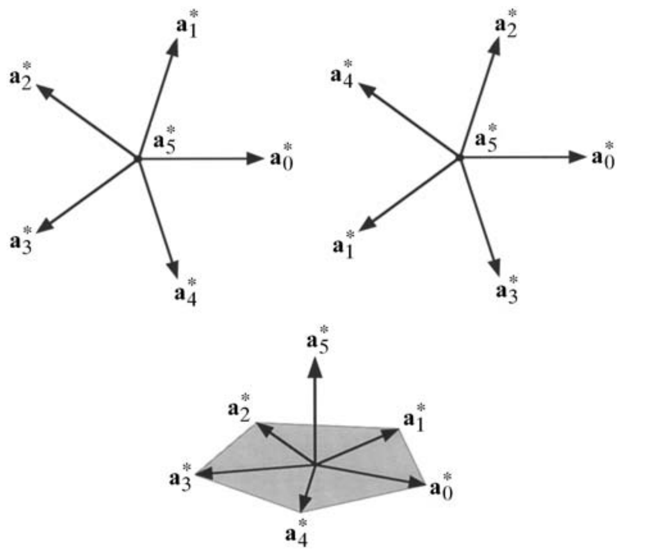

Fig. 4.6.3.12. Reciprocal basis of the decagonal phase in the 5D description projected upon $\mathbf{V}^{\parallel}$ (above left) and $\mathbf{V}^{\perp}$ (above right). Below, a perspective physical-space view is shown.

generators, the tenfold rotation $\alpha = 10$, the reflection plane $\beta = m_2$ (normal of the reflection plane along the vectors $\mathbf{a}_i^*{-}\mathbf{a}_{i+3}^*$ with $i = 1, \ldots, 4$ modulo 5) and the inversion operation $\Gamma(\gamma) = \bar{1}$ may be written in the form

$$\Gamma(\alpha) = \begin{pmatrix} 0 & 1 & \bar{1} & 0 & 0 \\ 0 & 1 & 0 & \bar{1} & 0 \\ 0 & 1 & 0 & 0 & 0 \\ \bar{1} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}_D \quad \Gamma(\beta) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}_D$$

$$\Gamma(\gamma) = \begin{pmatrix} \bar{1} & 0 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 & 0 \\ 0 & 0 & \bar{1} & 0 & 0 \\ 0 & 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & 0 & \bar{1} \end{pmatrix}_D .$$

By block-diagonalization, these reducible symmetry matrices can be decomposed into non-equivalent irreducible representations. These can be assigned to the two orthogonal subspaces forming the 5D embedding space $\mathbf{V} = \mathbf{V}^{\parallel} \oplus \mathbf{V}^{\perp}$, the 3D parallel (physical) subspace $\mathbf{V}^{\parallel}$ and the perpendicular 2D subspace $\mathbf{V}^{\perp}$. Thus, using $W\Gamma W^{-1} = \Gamma_V = \Gamma_V^{\parallel} \oplus \Gamma_V^{\perp}$, we obtain

$$\Gamma_V(\alpha) = \left(\begin{array}{ccc|cc} \cos(\pi/5) & -\sin(\pi/5) & 0 & 0 & 0 \\ \sin(\pi/5) & \cos(\pi/5) & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & \cos(3\pi/5) & -\sin(3\pi/5) \\ 0 & 0 & 0 & \sin(3\pi/5) & \cos(3\pi/5) \end{array}\right)_V = \left(\begin{array}{c|c} \Gamma^{\parallel}(\alpha) & 0 \\ \hline 0 & \Gamma^{\perp}(\alpha) \end{array}\right)_V ,$$

$$\Gamma_V(\beta) = \left(\begin{array}{ccc|cc} 1 & 0 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & \bar{1} \end{array}\right)_V , \quad \Gamma_V(\gamma) \left(\begin{array}{ccc|cc} \bar{1} & 0 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 & 0 \\ 0 & 0 & \bar{1} & 0 & 0 \\ \hline 0 & 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & 0 & \bar{1} \end{array}\right)_V ,$$

where

$$W = \left(\begin{array}{ccccc} a_1^* \cos(2\pi/5) & a_2^* \cos(4\pi/5) & a_3^* \cos(6\pi/5) & a_4^* \cos(8\pi/5) & 0 \\ a_1^* \sin(2\pi/5) & a_2^* \sin(4\pi/5) & a_3^* \sin(6\pi/5) & a_4^* \sin(8\pi/5) & 0 \\ 0 & 0 & 0 & 0 & a_5^* \\ \hline a_1^* \cos(6\pi/5) & a_2^* \cos(2\pi/5) & a_3^* \cos(8\pi/5) & a_4^* \cos(4\pi/5) & 0 \\ a_1^* \sin(6\pi/5) & a_2^* \sin(2\pi/5) & a_3^* \sin(8\pi/5) & a_4^* \sin(4\pi/5) & 0 \end{array}\right).$$

The column vectors of the matrix W give the parallel- (above the partition line) and perpendicular-space components (below the partition line) of a reciprocal basis in V space. Thus, W can be rewritten using the physical-space reciprocal basis defined above as

$$W = \left(\mathbf{d}_1^*, \quad \mathbf{d}_2^*, \quad \mathbf{d}_3^*, \quad \mathbf{d}_4^*, \quad \mathbf{d}_5^*\right),$$

yielding the reciprocal basis $\mathbf{d}_i^*$, $i = 1, \ldots, 5$, in the 5D embedding space (D space):

$$\mathbf{d}_i^* = a_i^* \begin{pmatrix} \cos(2\pi i/5) \\ \sin(2\pi i/5) \\ 0 \\ \cos(6\pi i/5) \\ \sin(6\pi i/5) \end{pmatrix}_V , \; i = 1, \ldots, 4 \text{ and } \mathbf{d}_5^* = a_5^* \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}_V .$$

The 5×5 symmetry matrices can each be decomposed into a 3×3 matrix and a 2×2 matrix. The first one, $\Gamma^{\parallel}$, acts on the parallel-space component, the second one, $\Gamma^{\perp}$, on the perpendicular-space component. In the case of $\Gamma(\alpha)$, the coupling factor between a rotation in parallel and perpendicular space is 3. Thus, a $\pi/5$ rotation in physical space is related to a $3\pi/5$ rotation in perpendicular space (Fig. 4.6.3.12).

With the condition $\mathbf{d}_i \cdot \mathbf{d}_j^* = \delta_{ij}$, a basis in direct 5D space is obtained:

$$\mathbf{d}_i = \frac{2}{5a_i^*} \begin{pmatrix} \cos(2\pi i/5) - 1 \\ \sin(2\pi i/5) \\ 0 \\ \cos(6\pi i/5) - 1 \\ \sin(6\pi i/5) \end{pmatrix}, \; i = 1, \ldots, 4, \text{ and } \mathbf{d}_5 = \frac{1}{a_5^*} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}.$$

The metric tensors G, G^* are of the type

$$\begin{pmatrix} A & C & C & C & 0 \\ C & A & C & C & 0 \\ C & C & A & C & 0 \\ C & C & C & A & 0 \\ 0 & 0 & 0 & 0 & B \end{pmatrix}$$

with $A = 2a_1^{*2}$, $B = a_5^{*2}$, $C = -(1/2)a_1^{*2}$ for the reciprocal space and $A = 4/5a_1^{*2}$, $B = 1/a_5^{*2}$, $C = 2/5a_1^{*2}$ for the direct space. Thus, for the lattice parameters in reciprocal space we obtain $d_i^* = a_i^*(2)^{1/2}$, $i = 1, \ldots, 4$; $d_5^* = a_5^*$; $\alpha_{ij}^* = 104.5°$, $i, j = 1, \ldots, 4$; $\alpha_{i5}^* = 90°$, $i = 1, \ldots, 4$, and for those in direct space $d_i = 2/[a_i^*(5)^{1/2}]$, $i = 1, \ldots, 4$; $d_5 = 1/a_5^*$; $\alpha_{ij} = 60°$, $i, j = 1, \ldots, 4$; $\alpha_{i5} = 90°$, $i = 1, \ldots, 4$. The volume of the 5D unit cell can be calculated from the metric tensor G:

$$V = [\det(G)]^{1/2} = \frac{4}{5(5)^{1/2}(a_1^*)^4 a_5^*} = \frac{(5)^{1/2}}{4}(d_1)^4 d_5.$$

Since decagonal phases are only quasiperiodic in two dimensions, it is sufficient to demonstrate their characteristics on a 2D

references