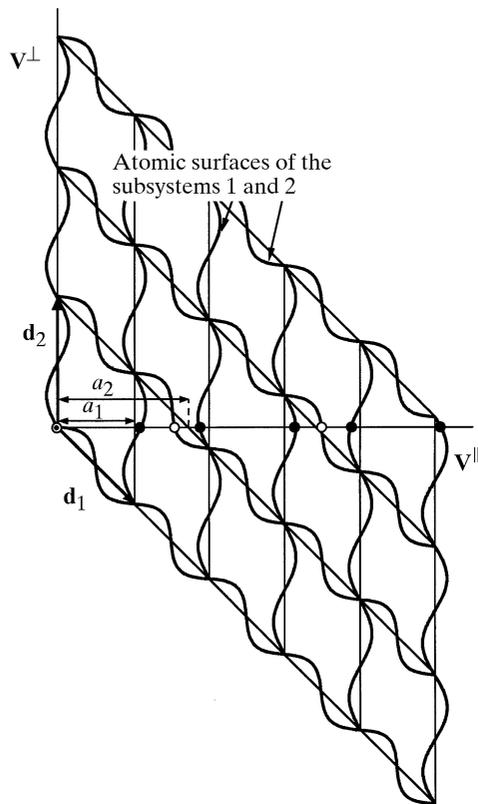4. DIFFUSE SCATTERING AND RELATED TOPICS

Fig. 4.6.2.5. 2D embedding of a 1D composite structure with mutual interaction of the subsystems causing modulations. Filled and empty circles represent the modulated substructures with periods a_1 and a_2 of the basic substructures, respectively. The atoms result from the parallel-space cut of the sinusoidal atomic surfaces running parallel to $\mathbf{d}_1$ and $\mathbf{d}_2$.

in both the 2D description $\mathbf{H} = h_1 \mathbf{d}_1^* + h_2 \mathbf{d}_2^*$ and in the 1D physical-space description with two parallel basis vectors $\mathbf{H}^{\parallel} = h_1 \mathbf{a}_1^* + h_2 \mathbf{a}_2^*$.

The reciprocal-lattice points $\mathbf{H} = h_1 \mathbf{d}_1^*$ and $\mathbf{H} = h_2 \mathbf{d}_2^*$, h_1, $h_2 \in \mathbb{Z}$, on the main axes $\mathbf{d}_1^*$ and $\mathbf{d}_2^*$ are the main reflections of the two substructures. All other reflections are referred to as satellite reflections. Their intensities differ from zero only in the case of modulated substructures. Each reflection of one subsystem coincides with exactly one reflection of the other subsystem.

4.6.2.4. 1D quasiperiodic structures

The Fibonacci sequence, the best investigated example of a 1D quasiperiodic structure, can be obtained from the substitution rule σ: S → L, L → LS, replacing the letter S by L and the letter L by the word LS (see *e.g.* Luck *et al.*, 1993). Applying the substitution matrix

$$S = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}$$

associated with σ, this rule can be written in the form

$$\begin{pmatrix} S \\ L \end{pmatrix} \rightarrow \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} S \\ L \end{pmatrix} = \begin{pmatrix} L \\ L + S \end{pmatrix}.$$

S gives the sum of letters, $L + S = S + L$, and not their order. Consequently, the same substitution matrix can also be applied, for instance, to the substitution σ': S → L, L → SL. The repeated action of S on the alphabet $A = \{S, L\}$ yields the words $A_n = \sigma^n(S)$ and $B_n = \sigma^n(L) = A_{n+1}$ as illustrated in Table 4.6.2.1. The frequencies of letters contained in the words A_n and B_n can
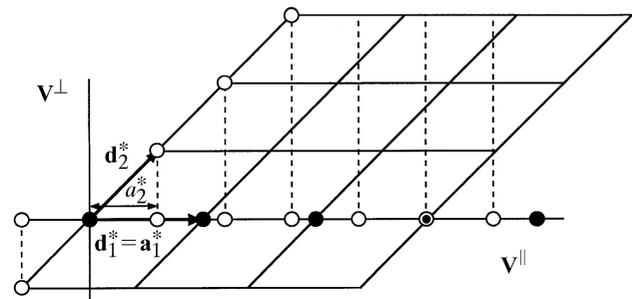

Fig. 4.6.2.6. Schematic representation of the reciprocal space of the embedded 1D composite structure depicted in Fig. 4.6.2.4. Filled and empty circles represent the reflections generated by the substructures with periods a_1 and a_2, respectively. The actual 1D diffraction pattern of the 1D CS results 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.

be calculated by applying the nth power of the transposed substitution matrix on the unit vector. From

$$\begin{pmatrix} v_{n+1}^A \\ v_{n+1}^B \end{pmatrix} = S^T \begin{pmatrix} v_n^A \\ v_n^B \end{pmatrix}$$

it follows that

$$\begin{pmatrix} v_n^A \\ v_n^B \end{pmatrix} = (S^T)^n \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

In the case of the Fibonacci sequence, v_n^B gives the total number of letters S and L, and v_n^A the number of letters L.

An infinite Fibonacci sequence, *i.e.* a word B_n with $n \to \infty$, remains invariant under inflation (deflation). Inflation (deflation) means that the number of letters L, S increases (decreases) under the action of the (inverted) substitution matrix S. Inflation and deflation represent self-similarity (scaling) symmetry operations on the infinite Fibonacci sequence. A more detailed discussion of the scaling properties of the Fibonacci chain in direct and reciprocal space will be given later.

The Fibonacci numbers $F_n = F_{n-1} + F_{n-2}$ form a series with $\lim_{n \to \infty}(F_{n+1}/F_n) = \tau$ {the golden mean $\tau = [1 + (5)^{1/2}]/2 = 2\cos(\pi/5) = 1.618\ldots$}. The ratio of the frequencies of L and S
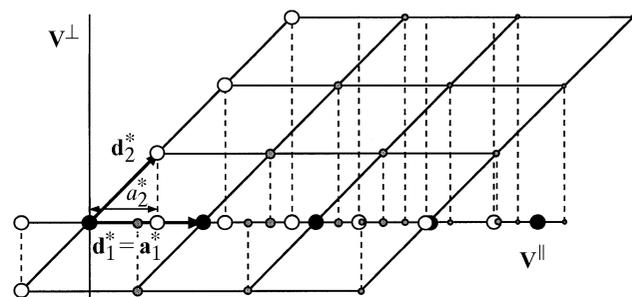

Fig. 4.6.2.7. Schematic representation of the reciprocal space of the embedded 1D composite structure depicted in Fig. 4.6.2.5. Filled and empty circles represent the main reflections of the two subsystems. The satellite reflections generated by the modulated substructures are shown as grey circles. The diameters of the circles are roughly proportional to the intensities of the reflections. The actual 1D diffraction pattern of the 1D CS 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.

references