

4.6. RECIPROCAL-SPACE IMAGES OF APERIODIC CRYSTALS

Table 4.6.2.1. Expansion of the Fibonacci sequence $B_n = \sigma^n(L)$ by repeated action of the substitution rule $\sigma: S \rightarrow L, L \rightarrow LS$

ν_L, ν_S are the frequencies of the letters L and S in word B_n .

B_n	ν_L	ν_S	n
L	1	0	0
LS	1	1	1
LSL	2	1	2
LSLLS	3	2	3
LSLLSLSL	5	3	4
LSLLSLSLLS	8	5	5
LSLLSLSLLSLSL	13	8	6
	\vdots	\vdots	\vdots
	F_{n+1}	F_n	n

in the Fibonacci sequence converges to τ if the sequence goes to infinity. The continued fraction expansion of the golden mean τ ,

$$\tau = 1 + \frac{1}{1 + \frac{1}{1 + \frac{1}{1 + \dots}}}$$

contains only the number 1. This means that τ is the ‘most irrational’ number, *i.e.* the irrational number with the worst truncated continued fraction approximation to it. This might be one of the reasons for the stability of quasiperiodic systems, where τ plays a role. The strong irrationality may impede the lock-in into commensurate systems (*rational approximants*).

By associating intervals (*e.g.* atomic distances) with length ratio τ to 1 to the letters L and S, a quasiperiodic structure $s(\mathbf{r})$ (*Fibonacci chain*) can be obtained. The invariance of the ratio of lengths $L/S = (L + S)/L = \tau$ is responsible for the invariance of the Fibonacci chain under scaling by a factor $\tau^n, n \in \mathbb{Z}$. Owing to a minimum atomic distance S in real crystal structures, the full set of inverse symmetry operators τ^{-n} does not exist. Consequently, the set of scaling operators $s = \{\tau^0 = 1, \tau^1, \dots\}$ forms only a semi-group, *i.e.* an associative groupoid. Groupoids are the most general algebraic sets satisfying only one of the group axioms: the associative law. The scaling properties of the Fibonacci sequence can be derived from the eigenvalues of the scaling matrix S . For this purpose the equation

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

with eigenvalue λ and unit matrix I has to be solved. The evaluation of the determinant yields the characteristic polynomial

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

yielding in turn the eigenvalues $\lambda_1 = [1 + (5)^{1/2}]/2 = \tau, \lambda_2 = [1 - (5)^{1/2}]/2 = -1/\tau$ and the eigenvectors

$$\mathbf{w}_1 = \begin{pmatrix} 1 \\ \tau \end{pmatrix}, \quad \mathbf{w}_2 = \begin{pmatrix} 1 \\ -1/\tau \end{pmatrix}.$$

Rewriting the eigenvalue equation gives for the first (*i.e.* the largest) eigenvalue

$$\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ \tau \end{pmatrix} = \begin{pmatrix} \tau \\ 1 + \tau \end{pmatrix} = \begin{pmatrix} \tau \\ \tau^2 \end{pmatrix} = \tau \begin{pmatrix} 1 \\ \tau \end{pmatrix}.$$

Identifying the eigenvector

$$\begin{pmatrix} 1 \\ \tau \end{pmatrix}$$

with

$$\begin{pmatrix} S \\ L \end{pmatrix}$$

shows that an infinite Fibonacci sequence $s(\mathbf{r})$ remains invariant under scaling by a factor τ . This scaling operation maps each new lattice vector $\tau\mathbf{r}$ upon a vector \mathbf{r} of the original lattice:

$$s(\tau\mathbf{r}) = s(\mathbf{r}).$$

Considering periodic lattices, these eigenvalues are integer numbers. For quasiperiodic ‘lattices’ (*quasilattices*) they always correspond to *algebraic numbers* (*Pisot numbers*). A Pisot number is the solution of a polynomial equation with integer coefficients. It is larger than one, whereas the modulus of its conjugate is smaller than unity: $\lambda_1 > 1$ and $|\lambda_2| < 1$ (Luck *et al.*, 1993). The total lengths l_n^A and l_n^B of the words A_n, B_n can be determined from the equations $l_n^A = \lambda_1^n l^A$ and $l_n^B = \lambda_1^n l^B$ with the eigenvalue λ_1 . The left Perron–Frobenius eigenvector \mathbf{w}_1 of S , *i.e.* the left eigenvector associated with λ_1 , determines the ratio S:L to 1: τ . The right Perron–Frobenius eigenvector \mathbf{w}_1 of S associated with λ_1 gives the relative frequencies, 1 and τ , for the letters S and L (for a definition of the Perron–Frobenius theorem see Luck *et al.*, 1993, and references therein).

The general case of an alphabet $A = \{L_1 \dots L_k\}$ with k letters (intervals) L_i , of which at least two are on incommensurate length scales and which transform with the substitution matrix S ,

$$L'_i \rightarrow \sum_{j=1}^k S_{ij} L_j,$$

can be treated analogously. S is a $k \times k$ matrix with non-negative integer coefficients. Its eigenvalues are solutions of a polynomial equation of rank k with integer coefficients (algebraic or Pisot numbers). The dimension n of the embedding space is generically equal to the number of letters (intervals) k involved by the substitution rule. From substitution rules, infinitely many different 1D quasiperiodic sequences can be generated. However, their atomic surfaces in the nD description are generically of fractal shape (see Section 4.6.2.5).

The quasiperiodic 1D density distribution $\rho(\mathbf{r})$ of the Fibonacci chain can be represented by the Fourier series

$$\rho(\mathbf{r}) = (1/V) \sum_{\mathbf{H}^\parallel} F(\mathbf{H}^\parallel) \exp(-2\pi i \mathbf{H}^\parallel \cdot \mathbf{r}),$$

with $\mathbf{H}^\parallel \in \mathbb{R}$ (the set of real numbers). The Fourier coefficients $F(\mathbf{H}^\parallel)$ form a Fourier module $M^* = \{\mathbf{H}^\parallel = \sum_{i=1}^2 h_i \mathbf{a}_i^* | h_i \in \mathbb{Z}\}$ equivalent to a \mathbb{Z} module of rank 2. Thus a periodic function in 2D space can be defined by

$$\rho(\mathbf{r}^\parallel, \mathbf{r}^\perp) = (1/V) \sum_{\mathbf{H}} F(\mathbf{H}) \exp[-2\pi i (\mathbf{H}^\parallel \cdot \mathbf{r}^\parallel + \mathbf{H}^\perp \cdot \mathbf{r}^\perp)],$$

where $\mathbf{r} = (\mathbf{r}^\parallel, \mathbf{r}^\perp) \in \Sigma$ and $\mathbf{H} = (\mathbf{H}^\parallel, \mathbf{H}^\perp) \in \Sigma^*$ are, by construction, direct- and reciprocal-lattice vectors (Figs. 4.6.2.8 and 4.6.2.9):