes of a point group are introduced. We develop, in section 4, a systematic method for enumerating special lines of a QL. In sections 5 and 6, we classify the special lines of irreducible QLs in three and two dimensions, respectively. In section 7, we investigate the interplay between a special line of a QL and its local structures. The final section, section 8, is devoted to discussions.

2. Irreducible quasilattices in two and three dimensions

The basis vectors e_i, $i=1,\ldots,D$, of a QL in d-dimensions are linearly independent over $\mathbb{Z}$, where $D>d$. Let G be the point group of the QL; G acts on the d-dimensional Euclidean space E_d. Then $e_i \in E_d$ are transformed linearly by any $\sigma \in \mathrm{G}$ among themselves with integer coefficients. We consider only the case where E_d is irreducible with respect to G. Then D is a multiple of d. The case where $D=2d$ is important. If we restrict our considerations to 2D and 3D QLs, this condition is satisfied only when $\mathrm{G}=\mathrm{D}_8(8m)$, $\mathrm{D}_{10}(10mm)$ and $\mathrm{D}_{12}(12mm)$ in two dimensions and $\mathrm{G}=\mathrm{Y}_h(\bar{5}\bar{3}m)$ in three dimensions. We shall confine our arguments to these cases only, i.e. the octagonal, decagonal and dodecagonal QLs in two dimensions and icosahedral ones in three dimensions.

There is only one Bravais class, $Pnmm$, of 2D QLs with the n-gonal point symmetry for $n=8$, 10 or 12. On the other hand, there are three Bravais classes, $P\bar{5}\bar{3}m$, $F\bar{5}\bar{3}m$ and $I\bar{5}\bar{3}m$, of 3D QLs with icosahedral point symmetry.

The set of vectors $L=\{\Sigma_i n_i e_i \mid n_i \in Z\}$ is called a pre-quasilattice (PQL), which is a dense set of point in E_d; a QL is a discrete subset of L. L is considered to be an additive group (a Z-module). L is left invariant by the action of G.

L and G can be lifted up to a D-dimensional periodic lattice $\tilde{L}$ and its point group $\tilde{\mathrm{G}}$. More precisely, there exists conjugate basis vectors e'_i, $i=1,\ldots,D$, such that

(i) e'_i are vectors in another Euclidean space E'_d in d-dimensions.

(ii) $\tilde{e}_i=(e_i, e_{i'}) \in E_D$ $(=E_d \oplus E_{d'})$, $i=1,\ldots,D$, are the basis vectors of $\tilde{L}$.

(iii) The action of $\tilde{\mathrm{G}}$ onto E_D is reducible into the action of G onto E_d and that of another point group G′ onto E'_d, where G, G′ and $\tilde{\mathrm{G}}$ are isomorphic to each other.

L is the projection of $\tilde{L}$ onto E_d. $L'=\{\Sigma_i n_i e'_i \mid n_i \in Z\}$, the conjugate PQL to L, is the projection of $\tilde{L}$ onto E'_d. There are one-to-one correspondences among L, L' and $\tilde{L}$. We shall call E_d the real space and E'_d the conjugate space.

Many trinities of the form $\langle T, T', \tilde{T}\rangle$, which are associated with the trinity $\langle E_d, E'_d, E_D\rangle$, will appear; T' is the conjugate to T. The case $T=\mathrm{G}$ or L has appeared in a preceding paragraph.

Let us introduce a quasi-space group $\mathscr{G}$ as a semidirect product of G and L; $\mathscr{G}=\mathrm{G} * L=\{\{\sigma|l\} \mid \sigma \in \mathrm{G}, l \in L\}$. $\mathscr{G}$ is a dense subgroup of the d-dimensional Euclidean group in contrast to the ordinary space group. $\mathscr{G}$ leaves L invariant. G and L is embedded in $\mathscr{G}$; $\mathrm{G} \simeq \{\{\sigma|0\} \mid \sigma \in \mathrm{G}\}$ $(\subset \mathscr{G})$ and L is the maximal Abelian subgroup of $\mathscr{G}$. $\mathscr{G}$ is a member of the trinity $\langle \mathscr{G}, \mathscr{G}', \tilde{\mathscr{G}}\rangle$; $\tilde{\mathscr{G}}$ $(=\tilde{\mathrm{G}} * \tilde{L})$ is an ordinary space group associated with the periodic lattice $\tilde{L}$. It can be shown generally that every algebraic structure associated with one member of the trinity can be translated into those of the other two (Katz and Duneau 1986).

A PQL has a self-similarity; that is there exists an algebraic integer τ such that $\tau L\ (=\{\tau \boldsymbol{l} \mid \boldsymbol{l} \in L\}) = L$ (in the case of the dodecagonal PQL in two dimensions; however, a rotation through $\pi/12$ must follow the scaling). The self-similarity gives rise to some arbitrariness in indexing a lattice vector of L (Elser 1985, Ostlund and Wright 1986, see also Niizeki 1989a).

Let $\boldsymbol{l}\ (=\Sigma_i n_i \boldsymbol{e}_i) \in L$. Then, the 1D subspace $D(\boldsymbol{l}) = \{x\boldsymbol{l} \mid x \in \boldsymbol{R}\}$ is called a lattice direction. Since $\hat{\boldsymbol{l}} \equiv \tau \boldsymbol{l}\ (\in L)$ is parallel to $\boldsymbol{l}$, $\hat{\boldsymbol{l}}$ defines the same lattice direction as $D(\boldsymbol{l})$. More generally, for any lattice direction D, $D \cap L$ is a submodule with two basis vectors $\boldsymbol{l}_1$ and $\boldsymbol{l}_2$; $D \cap L = \{n_1 \boldsymbol{l}_1 + n_2 \boldsymbol{l}_2 \mid n_1, n_2 \in \boldsymbol{Z}\}$ (Katz and Duneau 1986). This lattice direction is denoted by $D = \boldsymbol{l}_1/\boldsymbol{l}_2$. D is a member of the trinity $\langle D, D', \tilde{D} \rangle$, where $D' = \boldsymbol{l}'_1/\boldsymbol{l}'_2$ is a lattice direction of L' and $\tilde{D}$ is the lattice plane (not a direction) of $\tilde{L}$ spanned by $\tilde{\boldsymbol{l}}_1$ and $\tilde{\boldsymbol{l}}_2$.

A line is called a lattice line (more precisely, a quasilattice line) if it passes at least two lattice points. In fact, it passes an infinite number of lattice points because it is parallel to a lattice direction, which is a special lattice line.

3. The special manifolds of a point group

Let H be a non-trivial 3D point group which fixes the origin of E_3. It is then called a centring group if the origin is the only fixed point in E_3. However, if H is a mirror group, e.g. $C_s = \{E, \sigma_h\}$, the mirror plane is a fixed plane. The remaining case is the one in which H is a polar group; in this case, there exists a fixed line, which is nothing but the axis of the polar group. There are two series of polar point groups, i.e. C_n and C_{nv} with $n \geq 2$.

The fixed line of a polar subgroup of a point group G is called as a special line (SL) of G. Two polar subgroups of G can have a common fixed line. Then, they are subgroups of a maximal polar subgroup of G. Accordingly, there exists a one-to-one correspondence between the set of all the SLs of G and that of all the maximal polar subgroups of G. If two maximal polar subgroups of G are conjugate in G, the corresponding two SLs are equivalent. The number of inequivalent SLs is equal to the number of the maximal polar subgroups which are not conjugate to each other. On the other hand, the number of equivalent SLs whose point group H is given by $|G|/(2|H|)$, where $|*|$ stands for the order of the group $*$; the factor 2 in the denominator is due to the fact that an SL is tranformed into itself by the inversion operation. A similar conclusion is also derived for the case of special planes of G.

Let H be a polar subgroup of G and assume that there exists a mirror plane (a special plane) of G such that it does not include the axis of H. Then, H and the mirror generate a centring subgroup of G.

We assume that G is the point group of a Bravais lattice (or a PQL) L. Let H be a maximal polar subgroup of G and X the corresponding SL of G. Then, there exists a lattice vector $\boldsymbol{l}_0 \in L$ such that it is not parallel to X. It follows that $\boldsymbol{l} = \Sigma_\sigma \sigma \boldsymbol{l}_0\ (\sigma \in \mathrm{H})$ is a parallel lattice vector to X. Therefore, every SL of L is parallel to a lattice direction.

We shall apply the present theory to the three icosahedral Bravais QLs, $P\bar{5}\bar{3}m$, $F\bar{5}\bar{3}m$ and $I\bar{5}\bar{3}m$. The relevant point group $Y_h(\bar{5}\bar{3}m)$ has three inequivalent SLs corresponding to its three maximal polar subgroups, C_{5v}, C_{3v} and C_{2v}. The three SLs are denoted by

Δ, Λ and Σ, respectively, which agree with the 5-, 3- and 2-fold axes of the icosahedron constructed with twelve basis vectors, $\pm e_i$, $i = 1, \ldots, 6$, of $P\bar{5}\bar{3}m$. The three lattice directions $[100000]/[01111\bar{1}]$, $[111000]/[000111]$ and $[100\bar{1}00]/[00100\bar{1}]$ of $P\bar{5}\bar{3}m$ are parallel to Δ, Λ and Σ, respectively, where the index scheme in Niizeki (1989b) is used.

Y_h has only one class of equivalent special planes corresponding to the fifteen equivalent mirror planes.

It is an important property of the point group Y_h that each of its three inequivalent maximal polar subgroups has a companion mirror in Y_h, with which it generates Y_h; this is easily confirmed for each case of C_{5v}, C_{3v} and C_{2v}, separately. O_h also has a similar property.

The present consideration also applies to the case of point groups in two dimensions. Note, however, that a mirror group in two dimensions is considered to be a polar group because it is related to an SL. Then, $D_n(nmm)$ with even n has two inequivalent SLs corresponding to two inequivalent mirrors crossing with the angle π/n; the two mirrors generate D_n. The two SLs are denoted by Δ and Σ.

D_n is the point group of the 2D n-gonal PQL *Pnmm* with $n = 8$, 10 or 12. We assume that Δ is parallel to a basis vector of *Pnmm*. Then, representatives of Δ and Σ are indexed as $[1000]/[010\bar{1}]$ and $[1100]/[001\bar{1}]$ for $n = 8$, $[10000]/[01001]$ and $[0100\bar{1}]/[001\bar{1}0]$ for $n = 10$ and $[1000]/[020\bar{1}]$ and $[1100]/[011\bar{1}]$ for $n = 12$, where the index scheme in Niizeki (1990a) is used.

4. Special lines of a PQL

The main part of the theory in this section applies to both a periodic Bravais lattice and that of a PQL, so that we will not distinguish between the two cases, if unnecessary. The theory can be readily understood by frequent reference to the three cubic Bravais lattices (Koster 1957).

4.1. General theory

We consider the case of a 3D lattice, L, whose point group is G. Let $\mathscr{H}$ be a non-trivial subgroup of the space group $\mathscr{G}$ $(= G * L)$ of L and assume that it has a fixed point. Then $\mathscr{H}$ is a point group with respect to the fixed point. The fixed manifold X of $\mathscr{H}$ is a special manifold (SM) of L or, more precisely, a special point, line or plane depending on whether $\dim(X)$ is equal to 0, 1 or 2, respectively. If $\mathscr{H}$ is the maximal point group among those which are subgroups of $\mathscr{G}$ and leave X invariant, it is called the point group of X. Let H be the 'rotational part' of $\mathscr{H}$. Then, H is a subgroup of G and $H \simeq \mathscr{H}$. We shall sometimes identify $\mathscr{H}$ with H. Then, we will use the latter symbol.

Let $\alpha \in \mathscr{G}$. Then, $\hat{X} = \alpha X$ $(\equiv \{\alpha x \mid x \in X\})$ is an equivalent SM of L to X; the point group of $\hat{X}$ is given by $\hat{\mathscr{H}} = \alpha \mathscr{H} \alpha^{-1}$, which is conjugate to $\mathscr{H}$ in $\mathscr{G}$. In particular, if $\alpha = \{E \mid l\}$ with $l \in L$, then $\hat{X} = l + X$ $(= \{l + x \mid x \in X\})$ is translationally equivalent to X and $\hat{\mathscr{H}}$ is 'translationally equivalent' to $\mathscr{H}$; the rotational part is common between $\mathscr{H}$ and $\hat{\mathscr{H}}$. Two equivalent SMs usually have different orientations if they are not translationally equivalent. In particular, two equivalent special points can have different 'orientations' because the relevant point groups can be 'translationally inequivalent'. The set of all the equivalent SMs form a class; the point group of the class is defined by the point group of a representative of the class. We will see that a lattice has only finitely many classes of SMs.

$\mathcal{H}$ is a member of the trinity $\langle\mathcal{H}, \mathcal{H}', \tilde{\mathcal{H}}\rangle$, so that X is a member of the trinity $\langle X, X', \tilde{X}\rangle$, where X' (or $\tilde{X}$) is an SM of L' (or $\tilde{L}$); X (or X') is the projection of $\tilde{X}$ onto E_3 (or E_3'). Note, however, that $\dim(\tilde{X}) = 2\dim(X)$, so that an SL of L, for example, is a projection of a special plane of $\tilde{L}$.

We have presented a complete classification of the special points of important PQLs (or QLs) in two and three dimensions (Niizeki 1989a, b, 1990a). In every PQL, the lattice points form a class Γ of special points with the full symmetry. In some cases, there exists a class of non-trivial full symmetry points.

An SL of L is classified as type I or II according to whether it passes a lattice point of L or not, respectively. A class of type I (or II) SLs is denoted by a Greek (or Roman) letter following the convention from band theory (Koster 1957). A representative of a class of a type I SL passes the origin. Accordingly, it is simultaneously an SL of G because G is embedded in $\mathcal{G}$. Therefore, the theory developed in section 3 can be considered to give classifications of the type I SL of the QLs. A type I class of SL is denoted by the same symbol as that used for the corresponding SL of G though the two classes are logically different.

Let X be an SL of L. Then, we can choose a special plane Y of L in such a way that the axis of the point group H of X is not parallel to Y. It follows that $X \cap Y = \{x_0\}$, where x_0 is the crossing point between X and Y. x_0 is a special point of L; the point group of x_0 is equal to (or included in) the centring group generated by H and the mirror; that is every special line passes a special point. Conversely, let x_0 be a special point and assume that its point group K has a polar subgroup H. Then, a line which passes x_0 and is parallel to the axis of H is an SL. We can assume that H is a maximal polar subgroup of K. Then H is the point group of the SL. H as well as K is a subgroup of G. However, H is not always a maximal polar subgroup of G. Since a polar subgroup (exactly, its rotational part) of $\mathcal{G}$ is simultaneously a polar subgroup of G, an SL of L is parallel to an SL of G and, consequently, to a lattice direction. A type I SL is nothing but a high-symmetry lattice line.

This consideration shows that every SL is obtained from a special point and its maximal polar subgroup. Since an SL passing a special point x_0 is parallel to a lattice direction, it passes an infinite number of special points, which are translationally equivalent to x_0. Moreover, it is usual that the SL passes special points belonging to a different class from that of x_0. Therefore, SLs obtained from special points belonging to different classes may be equivalent. The total number of the classes of SLs of a lattice is usually smaller than that of special points. On the other hand, the number of translationally inequivalent SLs in a class of SLs is given by $|G|/(2|H|)$, where H is the point group of the class.

A necessary and sufficient condition for an SL X to pass a special point x_0 is that the point group of X is a maximal polar subgroup of the point group of x_0. As a corollary of this proposition, we can assert that an SL must be of type II if its point group is not a maximal polar subgroup of G. Let x_0 be a special point of L and assume that a maximal polar subgroup H of the point group of x_0 is not a maximal polar subgroup of G. Then, an SL obtained from x_0 and H is of type II on account of the corollary. We shall call a type II SL with this property a type IIb SL while the one without this property will be a type IIa SL. Two translationally inequivalent SLs in every class of type IIb SLs can be parallel. For example, the class Q of SLs of the BCC lattice is of type IIb (see Koster 1957).

Let X be an SL which passes a special point x_0 and is parallel to a lattice direction l_1/l_2. Then, the corresponding special plane $\tilde{X}$ of $\tilde{L}$ passes $\tilde{x}_0 = (x_0, x_0')$ and is parallel to the lattice plane $\{n_1\tilde{l}_1 + n_2\tilde{l}_2 | n_1, n_2 \in Z\}$.

Let H be a maximal polar subgroup of G and assume that G is generated by H and a mirror of G. Then, an SL whose point group is H passes a special point with the full symmetry; the point is the crossing point between the SL and a special plane associated with the mirror. Such an SL is of type I or type IIa; it must pass a non-trivial full symmetry point (NTFSP) in the latter case. If all the maximal polar subgroups of G have this property, e.g. the case of Y_h (or O_h), every type IIa SL passes a NTFSP.

4.2. *The dual transformation of SMs*

We consider the case where L has a NTFSP x_0. x_0 must be translationally equivalent to $-x_0$ or, equivalently, $2x_0 \in L$ because G has the inversion operation. The dual lattice† to L is defined by $L^{\#} = x_0 + L$. The space group is common between L and $L^{\#}$, so that all the SMs are also common between them. L is called self-dual because L and $L^{\#}$ are equivalent. Note that L and $L^{\#}$ form a black-and-white Bravais lattice (or PQL) (Niizeki 1990b). We do not define 'the dual lattice' for a non-self-dual lattice because it is of no use in this paper.

Let x_0 be a NTFSP of a self-dual lattice L and X an SM of L. Then, $X^{\#} = x_0 + X$ is also an SM with the same (exactly, isomorphic) point group as that of X. The transformation of X into $X^{\#}$ is called the dual transformation (DT); the double DT changes X into another SM which is translationally equivalent to X. If a class of SMs is invariant against the DT, it is self-dual and forms a singlet with respect to the DT. A non-self-dual class of SMs is a member of a doublet composed of a dual pair. In particular, Γ $(= L)$ and $L^{\#}$ form a doublet. On the contrary, C of $P8mm$, for example, forms a singlet (Niizeki 1989a).

A necessary and sufficient condition for a class of type I SLs to be self-dual is that every SL of the class passes a NTFSP in $L^{\#}$ or, equivalently, that the class is of type I also as a class of SLs of $L^{\#}$. On the other hand, if one member of a doublet of SLs is of type I, the other must be of type IIa.

From these considerations, we can concluded that a type IIa SL of a self-dual lattice L is obtained by a DT from a type I SL X which is non-self-dual; the dual $X^{\#}$ to X is parallel to X. All the type IIa SLs of the icosahedral PQLs (or the three cubic Bravais lattices) are obtained in this way for the reason mentioned at the end of section 4.1.

4.3. *Multiplet structures of SMs with respect to a self-similarity transformation*

We have shown previously (Niizeki 1989a, b) that the classes of special points of a PQL are divided into several multiplets with respect to the self-similarity transformation (ST) of the PQL; the members of a multiplet are permutated cyclically on the ST. In particular, Γ always forms a singlet. On the other hand, H, P and P′ of $F\bar{5}\bar{3}m$ or X_5, L_5 and L_5' of $I\bar{5}\bar{3}m$, for example, form a triplet. The classes of SLs are similarly divided into multiplets with respect to the ST. The point group must be common among the members of a multiplet because the ST is commutable with $\mathscr{G}$ $(= \mathrm{G} * L)$.

† Note that 'dual lattice' is sometimes used in conventional crystallography as the term representing the reciprocal lattice.

Since Γ is invariant against the ST, a type I (or II) SL is changed by the ST into another type I (or II) SL. More precisely, the members of a multiplet of SLs must be all type I, all type IIa or all type IIb.

4.4. *Compatibility between special points and special lines*

An SL belonging to a class C can pass a special point x_0 belonging to a class C' if the point group of C is a maximal polar subgroup of that of C'. Then, we shall say that the class C is compatible with C'. The compatibility relationships must be consistent with the multiplet structures of SMs with respect to both the ST and the DT: (i) if a class C of special lines (or points) forms a singlet and a class C' of special points (or lines) belonging to a multiplet is compatible with C then, other members of the multiplet are also compatible with C; and (ii) if different members of a multiplet of special points are compatible with those of SLs, both the multiplets must be consistent.

5. A classification of SLs icosahedral PQLs

In this section, we suppose that the results of Niizeki (1989b) are well known. The point groups of the special points of icosahedral QLs are Y_h, D_{2h}, D_{5d} and D_{3d}. Their maximal polar subgroups are C_{5v}, C_{3v}, C_{2v} and C_2. The last one, C_2, is maximal in D_{5d} and D_{3d} but not in Y_h and D_{2h}. Therefore, an SL associated with C_2 is of type IIb. It is parallel to Σ. We list in table 1 the classes of the SLs of the three icosahedral PQLs together with the compatibility relationships between them and the classes of special points. We later consider the three cases, $P\bar{5}\bar{3}m$, $F\bar{5}\bar{3}m$ and $I\bar{5}\bar{3}m$, separately.

$P\bar{5}\bar{3}m$ is a self-dual PQL with only one class, R, of NTFSPs. Of the three lattice directions Δ, Λ and Σ of Y_h, Δ and Λ give self-dual classes of type I SLs. On the other hand, Σ does not pass any NTFSP, so that its dual, S, is a class of type IIa SLs. Σ and S form a doublet. $P\bar{5}\bar{3}m$ has four classes, X_5, X_3, M_5 and M_3, of special points with point groups D_{5d} or D_{3d} but it has only one class, C, of the type IIb SL because this class is compatible with all the four classes of the special points. C is self-dual.

$F\bar{5}\bar{3}m$ is a self-dual PQL with three classes, H, P and P', of NTFSPs. Correspondingly, $F\bar{5}\bar{3}m$ has three kinds of DTs. Δ and Λ are self-dual as in $P\bar{5}\bar{3}m$. $F\bar{5}\bar{3}m$ has three classes, S, T and U, of type IIa SLs which are dual to Σ with respect to the three DTs. $F\bar{5}\bar{3}m$ has no type IIb SLs because the point groups of its special points are limited to Y_h and D_{2h}. Note that the indices of a special point of M' are mistaken in Niizeki (1989b) (a bar on an index should be deleted).

$I\bar{5}\bar{3}m$ is not self-dual, so that it has no type IIa SLs. $I\bar{5}\bar{3}m$ has six classes, X_5, X_3, L_5, L_5', L_3 and L_3', of special points with point groups D_{5d} or D_{3d}. By a similar argument as in the case of $P\bar{5}\bar{3}m$, we can conclude that $I\bar{5}\bar{3}m$ has three classes C, D and E, of type IIb SLs as listed in table 1(c). In the table we have exchanged the symbols L_3 and L_3' of the special points in comparison with those adopted in Niizeki (1989b), so that the consistency between the multiplet structure of the SLs and that of the special points becomes more symmetrical.

Each of the three classes, Δ, Λ and Σ, of type I SLs of an icosahedral PQL must form a singlet with respect to the ST. Also, S or C of $P\bar{5}\bar{3}m$ forms a singlet. S, T and U of $F\bar{5}\bar{3}m$ and C, D and E of $I\bar{5}\bar{3}m$ form triplets, respectively.

Table 1. The special lines of the three Bravais classes of icosahedral QLs and their compatibility relationships with the classes of special points.

Table 1(*a*), (*b*) or (*c*) refers to $P\bar{5}3m$, $F53m$ or $I53m$, respectively. The symbols of the special points are the same as those in Niizeki (1989b) but the L_3 and L'_3 of $I\bar{5}\bar{3}m$ have been exchanged for convenience. The symbol enclosed by parentheses stands for the point group of the relevant SL. An asterisk in each table represents that the relevant class of SLs is compatible with that of the special points; an SL belonging to the former class passes a special point to the latter.

An SL belonging to Δ (or Λ) is parallel to a 5(or 3)-fold axis of the icosahedron constructed with the twelve basis vectors, $\pm e_i$, $i=1,\ldots,6$, of $P\bar{5}\bar{3}m$. An SL belonging to another class is parallel to a 2-fold axis. More precisely, a representative SL in Δ, Λ or Σ is indexed as $[xyyyy\bar{y}]$, $[xxxyyy]$ or $[x0yx0\bar{y}]$, respectively, where $x, y \in \mathbb{R}$ and the index scheme in Niizeki (1989b) is used. On the other hand, SLs belonging to other classes are of type II and a representative SL in each class is represented as $x_0+[x0yx0\bar{y}]$, where x_0 is an appropriate special point on the SL. x_0 is listed in the last column in each table, where the symbol 'h' in an index stands for $\frac{1}{2}$.

	Γ	X_5	X_2	X_3	M_3	M_2	M_5	R	x_0
(*a*) $P\bar{5}\bar{3}m$									
$\Delta(C_{5v})$	*	*					*	*	
$\Lambda(C_{3v})$	*			*	*			*	
$\Sigma(C_{2v})$	*		*			*			
$S(C_{2v})$			*			*		*	$[0h00h0]$
$C(C_2)$		*		*	*		*		$[0h0000]$

	Γ	H	P	P'	M'	M	N	N'	x_0
(*b*) $F\bar{5}\bar{3}m$									
$\Delta(C_{5v})$	*	*	*	*					
$\Lambda(C_{3v})$	*	*	*	*					
$\Sigma(C_{2v})$	*					*	*	*	
$S(C_{2v})$		*			*		*	*	$[010000]$
$T(C_{2v})$			*		*	*		*	$[0h00h0]$
$U(C_{2v})$				*	*	*	*		$[0h00\bar{h}0]$

	Γ	X_2	X_5	L_5	L'_5	X_3	L_3	L'_3	x_0
(*c*) $I\bar{5}\bar{3}m$									
$\Delta(C_{5v})$	*		*	*	*				
$\Lambda(C_{3v})$	*					*	*	*	
$\Sigma(C_{2v})$	*	*							
$C(C_2)$			*			*			$[010000]$
$D(C_2)$				*			*		$[hhh\bar{h}hh]$
$E(C_2)$					*			*	$[h\bar{h}h\bar{h}hh]$

The subgroup D_{2h} of Y_h has three maximal polar subgroups which are isomorphic to C_{2v}. The three are conjugate to each other in Y_h but not in D_{2h}. Accordingly, special points belonging to a single class with point group D_{2h} (e.g. X_2 of $P\bar{5}\bar{3}m$) can be located on an SL (e.g. Σ or S of $P\bar{5}\bar{3}m$) in different orientations. In this respect, we remark that the quasi-dispersion relationship of an electron on $P\bar{5}\bar{3}m$ is displayed along a Σ and an S in Niizeki and Akamatsu (1990).

Prior to closing this section, we should remark that SLs of $P\bar{5}\bar{3}m$ have been classified by Janssen (1988). The compatibility relationships are, however, not presented.

6. Classification of SLs of the octagonal, decagonal and dodecagonal PQLs in two dimensions

Since a mirror subgroup of a 2D point group is always a maximal polar subgroup, an n-gonal PQL, *Pnmm*, cannot have any type IIb SLs. D_n with even n is generated by a pair of its inequivalent mirrors, so that a type II SL of *Pnmm* must pass a NTFSP. According to Niizeki (1989a), *P*10*mm* and *P*12*mm* are not self-dual, so that the two PQLs have only type I SLs. On the contrary, *P*8*mm* is self-dual and has one class, *O*, of NTFSPs. Σ of *P*8*mm* is self-dual with respect to the DT but Δ is not. The dual, *Y*, to Δ is the only class of type IIa SLs. The present result is similar to the fact that a 2D square lattice has one class of type IIa SLs but a 2D triangular lattice has none.

Both Δ and Σ form singlets in the case of *P*8*mm* or *P*10*mm* with respect to the ST. In contrast, Δ and Σ of *P*12*mm* form a doublet because the ST of the PQL accompanies a rotation through $\pi/12$ (Niizeki 1989a).

We list in table 2 the classes of the SLs of the 2D PQLs and their compatibility relationships with the classes of special points†. If a special point is compatible with both Δ and Σ it has a point group generated by two mirrors associated with Δ and Σ, where we have assumed that *Y* in the case of *P*8*mm* is merged into Δ. In contrast, if

Table 2. A similar table to table 1 but for octagonal (a), decagonal (b) and dodecagonal (c) QLs in two dimensions.

The symbols of the special points are the same as those in Niizeki (1989a) but the symbol C' has been changed into M. An SL belonging to Δ or Y is parallel to a basis vector of the relevant QL but the one to Σ is parallel to a direction with angle π/n from a basis vector with $n = 8$, 10 or 12.

A representative SL in each class of SLs is presented in the last column in each table. Note that the index scheme in Niizeki (1990a) has been used.

	Γ	*X*	*C*	*M*	*R*	*O*	Repres.
(a) *P*8*mm*							
Δ	*	*		*	*		$[xy0\bar{y}]$
Σ	*		*			*	$[yxxy]$
Y		*		*	*	*	$[xyh\bar{y}]$

	Γ	*X*	*C*	*M*	*P*	*P'*	Repres.
(b) *P*10*mm*							
Δ	*	*	*	*			$[xy00y]$
Σ	*	*	*	*	*	*	$[0xy\bar{y}\bar{x}]$

	Γ	*X*	*C*	*M*	*T*	*T'*	Repres.
(c) *P*12*mm*							
Δ	*	*		*	*		$[yxy0]$
Σ	*		*	*		*	$[yxxy]$

† The symbol C' of a class of special points in Niizeki (1989a) has been replaced by M in this paper. Note also that bars should be put on the first and last indices of P' in the table of the special points of *P*10*mm* in Niizeki (1989a).

a special point is compatible with only Δ (or Σ) it has a point group generated by two mirrors both of which are associated with Δ (or Σ).

7. Special manifolds of a QL

A PQL, L, in d-dimensions is a dense set of points in E_d. A QL is its discrete subset, $Q \equiv Q(\boldsymbol{\phi}, W) = \{\boldsymbol{l} \mid \boldsymbol{l} \in L, \boldsymbol{l}' \in \boldsymbol{\phi} + W\}$, where $\boldsymbol{l}'$ is the conjugate of $\boldsymbol{l}$, $\boldsymbol{\phi}$ the phase vector in E'_d and W the window; W is a symmetrical domain in E'_d. Q is a member of the trinity $\langle Q, Q', \tilde{Q}\rangle$, where $\tilde{Q}$ is obtained from $\tilde{L}$ by cutting it with the strip, $S(\boldsymbol{\phi}, W) = E_d + (\boldsymbol{\phi} + W)$ (Katz and Duneau 1986).

Since L is identical to the class Γ of special points of L, we consider the lattice points of Q (= $Q(\boldsymbol{\phi}, W)$) to be special points of Q; they form the class Γ of Q (Niizeki 1989a). In the general case, a class of special points of Q is similarly obtained from a class X of L; it is natural (but not compulsory) to use the same strip, $S(\boldsymbol{\phi}, W)$, for the cutting procedure. The resulting set of special points is denoted as $Q_X(\boldsymbol{\phi}, W)$, which is also a QL with the same point group as that of Q. Q_X is of the non-Bravais-type except for the case in which X is a class of NTFSPs (Niizeki 1989a). In the exceptional case, Q_X is the dual QL to Q and is locally isomorphic to Q; Q and Q_X form a black-and-white Bravais QL (Niizeki 1990b).

A special point is usually located on the centre of a local symmetry of Q; the local symmetry should be consistent with the point group of the special point but is sometimes broken 'spontaneously' (Niizeki 1989a). For example, X, C, M, R or O of the 2D octagonal QL ($P8mm$) as presented in figure 1 is located on the centre of a bond, a rhombus, a square, a thin hexagon or a regular octagon, respectively, where a hexagon (or an octagon) is formed of two (or four) rhombi and one (or two) square(s); the interior structure of a hexagon (or an octagon) breaks the point symmetry D_2 (or D_8) of R (or O).

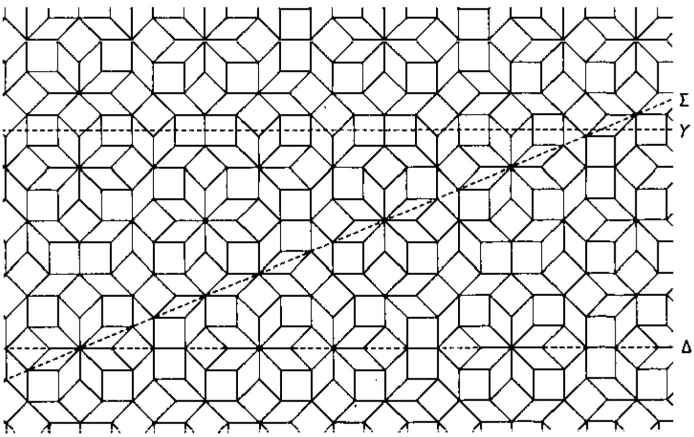

Figure 1. The 2D octagonal QL ($P8mm$) obtained from a simple hypercubic lattice in four dimensions. The centre of a bond, a rhombus, a square, a thin hexagon or a regular octagon is a special point of type X, C, M, R or O, respectively, where a hexagon or an octagon is a composite of rhombi and square(s). The lines show representatives of three classes, Δ, Σ and Y, of SLs of the QL. We can confirm the compatibility relationships in table 2(a).

We consider next the case of SLs. SLs of a single class C are also embedded densely into E_d. Let $Q(\boldsymbol{\phi}, W)$ be a QL derived from L. Then, $C(\boldsymbol{\phi}, W) = \{X \mid X \in C, X' \cap (\boldsymbol{\phi} + W) \neq \varnothing\}$ is a 'discrete' subset of C in the sense that only a finite number of SLs included in $C(\boldsymbol{\phi}, W)$ can pass a given finite domain in E_d.

In the case where C is of type I, an SL in $C(\boldsymbol{\phi}, W)$ passes an infinite number of lattice points of $Q(\boldsymbol{\phi}, W)$ but the one in $C - C(\boldsymbol{\phi}, W)$ passes none; an SL in $C(\boldsymbol{\phi}, W)$ represents a lattice line of $Q(\boldsymbol{\phi}, W)$. It can be shown that the lattice points on an SL X of $C(\boldsymbol{\phi}, W)$ form a 1D QL obtained from a 2D lattice $\tilde{L} \cap \tilde{X}$ with the strip $S(\boldsymbol{\phi}, W) \cap \tilde{X}$. From these arguments, it is natural to consider $C(\boldsymbol{\phi}, W)$ as a class of SLs of $Q(\boldsymbol{\phi}, W)$ irrespective of whether C is of type I or II.

We show, in figure 1, representatives of three classes of SLs of the 2D octagonal QL. We can confirm the compatibility relationships in table 2(a). Note that the SL belonging to Σ cuts the rhombi in two ways, which implies that special points belonging to C are located on the SL in two orientations.

8. Discussions

A symmorphic space group is a subgroup of the space group of a Bravais lattice which represents the translational part of the former group. Therefore, the SLs of the former must be simultaneously those of the latter (but the converse is not always true). The remaining task in this case is to determine the point group of each class of SLs; it is a subgroup of the point group of the relevant class of SLs of the Bravais lattice. This can be readily implemented.

However, the situation is more complicated in the case of a non-symmorphic space group. Nevertheless, the classification of its SLs (more generally, special manifolds) is reduced to the case of a Bravais lattice because it is a subgroup of the space group of an appropriate Bravais lattice.

The classification of the SLs of a PQL, L, is equivalent to that of the special planes of $\tilde{L}$. The latter task is, however, not easier than the former in contrast to the case of special points (Niizeki 1989a, b). This is the reason why the present classification of the SLs of a PQL is implemented in E_d, the real space, but not in E_D.

In the present paper, we have concentrated mainly on SLs. A similar consideration applies to the case of special planes. We can conclude that each of the three icosahedral PQLs has only one class of special planes, which are lattice planes with the mirror symmetry; every special plane is perpendicular to a 2-fold axis. Every SL of type I or IIa is included in a special plane because its point group includes a mirror but an SL of type IIb is not. By a similar reason, every special point is located on a special plane.

We have defined in section 7 $C(\boldsymbol{\phi}, W)$, i.e. a class of SLs of a $Q(\boldsymbol{\phi}, W)$. Let $\mathscr{L}(\boldsymbol{\phi}, W)$ be the union of all SLs in $C(\boldsymbol{\phi}, W)$. Then, it represents a quasiperiodic linear grid in E_d. In the case of a 3D QL, we can define also a quasiperiodic planer grid from a class of special planes. These grids are closely related to the structure of the relevant QL. The details of this subject will be discussed elsewhere.

Let X be an SM of a PQL, L, and let $\tilde{\boldsymbol{x}} = (\boldsymbol{x}, \boldsymbol{x}') \in \tilde{X}$. Then, the shifted QL, $Q = \boldsymbol{x} + Q(-\boldsymbol{x}', W)$, has a global point symmetry, whose point group is the same as that of X; the centre of the symmetry is located at the origin. Note, however, that the point symmetry of Q is broken spontaneously in the case where $S(-\boldsymbol{x}', W)$ is a singular strip (Niizeki 1989a). If X is a special point, Q has the centre of the global symmetry. On the other hand, if X is an SL, Q has an axial symmetry. In the final case where X

is a special plane, Q has a mirror symmetry. Therefore, the present investigation together with those in Niizeki (1989a, b) provides us with a complete list of QLs with global point symmetries, though limited to the cases of irreducible QLs in two and three dimensions. In this respect, we should remark that the 2D Penrose tilings with global point symmetries have been classified by de Bruijn (1981).

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