

4. DIFFUSE SCATTERING AND RELATED TOPICS

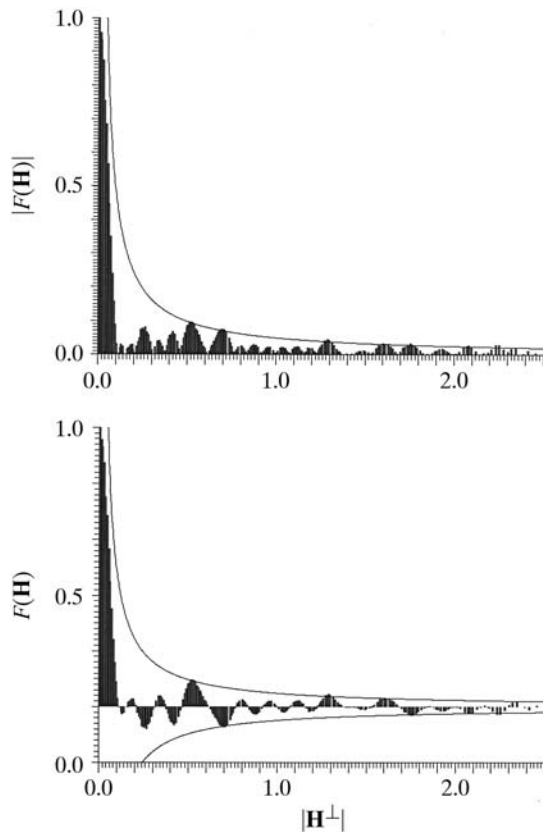


Fig. 4.6.3.9. The structure factors  $F(\mathbf{H})$  (below) and their magnitudes  $|F(\mathbf{H})|$  (above) of the squared Fibonacci chain decorated with equal point atoms are shown as a function of the perpendicular-space component  $|\mathbf{H}^\perp|$  of the diffraction vector. The short distance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

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  $\mathbf{H}$ ,

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

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  $\tau^n$  according to the eigenvalues  $\tau$  and  $-\tau^{-1}$  of  $S$  acting in the two eigenspaces  $\mathbf{V}^\parallel$  and  $\mathbf{V}^\perp$ :

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

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

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

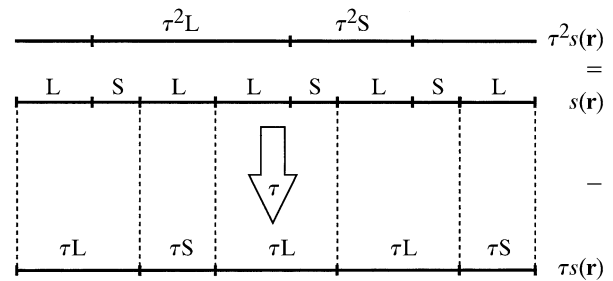


Fig. 4.6.3.10. Part . . . L S L L S L S L . . . of a Fibonacci sequence  $s(\mathbf{r})$  before and after scaling by the factor  $\tau$ . L is mapped onto  $\tau L$ , S onto  $\tau S = L$ . The vertices of the new sequence are a subset of those of the original sequence (the correspondence is indicated 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  $\tau^2$ .

Thus, for scaling  $n$  times we obtain

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

with

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

yielding eventually

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

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):

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

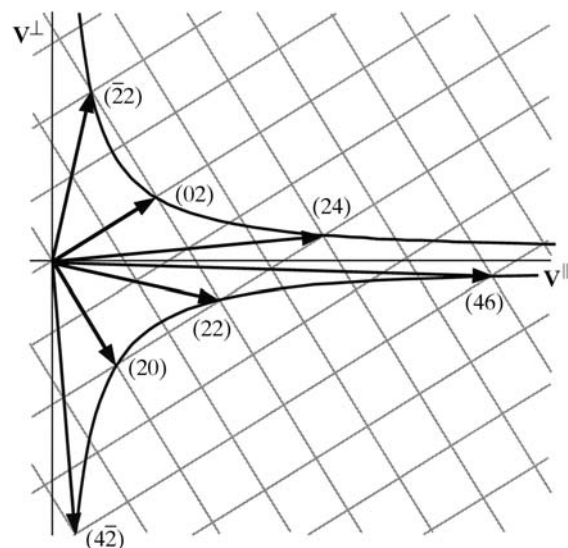


Fig. 4.6.3.11. Scaling operations of the Fibonacci sequence. The scaling operation  $S$  acts six times on the diffraction vector  $\mathbf{H} = (4\bar{2})$  yielding the sequence  $(4\bar{2}) \rightarrow (2\bar{2}) \rightarrow (20) \rightarrow (02) \rightarrow (22) \rightarrow (24) \rightarrow (46)$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