International Tables for Crystallography (2010). Vol. B, Figure 4.6.2.10, p. 597.

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

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

$$\begin{aligned}
\mathbf{d}'_i &= \sum_{j=1}^{2} S_{mij}\mathbf{d}_j;\\
\mathbf{d}'_1 &= \frac{1}{2+\tau}\left[(\tau^2 + x\tau + 1)\mathbf{d}_1 - x\mathbf{d}_2\right]\\
&= \frac{1}{(2+\tau)a^*}\begin{pmatrix} 1 \\ -\tau - x \end{pmatrix}_V\\
&= \frac{1}{(2+\tau)a^*}\begin{pmatrix} 1 \\ -\dfrac{2n\tau + m\tau}{m\tau + n} \end{pmatrix}_V,\\
\mathbf{d}'_2 &= \frac{1}{2+\tau}\left[x\tau^2\mathbf{d}_1 + (\tau^2 - x\tau + 1)\mathbf{d}_2\right]\\
&= \frac{1}{(2+\tau)a^*}\begin{pmatrix} \tau \\ -x\tau + 1 \end{pmatrix}_V\\
&= \frac{1}{(2+\tau)a^*}\begin{pmatrix} \tau \\ \dfrac{2m\tau - n\tau}{m\tau + n} \end{pmatrix}_V.
\end{aligned}$$

This shear matrix does not change the magnitudes of the intervals L and S. In reciprocal space the inverted and transposed shear matrix is applied on the reciprocal basis,

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

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

$$\begin{aligned}
\mathbf{d}^{*'}_i &= \sum_{j=1}^{2} (S_m^{-1})^T_{ij}\mathbf{d}^*_j;\\
\mathbf{d}^{*'}_1 &= \frac{1}{2+\tau}\left[(\tau^2 - x\tau + 1)\mathbf{d}^*_1 - x\tau^2\mathbf{d}^*_2\right]\\
&= a^*\begin{pmatrix} 1 - x\tau \\ -\tau \end{pmatrix}_V\\
&= a^*\begin{pmatrix} \dfrac{2m\tau - n\tau}{m\tau + n} \\ -\tau \end{pmatrix}_V,\\
\mathbf{d}^{*'}_2 &= \frac{1}{2+\tau}\left[x\mathbf{d}^*_1 + (\tau^2 + x\tau + 1)\mathbf{d}^*_2\right]\\
&= a^*\begin{pmatrix} \tau + x \\ 1 \end{pmatrix}_V\\
&= a^*\begin{pmatrix} \dfrac{2n\tau + m\tau}{m\tau + n} \\ 1 \end{pmatrix}_V.
\end{aligned}$$

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.

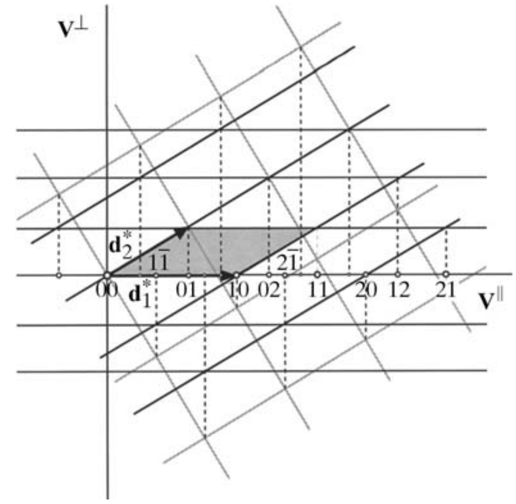

Fig. 4.6.2.10. Reciprocal space of the embedded Fibonacci chain as a modulated structure. Several main and satellite reflections are indexed. The square reciprocal lattice of the quasicrystal description illustrated in Fig. 4.6.2.9 is indicated by grey lines. The reflections located on $\mathbf{V}^{\parallel}$ 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.

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:

references