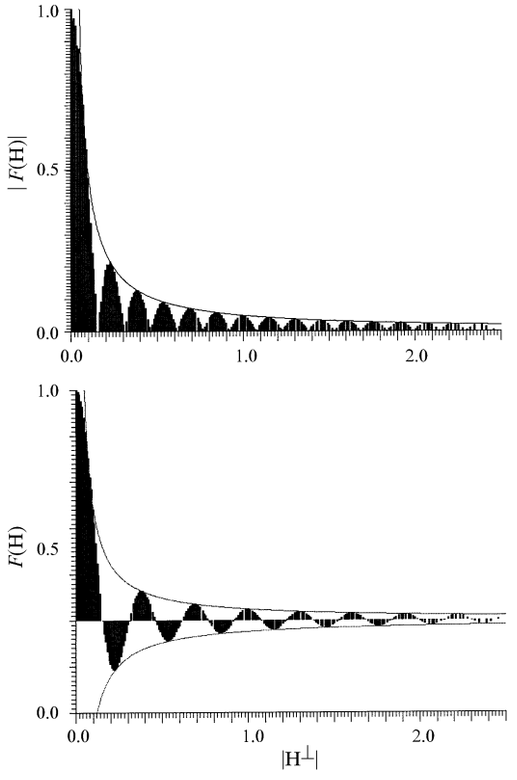

Fig. 4.6.3.6. The structure factors $F(\mathbf{H})$ (below) and their magnitudes $|F(\mathbf{H})|$ (above) of a Fibonacci chain decorated with equal point atoms are shown as a function of the perpendicular-space component $|\mathbf{H}^{\perp}|$ of the diffraction vector. The short distance in the Fibonacci chain is S = 2.5 Å, all structure factors within $0 \leq |\mathbf{H}| \leq 2.5$ Å^{-1} have been calculated and normalized to $F(00) = 1$.

4.6.3.3.1.3. *Structure factor*

The structure factor of a periodic structure is defined as the Fourier transform of the density distribution $\rho(\mathbf{r})$ of its unit cell (UC):

$$F(\mathbf{H}) = \int_{\mathrm{UC}} \rho(\mathbf{r}) \exp(2\pi i \mathbf{H} \cdot \mathbf{r})\, \mathrm{d}\mathbf{r}.$$

The same is valid in the case of the nD description of a quasiperiodic structure. The parallel- and perpendicular-space components are orthogonal to each other and can be separated. In the case of the 1D Fibonacci sequence, the Fourier transform of the parallel-space component of the electron-density distribution of a single atom gives the usual atomic scattering factor $f(\mathbf{H}^{\parallel})$. Parallel to $x^{\perp}$, $\rho(\mathbf{r})$ adopts values $\neq 0$ only within the interval $-(1+\tau)/[2a^*(2+\tau)] \leq x^{\perp} \leq (1+\tau)/[2a^*(2+\tau)]$ and one obtains

$$F(\mathbf{H}) = f(\mathbf{H}^{\parallel})[a^*(2+\tau)]/(1+\tau) \times \int_{-(1+\tau)/[2a^*(2+\tau)]}^{+(1+\tau)/[2a^*(2+\tau)]} \exp(2\pi i \mathbf{H}^{\perp} \cdot x^{\perp})\, \mathrm{d}x^{\perp}.$$

The factor $[a^*(2+\tau)]/(1+\tau)$ results from the normalization of the structure factors to $F(\mathbf{0}) = f(0)$. With

$$\mathbf{H} = h_1\mathbf{d}_1^* + h_2\mathbf{d}_2^* + h_3\mathbf{d}_3^* + h_4\mathbf{d}_4^* = h_1 a_1^* \begin{pmatrix} 1 \\ -\tau \\ 0 \\ 0 \end{pmatrix} + h_2 a_1^* \begin{pmatrix} \tau \\ 1 \\ 0 \\ 0 \end{pmatrix} + h_3 a_3^* \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} + h_4 a_4^* \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

and $\mathbf{H}^{\perp} = a_1^*(-\tau h_1 + h_2)$ the integrand can be rewritten as

$$F(\mathbf{H}) = f(\mathbf{H}^{\parallel})[a^*(2+\tau)]/(1+\tau) \times \int_{-(1+\tau)/[2a^*(2+\tau)]}^{+(1+\tau)/[2a^*(2+\tau)]} \exp[2\pi i(-\tau h_1 + h_2)x^{\perp}]\, \mathrm{d}x^{\perp},$$

yielding

$$F(\mathbf{H}) = f(\mathbf{H}^{\parallel})(2+\tau)/[2\pi i(-\tau h_1 + h_2)(1+\tau)] \times \exp[2\pi i(-\tau h_1 + h_2)x^{\perp}]\big|_{-(1+\tau)/[2a^*(2+\tau)]}^{+(1+\tau)/[2a^*(2+\tau)]}.$$

Using $\sin x = (\mathrm{e}^{ix} - \mathrm{e}^{-ix})/2i$ gives

$$F(\mathbf{H}) = f(\mathbf{H}^{\parallel})(2+\tau)/[\pi(-\tau h_1 + h_2)(1+\tau)] \times \sin[\pi(1+\tau)(-\tau h_1 + h_2)]/(2+\tau).$$

Thus, the structure factor has the form of the function $\sin(x)/x$ with x a perpendicular reciprocal-space coordinate. The upper and lower limiting curves of this function are given by the hyperbolae $\pm 1/x$ (Fig. 4.6.3.6). The continuous shape of $F(\mathbf{H})$ as a function of $\mathbf{H}^{\perp}$ allows the estimation of an overall temperature factor and atomic scattering factor for reflection-data normalization (compare Figs. 4.6.3.6 and 4.6.3.7).

In the case of a 3D crystal structure which is quasiperiodic in one direction, the structure factor can be written in the form

$$F(\mathbf{H}) = \sum_{k=1}^{n} \Big[T_k(\mathbf{H}) f_k(\mathbf{H}^{\parallel}) g_k(\mathbf{H}^{\perp}) \exp(2\pi i \mathbf{H} \cdot \mathbf{r}_k) \Big].$$

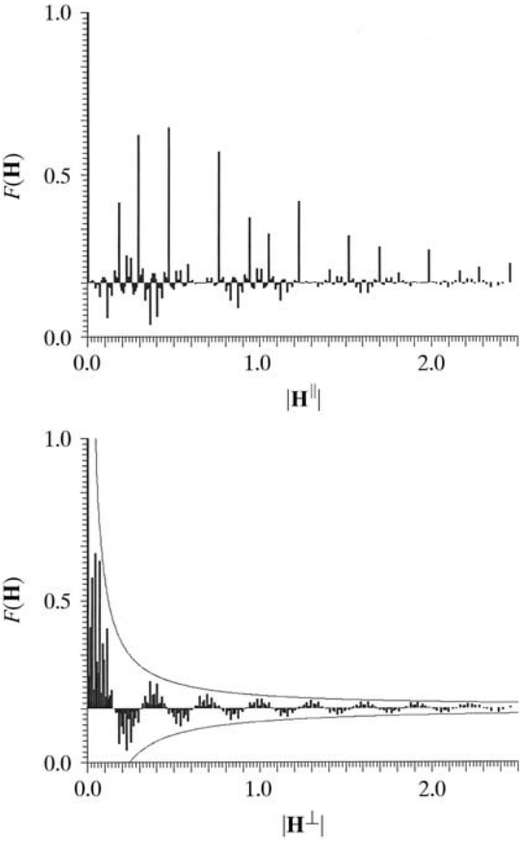

Fig. 4.6.3.7. The structure factors $F(\mathbf{H})$ of the Fibonacci chain decorated with aluminium atoms ($U_{\mathrm{overall}} = 0.005$ Å^2) as a function of the parallel (above) and the perpendicular (below) component of the diffraction vector. The short distance is S = 2.5 Å, all structure factors within $0 \leq |\mathbf{H}| \leq 2.5$ Å^{-1} have been calculated and normalized to $F(00) = 1$.

references