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Special points of (2+1)-reducible quasilattices in three dimensions

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Abstract. We present a complete classification of special points of five-dimensional (5D) Bravais lattices which yield with the cut-and-projection method (2+1)-reducible quasilattices in 3D; the quasilattices are periodic along the c axis but quasiperiodic only along the plane perpendicular to it. There exist five Bravais classes of 5D lattices associated with the (2+1)-reducible quasilattices, namely primitive octagonal, decagonal and dodecagonal lattices, the centred octagonal lattice and the pentagonal lattice. We discuss also the special points of the reciprocal lattices of these 5D lattices.

1. Introduction

A point in three-dimensional (3D) Euclidean space is called a special point of a lattice if its point symmetry with respect to the lattice has the centre of symmetry. In other words, a special point is an isolated point whose point symmetry is higher than those of neighbouring sites. The atoms in a crystal with a simple chemical formula occupy special points of a lattice.

The special points of the reciprocal lattice of a periodic lattice are important in the band theory of solids because the dispersion relation of electron or phonon is stationary at these points and, moreover, the band degeneracy can occur at these points.

The quasicrystal has a novel structure which has a 3D positional long-range order but has a non-crystallographic point symmetry (Henley 1987). It cannot be periodic but quasiperiodic. The quasilattice (QL) is a basic geometrical object which is useful in analysing the structure of a quasicrystal. A QL is usually obtained with the cut-and-projection method from a higher-dimensional periodic lattice (Janssen 1988). A QL has at most one point with a global point symmetry but an infinite number of points with local point symmetries. The centres of the local symmetries of a QL are the projections of the special points of the higher-dimensional lattice (Niizeki 1989c, d; to be referred to as I and II, respectively). It has been shown that the special points in the reciprocal space of a QL are useful in understanding the reciprocal space properties of electronic wavefunctions in a quasicrystal (Niizeki and Akamatsu 1990).

We have presented in I and II complete classifications of three Bravais classes of 4D lattices associated with octagonal, decagonal and dodecagonal QL in 2D and the three Bravais classes of 6D lattices associated with the 3D icosahedral QL†.

Actual octagonal, decagonal and dodecagonal quasicrystals are obviously three-dimensional; they are periodic along the c axis but quasiperiodic only along the plane

† The special points of the 4D decagonal lattice and the 6D primitive icosahedral lattice are given also in Janssen (1988).

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perpendicular to it (Janssen 1988). The point groups of these quasicrystals are D_{mh} with $m=8$, 10 or 12, or their non-crystallographic subgroups. D_{mh} is represented as a direct product, $D_{mh}=C_{mv}\times C_s$, where C_{mv} acts on the plane (the 2D subspace) and $C_s=\{E,\sigma_h\}$ on the axis (the 1D subspace). Accordingly, the 3D quasilattices with these symmetries are called (2+1)-reducible. The (2+1)-reducible QL are obtained from (2+1)-reducible 5D Bravais lattices with appropriate point symmetries (exactly speaking, the 5D lattices are (2+2+1)-reducible). There exist five Bravais classes of (2+1)-reducible 5D Bravais lattices, i.e. the primitive octagonal, decagonal and dodecagonal lattices, the centred octagonal lattice and the pentagonal lattice (Janssen 1988, Gähler 1989). The object of the present paper is to present a complete classification of the special points of these lattices and their reciprocal lattices.

In section 2, we will review the properties of m-gonal lattices in 4D and 5D (Janssen 1988, Niizeki 1989a, b and Gähler 1989). Since the relationships between m-gonal lattices in 4D (or 5D) and their reciprocal lattices have not been presented systematically to date, we present them in section 3. We develop in section 4 a general theory of special points, most of which will be summaries of the theories presented in I and II. The special points of the (2+1)-reducible Bravais lattices in 5D are classified in section 5. The content of this section is the main contribution of this paper. We investigate in section 6 the transformation among the special points of a 5D lattice under its automorphism which is related to self-similarity of the QL derived from the 5D lattice. In section 7 we discuss briefly the special points of the reciprocal lattices of the 5D lattices. We also discuss the special points of (2+1)-reducible QL derived from the 5D lattices.

2. The (2+1)-reducible Bravais lattices in 5D

The point group of a (2+1)-reducible Bravais lattice in 5D is isomorphic with that of a 3D QL derived from the lattice and we shall identify the former with the latter. A (2+1)-reducible Bravais lattice in 5D is a periodic stacking of 4D m-gonal lattices with $m=8$, 10 or 12 along the fifth axis. The fifth axis is called the c axis (or the z axis) because it turns to the c axis of the 3D (2+1)-reducible QL derived from the 5D lattice. We introduce the 4D lattices before introducing the 5D lattices.

2.1. *The octagonal, decagonal and dodecagonal lattices in 4D*

The 4D Euclidean space, E_4, is divided into the parallel (or real) subspace $E_\parallel$ and the perpendicular (or internal) subspace $E_\perp$ as $E_4=E_\parallel\oplus E_\perp$; both of $E_\parallel$ and $E_\perp$ are 2D Euclidean spaces. We shall identify a 2D Euclidean space with the complex plane and a 2D vector with a complex number. Then, $E_4=E_\parallel\oplus E_\perp$ is identified with the complex 2D space $E_4\simeq \boldsymbol{C}\oplus\boldsymbol{C}\equiv\boldsymbol{C}^2$ and $\boldsymbol{x}\in E_4$ is represented as $\boldsymbol{x}=(z_\parallel, z_\perp)\in\boldsymbol{C}^2$.

The point group of the m-gonal lattice in 4D is (2+2)-reducible and the first component of the reduction is equal to C_{mv} ($\simeq D_m$), which acts on the parallel space (the second component C'_{mv} is isomorphic to the first, but this isomorphism is external, i.e. $C'_{mv}\neq\sigma C_{mv}\sigma^{-1}\ \forall\sigma\in C_{mv}$). The 4D point group is identified with the 2D one.

The basis vectors $\boldsymbol{e}_i$, $i=0$–3, of the 4D octagonal or dodecagonal lattice L_m with $m=8$ or 12 are given by

$$\boldsymbol{e}_i=(a_\parallel\zeta^i, a_\perp(-\zeta)^i) \qquad (1)$$

with $\zeta = \exp(2\pi i/m)$. The m-gonal lattice is represented with respect to these basis vectors as

$$L_m = \left\{ \sum_{i=0}^{3} n_i \boldsymbol{e}_i \mid n_i \in \boldsymbol{Z} \right\}. \tag{2}$$

In the special case where $a_\parallel = a_\perp$, L_8 coincides with a 4D simple hypercubic lattice $L_{4,\mathrm{hc}}$. A general octagonal lattice is an octagonal affine distortion of $L_{4,\mathrm{hc}}$; the affine transformation scales $E_\parallel$ and $E_\perp$ differently. Note that the lattice constant $a_\perp$ can be chosen arbitrarily because L_m is to be projected along $E_\perp$.

We adopt in this paper an overcomplete but symmetrical basis system, $\boldsymbol{e}_i$, $i = 0$–4, for the decagonal lattice L_{10}, where

$$\boldsymbol{e}_i = (a_\parallel \zeta^i, a_\perp \zeta^{2i}) \tag{3}$$

with $\zeta = \exp(2\pi i/5)$. Then, L_{10} is given by

$$L_{10} = \left\{ \sum_{i=0}^{4} n_i \boldsymbol{e}_i \mid n_i \in \boldsymbol{Z} \text{ and } 0 \leq n_0 + n_1 + \ldots + n_4 \leq 4 \right\}. \tag{4}$$

The volume of the unit cell of L_m is given by $\Omega_m = |\det(\boldsymbol{e}_0 \boldsymbol{e}_1 \boldsymbol{e}_2 \boldsymbol{e}_3)|$. It is written as $\Omega_m = \omega_m (a_\parallel a_\perp)^2$, where the numerical factor ω_m takes on the values 4, $5\sqrt{5}/4$ or 3 according as $m = 8$, 10 or 12, respectively.

The projection of L_m onto $E_\parallel$ is equal to $a_\parallel \boldsymbol{Z}_m(\zeta)$ with $\zeta = \exp(2\pi i/m)$ for $m = 8$ and 12 or $\zeta = \exp(2\pi i/5)$ for $m = 10$, where

$$\boldsymbol{Z}_m(\zeta) = \left\{ \sum_{i=0}^{4} n_i \zeta^i \mid n_i \in \boldsymbol{Z} \right\} \tag{5}$$

is an integral domain of biquadratic algebraic integers. Let $\zeta' = -\zeta$ for $m = 8$ and 12 or $\zeta' = \zeta^2$ for $m = 10$. Then, ζ' is an algebraic conjugate (not the complex conjugate) of ζ in $\boldsymbol{Z}_m(\zeta)$ and $\boldsymbol{Z}_m(\zeta) = \boldsymbol{Z}_m(\zeta')$. Note that $\zeta^{m/2} = -1$ for $m = 8$ and 12 but $= 1$ for $m = 10$. More precisely, $P_m(\zeta) = 0$ with $P_8(x) = x^4 + 1$, $P_{10}(x) = x^4 + x^3 + x^2 + x + 1$ and $P_{12}(x) = x^4 - x^2 + 1$.

Let $\sigma = \Sigma_i k_i \zeta^i \in \boldsymbol{Z}_m(\zeta)$. Then, a special 4D affine transformation $\hat{\sigma}$ is defined as follows: $\boldsymbol{x} = (z_\parallel, z_\perp) \to \hat{\sigma}\boldsymbol{x} = (\sigma z_\parallel, \sigma' z_\perp)$ with $\sigma' = \Sigma_i k_i (\zeta')^i$ being the algebraic conjugate of σ. $\hat{\sigma}$ acts as a similarity transformation onto $E_\parallel$ (or $E_\perp$) with the ratio $|\sigma|$ (or $|\sigma'|$). L_m is transformed by $\hat{\sigma}$ to its superlattice $\hat{\sigma}L_m$ ($\subset L_m$), which is another m-gonal lattice (Niizeki 1989b). Then, the volume of the unit cell is multiplied by $\det \hat{\sigma} = |\sigma\sigma'|^2 \equiv N(\sigma)$, which takes a positive integer value. $\hat{\sigma}$ is an automorphism of L_m if $N(\sigma) = 1$ (i.e. σ is a unit of $\boldsymbol{Z}_m(\zeta)$). $\hat{\sigma}$ is an orthogonal transformation in 4D if $|\sigma| = |\sigma'| = 1$. The action of $\hat{\sigma}$ on L_m is isomorphic to the action of σ on $\boldsymbol{Z}_m(\zeta)$. Note that $\hat{\sigma} = \Sigma_i k_i (\hat{\zeta})^i \in \boldsymbol{Z}(\hat{\zeta})$ $(\simeq \boldsymbol{Z}_m(\zeta))$.

The 4D m-fold rotation in the point group C_{mv} of L_m is given by $C_m = \hat{\zeta}$ for $m = 8$ and 12 or $C_{10} = \hat{\eta}$ with $\eta = -\zeta^3 = \exp(\pi i/5)$. Accordingly, $C_5 = (C_{10})^2 = \hat{\zeta}$. On the other hand, the 4D mirror σ_v in C_{mv} is represented by the complex conjugate operation on $E_4 \simeq \boldsymbol{C}^2$. The action of σ_v on L_m is isomorphic to that of the complex conjugate operation on $\boldsymbol{Z}_m(\zeta)$.

There exists a 4D unimodular matrix R_m such that $\hat{\zeta}(\boldsymbol{e}_0 \boldsymbol{e}_1 \boldsymbol{e}_2 \boldsymbol{e}_3) = (\boldsymbol{e}_0 \boldsymbol{e}_1 \boldsymbol{e}_2 \boldsymbol{e}_3) R_m$. It satisfies $P_m(R_m) = 0$. R_8 is anticyclic because $\hat{\zeta}\boldsymbol{e}_i = \boldsymbol{e}_{i+1}$ with $\boldsymbol{e}_4 = -\boldsymbol{e}_0$. If $\sigma = \Sigma_i k_i \zeta^i \in \boldsymbol{Z}_m(\zeta)$, then $\hat{\sigma}(\boldsymbol{e}_0 \boldsymbol{e}_1 \boldsymbol{e}_2 \boldsymbol{e}_3) = (\boldsymbol{e}_0 \boldsymbol{e}_1 \boldsymbol{e}_2 \boldsymbol{e}_3) K$ with $K = \Sigma_i k_i (R_m)^i \in \boldsymbol{Z}(R_m)$ and $\det \hat{\sigma} = \det K$. The commutable ring $\boldsymbol{Z}(R_m)$ is isomorphic to $\boldsymbol{Z}_m(\zeta)$ and $\boldsymbol{Z}(\hat{\zeta})$; $\hat{\zeta}$ and R_m are related by a similarity transformation with the 4×4 matrix $(\boldsymbol{e}_0 \boldsymbol{e}_1 \boldsymbol{e}_2 \boldsymbol{e}_3)$.

L_8 is divided into two sublattices $L_8^{(0)}$ and $L_8^{(1)}$ $(=e_0+L_8^{(0)})$ by the parity of the sum of the indices of the lattice vectors. $L_8^{(0)}$ is a face-centred type sublattice of L_8 but belongs to a primitive octagonal Bravais class (Niizeki 1989b) because $L_8^{(0)}=\hat{\sigma}L_8$ with $\sigma=1+\zeta=2\cos(\pi/8)\exp(\mathrm{i}\pi/8)$, $\sigma'=1-\zeta=2\sin(\pi/8)\exp(-3\mathrm{i}\pi/8)$ and $\det\hat{\sigma}=2$. Note that $\hat{\sigma}e_i=e_i+e_{i+1}$. Incidentally, a body-centred sublattice of L_8 belongs also to a primitive octagonal Bravais class because

$$2(\hat{\sigma})^{-1}L_8=\left\{\sum_i n_i e_i \mid n_i\in \boldsymbol{Z},\, n_i\equiv n_j \bmod 2\right\}$$

on account of $2/\sigma=1-\zeta+\zeta^2-\zeta^3$.

L_{10} is divided naturally into five sublattices $L_{10}^{(p)}$, $p=0$–4, where each sublattice is composed of the lattice vectors whose indices sum to p. The five sublattices are translated to each other; $L_{10}^{(p)}=pe_0+L_{10}^{(0)}$, $p=1$–4. $L_{10}^{(0)}$ is another 4D decagonal Bravais lattice (Niizeki 1989b), which is written as $\hat{\sigma}L_{10}$ with $\sigma=\zeta^2-\zeta^3=2\mathrm{i}\sin(\pi/5)$, $\sigma'=\zeta^4-\zeta=-2\mathrm{i}\sin(2\pi/5)$ and $\det\hat{\sigma}=5$. Basis vectors of $L_{10}^{(0)}$ are given by $\hat{\sigma}e_i$ $(=e_{i+2}-e_{i+3})$, $i=0$–4, so that the axes of $L_{10}^{(0)}$ are rotated by $\pi/2$ (or $-\pi/2$) in $E_\parallel$ (or $E_\perp$) from those of L_{10}. The relation between L_{10} and $L_{10}^{(0)}$ is similar to that between the 2D triangular lattice and one of its three sublattices into which it is divided.

2.2. (2+1)-reducible Bravais lattices in 5D

A primitive m-gonal Bravais lattice in 5D with $m=8$, 10 or 12 is defined by the direct product of the 4D m-gonal lattice L_m and the 1D lattice $L_1=\{nc \mid n\in\boldsymbol{Z}\}$; $L_{m,1}=L_m\times L_1=\{(\boldsymbol{l},nc)\mid \boldsymbol{l}\in L_m \text{ and } n\in\boldsymbol{Z}\}$. The point group of $L_{m,1}$ is given by $D_{mh}=C_{mv}\times C_s=D_m+ID_m$ with I being the 5D inversion. Basis vectors ε_i of $L_{m,1}$ are given by $\varepsilon_i=(e_i,0)$, $i=0,1,\ldots,k-1$, and $\varepsilon_k=(0,c)$ with $k=4$ for $m=8$ and 12 but $k=5$ for $m=10$. Accordingly, a lattice vector $\boldsymbol{l}=\sum_i n_i\varepsilon_i$ is indexed as $\boldsymbol{l}=[n_0n_1\ldots n_k]$. Note that $L_{8,1}$ is an octagonal affine distortion of the 5D simple hypercubic lattice, $L_{5,\mathrm{hc}}$.

The centred octagonal lattice in 5D, $L_{8,\mathrm{c}}$, is given as one of the two face-centred sublattices of the primitive octagonal lattice $L_{8,1}$ and is represented with the basis vectors of $L_{8,\mathrm{c}}$ as

$$L_{8,\mathrm{c}}=\left\{\sum_{i=0}^{4} n_i\varepsilon_i \mid n_i\in\boldsymbol{Z} \text{ and } n_0+n_1+\ldots+n_4=\text{even}\right\}. \tag{6}$$

The point group of $L_{8,\mathrm{c}}$ is D_{8h}. The volume of the unit cell of $L_{8,\mathrm{c}}$ is twice that of $L_{8,1}$. $L_{8,\mathrm{c}}$ is an alternating stacking of two 4D octagonal lattices $L_8^{(0)}$ and $L_8^{(1)}$. The relation between $L_{8,1}$ and $L_{8,\mathrm{c}}$ is similar to that between the primitive and the face-centred tetragonal lattices in 3D.

The pentagonal lattice L_5 is a non-primitive (2+1)-reducible lattice, which is one of the five equivalent sublattices into which $L_{10,1}$ is divided. Its basis vectors $\tilde{\varepsilon}_i$, $i=0$–4, are related to those of $L_{10,1}$ by $\tilde{\varepsilon}_i=\varepsilon_i+\varepsilon_5=(e_i,c)$. The point group of L_5 is $D_{5d}=D_5+ID_5\subset D_{10h}$. The remaining four sublattices are given by $p\varepsilon_0+L_5$, $p=1$–4.

If $a_\parallel=a_\perp=\sqrt{2}c$, we obtain $\tilde{\varepsilon}_i\cdot\tilde{\varepsilon}_j=5c^2\delta_{i,j}$, so that L_5 coincides in this case with $L_{5,\mathrm{hc}}$. Therefore, a general pentagonal lattice is a pentagonal affine distortion of $L_{5,\mathrm{hc}}$.

L_5 is a periodic stacking along the c axis of 4D decagonal lattices $L_{10}^{(p)}$, which are sublattices of L_{10}. If these five 4D lattices are denoted by A, B, C, D and E, respectively, the one period of the stacking is given by $ABCDE$. Consequently, L_5 degenerates into L_{10} if it is projected along the c axis. The relation between L_5 and $L_{10,1}$ is very similar to that between the rhombohedral lattice and the hexagonal lattice in 3D.

There are no non-primitive dodecagonal lattices in 5D.

3. The reciprocal lattices

Let $L=\{\Sigma_i n_i \boldsymbol{e}_i \mid n_i \in \boldsymbol{Z}\}$ be a d-dimensional Bravais lattice with point group G. Then, the reciprocal lattice L^* of L is the set of all the vectors $\boldsymbol{g}$ satisfying the condition, $\boldsymbol{g}\cdot\boldsymbol{l}\in \boldsymbol{Z}\ \forall \boldsymbol{l}\in L$. It follows that L^* is a Bravais lattice whose point group is G. A necessary and sufficient condition for $\boldsymbol{e}_i^*$ to be basis vectors of L^* is that the $d\times d$ matrix $(\boldsymbol{e}_i\cdot\boldsymbol{e}_j^*)$ is a unimodular matrix. $\boldsymbol{e}_i^*$ are called dual basis vectors to $\boldsymbol{e}_i$ if they satisfy the conditions $\boldsymbol{e}_i\cdot\boldsymbol{e}_j^*=\delta_{i,j}$. The dual basis vectors are, however, not always convenient because they may not explicitly conform to the symmetry of L^*. In this paper, we shall use symmetry-adopted basis vectors. Note that volumes Ω and Ω^* of the unit cells of L and L^*, respectively, are related by $\Omega\Omega^*=1$.

A reciprocal lattice vector $\boldsymbol{g}=\Sigma_i n_i\boldsymbol{e}_i^*\in L^*$ is indexed with parentheses as $\boldsymbol{g}=(n_0 n_1 \ldots n_k)$.

It follows from the general argument that the reciprocal lattices of the octagonal, decagonal, dodecagonal and pentagonal lattices in 4D or 5D are 4D or 5D lattices with the same point symmetries.

3.1. *The case of 4D lattices*

The basis vectors e_i^* of the reciprocal 4D octagonal lattice L_8^* and the dodecagonal one L_{12}^* are given by similar equations to equations (1) but the lattice constants are replaced by $a_\parallel^*=1/(2a_\parallel)$ and $a_\perp^*=1/(2a_\perp)$ for L_8^* and $a_\parallel^*=1/(\sqrt{3}a_\parallel)$ and $a_\perp^*=-1/(\sqrt{3}a_\perp)$ (<0) for L_{12}^*. The numerical factors in these relations of the lattice constants are consistent with the relation $\Omega_m\Omega_m^*=1$. $\boldsymbol{e}_i^*$ are dual to $\boldsymbol{e}_i$ for the octagonal case.

It is well known that the axes of the reciprocal triangular lattice in 2D are rotated by $\pi/2$ from those of the one in the real space. A similar relation exists between L_{10} and its reciprocal lattice L_{10}^*; L_{10}^* is given by $L_{10}^{(0)}$ (not by L_{10}) but with the lattice constants being replaced by $a_\parallel^*=2/(5a_\parallel)$ and $a_\perp^*=2/(5a_\perp)$. That is, the basis vectors of L_{10}^* are given by $\boldsymbol{e}_i^*=(a_\parallel^*\sigma\zeta^i, a_\perp^*\sigma'\zeta^{2i})$ with $\sigma=\zeta^2-\zeta^3$.

The matrices $(\boldsymbol{e}_i\cdot\boldsymbol{e}_j^*)$ for the decagonal and the dodecagonal cases are presented in appendix 1.

3.2. *The case of 5D lattices*

The reciprocal lattice of the primitive lattice $L_{m,1}=L_m\times L_1$ is also a primitive m-gonal lattice because $L_{m,1}^*=L_m^*\times L_1^*$, where $L_1^*=\{nc^*\mid n\in\boldsymbol{Z}\}$ with $c^*=1/c$. The basis vectors of $L_{m,1}^*$ are given by $\boldsymbol{\varepsilon}_i^*=(\boldsymbol{e}_i^*,0)$, $i=0,1,\ldots,k-1$, and $\boldsymbol{\varepsilon}_k^*=(0,c^*)$.

The centred octagonal Bravais lattice $L_{8,\mathrm{c}}$ is a face-centred sublattice of $L_{8,1}$ so that its reciprocal lattice $L_{8,\mathrm{c}}^*$ is the body-centred lattice $L_8^*\cup\{(11111)/2+L_8^*\}$, i.e.

$$L_{8,\mathrm{c}}^*=\{\tfrac{1}{2}(n_0n_1n_2n_3n_4)\mid n_i\in\boldsymbol{Z} \text{ and } n_i\equiv n_j \bmod 2\} \tag{7}$$

where the index scheme for $L_{8,1}^*$ is used.

It is shown easily that $L_{8,\mathrm{c}}^*$ can be indexed, alternatively, as a face-centred octagonal lattice if the basis vectors $\tilde{\boldsymbol{e}}_i^*=((\hat{\sigma})^{-1}\boldsymbol{e}_i^*,0)$, $i=0$–3, and $\tilde{\boldsymbol{\varepsilon}}_4^*=(0,c/2)$ are used, where $\sigma=1+\zeta$. This means that a body-centred octagonal lattice in 5D and the face-centred lattice belong to the same Bravais class but, however, $\tilde{\boldsymbol{\varepsilon}}_i^*$ are rotated from $\boldsymbol{\varepsilon}_i^*$. This is similar to the fact that the face-centred tetragonal lattice in 3D can be indexed as a body-centred lattice if the basis vectors are changed. However, the index scheme with $\boldsymbol{\varepsilon}_i^*$ is superior to that with $\tilde{\boldsymbol{\varepsilon}}_i^*$ because $\boldsymbol{\varepsilon}_{i,\parallel}^*$ are parallel to $\boldsymbol{\varepsilon}_{i,\parallel}$.

The reciprocal lattice of L_5 is also a pentagonal Bravais lattice L_5^* whose lattice constants are related to those of L_5 by $a_\parallel^* = 2/(5a_\parallel)$, $a_\perp^* = 2/(5a_\perp)$ and $c^* = 1/(5c)$. The basis vectors of L_5^* are dual to those of L_5.

4. A general theory of the special points

A point group is called a centring group if the origin is its only fixed point. A group is a centring group if it includes I, the inversion operator. A point $\boldsymbol{x}$ in E_d is called a special point of a lattice $L \subset E_d$ if its point group $\mathrm{G}(\boldsymbol{x})$ with respect to the space group $\mathscr{G} = \{\{\rho|\boldsymbol{l}\}|\rho \in \mathrm{G}$ and $\boldsymbol{l} \in L\}$ is a centring subgroup of G. Two special points are equivalent if they are transformed to each other by $\mathscr{G}$. A set of equivalent special points (mathematically, an orbit) form a class of special points. We can choose a representative $\boldsymbol{x}_0$ in a unit cell from each class. The number of special points of a class in the unit cell is given by $r = |\mathrm{G}|/|\mathrm{G}(\boldsymbol{x}_0)|$ where $|\cdot|$ stands for the order of the group. r is called the order of the class.

We assume hereafter that L is a Bravais lattice. Then, G includes I. A subgroup of G is classified into type-I or type-II according as it includes I or not, respectively, and, correspondingly, a special point of L is classified similarly. A necessary and sufficient condition for a point to be a type-I special point is that it is a lattice vector of the 'half lattice', $L^{(\mathrm{H})} \equiv \{\boldsymbol{l}/2|\boldsymbol{l} \in L\}$. Accordingly, the sum of the order over all the classes of type-I special points of L is equal to 2^d. The problem remaining for the type-I special points is to determine their point groups. The lattice points of L form one class of type-I special points with the full symmetry. This class is denoted by Γ following the convention in the band theory. We shall call a Bravais lattice a type-I lattice if it has no type-II special points but a type-II lattice, otherwise.

E_d is divided into fundamental domains which are translationally equivalent. A representative of the domains is the one, V, which includes the origin $\mathbf{0} \in L$. We assume that V (exactly, its closure) is a symmetrical convex polytope which is invariant against G. For example, the fundamental domain derived from the Voronoi partitioning with respect to L has this property. Then, all the special points in V except Γ at the origin are located on the centres of k-dimensional surfaces of V with $0 \leqslant k \leqslant d-1$. We take the symmetrical fundamental domains to be unit cells of L. The parallelotope formed by the basis vectors is not usually symmetrical.

The Voronoi cell at the origin of a simple hypercubic lattice $L_{d,\mathrm{hc}}$ is a hypercube. Therefore, its special point is indexed as $[h_0 h_1 \ldots h_{d-1}]$ in which h_i can take 0, $\frac{1}{2}$ or $-\frac{1}{2}$. Consequently, all the special points are type I and $L_{d,\mathrm{hc}}$ is a type-I lattice. The simplest case is the 1D lattice $L_1 = \{nc|n \in \boldsymbol{Z}\}$, which has two classes of special points with the full symmetry C_s; the representatives are 0 and $c/2$.

Assume that L is an affine distortion of $L_{d,\mathrm{hc}}$, whose point symmetry is higher than that of L. Then, all the special points of L are derived from those of $L_{d,\mathrm{hc}}$ and, consequently, L as well as $L_{d,\mathrm{hc}}$ is a type-I lattice. However, two equivalent special points of $L_{d,\mathrm{hc}}$ are not necessarily equivalent as special points of L. Note that the parallelotope formed by the basis vectors of L is a symmetrical unit cell but is not a Voronoi cell.

Assume that L is a direct product of lower-dimensional lattices $L' \subset E_{d'}$ and $L'' \subset E_{d''}$, $L = L' \times L''$ $(= \{(\boldsymbol{l}', \boldsymbol{l}'')|\boldsymbol{l}' \in L', \boldsymbol{l}'' \in L''\}$ and that G is also a direct product, $\mathrm{G} = \mathrm{G}' \times \mathrm{G}''$

with G′ and G″ being the point groups of L' and L''. Then, it can be shown easily that a necessary and sufficient condition for $\boldsymbol{x} = (\boldsymbol{x}', \boldsymbol{x}'') \in E_D = E_{d'} \oplus E_{d''}$ to be a special point of L is that $\boldsymbol{x}'$ and $\boldsymbol{x}''$ are special points of L' and L'', respectively. Then $\mathrm{G}(\boldsymbol{x}) = \mathrm{G}'(\boldsymbol{x}') \times \mathrm{G}''(\boldsymbol{x}'')$. L is a type-I lattice only if L' and L'' are type-I lattices. Note that the fundamental domain of L is a direct product of those of L' and L''; $V = V' \times V'' = \{(\boldsymbol{x}', \boldsymbol{x}'') \mid \boldsymbol{x}' \in V', \boldsymbol{x}'' \in V''\}$. The boundary of V is given by $\partial V = \partial V' \times V'' + V' \times \partial V''$.

The simplest case of the above theorem is where $d' = d - 1$ and $d'' = 1$, i.e. $L'' = L_1$. Then, $V'' = V_1 = [-c/2, c/2]$ and $V = V' \times V_1$ is a hyperprism whose base hypersurface is V'. A special point of L is given by $\boldsymbol{x} = (\boldsymbol{x}', 0)$ or $(\boldsymbol{x}', c/2)$ with $\boldsymbol{x}'$ being a special point of L'. In the former case, $\boldsymbol{x}$ (except the case $\boldsymbol{x} = 0$) is located on the boundary of $V' \times \{0\}$, which is the horizontal cross section of V through the origin, and, in the latter case, $\boldsymbol{x}$ is on the top hypersurface of V. The point group of a special point $\boldsymbol{x}$ is given by $\mathrm{G}(\boldsymbol{x}) = \mathrm{G}(\boldsymbol{x}') \times C_s$.

Assume that L is a sublattice of a type-I lattice $\tilde{L}$ as is in the case of $L_{8,c}$. Then, $\mathscr{G}$ is a subgroup of the space group of $\tilde{L}$. Consequently, all the special points of L are simultaneously special points of $\tilde{L}$, so that the former are searched by examining the latter, which are known already. The point group of a special point of L is a subgroup of that of $\tilde{L}$. Moreover, two equivalent special points of $\tilde{L}$ are not necessarily equivalent as special points of L.

Before closing this section, we add a remark. If $\boldsymbol{x}$ is a type-II special point, $I\boldsymbol{x}$ is an equivalent special point to $\boldsymbol{x}$ but is not translationally equivalent to $\boldsymbol{x}$.

5. The special points of the 5D Bravais lattices

The special points of 4D lattices L_m with $m = 8$, 10 and 12 have been listed in I. Therefore, the special points of the primitive m-gonal lattices in 5D are easily enumerated because the 5D lattices are direct products of L_m and L_1. The results are listed in table 1. The special point of the type $\boldsymbol{x} = (\boldsymbol{x}', 0)$, where $\boldsymbol{x}'$ is a special point of L_m, is represented by the same symbol as that used in I for $\boldsymbol{x}'$ (note, however, that the symbol C' in I is replaced by M in this paper). On the other hand, the special point of the type $\boldsymbol{x} = (\boldsymbol{x}', c/2)$ is represented in most cases by the second alphabet to that of the symbol for $(\boldsymbol{x}', 0)$. Since the present index scheme for L_{10} is different from that in I, the indices of the special points of $L_{10,1}$ are transformed appropriately from those presented in I†. In the case of $L_{8,1}$, different special points with a same number of zero indices are derived from a single class of special points of $L_{5,\mathrm{hc}}$.

The type-I special points of the centred octagonal lattice $L_{8,c}$ are classified as in table 2. The representative of each class is indexed as $\frac{1}{2}[n_0 n_1 n_2 n_3 n_4]$ with $0 \leqslant n_i \leqslant 1$ and $\Sigma_i\, n_i =$ even. Since the unit cell of $L_{8,c}$ is twice that of $L_{8,1}$, two classes of special points of $L_{8,c}$ may become a single class of special points of $L_{8,1}$ given in table 1. A special point of $L_{8,c}$ is denoted by the same symbol as that of $L_{8,1}$ if indices are common.

The remaining task for $L_{8,c}$ is to enumerate its type-II special points. There exist seven type-II centring subgroups of D_{8h}: D_2, D_4, D_8, S_4, S_8, D_{2d} and D_{4d}. None of them includes σ_h. Special points of $L_{8,c}$ are derived from those of $L_{8,1}$ and we can assume that a representative of a class of type-II special points takes the form: $\boldsymbol{x} = \frac{1}{2}[n_0 n_1 n_2 n_3 n_4]$ with $0 \leqslant n_i \leqslant 1$ and $\Sigma_i\, n_i =$ odd; if $\boldsymbol{x}$ cannot be reduced to this form by a translation in $L_{8,c}$, $-\boldsymbol{x}$ $(= I\boldsymbol{x})$ can be. If $n_4 = 0$, then, $\sigma_h \in \mathrm{G}(\boldsymbol{x})$. Therefore, X and

† The bars on some indices of special point P' were missed in I.

Table 1. Classifications of special points of the primitive octagonal (a), decagonal (b) and dodecagonal (c) lattices in 5D. The first row shows a symbol assigned to each class of the special points. The second and the third rows show its point group and its order, respectively. The fourth row shows indices of a representative of each class. A class in the last half of each table differs from the corresponding one in the first half in that the last index of the representative is changed from 0 to $\frac{1}{2}$.

(a)

Γ	X	C	M	R	O	Z	W	D	N	S	P
D_{8h}	D_{2h}	D_{2h}	D_{4h}	D_{2h}	D_{8h}	D_{8h}	D_{2h}	D_{2h}	D_{4h}	D_{2h}	D_{8h}
1	4	4	2	4	1	1	4	4	2	4	1
00000	$\frac{1}{2}0000$	$\frac{1}{2}\frac{1}{2}000$	$0\frac{1}{2}0\frac{1}{2}0$	$0\frac{1}{2}\frac{1}{2}\frac{1}{2}0$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}0$	$0000\frac{1}{2}$	$\frac{1}{2}000\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}00\frac{1}{2}$	$0\frac{1}{2}0\frac{1}{2}\frac{1}{2}$	$0\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$

(b)

Γ	X	C	M	P	P'	Z	W	D	N	Q	Q'
D_{10h}	D_{2h}	D_{2h}	D_{2h}	D_{5h}	D_{5h}	D_{10h}	D_{2h}	D_{2h}	D_{2h}	D_{5h}	D_{5h}
1	5	5	5	2	2	1	5	5	5	2	2
000000	$\frac{1}{2}00000$	$0\frac{1}{2}0\frac{1}{2}00$	$00\frac{1}{2}\frac{1}{2}00$	$0\frac{1}{5}\frac{2}{5}\frac{\bar{2}}{5}\frac{\bar{1}}{5}0$	$0\frac{2}{5}\frac{\bar{1}}{5}\frac{1}{5}\frac{\bar{2}}{5}0$	$00000\frac{1}{2}$	$\frac{1}{2}0000\frac{1}{2}$	$0\frac{1}{2}00\frac{1}{2}\frac{1}{2}$	$00\frac{1}{2}\frac{1}{2}0\frac{1}{2}$	$0\frac{1}{5}\frac{2}{5}\frac{\bar{2}}{5}\frac{\bar{1}}{5}\frac{1}{2}$	$0\frac{2}{5}\frac{\bar{1}}{5}\frac{1}{5}\frac{\bar{2}}{5}\frac{1}{2}$

(c)

Γ	X	C	M	T	T'	Z	W	D	N	U	U'
D_{12h}	D_{2h}	D_{2h}	D_{4h}	D_{3h}	D_{3h}	D_{12h}	D_{2h}	D_{2h}	D_{4h}	D_{3h}	D_{3h}
1	6	6	3	4	4	1	6	6	3	4	4
00000	$\frac{1}{2}0000$	$\frac{1}{2}\frac{1}{2}000$	$\frac{1}{2}00\frac{1}{2}0$	$\frac{1}{3}0\frac{1}{3}00$	$\frac{1}{3}\frac{1}{3}\frac{1}{3}\frac{1}{3}0$	$0000\frac{1}{2}$	$\frac{1}{2}000\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}00\frac{1}{2}$	$\frac{1}{2}00\frac{1}{2}\frac{1}{2}$	$\frac{1}{3}0\frac{1}{3}0\frac{1}{2}$	$\frac{1}{3}\frac{1}{3}\frac{1}{3}\frac{1}{3}\frac{1}{2}$

Table 2. A classification of special points of the centred octagonal lattice in 5D. The first four rows are similar to those in table 1. The fifth row shows indices of a representative in the basis system as a body-centred octagonal lattice. The last two columns (N and P) show type-II special points.

Γ	Z	C	M	C'	O	W	S	N	P
D_{8h}	D_{8h}	D_{2h}	D_{2h}	D_{2h}	D_{4h}	C_{2h}	C_{2h}	D_{2d}	D_{4d}
1	1	4	4	4	2	8	8	4	2
00000	00001	$\frac{1}{2}\frac{1}{2}000$	$0\frac{1}{2}0\frac{1}{2}0$	$\frac{1}{2}00\frac{1}{2}0$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}0$	$\frac{1}{2}000\frac{1}{2}$	$0\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$0\frac{1}{2}0\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$
00000	$0000\frac{1}{2}$	$\frac{1}{2}0000$	$\frac{1}{2}00\frac{1}{2}0$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}00$	$\frac{1}{2}0\frac{1}{2}00$	$\frac{1}{4}\frac{\bar{1}}{4}\frac{1}{4}\frac{\bar{1}}{4}\frac{1}{4}$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\frac{1}{4}\frac{1}{4}$	$\frac{1}{2}00\frac{1}{2}\frac{1}{4}$	$\frac{1}{2}0\frac{1}{2}0\frac{1}{4}$

R in table 1(a) cannot be special points of $L_{8,c}$. Z ($=\frac{1}{2}[00001]$) is also excluded because its point group is C_{8v}.

There remain only three candidates for type-II special points of $L_{8,c}$, namely, D, N and P in table 1(a). Of the three, D is excluded because its point group is C_{2v}. The point group of N (or P) includes $S_4 = C_4\sigma_h$ (or $S_8 = C_8\sigma_h$), so that N (or P) is a type-II special point. The point groups of N and P are D_{2d} and D_{4d}, respectively, as given in table 2.

The pentagonal lattice L_5 is a type-I lattice and the point groups of the special points are determined as presented in table 3. Note that C and M (or O and P) would be equivalent if L_5 were $L_{5,\mathrm{hc}}$. Table 3 has a mirror symmetry with respect to the interchange of indices, $0 \leftrightarrow \frac{1}{2}$, which follows from self-duality of L_5.

Table 3. A classification of special points of the pentagonal lattice in 5D.

Γ	X	C	M	O	P	D	I
D_{5d}	C_{2h}	C_{2h}	C_{2h}	C_{2h}	C_{2h}	C_{2h}	D_{5d}
1	5	5	5	5	5	5	1
00000	$\frac{1}{2}0000$	$0\frac{1}{2}00\frac{1}{2}$	$00\frac{1}{2}\frac{1}{2}0$	$\frac{1}{2}\frac{1}{2}00\frac{1}{2}$	$\frac{1}{2}0\frac{1}{2}\frac{1}{2}0$	$0\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$

6. Transformation among the special points

An m-gonal QL in 2D has self-similarity characterized by a complex number τ_m, which is a unit of $\boldsymbol{Z}_m(\zeta)$; on the inflation the QL is scaled by $|\tau_m|$ and, subsequently, rotated by $\arg \tau_m$. τ_m is given by $1+\zeta+\zeta^{-1}$ ($=1+\sqrt{2}$), $-\zeta^2-\zeta^{-2}$ ($=\frac{1}{2}(1+\sqrt{5})$) and $1+\zeta$ for $m=8$, 10 and 12, respectively (Niizeki 1989a).

The affine transformation $\hat{\tau}_m$ is an automorphism of L_m and satisfies $\hat{\tau}_m C_{mv} \hat{\tau}_m^{-1} = C_{mv}$. Therefore, there exists a unimodular matrix K_m such that $\hat{\tau}_m(e_0e_1e_2e_3) = (e_0e_1e_2e_3)K_m$. Then, the indices of a special point are transformed by K_m on the inflation procedure. It follows that (i) all the classes of the special points of L_m can be grouped into multiplets, (ii) different members of a single multiplet are permuted cyclically by the inflation and (iii) the point group is common among the members of the multiplet. Γ always forms a singlet. A class must form a singlet if there are no classes (other than Γ) with the same point symmetry as that of the class.

The above results are discussed in I. We consider here a similar question in the case of (2+1)-reducible Bravais lattices in 5D. Since (2+1)-reducible QL associated with these 5D lattices are periodic along the c axis, the present automorphism α must be (4+1)-reducible; $\alpha = \hat{\sigma} \oplus (1)$, where $\hat{\sigma}$ ($\sigma \in \boldsymbol{Z}(\zeta)$) is an automorphism of the 4D hyperlayers perpendicular to the c axis. A 5D unimodular matrix K is associated with α. We can take $\sigma = \tau_m$ for the case of $L_{m,1}$ because $L_{m,1} = L_m \times L_1$. This choice also works well for $L_{8,c}$, as proved in appendix 2.1. However, this choice is wrong for L_5 and we have to choose $\sigma = -(\tau_{10})^2$ as shown in appendix 2.2. This automorphism of L_5 was found by Gähler (1986) in connection with self-similarity of a decagonal QL in 2D. Note that the unimodular matrix K associated with α can be treated in modulo 2 when the indices of a type-I special point $\boldsymbol{x}$ of L_m are transformed because $2\boldsymbol{x} \equiv 0 \bmod L_m$.

Grouping the special points of $L_{m,1}$ into multiplets is performed straightforwardly because the multiplets are derived from those of L_m; the latter multiplets are listed in I. It can be shown easily that $L_{8,c}$ has two doublets $\{C, C'\}$ and $\{W, S\}$ but other classes are singlets. The presence of a doublet is due to the fact that the relevant unimodular matrix K satisfies $K^2 \equiv E \bmod 2$ with E being the unit matrix. On the other hand, L_5 has two triplets $\{X, P, O\}$ and $\{D, C, M\}$ but Γ and I are singlets. The triplets are allowed because $K^3 \equiv E \bmod 2$.

7. Discussion

We have shown in section 3 that the reciprocal lattice of a $(2+1)$-reducible Bravais lattice in 5D is also a $(2+1)$-reducible Bravais lattice with the same point symmetry. Therefore, the results of the preceding section apply equally to the classification of the special points in the reciprocal space of the $(2+1)$-reducible Bravais lattices. The only task remaining is to reindex the special points of the centred octagonal lattice as a body-centred lattice. The transformation matrix which transforms the indices from the face-centred lattice to the body-centred one is given by

$$\frac{1}{2}\begin{pmatrix} 1 & 1 & -1 & 1 & 0 \\ -1 & 1 & 1 & -1 & 0 \\ 1 & -1 & 1 & 1 & 0 \\ -1 & 1 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

The indices as a body-centred lattice are listed in the fifth row of table 2.

A $(2+1)$-reducible QL derived from $L_{m,1}$ takes the form $Q_{m,1} = Q_m \times L_1$ with Q_m being a 2D QL derived from L_m. An m-gonal quasiperiodic tiling (QPT) in 2D is associated with Q_m and, accordingly, $Q_{m,1}$ yields a 3D $(2+1)$-reducible QPT composed of prisms, each of which is given by $T \times S$ with T being a tile in the 2D QPT and $S = [nc, (n+1)c]$ being a segment of L_1. The vertices, the edge centres, the surface centres and the body centres of the prisms are special points of $Q_{m,1}$. The base centre and the body centre of a symmetrical prism (e.g., the case of the octagonal prism of $Q_{8,1}$) formed of several basic prisms are also special points.

The centred octagonal QL, $Q_{8,c}$, obtained from $L_{8,c}$ is given, alternatively, as a sublattice of $Q_{8,1}$. It is an alternating stacking of two 2D octagonal QL derived from $L_8^{(0)}$ and $L_8^{(1)}$. The special points of $Q_{8,c}$ are obtained from those of $Q_{8,1}$.

The pentagonal lattice L_5 is an affine distortion of $L_{5,\mathrm{hc}}$. Therefore, the pentagonal QL, Q_5, obtained from L_5 yields naturally a 3D pentagonal QPT with parallelepipeds (Lück 1987). The vertices, the edge centres, the face centres and the body centres of the parallelepipeds are special points of Q_5. More precisely, the special points of type O and P are located on the body centres of the two kinds of parallelepipeds of the QPT; O (or P) becomes an oblate (or prolate) rhombohedron when $a_{\parallel} = 2c$. A parallelepiped of type P (or O) has four (or two) faces of type C and two (or four) faces of type M. Four (or ten) parallelepipeds may form a dodecahedron (or an icosahedron), which is an affine distortion of a rhombic dodecahedron (or icosahedron) in the primitive icosahedral QL in 3D. The centre of the dodecahedron (or icosahedron) is a special point of type D (or I). These polyhedra (as well as the two parallelepipeds) are so-called zonohedra, which are projections of a 5D hypercube and a 4D hypercube which is one of the hypersurfaces of the former (Coxeter 1973).

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Appendix 1

The matrices $(e_i \cdot e_j^*)$ are given by the left-hand matrix below for the decagonal case and by the right-hand matrix below for the dodecagonal case:

$$\begin{pmatrix} 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 1 & -1 \\ -1 & 0 & 0 & 0 & 1 \\ 1 & -1 & 0 & 0 & 0 \end{pmatrix} \qquad \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

Appendix 2

2.1.

The 5D unimodular matrix associated with $\alpha = \hat{\sigma} \oplus (1)$ is $K = K_8 \oplus (1)$, which is given by the left-hand matrix below:

$$\begin{pmatrix} 1 & 1 & 0 & -1 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ -1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \qquad \begin{pmatrix} -1 & 0 & 1 & 1 & 0 \\ 0 & -1 & 0 & 1 & 1 \\ 1 & 0 & -1 & 0 & 1 \\ 1 & 1 & 0 & -1 & 0 \\ 0 & 1 & 1 & 0 & -1 \end{pmatrix}.$$

The parity of the sum of the indices of $\boldsymbol{l} \in L_{8,1}$ is not changed by $K = (k_{ij})$ because $\Sigma_i k_{ij} \equiv 1 \bmod 2$. Therefore, α is an automorphism of $L_{8,c}$.

2.2.

$\hat{\tau}_{10}$ transforms $L_{10}^{(p)}$ into $L_{10}^{(q)}$ with $q \equiv -2p \bmod 5$ (Niizeki 1989b). Therefore, it changes the stacking *ABCDE* of L_5 into *ADBEC*, which cannot be transformed to *ABCDE* by a rotation around the c axis. Thus, $\alpha = \hat{\tau}_{10} \oplus (1)$ is not an automorphism of L_5. On the other hand, $(-\hat{\tau}_{10}^2) L_{10}^{(p)} = L_{10}^{(p)}$ because $-(-2)^2 \equiv 1 \bmod 5$. It follows that $\alpha = (-\hat{\tau}_{10}^2) \oplus (1)$ is an automorphism of L_5. The 5D unimodular matrix K associated with α is given by the right-hand matrix above.

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