

4. DIFFUSE SCATTERING AND RELATED TOPICS

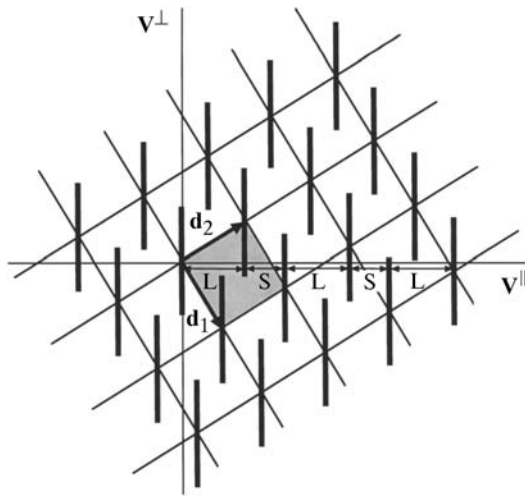


Fig. 4.6.2.8. 2D embedding of the Fibonacci chain. The short and long distances S and L , generated by the intersection of the atomic surfaces with the physical space \mathbf{V}^{\parallel} , are indicated. The atomic surfaces are represented by bars parallel to \mathbf{V}^{\perp} . Their lengths correspond to the projection of one unit cell (shaded) upon \mathbf{V}^{\perp} .

$$\mathbf{r} = n_1 \mathbf{d}_1 + n_2 \mathbf{d}_2, \text{ with } \mathbf{d}_1 = \frac{1}{a^*(2+\tau)} \begin{pmatrix} 1 \\ -\tau \end{pmatrix}_V,$$

$$\mathbf{d}_2 = \frac{1}{a^*(2+\tau)} \begin{pmatrix} \tau \\ 1 \end{pmatrix}_V;$$

$$\mathbf{H} = h_1 \mathbf{d}_1^* + h_2 \mathbf{d}_2^*, \text{ with } \mathbf{d}_1^* = a^* \begin{pmatrix} 1 \\ -\tau \end{pmatrix}_V, \mathbf{d}_2^* = a^* \begin{pmatrix} \tau \\ 1 \end{pmatrix}_V.$$

The 1D Fibonacci chain results from the cut of the parallel (physical) space with the 2D lattice Σ decorated with line elements for the *atomic surfaces* (*acceptance domains*). In this description, the atomic surfaces correspond simply to the projection of one 2D unit cell upon the perpendicular-space coordinate. This satisfies the condition that each unit cell contributes exactly to one point of the Fibonacci chain (*primitive unit cell*). The physical space \mathbf{V}^{\parallel} is related to the eigenspace of the substitution matrix S associated with its eigenvalue $\lambda_1 = \tau$. The perpendicular space \mathbf{V}^{\perp} corresponds to the eigenspace of the substitution matrix S associated with its eigenvalue $\lambda_2 = -1/\tau$. Thus, the physical space scales to powers of τ and the perpendicular space to powers of $-1/\tau$.

By block-diagonalization, the reducible substitution (scaling) matrix S can be decomposed into two non-equivalent irreducible representations. These can be assigned to the two 1D orthogonal subspaces \mathbf{V}^{\parallel} and \mathbf{V}^{\perp} forming the 2D embedding space $\mathbf{V} = \mathbf{V}^{\parallel} \oplus \mathbf{V}^{\perp}$. Thus, using $WSW^{-1} = S_V = S_V^{\parallel} \oplus S_V^{\perp}$, where

$$W = \begin{pmatrix} 1 & \tau \\ -\tau & 1 \end{pmatrix} = (\mathbf{d}_1^* \quad \mathbf{d}_2^*),$$

one obtains

$$\begin{pmatrix} 1 & \tau \\ -\tau & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}_D \begin{pmatrix} 1 & \tau \\ -\tau & 1 \end{pmatrix}^{-1} = \begin{pmatrix} \tau & 0 \\ 0 & -1/\tau \end{pmatrix}_V$$

$$= \begin{pmatrix} S^{\parallel} & 0 \\ 0 & S^{\perp} \end{pmatrix}_V,$$

the scaling operations S^{\parallel} and S^{\perp} in parallel and in perpendicular space as indicated by the partition lines.

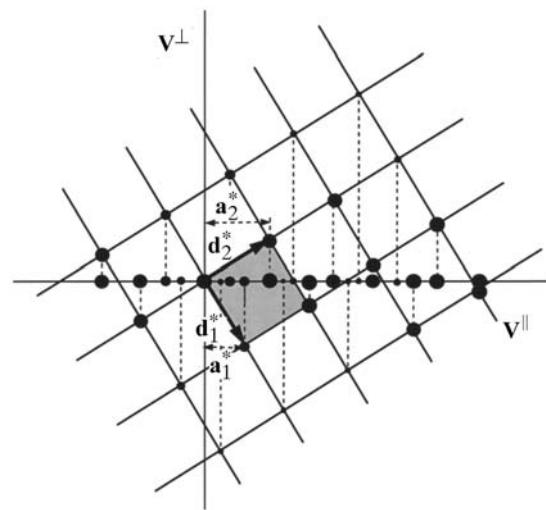


Fig. 4.6.2.9. Schematic representation of the reciprocal space of the embedded Fibonacci chain depicted in Fig. 4.6.2.8. The physical-space reciprocal basis \mathbf{a}_1^* and \mathbf{a}_2^* is marked. The diameters of the filled circles are roughly proportional to the reflection intensities. One 2D reciprocal-lattice unit cell is shadowed. The actual 1D diffraction pattern of the 1D Fibonacci chain results from a projection of the 2D reciprocal space onto the parallel space. The correspondence between 2D reciprocal-lattice positions and their projected images is indicated by dashed lines.

The metric tensors for the reciprocal and the direct 2D square lattices read

$$G^* = |a^*|^2(2+\tau) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ and } G = \frac{1}{|a^*|^2(2+\tau)} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

The short distance S of the Fibonacci sequence is related to a^* by

$$S = 1/[a^*(2+\tau)]$$

$$= \min \left\{ |\pi^{\parallel}(\mathbf{d}_i - \mathbf{d}_j)| \mid |\pi^{\perp}(\mathbf{d}_i - \mathbf{d}_j)| < \Omega_{AS} \wedge i, j \in \mathbb{Z} \right\},$$

with the projectors π^{\parallel} and π^{\perp} onto \mathbf{V}^{\parallel} and \mathbf{V}^{\perp} . The *point density* ρ_p of the Fibonacci chain, *i.e.* the number of vertices per unit length, can be calculated using the formula

$$\rho_p = \frac{\Omega_{AS}}{\Omega_{UC}} = \frac{(1+\tau)/[a^*(2+\tau)]}{1/[|a^*|^2(2+\tau)]} = a^* \tau^2,$$

where Ω_{AS} and Ω_{UC} are the areas of the atomic surface and of the 2D unit cell, respectively.

For an infinite Fibonacci sequence generated from the intervals S and L an average distance d can be calculated:

$$d = \lim_{n \rightarrow \infty} \frac{F_n S + F_{n+1} L}{F_n + F_{n+1}} = \lim_{n \rightarrow \infty} \frac{F_n(S + \tau L)}{F_n(1 + \tau)} = \frac{S(1 + \tau^2)}{(1 + \tau)} = (3 - \tau)S.$$

Therefrom, the point density can also be calculated:

$$\rho_p = 1/d = 1/[(3 - \tau)S] = [a^*(2 + \tau)]/(3 - \tau) = a^* \tau^2.$$

An approximant structure of the Fibonacci sequence with a unit cell containing m intervals L and n intervals S can be generated by shearing the 2D lattice Σ by the shear matrix S_m ,