

4. DIFFUSE SCATTERING AND RELATED TOPICS

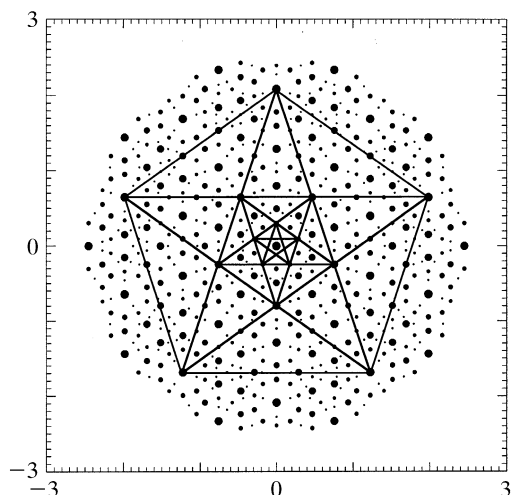


Fig. 4.6.3.24. Pentagrammatic relationships between scaling symmetry-related positive structure factors  $F(\mathbf{H})$  of the Penrose tiling (edge length  $a_r = 4.04 \text{ \AA}$ ) in parallel space. The magnitudes of the structure factors are indicated by the diameters of the filled circles.

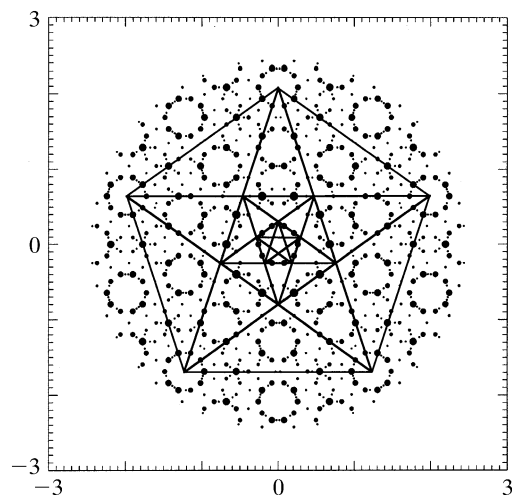


Fig. 4.6.3.25. Pentagrammatic relationships between scaling symmetry-related negative structure factors  $F(\mathbf{H})$  of the Penrose tiling (edge length  $a_r = 4.04 \text{ \AA}$ ) in parallel space. The magnitudes of the structure factors are indicated by the diameters of the filled circles.

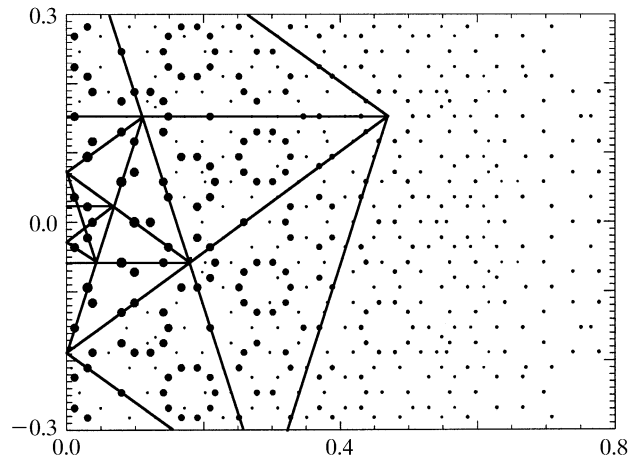
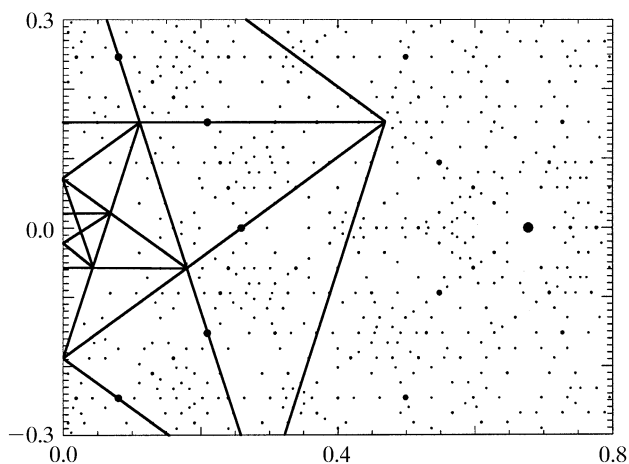
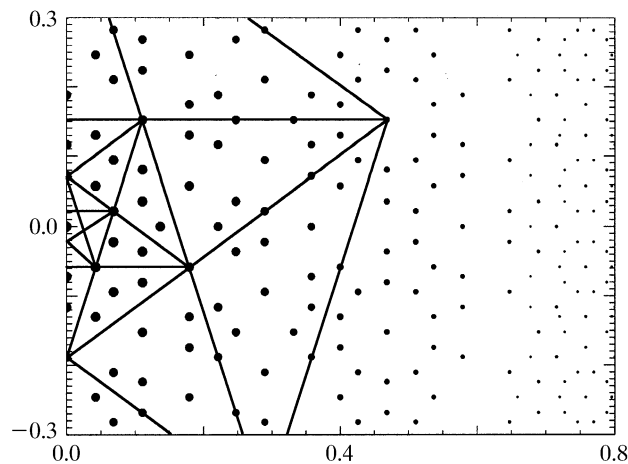
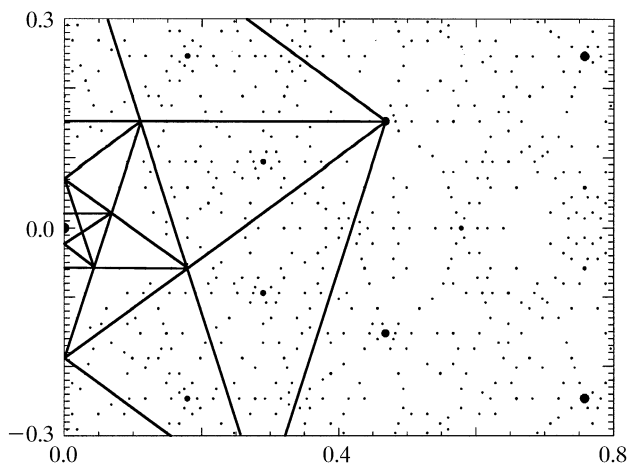


Fig. 4.6.3.26. Pentagrammatic relationships between scaling symmetry-related structure factors  $F(\mathbf{H})$  of the Penrose tiling (edge length  $a_r = 4.04 \text{ \AA}$ ) in parallel space. Enlarged sections of Figs. 4.6.3.24 (above) and 4.6.3.25 (below) are shown.

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

$$\begin{pmatrix} \mathbf{a}_1^* \\ \mathbf{a}_2^* \\ \mathbf{a}_3^* \\ \mathbf{a}_4^* \\ \mathbf{a}_5^* \\ \mathbf{a}_6^* \end{pmatrix} = a^* \begin{pmatrix} 0 & 0 & 1 \\ \sin \theta \cos(4\pi/5) & \sin \theta \sin(4\pi/5) & \cos \theta \\ \sin \theta \cos(6\pi/5) & \sin \theta \sin(6\pi/5) & \cos \theta \\ \sin \theta \cos(8\pi/5) & \sin \theta \sin(8\pi/5) & \cos \theta \\ \sin \theta & 0 & \cos \theta \\ \sin \theta \cos(2\pi/5) & \sin \theta \sin(2\pi/5) & \cos \theta \end{pmatrix} \begin{pmatrix} \mathbf{e}_1^V \\ \mathbf{e}_2^V \\ \mathbf{e}_3^V \end{pmatrix},$$

where  $\mathbf{e}_i^V$  are Cartesian basis vectors. Thus, from the number of independent reciprocal-basis vectors needed to index the Bragg reflections with integer numbers, the dimension of the embedding space has to be six. The vector components refer to a Cartesian coordinate system ( $V$  basis) in the physical (parallel) space.

The set  $M^* = \{\mathbf{H}^{\parallel} = \sum_{i=1}^6 h_i \mathbf{a}_i^* | h_i \in \mathbb{Z}\}$  of all diffraction vectors remains invariant under the action of the symmetry operators of the icosahedral point group  $K = m\bar{3}5$ . The symmetry-adapted matrix representations for the point-group generators, one five-