International Tables for Crystallography (2006). Vol. B, Figure 4.6.2.10, p. 493.

$$(S_m^{-1})^T = \frac{1}{2+\tau}\begin{pmatrix} \tau^2 - x\tau + 1 & -x\tau^2 \\ x & \tau^2 + x\tau + 1 \end{pmatrix}_D,$$

where $x = (n\tau - m)/(m\tau + n)$:

$$\mathbf{d}_i^{*'} = \sum_{j=1}^{2}(S_m^{-1})_{ij}^T\mathbf{d}_j^*;$$

$$\mathbf{d}_1^{*'} = \frac{1}{2+\tau}\left[(\tau^2 - x\tau + 1)\mathbf{d}_1^* - x\tau^2\mathbf{d}_2^*\right]$$

$$= a^*\begin{pmatrix} 1 - x\tau \\ -\tau \end{pmatrix}_V$$

$$= a^*\begin{pmatrix} \dfrac{2m\tau - n\tau}{m\tau + n} \\ -\tau \end{pmatrix}_V,$$

$$\mathbf{d}_2^{*'} = \frac{1}{2+\tau}\left[x\mathbf{d}_1^* + (\tau^2 + x\tau + 1)\mathbf{d}_2^*\right]$$

$$= a^*\begin{pmatrix} \tau + x \\ 1 \end{pmatrix}_V$$

$$= a^*\begin{pmatrix} \dfrac{2n\tau + m\tau}{m\tau + n} \\ 1 \end{pmatrix}_V.$$

The point $x_n(t)$ of the nth interval L or S of an infinite Fibonacci sequence is given by

$$x_n(t) = \{x_0 + n(3 - \tau) - (\tau - 1)[\mathrm{frac}(n\tau + t) - (1/2)]\}\mathrm{S},$$

where t is the phase of the modulation function $y(t) = (\tau - 1)[\mathrm{frac}(n\tau + t) - (1/2)]$ (Janssen, 1986). Thus, the Fibonacci sequence can also be dealt with as an incommensurately modulated structure. This is a consequence of the fact that for 1D structures only the crystallographic point symmetries 1 and $\bar{1}$ allow the existence of a periodic average structure.

The embedding of the Fibonacci chain as an incommensurately modulated structure can be performed as follows:

(1) select a subset $\Lambda^* \subset M^*$ of strong reflections for main reflections $\mathbf{H} = h\mathbf{a}^*, h \in \mathbb{Z}$;

(2) define a satellite vector $\mathbf{q} = \alpha\mathbf{a}^*$ pointing from each main reflection to the next satellite reflection.

One possible way of indexing based on the same $\mathbf{a}^*$ as defined above is illustrated in Fig. 4.6.2.10. The scattering vector is given by $\mathbf{H}^{\parallel} = h(\tau + 1)\mathbf{a}^* + mq$, where $\mathbf{q} = \tau\mathbf{a}^*$, or, in the 2D representation, $\mathbf{H} = h_1\mathbf{d}_1^* + h_2\mathbf{d}_2^*$, where $\mathbf{d}_1^* = a^*\begin{pmatrix} 1+\tau \\ 0 \end{pmatrix}_V$ and $\mathbf{d}_2^* = a^*\begin{pmatrix} \tau \\ 1 \end{pmatrix}_v$, with the direct basis

$$\mathbf{d}_1 = \frac{1}{a^*(1+\tau)}\begin{pmatrix} 1 \\ -\tau \end{pmatrix}_V, \quad \mathbf{d}_2 = \frac{1}{a^*}\begin{pmatrix} 0 \\ 1 \end{pmatrix}_V.$$

The modulation function is saw-tooth-like (Fig. 4.6.2.11).

4.6.2.5. *1D structures with fractal atomic surfaces*

A 1D structure with a *fractal atomic surface* (Hausdorff dimension 0.9157. . .) can be derived from the Fibonacci sequence by squaring its substitution matrix S:

$$\begin{pmatrix} \mathrm{S} \\ \mathrm{L} \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} \mathrm{S} \\ \mathrm{L} \end{pmatrix} = \begin{pmatrix} \mathrm{S+L} \\ \mathrm{S+2L} \end{pmatrix}$$

$$\text{with } S^2 = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix},$$

corresponding to the substitution rule S $\rightarrow$ SL, L $\rightarrow$ LLS as well as two other non-equivalent ones (see Janssen, 1995). The eigenvalues λ_i are obtained by calculating

$$\det|S - \lambda I| = 0.$$

The evaluation of the determinant gives the characteristic polynomial

$$\lambda^2 - 3\lambda + 1 = 0,$$

with the solutions $\lambda_{1,2} = [3 \pm (5)^{1/2}]/2$, with $\lambda_1 = \tau^2$ and $\lambda_2 = 1/\tau^2 = 2 - \tau$, and the same eigenvectors $\mathbf{w}_1 = \begin{pmatrix} 1 \\ \tau \end{pmatrix}, \mathbf{w}_2 = \begin{pmatrix} 1 \\ -1/\tau \end{pmatrix}$ as for the Fibonacci sequence. Rewriting the eigenvalue equation gives

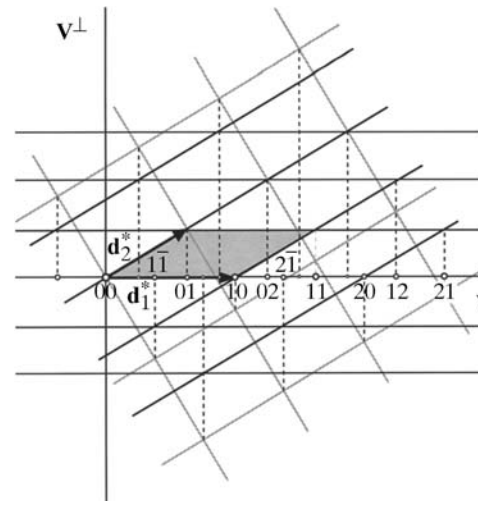

Fig. 4.6.2.10. Reciprocal space of the embedded Fibonacci chain as a modulated structure. Several main and satellite reflections are indexed. The square reciprocal lattice of the quasicrystal description illustrated in Fig. 4.6.2.9 is indicated by grey lines. The reflections located on $\mathbf{V}^{\parallel}$ can be considered to be projected either from the 2D square lattice of the embedding as for a QS or from the 2D oblique lattice of the embedding as for an IMS.

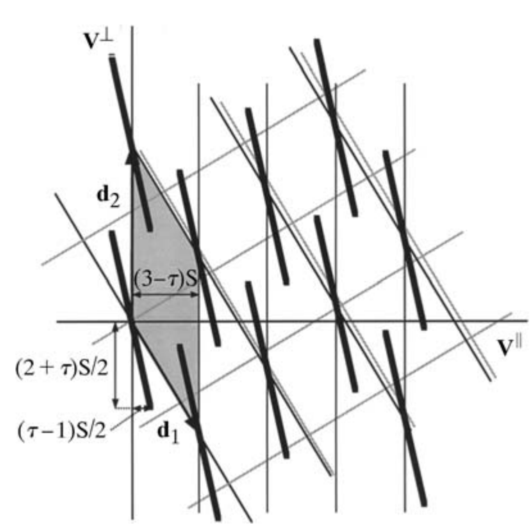

Fig. 4.6.2.11. 2D direct-space embedding of the Fibonacci chain as a modulated structure. The average period is $(3 - \tau)$S. The square lattice in the quasicrystal description shown in Fig. 4.6.2.8 is indicated by grey lines. The rod-like atomic surfaces are now inclined relative to $\mathbf{V}^{\parallel}$ and arranged so as to give a saw-tooth modulation wave.

references