International Tables for Crystallography (2006). Vol. B, Section 4.6.3.3.2.5, pp. 508–509.

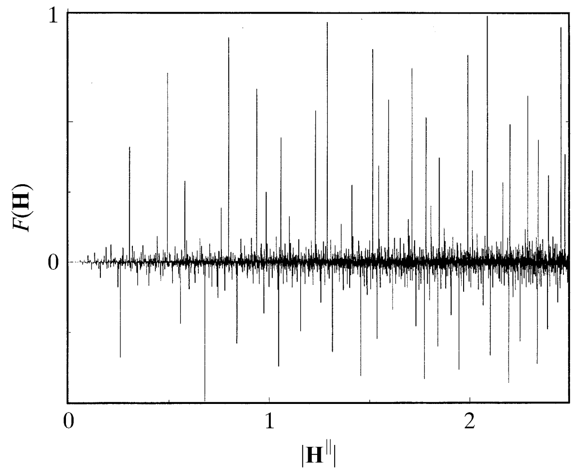

Fig. 4.6.3.21. Radial distribution function of the structure factors $F(\mathbf{H})$ of the Penrose tiling (edge length of the Penrose unit rhombs $a_r = 4.04$ Å) decorated with point atoms as a function of $\mathbf{H}^{\parallel}$. All structure factors within $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$ and $0 \leq |\mathbf{H}^{\parallel}| \leq 2.5$ Å^{-1} have been used and normalized to $F(0000) = 1$.

4.6.3.3.2.5. *Relationships between structure factors at symmetry-related points of the Fourier image*

Scaling the Penrose tiling by a factor τ^{-n} by employing the matrix S^{-n} scales at the same time its reciprocal space by a factor τ^n:

$$S\mathbf{H} = \begin{pmatrix} 0 & 1 & 0 & \bar{1} & 0 \\ 0 & 1 & 1 & \bar{1} & 0 \\ \bar{1} & 1 & 1 & 0 & 0 \\ \bar{1} & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}_D \begin{pmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \\ h_5 \end{pmatrix} = \begin{pmatrix} h_2 - h_4 \\ h_2 + h_3 - h_4 \\ -h_1 + h_2 + h_3 \\ -h_1 + h_3 \\ h_5 \end{pmatrix}.$$

Since this operation increases the lengths of the diffraction vectors by the factor τ in parallel space and decreases them by the factor $1/\tau$ in perpendicular space, the following distribution of structure-factor magnitudes (for point atoms at rest) is obtained:

$$|F(S^n\mathbf{H})| > |F(S^{n-1}\mathbf{H})| > \ldots > |F(S^1\mathbf{H})| > |F(\mathbf{H})|,$$
$$|F(\tau^n\mathbf{H}^{\parallel})| > |F(\tau^{n-1}\mathbf{H}^{\parallel})| > \ldots > |F(\tau\mathbf{H}^{\parallel})| > |F(\mathbf{H})|.$$

The scaling operations S^n, $n \in \mathbb{Z}$, the rotoscaling operations $(\Gamma(\alpha)S^2)^n$ (Fig. 4.6.3.14) and the tenfold rotation $(\Gamma(\alpha))^n$, where

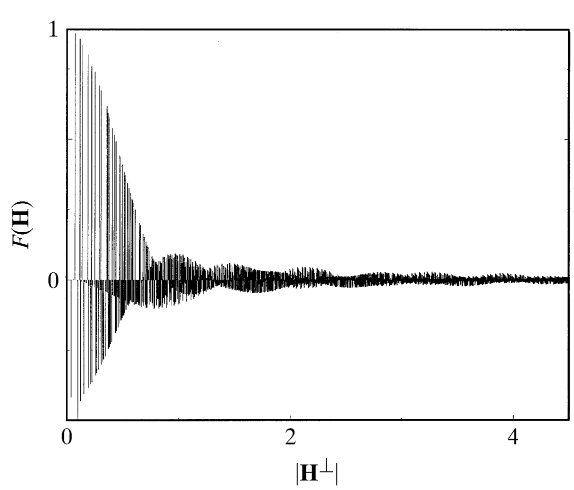

Fig. 4.6.3.22. Radial distribution function of the structure factors $F(\mathbf{H})$ of the Penrose tiling (edge length of the Penrose unit rhombs $a_r = 4.04$ Å) decorated with point atoms as a function of $\mathbf{H}^{\perp}$. All structure factors within $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$ and $0 \leq |\mathbf{H}^{\parallel}| \leq 2.5$ Å^{-1} have been used and normalized to $F(0000) = 1$.

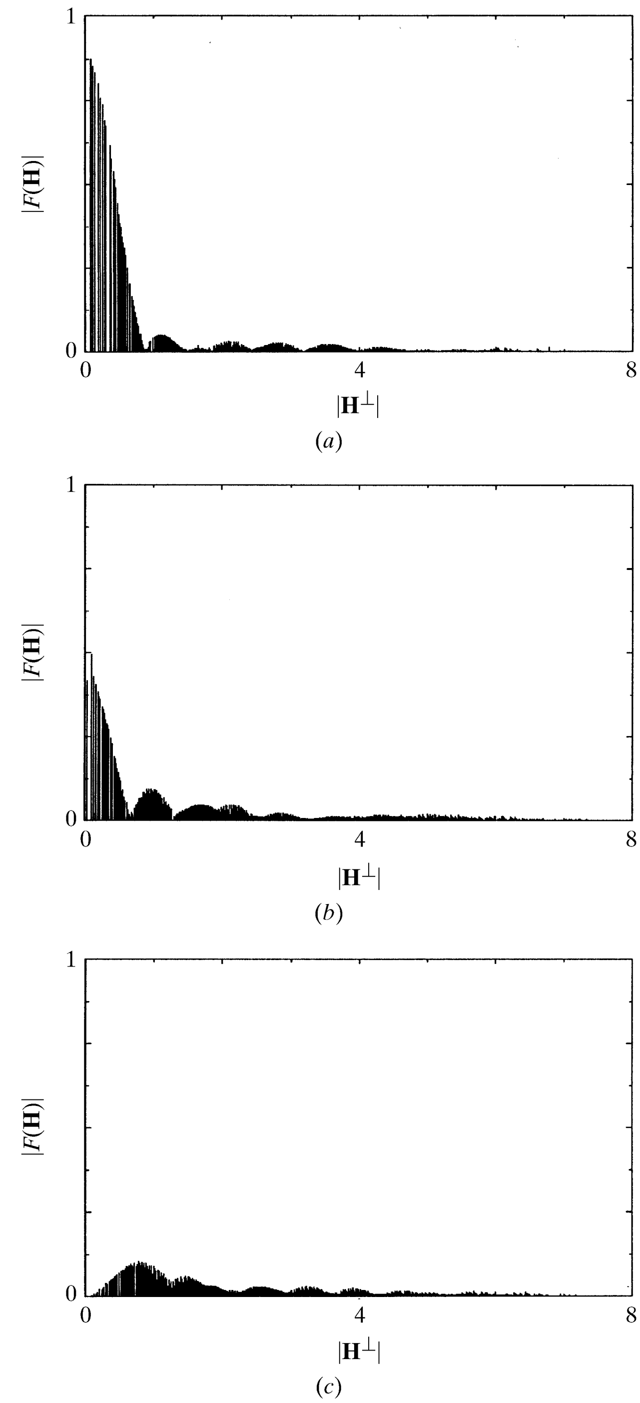

Fig. 4.6.3.23. Radial distribution function of the structure-factor magnitudes $|F(\mathbf{H})|$ of the Penrose tiling (edge length of the Penrose unit rhombs $a_r = 4.04$ Å) decorated with point atoms as a function of $\mathbf{H}^{\perp}$. All structure factors within $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$ and $0 \leq |\mathbf{H}^{\parallel}| \leq 2.5$ Å^{-1} have been used and normalized to $F(0000) = 1$. The branches with (*a*) $\left|\sum_{i=1}^{4} h_i\right| = 0 \bmod 5$, (*b*) $\left|\sum_{i=1}^{4} h_i\right| = 1 \bmod 5$ and (*c*) $\left|\sum_{i=1}^{4} h_i\right| = 2 \bmod 5$ are shown.

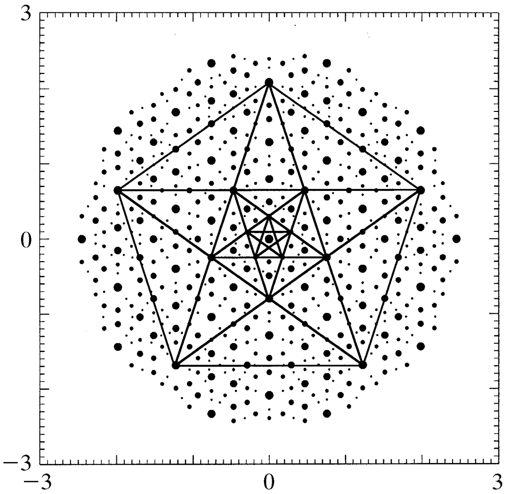

Fig. 4.6.3.24. Pentagrammal relationships between scaling symmetry-related positive structure factors $F(\mathbf{H})$ of the Penrose tiling (edge length $a_r = 4.04$ Å) in parallel space. The magnitudes of the structure factors are indicated by the diameters of the filled circles.

$$(\Gamma(\alpha)S^2)^n = \begin{pmatrix} 1 & 1 & \bar{1} & \bar{1} & 0 \\ 1 & 2 & 0 & \bar{2} & 0 \\ 0 & 2 & 1 & \bar{1} & 0 \\ \bar{1} & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}^n_D,$$

connect all structure factors with diffraction vectors pointing to the nodes of an infinite series of pentagrams. The structure factors with positive signs are predominantly on the vertices of the pentagram while the ones with negative signs are arranged on circles around the vertices (Figs. 4.6.3.24 to 4.6.3.27).

4.6.3.3.3. *Icosahedral phases*

A structure that is quasiperiodic in three dimensions and exhibits icosahedral diffraction symmetry is called an icosahedral phase. Its holohedral Laue symmetry group is $K = m\bar{3}\bar{5}$. All reciprocal-space vectors $\mathbf{H} = \sum_{i=1}^{6} h_i \mathbf{a}_i^* \in M^*$ can be represented on a basis

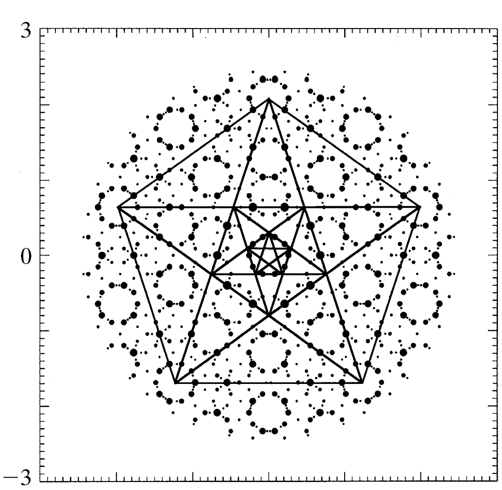

Fig. 4.6.3.25. Pentagrammal relationships between scaling symmetry-related negative structure factors $F(\mathbf{H})$ of the Penrose tiling (edge length $a_r = 4.04$ Å) in parallel space. The magnitudes of the structure factors are indicated by the diameters of the filled circles.

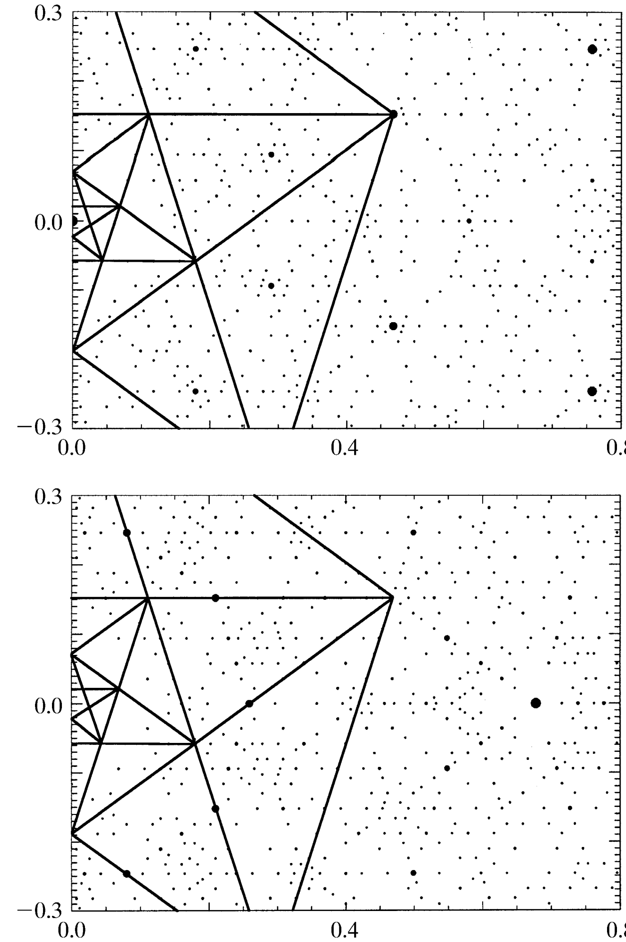

Fig. 4.6.3.26. Pentagrammal relationships between scaling symmetry-related structure factors $F(\mathbf{H})$ of the Penrose tiling (edge length $a_r = 4.04$ Å) in parallel space. Enlarged sections of Figs. 4.6.3.24 (above) and 4.6.3.25 (below) are shown.

$\mathbf{a}_1^* = a^*(0, 0, 1)$, $\mathbf{a}_i^* = a^*[\sin\theta\cos(2\pi i/5), \sin\theta\sin(2\pi i/5), \cos\theta]$, $i = 2, \ldots, 6$ where $\sin\theta = 2/(5)^{1/2}$, $\cos\theta = 1/(5)^{1/2}$ and $\theta \simeq 63.44°$, the angle between two neighbouring fivefold axes (Fig. 4.6.3.28). This can be rewritten as

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

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 $K = m\bar{3}\bar{5}$. The symmetry-adapted matrix representations for the point-group generators, one fivefold rotation α, a threefold rotation β and the inversion operation γ, can be written in the form