

4.6. RECIPROCAL-SPACE IMAGES OF APERIODIC CRYSTALS

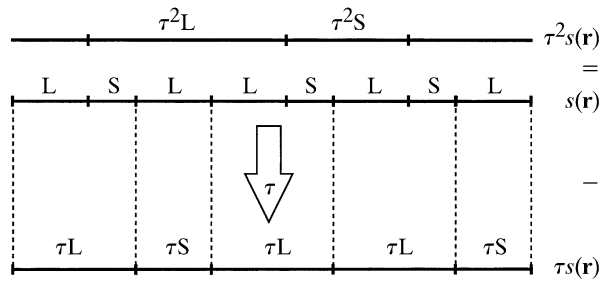


Fig. 4.6.3.10. Part ... LSLLSLSL ... of a Fibonacci sequence $s(\mathbf{r})$ before and after scaling by the factor τ . L is mapped onto τL , S onto $\tau S = L$. The vertices of the new sequence are a subset of those of the original sequence (the correspondence is indicated by dashed lines). The residual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

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

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} ,

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

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} :

$$\pi^{\parallel}(S \mathbf{H}) = (h_2 + \tau(h_1 + h_2)) a^* = (\tau h_1 + h_2(\tau + 1)) a^* \\ = \tau(h_1 + \tau h_2) a^*,$$

$$\pi^{\perp}(S \mathbf{H}) = (-\tau h_2 + h_1 + h_2) a^* = (h_1 - h_2(\tau - 1)) a^* \\ = -(1/\tau)(-\tau h_1 + h_2) a^*,$$

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

Thus, for scaling n times we obtain

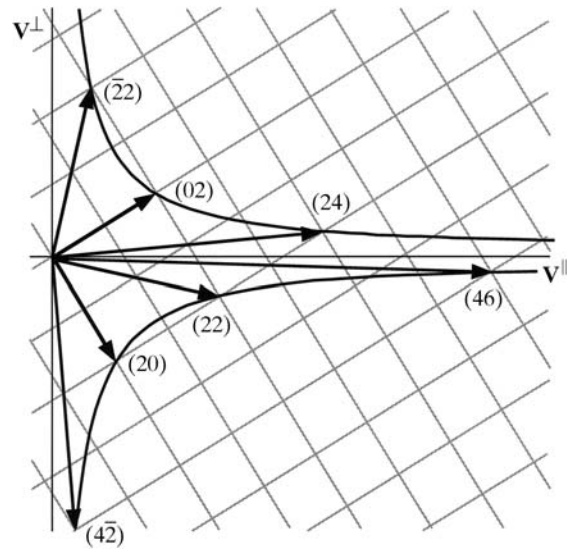


Fig. 4.6.3.11. Scaling operations of the Fibonacci sequence. The scaling operation S acts six times on the diffraction vector $\mathbf{H} = (42)$ yielding the sequence $(\bar{4}2) \rightarrow (\bar{2}2) \rightarrow (20) \rightarrow (02) \rightarrow (22) \rightarrow (24) \rightarrow (46)$.

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

with

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

yielding eventually

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

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) $\mathbf{a}_i^* = a_i^* (\cos 2\pi i/5, \sin 2\pi i/5, 0)$, $i = 1, \dots, 4$ 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