*International Tables for Crystallography* (2006). Vol. B, Figure 4.6.2.8, p. 491.



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

$\nu_\mathrm{L}$, $\nu_\mathrm{S}$ are the frequencies of the letters L and S in word $B_n$.

| $B_n$ | $\nu_\mathrm{L}$ | $\nu_\mathrm{S}$ | $n$ |
|---|---|---|---|
| L | 1 | 0 | 0 |
| LS | 1 | 1 | 1 |
| LSL | 2 | 1 | 2 |
| LSLLS | 3 | 2 | 3 |
| LSLLSLSL | 5 | 3 | 4 |
| LSLLSLSLLSLLS | 8 | 5 | 5 |
| LSLLSLSLLSLLSLSLLSLSL | 13 | 8 | 6 |
| | ⋮ | ⋮ | ⋮ |
| | $F_{n+1}$ | $F_n$ | $n$ |

$$\tau = 1 + \cfrac{1}{1 + \cfrac{1}{1 + \cfrac{1}{1 + \ldots}}},$$

contains only the number 1. This means that $\tau$ 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 $\tau$ 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 $\tau$ 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 $\mathrm{L/S} = (\mathrm{L}+\mathrm{S})/\mathrm{L} = \tau$ 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 $\tau^{-n}$ does not exist. Consequently, the set of scaling operators $s = \{\tau^0 = 1, \tau^1, \ldots\}$ forms only a semigroup, *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 $\lambda$ 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 $\mathbf{w}_1 = \begin{pmatrix} 1 \\ \tau \end{pmatrix}$, $\mathbf{w}_2 = \begin{pmatrix} 1 \\ -1/\tau \end{pmatrix}$. 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 $\begin{pmatrix} \mathrm{S} \\ \mathrm{L} \end{pmatrix}$ shows that an infinite Fibonacci sequence $s(\mathbf{r})$ remains invariant under scaling by a factor $\tau$. 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 $\lambda_1$. The left Perron–Frobenius eigenvector $\mathbf{w}_1$ of *S*, *i.e.* the left eigenvector associated with $\lambda_1$, determines the ratio S:L to 1:$\tau$. The right Perron–Frobenius eigenvector $\mathbf{w}_1$ of *S* associated with $\lambda_1$ gives the relative frequencies, 1 and $\tau$, 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 $A = \{\mathrm{L}_1 \ldots \mathrm{L}_k\}$ with *k* letters (intervals) $\mathrm{L}_i$, of which at least two are on incommensurate length scales and which transform with the substitution matrix *S*,

$$\mathrm{L}_i' \to \sum_{j=1}^{k} S_{ij}\mathrm{L}_j,$$

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 *n*D 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):

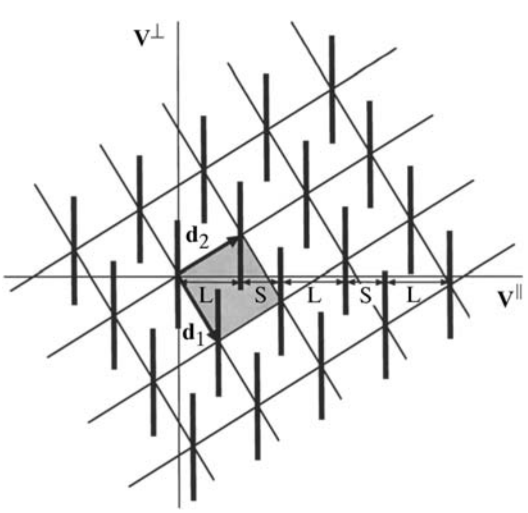


Fig. 4.6.2.8. 2D embedding of the Fibonacci chain. The short and long distances S and L, generated by the intersection of the atomic surfaces with the physical space $\mathbf{V}^\parallel$, are indicated. The atomic surfaces are represented by bars parallel to $\mathbf{V}^\perp$. Their lengths correspond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





references