

4.6. RECIPROCAL-SPACE IMAGES OF APERIODIC CRYSTALS

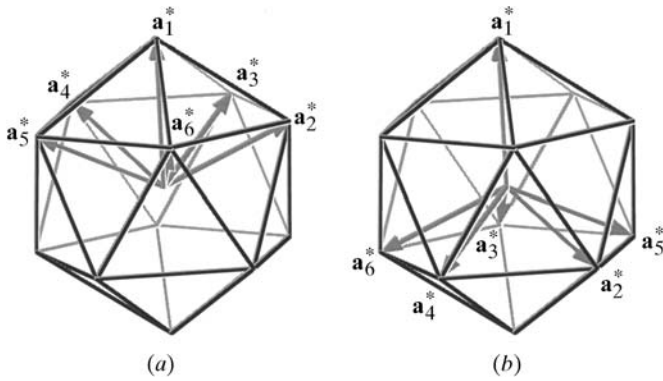


Fig. 4.6.3.28. Perspective (a) parallel- and (b) perpendicular-space views of the reciprocal basis of the 3D Penrose tiling. The six rationally independent vectors \mathbf{a}_i^* point to the edges of an icosahedron.

fold rotation α , a threefold rotation β and the inversion operation γ , can be written in the form

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

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

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 $W\Gamma W^{-1} = \Gamma^{\text{red}} = \Gamma^{\parallel} \oplus \Gamma^{\perp}$, we obtain

$$\Gamma(\alpha) = \begin{pmatrix} \cos(2\pi/5) & -\sin(2\pi/5) & 0 & 0 & 0 & 0 \\ \sin(2\pi/5) & \cos(2\pi/5) & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \cos(4\pi/5) & -\sin(4\pi/5) & 0 \\ 0 & 0 & 0 & \sin(4\pi/5) & \cos(4\pi/5) & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}_V = \begin{pmatrix} \Gamma^{\parallel} & 0 \\ 0 & \Gamma^{\perp} \end{pmatrix}_V,$$

where

$$W = a^* \begin{pmatrix} 0 & sc4 & sc6 & sc8 & s & sc2 \\ 0 & ss4 & ss6 & ss8 & 0 & ss2 \\ 1 & c & c & c & c & c \\ 0 & -sc8 & -sc2 & -sc6 & -s & -sc4 \\ 0 & -ss8 & -ss2 & -ss6 & 0 & -ss4 \\ 1 & -c & -c & -c & -c & -c \end{pmatrix}_V,$$

$c = \cos \theta$, $s = \sin \theta$, $scn = \sin \theta \cos(n\pi/5)$, $ssn = \sin \theta \sin(n\pi/5)$. The column vectors of the matrix W give the parallel- (above the partition line) and perpendicular-space components (below the

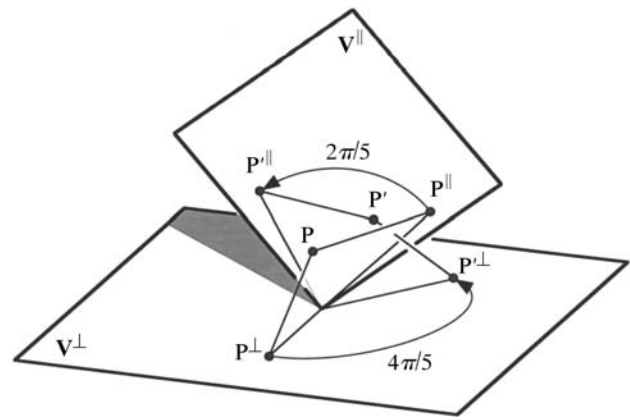


Fig. 4.6.3.29. Schematic representation of a rotation in 6D space. The point P is rotated to P' . The component rotations in parallel and perpendicular space are illustrated.

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^* , $i = 1, \dots, 6$, in the 6D embedding space (D space)

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

The 6×6 symmetry matrices can each be decomposed into two 3×3 matrices. The first one, Γ^{\parallel} , acts on the parallel-space component, the second one, Γ^{\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 $2\pi/5$ rotation in physical space is related to a $4\pi/5$ rotation in perpendicular space (Figs. 4.6.3.28 and 4.6.3.29).

With the condition $\mathbf{d}_i \cdot \mathbf{d}_j^* = \delta_{ij}$, the basis in direct 6D space is obtained:

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

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