International Tables for Crystallography (2006). Vol. B, Figure 4.6.3.27, p. 510.

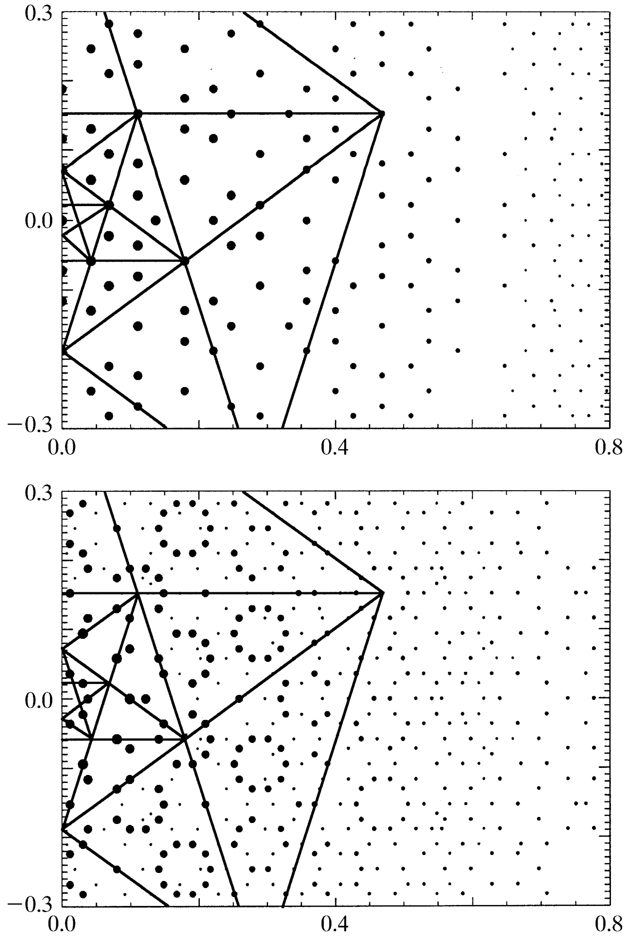

Fig. 4.6.3.27. Pentagrammal relationships between scaling symmetry-related structure factors $F(\mathbf{H})$ of the Penrose tiling (edge length $a_r = 4.04$ Å) in perpendicular space. Enlarged sections of positive (above) and negative structure factors (below) are shown.

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

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

Block-diagonalization of these reducible symmetry matrices decomposes them into non-equivalent irreducible representations. These can be assigned to the two orthogonal subspaces forming the 6D embedding space $\mathbf{V} = \mathbf{V}^{\parallel} \oplus \mathbf{V}^{\perp}$, the 3D parallel (physical) subspace $\mathbf{V}^{\parallel}$ and the perpendicular 3D subspace $\mathbf{V}^{\perp}$. Thus, using $W\Gamma W^{-1} = \Gamma^{\rm red} = \Gamma^{\parallel} \oplus \Gamma^{\perp}$, we obtain

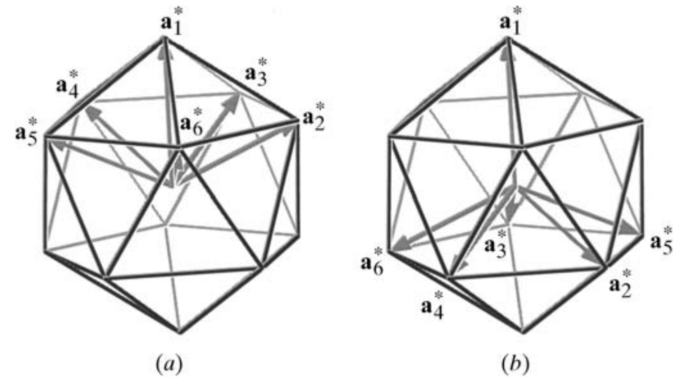

Fig. 4.6.3.28. Perspective (*a*) parallel- and (*b*) perpendicular-space views of the reciprocal basis of the 3D Penrose tiling. The six rationally independent vectors $\mathbf{a}_i^*$ point to the edges of an icosahedron.

$$\Gamma(\alpha) = \left(\begin{array}{ccc|ccc} \cos(2\pi/5) & -\sin(2\pi/5) & 0 & 0 & 0 & 0 \\ \sin(2\pi/5) & \cos(2\pi/5) & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & \cos(4\pi/5) & -\sin(4\pi/5) & 0 \\ 0 & 0 & 0 & \sin(4\pi/5) & \cos(4\pi/5) & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right)_V = \left(\begin{array}{c|c} \Gamma^{\parallel} & 0 \\ \hline 0 & \Gamma^{\perp} \end{array}\right)_V,$$

where

$$W = a^* \left(\begin{array}{cccccc} 0 & sc4 & sc6 & sc8 & s & sc2 \\ 0 & ss4 & ss6 & ss8 & 0 & ss2 \\ 1 & c & c & c & c & c \\ \hline 0 & -sc8 & -sc2 & -sc6 & -s & -sc4 \\ 0 & -ss8 & -ss2 & -ss6 & 0 & -ss4 \\ 1 & -c & -c & -c & -c & -c \end{array}\right)_V,$$

$c = \cos\theta$, $s = \sin\theta$, $scn = \sin\theta\cos(n\pi/5)$, $ssn = \sin\theta\sin(n\pi/5)$. 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 $\mathbf{V}$. Thus, W can be rewritten using the physical-space reciprocal basis defined above and an arbitrary constant c,

$$W = \begin{pmatrix} \mathbf{a}_1^* & \mathbf{a}_2^* & \mathbf{a}_3^* & \mathbf{a}_4^* & \mathbf{a}_5^* & \mathbf{a}_6^* \\ c\mathbf{a}_1^* & -c\mathbf{a}_4^* & -c\mathbf{a}_6^* & -c\mathbf{a}_3^* & -c\mathbf{a}_5^* & -c\mathbf{a}_2^* \end{pmatrix} = (\mathbf{d}_1^* \ \ \mathbf{d}_2^* \ \ \mathbf{d}_3^* \ \ \mathbf{d}_4^* \ \ \mathbf{d}_5^* \ \ \mathbf{d}_6^*),$$

yielding the reciprocal basis $\mathbf{d}_i^*, i = 1, \ldots, 6$, in the 6D embedding space (D space)

$$\mathbf{d}_1^* = a^* \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ c \end{pmatrix} \text{ and } \mathbf{d}_i^* = a^* \begin{pmatrix} \sin\theta\cos(2\pi i/5) \\ \sin\theta\sin(2\pi i/5) \\ \cos\theta \\ -c\sin\theta\cos(4\pi i/5) \\ -c\sin\theta\sin(4\pi i/5) \\ -c\cos\theta \end{pmatrix}, i = 2, \ldots, 6.$$

The 6×6 symmetry matrices can each be decomposed into two 3×3 matrices. 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 2. Thus a $2\pi/5$

references