International Tables for Crystallography (2010). Vol. B, Section 4.6.3.3.1.5, pp. 606–607.

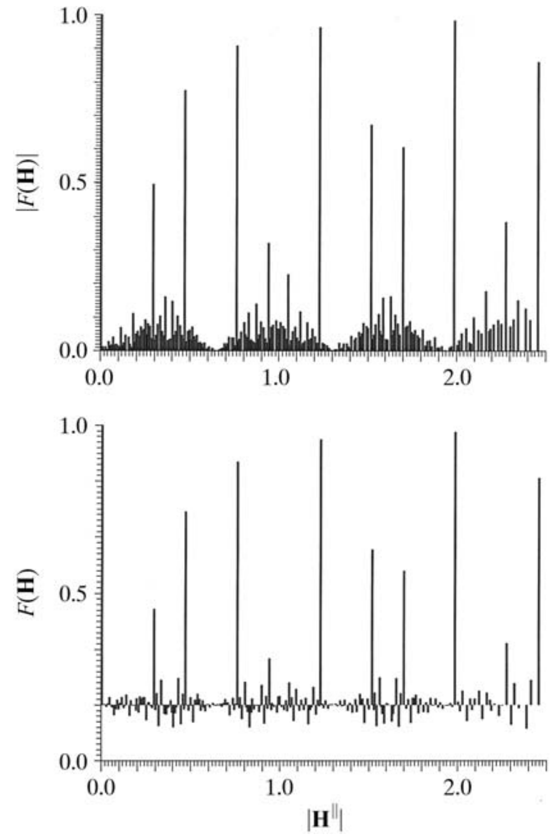

Fig. 4.6.3.8. The structure factors $F(\mathbf{H})$ (below) and their magnitudes $|F(\mathbf{H})|$ (above) of the squared Fibonacci chain decorated with equal point atoms are shown as a function of the parallel-space component $|\mathbf{H}^{\parallel}|$ of the diffraction vector. The short distance is $\text{S} = 2.5$ Å, all structure factors within $0 \le |\mathbf{H}| \le 2.5$ Å^{-1} have been calculated and normalized to $F(00) = 1$.

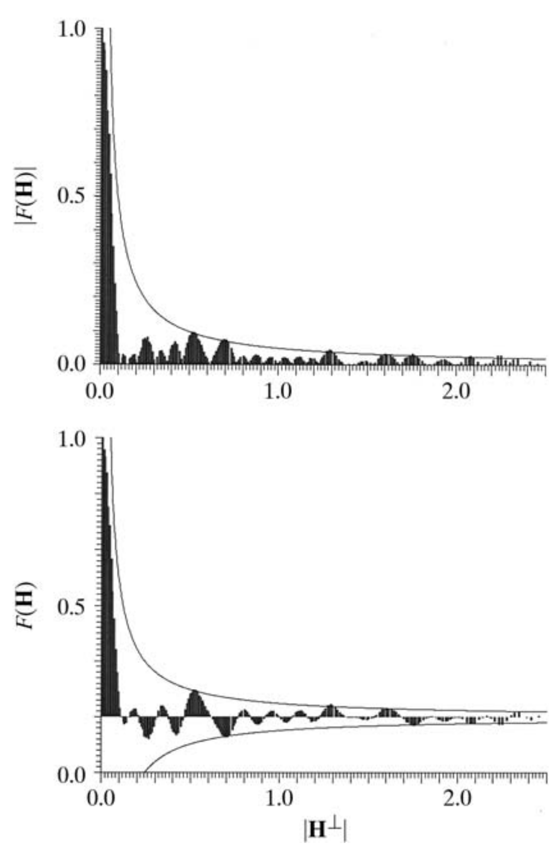

Fig. 4.6.3.9. The structure factors $F(\mathbf{H})$ (below) and their magnitudes $|F(\mathbf{H})|$ (above) of the squared Fibonacci chain decorated with equal point atoms are shown as a function of the perpendicular-space component $|\mathbf{H}^{\perp}|$ of the diffraction vector. The short distance is $\text{S} = 2.5$ Å, all structure factors within $0 \le |\mathbf{H}| \le 2.5$ Å^{-1} have been calculated and normalized to $F(00) = 1$.

are discussed. The intensities $I(\mathbf{H})$ of the Fibonacci chain decorated with point atoms are only a function of the perpendicular-space component of the diffraction vector. $|F(\mathbf{H})|$ and $F(\mathbf{H})$ are illustrated in Figs. 4.6.3.5 and 4.6.3.6 as a function of $\mathbf{H}^{\parallel}$ and of $\mathbf{H}^{\perp}$. The distribution of $|F(\mathbf{H})|$ as a function of their frequencies clearly resembles a centric distribution, as can be expected from the centrosymmetric 2D subunit cell. The shape of the distribution function depends on the radius $H_{\max}$ of the limiting sphere in reciprocal space. The number of weak reflections increases with the square of $H_{\max}$, that of strong reflections only linearly (strong reflections always have small $\mathbf{H}^{\perp}$ components).

The weighted reciprocal space of the Fibonacci sequence contains an infinite number of Bragg reflections within a limited region of the physical space. Contrary to the diffraction pattern of a periodic structure consisting of point atoms on the lattice nodes, the Bragg reflections show intensities depending on the perpendicular-space components of their diffraction vectors.

The reciprocal space of a sequence generated from hyperatoms with fractally shaped atomic surfaces (squared Fibonacci sequence) is very similar to that of the Fibonacci sequence (Figs. 4.6.3.8 and 4.6.3.9). However, there are significantly more weak reflections in the diffraction pattern of the 'fractal' sequence, caused by the geometric form factor.

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

The two possible point-symmetry groups in the 1D quasiperiodic case, $K^{1\text{D}} = 1$ and $K^{1\text{D}} = \bar{1}$, relate the structure factors to

$$1: \qquad F(\mathbf{H}) = -F(\bar{\mathbf{H}}),$$
$$\bar{1}: \qquad F(\mathbf{H}) = F(\bar{\mathbf{H}}).$$

A 3D structure with 1D quasiperiodicity results from the stacking of atomic layers with distances following a quasiperiodic sequence. The point groups $K^{3\text{D}}$ describing the symmetry of such structures result from the direct product $K^{3\text{D}} = K^{2\text{D}} \otimes K^{1\text{D}}$. $K^{2\text{D}}$ corresponds to one of the ten crystallographic 2D point groups, $K^{1\text{D}}$ can be $\{1\}$ or $\{1, m\}$. Consequently, 18 3D point groups are possible.

Since 1D quasiperiodic sequences can be described generically as incommensurately modulated structures, their possible point and space groups are equivalent to a subset of the $(3+1)$D superspace groups for IMSs with satellite vectors of the type (00γ), *i.e.* $\mathbf{q} = \gamma\mathbf{c}^*$, for the quasiperiodic direction [001] (Janssen *et al.*, 2004).

From the scaling properties of the Fibonacci sequence, some relationships between structure factors can be derived. Scaling the physical-space structure by a factor τ^n, $n \in \mathbb{Z}$, corresponds to a scaling of the perpendicular space by the inverse factor $(-\tau)^{-n}$. For the scaling of the corresponding reciprocal subspaces, the inverse factors compared to the direct spaces have to be applied.

The set of vectors $\mathbf{r}$, defining the vertices of a Fibonacci sequence $s(\mathbf{r})$, multiplied by a factor τ coincides with a subset of the vectors defining the vertices of the original sequence (Fig. 4.6.3.10). The residual vertices correspond to a particular decoration of the scaled sequence, *i.e.* the sequence $\tau^2 s(\mathbf{r})$. The Fourier transform of the sequence $s(\mathbf{r})$ then can be written as the sum of the Fourier transforms of the sequences $\tau s(\mathbf{r})$ and $\tau^2 s(\mathbf{r})$;

$$\sum_k \exp(2\pi i\mathbf{H}\cdot\mathbf{r}_k) = \sum_k \exp(2\pi i\mathbf{H}\tau\mathbf{r}_k) + \sum_k \exp[2\pi i\mathbf{H}(\tau^2\mathbf{r}_k + \tau)].$$

In terms of structure factors, this can be reformulated as

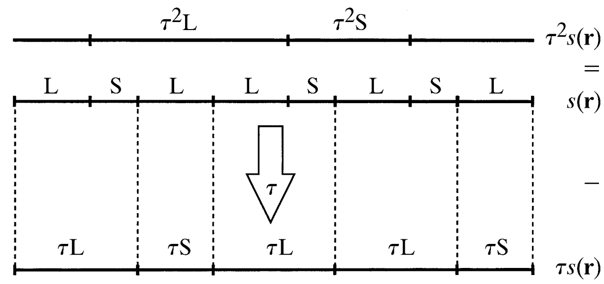

Fig. 4.6.3.10. Part ... LSLLSLSL ... of a Fibonacci sequence $s(\mathbf{r})$ before and after scaling by the factor τ. L is mapped onto τL, S onto τS = L. The vertices of the new sequence are a subset of those of the original sequence (the correspondence is indicated by dashed lines). The residual vertices $\tau^2 s(\mathbf{r})$, which give when decorating $\tau s(\mathbf{r})$ the Fibonacci sequence $s(\mathbf{r})$, form a Fibonacci sequence scaled by a factor τ^2.

$$F(\mathbf{H}) = F(\tau\mathbf{H}) + \exp(2\pi i\tau\mathbf{H})F(\tau^2\mathbf{H}).$$

Hence, phases of structure factors that are related by scaling symmetry can be determined from each other.

Further scaling relationships in reciprocal space exist: scaling a diffraction vector

$$\mathbf{H} = h_1\mathbf{d}_1^* + h_2\mathbf{d}_2^* = h_1 a^* \begin{pmatrix} 1 \\ -\tau \end{pmatrix}_V + h_2 a^* \begin{pmatrix} \tau \\ 1 \end{pmatrix}_V$$

with the matrix

$$S = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}_D,$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}_D \begin{pmatrix} h_1 \\ h_2 \end{pmatrix}_D = \begin{pmatrix} F_n & F_{n+1} \\ F_{n+1} & F_{n+2} \end{pmatrix}_D \begin{pmatrix} h_1 \\ h_2 \end{pmatrix}_D = \begin{pmatrix} F_n h_1 + F_{n+1} h_2 \\ F_{n+1} h_1 + F_{n+2} h_2 \end{pmatrix}_D,$$

increases the magnitudes of structure factors assigned to this particular diffraction vector $\mathbf{H}$,

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

This is due to the shrinking of the perpendicular-space component of the diffraction vector by powers of $(-\tau)^{-n}$ while expanding the parallel-space component by τ^n according to the eigenvalues τ and $-\tau^{-1}$ of S acting in the two eigenspaces $\mathbf{V}^\parallel$ and $\mathbf{V}^\perp$:

$$\begin{aligned} \pi^\parallel(S\mathbf{H}) &= (h_2 + \tau(h_1 + h_2))a^* = (\tau h_1 + h_2(\tau + 1))a^* \\ &= \tau(h_1 + \tau h_2)a^*, \\ \pi^\perp(S\mathbf{H}) &= (-\tau h_2 + h_1 + h_2)a^* = (h_1 - h_2(\tau - 1))a^* \\ &= -(1/\tau)(-\tau h_1 + h_2)a^*, \\ |F(\tau^n\mathbf{H}^\parallel)| &> |F(\tau^{n-1}\mathbf{H}^\parallel)| > \ldots > |F(\tau\mathbf{H}^\parallel)| > |F(\mathbf{H}^\parallel)|. \end{aligned}$$

Thus, for scaling n times we obtain

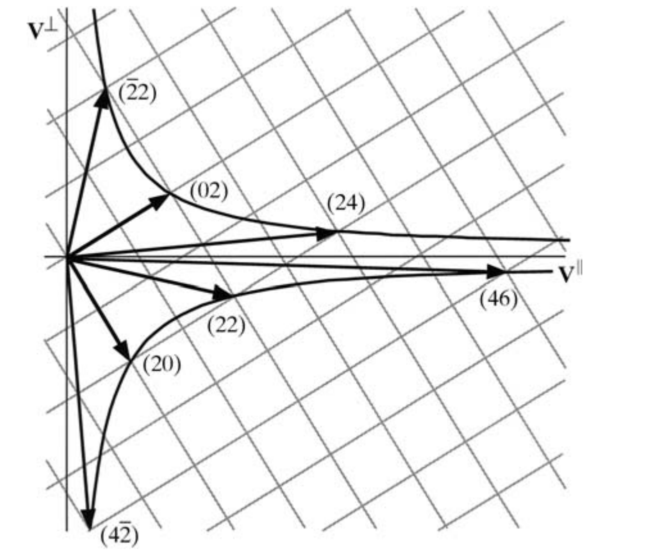

Fig. 4.6.3.11. Scaling operations of the Fibonacci sequence. The scaling operation S acts six times on the diffraction vector $\mathbf{H} = (4\bar{2})$ yielding the sequence $(4\bar{2}) \to (\bar{2}2) \to (20) \to (02) \to (22) \to (24) \to (46)$.

$$\begin{aligned} \pi^\perp(S^n\mathbf{H}) &= \big(-\tau\big(F_n h_1 + F_{n+1}h_2\big) + \big(F_{n+1}h_1 + F_{n+2}h_2\big)\big)a^* \\ &= \big(h_1\big(-\tau F_n + F_{n+1}\big) + h_2\big(-\tau F_{n+1} + F_{n+2}\big)\big)a^* \end{aligned}$$

with

$$\lim_{n\to\infty}\big(-\tau F_n + F_{n+1}\big) = 0 \text{ and } \lim_{n\to\infty}\big(-\tau F_{n+1} + F_{n+2}\big) = 0,$$

yielding eventually

$$\lim_{n\to\infty}\big(\pi^\perp(S^n\mathbf{H})\big) = 0 \text{ and } \lim_{n\to\infty}(F(S^n\mathbf{H})) = F(\mathbf{0}).$$

The scaling of the diffraction vectors $\mathbf{H}$ by S^n corresponds to a hyperbolic rotation (Janner, 1992) with angle $n\varphi$, where $\sinh\varphi = 1/2$ (Fig. 4.6.3.11):

$$\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}^{2n} = \begin{pmatrix} \cosh 2n\varphi & \sinh 2n\varphi \\ \sinh 2n\varphi & \cosh 2n\varphi \end{pmatrix},$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}^{2n+1} = \begin{pmatrix} \sinh[(2n+1)\varphi] & \cosh[(2n+1)\varphi] \\ \cosh[(2n+1)\varphi] & \sinh[(2n+1)\varphi] \end{pmatrix}.$$

4.6.3.3.2. Decagonal phases

A structure quasiperiodic in two dimensions, periodic in the third dimension and with decagonal diffraction symmetry is called a decagonal phase. Its holohedral Laue symmetry group is $K = 10/mmm$. All reciprocal-space vectors $\mathbf{H} \in M^*$ can be represented on a basis (V basis) $\mathbf{a}_i^* = a_i^*\,(\cos 2\pi i/5, \sin 2\pi i/5, 0)$, $i = 1, \ldots, 4$ and $\mathbf{a}_5^* = a_5^*(0, 0, 1)$ (Fig. 4.6.3.12) as $\mathbf{H} = \sum_{i=1}^{5} h_i\mathbf{a}_i^*$. The vector components refer to a Cartesian coordinate system in physical (parallel) space. Thus, from the number of independent reciprocal-basis vectors necessary to index the Bragg reflections with integer numbers, the dimension of the embedding space has to be at least five. This can also be shown in a different way (Hermann, 1949).

The set M^* of all vectors $\mathbf{H}$ remains invariant under the action of the symmetry operators of the point group $10/mmm$. The symmetry-adapted matrix representations for the point-group