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

$$\mathbf{H} = h_1\mathbf{d}_1^* + h_2\mathbf{d}_2^* + h_3\mathbf{d}_3^* + h_4\mathbf{d}_4^* = h_1a_1^*\begin{pmatrix}1\\-\tau\\0\\0\end{pmatrix} + h_2a_1^*\begin{pmatrix}\tau\\1\\0\\0\end{pmatrix} + h_3a_3^*\begin{pmatrix}0\\0\\1\\0\end{pmatrix} + h_4a_4^*\begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

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

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

The sum runs over all n averaged hyperatoms in the 4D unit cell of the structure. The *geometric form factor* $g_k(\mathbf{H}^{\perp})$ corresponds to the Fourier transform of the kth atomic surface,

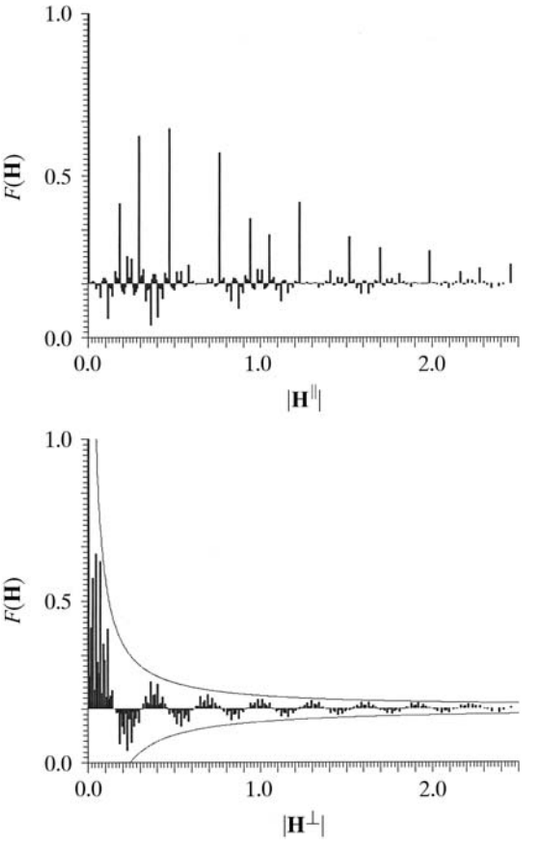

Fig. 4.6.3.7. The structure factors $F(\mathbf{H})$ of the Fibonacci chain decorated with aluminium atoms (U_{overall} = 0.005 Å^2) as a function of the parallel (above) and the perpendicular (below) component of the diffraction vector. The short distance is S = 2.5 Å, all structure factors within $0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

$$g_k(\mathbf{H}^{\perp}) = (1/A_{\mathrm{UC}}^{\perp}) \int_{A_k} \exp(2\pi i \mathbf{H}^{\perp} \cdot \mathbf{r}^{\perp})\, \mathrm{d}\mathbf{r}^{\perp},$$

normalized to $A_{\mathrm{UC}}^{\perp}$, the area of the 2D unit cell projected upon $\mathbf{V}^{\perp}$, and A_k, the area of the kth atomic surface.

The atomic temperature factor $T_k(\mathbf{H})$ can also have perpendicular-space components. Assuming only harmonic (static or dynamic) displacements in parallel and perpendicular space one obtains, in analogy to the usual expression (Willis & Pryor, 1975),

$$T_k(\mathbf{H}) = T_k(\mathbf{H}^{\parallel}, \mathbf{H}^{\perp}) = \exp(-2\pi^2 \mathbf{H}^{\parallel T} \langle \mathbf{u}_i^{\parallel} \mathbf{u}_j^{\parallel T} \rangle \mathbf{H}^{\parallel}) \exp(-2\pi^2 \mathbf{H}^{\perp T} \langle \mathbf{u}_i^{\perp} \mathbf{u}_j^{\perp T} \rangle \mathbf{H}^{\perp}),$$

with

$$\langle \mathbf{u}_i^{\parallel} \mathbf{u}_j^{\parallel T} \rangle = \begin{pmatrix} \langle \mathbf{u}_1^{\parallel 2} \rangle & \langle \mathbf{u}_1^{\parallel} \cdot \mathbf{u}_2^{\parallel T} \rangle & \langle \mathbf{u}_1^{\parallel} \cdot \mathbf{u}_3^{\parallel T} \rangle \\ \langle \mathbf{u}_2^{\parallel} \cdot \mathbf{u}_1^{\parallel T} \rangle & \langle \mathbf{u}_2^{\parallel 2} \rangle & \langle \mathbf{u}_2^{\parallel} \cdot \mathbf{u}_3^{\parallel T} \rangle \\ \langle \mathbf{u}_3^{\parallel} \cdot \mathbf{u}_1^{\parallel T} \rangle & \langle \mathbf{u}_3^{\parallel} \cdot \mathbf{u}_2^{\parallel T} \rangle & \langle \mathbf{u}_3^{\parallel 2} \rangle \end{pmatrix}$$

and $\langle \mathbf{u}_i^{\perp} \mathbf{u}_j^{\perp T} \rangle = \langle \mathbf{u}_4^{\perp} \rangle$.

The elements of the type $\langle \mathbf{u}_i \cdot \mathbf{u}_j^T \rangle$ represent the average values of the atomic displacements along the ith axis times the displacement along the jth axis on the V basis.

4.6.3.3.1.4. Intensity statistics

In the following, only the properties of the quasiperiodic component of the 3D structure, namely the Fourier module M_1^*,