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Fibonacci chain as a periodic chain with discommensurations

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Abstract. The quasiperiodic Fibonacci chain can be obtained by finite displacements from a periodic chain if one introduces ordered defects that are similar to discommensurations in incommensurate crystal phases. It is shown that the chain with discommensurations can also be constructed by means of a substitution rule having the Pisot property. In superspace the defect structure is a superstructure for the two-dimensional array that corresponds to the Fibonacci chain.

1. Introduction

Both in experiment (Spaepen et al 1990) and in theory (Kramer 1985, Janssen 1991, Coddens and Launois 1991, Mosseri 1993) periodic structures that resemble quasicrystals, the so-called approximants, have been studied. Transitions between them may occur via an intermediate modulated quasicrystalline phase (Janssen 1991, Duneau 1992, Audier et al 1993, Menguy et al 1993). Mathematically an approximant may be obtained from a quasicrystal by a deformation, for example a strain, of the higher-dimensional structure whose intersection with physical space yields the quasicrystal. The kinetics of such a transformation, however, is more difficult to understand. If one insists on a process via phason hopping, the frequency of the different tiles remains constant and therefore the transformation to a periodic structure can only be realized locally. This means that one has to introduce structural defects in the periodic structure. We study these defects in a simple one-dimensional model and show that they are related to the singular words introduced in (Wen and Wen 1993) for the decomposition of the infinite Fibonacci word.

We start by recalling some elementary properties of the Fibonacci chain and some results from (Wen and Wen 1993). Then we study the question of what happens to a chain obtained by a substitution rule (replacing the letters (or intervals) in the chain by words). It will be shown that the new chain can be obtained by a substitution rule as well. Then we apply this result to study the structure and Fourier transform of the periodic chain with defects obtained by finite displacements from the Fibonacci chain.

Let $w = w_1 w_2 \dots$ be an infinite sequence of letters a or b, i.e. $w_i \in \{a, b\}$. Let $S_n(w) := S_n = w_1 w_2 \dots w_n$ be the word composed of the first n letters of w. We write $a_n = |S_n|_a$ for the number of letters a in S_n , and $b_n = |S_n|_b$. Let $\ell_a, \ell_b \in \mathbb{R}^+$ be the lengths of two intervals with $\ell_a \neq \ell_b$. Consider the one-dimensional chain $\{x_n\}$ defined by

$$x_{0} = 0 x_{n} - x_{n-1} = \begin{cases} \ell_{a} & \text{if } w_{n} = a \\ \ell_{b} & \text{if } w_{n} = b \end{cases}.$$
(1)

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Thus $x_n = a_n \ell_a + b_n \ell_b$. If the limit a_n/n exists, we can define an average length (or inverse density) Δ :

$$\frac{x_n}{n} = \frac{a_n}{n} \ell_a + \frac{b_n}{n} \ell_b \to \mu_a \ell_a + \mu_b \ell_b := \Delta.$$
⁽²⁾

From the sequence $\{x_n\}$ one gets a sequence $\{u_n\}$ (the modulation sequence) by

$$u_n := \frac{x_n - n\Delta}{\ell_a - \ell_b}.$$
(3)

From (1)–(3) and the relation $\mu_a + \mu_b = 1$ follows

$$u_{n} = a_{n} - n\mu_{a} = a_{n}\mu_{b} - b_{n}\mu_{a} = \mu_{b}\left(a_{n} - b_{n}\frac{\mu_{a}}{\mu_{b}}\right).$$
(4)

Notice from (4) that:

- (1) u_n is independent of the choice of ℓ_a and ℓ_b ;
- (2) if $\mu_a/\mu_b = \mu$ the sequence obtained by replacing a by 1 and b by μ is equivalent to the geometric embedding model of (Luck *et al* 1993);
- (3) the asymptotic properties of u_n are completely determined by μ_a and the rate with which a_n/n tends to μ_a.

Let $x = x_1, x_2, ...$ be a sequence over the alphabet $S = \{a, b\}$, such that the frequencies μ_a and μ_b of a and b in x exist. Consider then a substitution τ given by $\tau(a) = A$ and $\tau(b) = B$, where A and B are words in S^* . With $\alpha = |A|_a$, $\beta = |A|_b$, $\gamma = |B|_a$ and $\delta = |B|_b$ we get the substitution matrix

$$M_{\tau} = \begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix}$$
(5)

If we apply τ to x we get another sequence over $\{a, b\}$

$$y = \tau(x) = \tau(x_1)\tau(x_2) \ldots = y_1 y_2 \ldots$$

Our aim is to compare the properties of x and y. In the sequel we assume that $0 < \mu_a < 1$ and that $\alpha + \beta + \gamma + \delta > 0$ (otherwise y is not defined).

Proposition 1. Let $\mu = \mu_a/\mu_b$ and let ν_a, ν_b frequencies of a and b in y, $\nu = \nu_a/\nu_b$. Then

$$\nu_a = \frac{\alpha \mu_a + \gamma \mu_b}{(\alpha + \beta)\mu_a + (\gamma + \delta)\mu_b} \qquad \nu_b = \frac{\beta \mu_a + \delta \mu_b}{(\alpha + \beta)\mu_a + (\gamma + \delta)\mu_b} \tag{6}$$

$$\nu = \frac{\alpha \mu + \gamma}{\beta \mu + \delta} \,. \tag{7}$$

Proof. Notice that

$$y = \tau(x_1)\tau(x_2)... = c_1c_2...$$
 $c_j \in \{A, B\}$ (8)

with

$$c_j = \begin{cases} A & \text{if } x_j = a \\ B & \text{if } x_j = b \end{cases}.$$
(9)

Let A_N , B_N be the number of occurences of A and B, respectively, in the first N terms. Then

$$\frac{A_N}{N} \to \mu_a \qquad \frac{B_N}{N} \to \mu_b \,.$$

On the other hand, the number of the letters a and b in the first N blocks of A and B are $\alpha A_N + \gamma B_N$ and $\beta A_N + \delta B_N$, respectively. Therefore,

$$\nu_a = \lim_{N \to \infty} \frac{\alpha A_N + \gamma B_N}{(\alpha + \beta)A_N + (\gamma + \delta)B_N} = \frac{\alpha \mu_\alpha + \gamma \mu_b}{(\alpha + \beta)\mu_\alpha + (\gamma + \delta)\mu_b}.$$
 (10)

From this the other formulae follow immediately.

Notice that for the fixed point $\mu = (\alpha \mu + \gamma)/(\beta \mu + \delta)$ of the fractional linear transformation $\nu = (\alpha \mu + \gamma)/(\beta \mu + \delta)$ the frequency will not change.

Proposition 2. Let $\{u_n(x)\}$ and $\{u_n(y)\}$ be the modulation sequences of the chains corresponding to x and y. Then $\{u_n(x)\}$ is bounded if and only if $\{u_n(y)\}$ is bounded.

Proof. Consider the subsequence $\{u_{|\tau(S_n)|}(y)\}_{n\geq 1}$ of the sequence $\{u_n(y)\}$, where $S_n := x_1x_2...x_n$. Notice that $|\tau(S_n)|_a = \alpha a_n + \gamma b_n$ and $|\tau(S_n)|_b = \beta a_n + \delta b_n$. Putting $c = \{(\alpha + \beta)\mu_a + (\gamma + \delta)\mu_b\}^{-1}$, we obtain from (4) and (6)

$$u_{|\tau(S_n)|}(y) = c\{(\alpha a_n + \gamma b_n)(\beta \mu_a + \delta \mu_b) - (\beta a_n + \delta b_n)(\alpha \mu_a + \gamma \mu_b)\}$$
$$= c\{(\alpha \delta - \beta \gamma)(a_n \mu_b - b_n \mu_a)\} = c(\alpha \delta - \beta \gamma)u_n(x).$$
(11)

Hence $u_{|\tau(S_n)|}(y)$ and $u_n(x)$ differ only by a constant factor which is independent of n. Now let

$$M_{A} = \max\{u_{j}(A), A = s_{1}s_{2}\dots s_{|A|}\} \qquad M_{B} = \max\{u_{j}(B), B = t_{1}t_{2}\dots t_{|B|}\}$$

$$m_{A} = \min\{u_{j}(A), A = s_{1}s_{2}\dots s_{|A|}\} \qquad m_{B} = \min\{u_{j}(B), B = t_{1}t_{2}\dots t_{|B|}\}.$$
(12)

Then for any *n* there is an integer k such that $|\tau(S_k)| \leq n < |\tau(S_{k+1})|$. Thus

$$\min(m_A, m_B) \leqslant u_n(y) - u_{|\tau(S_k)|}(y) \leqslant \max(M_A, M_B).$$

We obtain the result that $\{u_{\tau(S_n)}(y)\}_{n\geq 1}$ is bounded if and only if $\{u_n(y)\}$ is bounded.

Remark 1. Let $\lambda = {\lambda_n}_{n \ge 1}$ be a bounded sequence of real numbers. We define the variation of λ as $var(\lambda) = \sup_n \lambda_n - \inf_n \lambda_n$.

Then a more detailed analysis leads to the following result.

Let $u(x) = \{u_n(x)\}_{n \ge 1}$ and $u(y) = \{u_n(y)\}_{n \ge 1}$. Then

$$\operatorname{var}(u(y)) = \begin{cases} C\operatorname{var}(u(x)) + M_A - m_A & \text{if } M_A - u_{|A|} \ge M_B & m_A - u_{|A|} \le m_B \\ C\operatorname{var}(u(x)) + M_A - u_{|A|}(x) - m_B & \text{if } M_A - u_{|A|} \ge M_B & m_A - u_{|A|} \ge m_B \\ C\operatorname{var}(u(x)) + M_B - m_A + u_{|A|}(x) & \text{if } M_A - u_{|A|} \le M_B & m_A - u_{|A|} \le m_B \\ C\operatorname{var}(u(x)) + M_B - m_B & \text{if } M_A - u_{|A|} \le M_B & m_A - u_{|A|} \ge m_B \end{cases}$$

where $C = (\alpha \delta - \beta \gamma) / \{(\alpha + \beta)\mu_a + (\gamma + \delta)\mu_b\}.$

Remark 2. By (6) one has, in the case det $\begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix} \neq 0$, that ν , ν_a and ν_b belong to $Q(\mu) \setminus Q$. If the determinant is equal to zero at least either β or δ is different from zero. Suppose $\delta \neq 0$. Then

$$\nu = \frac{\alpha \mu + \gamma}{\beta \mu + \delta} = \frac{\alpha \delta \mu + \gamma \delta}{\delta(\beta \mu + \delta)} = \frac{\beta \gamma \mu + \gamma \delta}{\delta(\beta \mu + \delta)} = \frac{\gamma}{\delta}.$$

and

$$v_a = rac{\gamma}{\gamma + \delta}$$
 $v_b = rac{\delta}{\delta + \gamma}$ $v, v_a, v_b \in Q$.

Example 1. Let $x = x_1 x_2 x_3 \dots$ be the Fibonacci chain and $y = \tau(x_1) \tau(x_2) \dots = y_1 y_2 \dots$ with $\tau(a) = aba$ and $\tau(b) = a^2b$. Then

$$M_{\tau} = \begin{pmatrix} 2 & 2 \\ 1 & 1 \end{pmatrix}$$
 $\nu = 2$ $\nu_a = \frac{2}{3}$ $\nu_b = \frac{1}{3}$

The frequencies of this chain are the same as those of the Toeplitz chain which can be obtained from the substitution $a \rightarrow ab$, $b \rightarrow aa$.

Example 2. Again we consider the Fibonacci chain $x = x_1 x_2 \dots$, now with a substitution $\tau(a) = bbb$, $\tau(b) = ab$. In this case

$$\begin{aligned} \nu &= (3\sqrt{5} - 5)/10 \qquad \nu_a = (3 - \sqrt{5})/(3 + \sqrt{5}) \qquad \nu_b = 2\sqrt{5}/(3 + \sqrt{5}) \\ M_\tau &= \begin{pmatrix} 0 & 1 \\ 3 & 1 \end{pmatrix} \,. \end{aligned}$$

Compare this result with the substitution

$$\sigma(a) = bbbbb \qquad \sigma(b) = abbbbb \qquad M_{\sigma} = \begin{pmatrix} 0 & 1 \\ 5 & 5 \end{pmatrix}.$$

For this chain the Fourier module is given by

$$\mathcal{F}_{\sigma} = \frac{2\pi}{K} \mathbb{Z}(\lambda_1^{-1}, \lambda_1^{-2}, \ldots) \qquad \lambda_1 = 1 + 3\sqrt{5}$$

where K is the lattice constant. This is a \mathbb{Z} -module of infinite rank, also called a limit quasiperiodic system.

2. Defects and singular words

A Fibonacci chain may successively be approximated in the following way. Let $\{f_m\}_{m\geq 1}$ be the Fibonacci numbers defined by $f_m = f_{m-1} + f_{m-2}$ with $f_{-1} = f_0 = 1$ and $F_{\infty} = abaab \dots$ the unique fixed point of the Fibonacci substitution: $\sigma(a) = ab$, $\sigma(b) = a$.

We call the cyclic permutations of a word w its conjugates, and denote the set of these by C(w). Let Ω_n denote the set of words of length n occuring in F_{∞} .

Clearly $F_m = \sigma^m(a) \in \Omega_{f_m}$. It is shown in (Wen and Wen 1993) that actually

$$\Omega_{f_m} = C(F_m) \cup \{w_m\}. \tag{13}$$

$$L(w) = (f_{m-1}, f_{m-2})$$
(14)

if $w \in C(F_m)$, and

$$L(w_{2n}) = (f_{2n-1} + 1, f_{2n-2} - 1), L(w_{2n+1}) = (f_{2n} - 1, f_{2n} + 1).$$
(15)

Now we split the infinite word F_{∞} into words of length f_m from $C(F_m)$ and the letter *a* (if *m* odd) or *b* (for *m* even) according to the following rule, which we call the periodic approximation algorithm (of order *m*). Suppose the first *k* letters have already been partitioned into words. If $x_{k+1}x_{k+2}...x_{k+f_m}$ belongs to $C(F_m)$ we add this word to the partitioning, otherwise we add simply x_{k+1} .

For example for m = 2 (then $F_2 = aba$) the periodic approximation algorithm yields the splitting

$$F_{\infty} = (aba)(aba)(baa)(baa)(b)(aba)(aba)(baa) \dots$$

Now suppose we code the words from $C(F_m)$ in this splitting by letters X_1, X_2, \ldots and b by the letter Y. We shall prove that the new sequence obtained in this way can be obtained by a substitution Σ_m , e.g. for m = 2 we code $aba \to X_1$, $baa \to X_2$, $b \to Y$ and the coded sequence $X_1X_1X_2X_2YX_1X_2\ldots$ will turn out to be the fixed point of the substitution Σ_2 given by

$$\Sigma_2(X_1) = X_1 X_1 X_2 X_2 Y$$
 $\Sigma_2(X_2) = X_1 X_1 X_1 X_2 Y$ $\Sigma_2(Y) = X_1$.

To define this substitution we need to find multiples of the Fibonacci numbers which are one less than another Fibonacci number. A solution to this problem is given by the Lucas numbers $(\ell_n)_{n\geq 0}$ defined by

$$\ell_0 = 1$$
 $\ell_1 = 3$ $\ell_{n+1} = \ell_n + \ell_{n-1}$ $n \ge 1$.

Lemma 1. Let (f_n) be the Fibonacci numbers, (ℓ_n) the Lucas numbers. Then for all $n \ge 0$

$$\ell_{2n}f_{2n} + 1 = f_{4n+1} \tag{16}$$

$$\ell_{2n}f_{2n+1} + 1 = f_{4n+2} \tag{17}$$

Proof. For the induction proof it is useful to supplement (16) and (17) with

$$\ell_{2n+1}f_{2n+1} - 1 = f_{4n+3} \tag{18}$$

$$\ell_{2n+1}f_{2n+2} - 1 = f_{4n+4}. \tag{19}$$

Now (16)–(19) are easily checked for n = 0. Suppose (16)–(19) are correct for n. Then

$$f_{4(n+1)+1} = f_{4n+4} + f_{4n+3} = f_{4n+4} + f_{4n+2} + f_{4n+1}$$
$$= \ell_{2n+1} f_{2n+2} - 1 + \ell_{2n} f_{2n+1} + 1 + \ell_{2n} f_{2n} + 1$$
$$= \ell_{2n+1} f_{2n+2} + \ell_{2n} f_{2n+2} + 1$$
$$= \ell_{2n+3} f_{2n+2} + 1.$$

Similarly (17)–(19) will follow for n+1. The lemma follows as well from standard identities

$$\ell_n = \tau^n + (1-\tau)^n$$
 $f_n = \frac{\tau^n - (1-\tau)^n}{2\tau - 1}$.

Since $L(F_m) = (f_{m-1}, f_{m-2})$, there are f_{m-1} words of $C(F_m)$ with last letter a and f_{m-2} words with last letter b. We denote these sets of words by, respectively, $C(F_m, a) := \{A_1, A_2, \ldots, A_{f_{m-1}}\}$ and $C(F_m, b)$. We now consider the case m = 2n even.

Lemma 2. Let $A_j \in C(F_{2n}, a)$. Then $\sigma^{2n+1}(A_i) = A_{i1}A_{i2}\dots A_{i\ell_n}b$

where $A_{ji} \in C(F_{2n}, a)$.

Proof.

- (1) If u is a suffix of v we write $u \triangleright v$. Since $a \triangleright A_j$ by definition of A_j and $b \triangleright \sigma^{2n+1}(a)$, one has $b \triangleright \sigma^{2n+1}(A_j)$. Clearly, $L(A_j) = L(F_{2n})$. Therefore, $|\sigma^{2n+1}(A_j)| = |\sigma^{2n+1}(F_{2n})| = |F_{4n+1}| = f_{4n+1}$. By (16) one has $f_{4n+1} 1 = \ell_{2n} f_{2n}$. Hence $\sigma^{2n+1}(A_j)$ may be written as $A_{j1}A_{j2} \dots A_{j\ell_{2n}}b$ such that $|A_{jk}| = f_{2n}$.
- (2) If there is an index k such that A_{jk} does not belong to $C(F_{2n})$, then by (13) $A_{jk} = w_{2n}$. So one has by (14)

$$|A_{jk}|_a = f_{2n-1} - 1. (20)$$

On the other hand $|\sigma^{2n+1}(A_j)|_a = |F_{4n+1}|_a = f_{4n}$. Substracting (16) from (17) in lemma 1, we obtain

$$f_{4n} = \ell_{2n} f_{2n-1} \,. \tag{21}$$

Hence by (20), (21) there will be among the ℓ_{2n} words A_{ji} at least an index $k', k \neq k'$, such that $|A_{jk'}|_a \ge f_{2n-1} + 1$. This is impossible because of (14). This means that for any *i* holds: $A_{ji} \in C(F_{2n})$.

(3) Now we shall prove furthermore that for any $i: A_{ji} \in C(F_{2n}, a)$. Assume that $b \triangleright A_{jk}$ for some k. Because of (2) one has $L(A_{jk}) = (f_{2n-1}, f_{2n-2})$ and $L(A_{jk}b^{-1}) = (f_{2n-1}, f_{2n-2} - 1)$. If $a \triangleright A_{jk-1}$, $aA_{jk}b^{-1}$ is a factor of F_{∞} . Notice that $L(aA_{jk}b^{-1}) = (f_{2n-1} + 1, f_{2n-2} - 1)$, and this is impossible because of (13) and (14). Thus $b \triangleright A_{jk-1}$. Continuing we find that $b \triangleright A_{j1}$. But we have always $a \triangleright A_{j1}$ from the fact that $\sigma^{2n+1}(a) = F_{2n}F_{2n-1}, \sigma^{2n+1}(b) = F_{2n}$ and $a \triangleright F_{2n}$, this contradiction leads to the conclusion that for any i one has $a \triangleright A_{ji}$.

Now we are going to prove the main result which concludes that the splitting of the chain F_{∞} described at the beginning of this section can be generated by a substitution rule. For this, let the alphabet S_{2n} be given by

$$S_{2n} = \{X_1, X_2, \dots, X_{f_{2n-1}}, Y\}$$

(the case for m = 2n+1 odd goes analogously). Recall that by lemma 3, if $A_j \in C(F_{2n}, a)$, then

$$\sigma^{2n+1}(A_j) = A_{j1}A_{j2}\dots A_{j\ell_{2n}}b$$
(22)

where $A_{ji} \in C(F_{2n}, a)$. (Here we put $A_1 := F_{2n}$.)

Now define a substitution rule: $\Sigma_{2n} : S_{2n} \to S_{2n}^*$ by

$$\Sigma_{2n}(X_j) = X_{j1}X_{j2}\ldots X_{j\ell_{2n}}Y \qquad \Sigma_{2n}(Y) = X_1$$

where $X_{ji} = X_k$ if $A_{ji} = A_k$. Let $W = W_1 W_2 \dots$ be the unique fixed point of Σ_{2n} which is obtained by iterating Σ_{2n} an infinite number of times, starting from X_1 . So $\Sigma_{2n}(W) = W$. Now define another substitution $\phi : S_{2n}^* \to S^*$ by $\phi(X_j) = A_j$ for $1 \leq j \leq \ell_{2n}$ and $\phi(Y) = b$. Theorem 1. With the notations as above we have

$$\phi(W)=F_{\infty}.$$

Moreover, the splitting in words $\phi(W_1)\phi(W_2)\dots$ is equal to the splitting obtained by the periodic approximation algorithm.

Proof. It is easy to check that $\phi \circ \Sigma_{2n} = \sigma^{2n+1} \circ \phi$ on S_{2n} , using the definitions. Hence $\phi \circ \Sigma_{2n} = \sigma^{2n+1} \circ \phi$ on S_{2n}^* , which in turn implies that $\phi \circ (\Sigma_{2n})^k (X_1) = \sigma^{(2n+1)k}(A_1)$ for all k.

Notice that $(\Sigma_{2n})^k(X_1) \to W$ and $\lim_{k\to\infty} \sigma^{(2n+1)k}(A_1) = F_{\infty}$. Hence $\phi(W) = F_{\infty}$. To prove the second statement, we only have to check that if there is a $b = \phi(Y)$ in the splitting induced by $\phi(W_1)\phi(W_2)\ldots$, that the block of length 2n which starts with this b is singular. But this is true, because the word of length 2n following this b ends in an a by lemma 3.

Remark. We only proved theorem 1 for m = 2n even, but the case of m odd can be proved in a similar way. In that case $S_{2n+1} = \{X_1, X_2, \dots, X_{f_{2n-1}}, Y\}$ with $X_j \in C(F_{2n+1}, b)$.

Example 3.
$$m=1, C(F_1, b) = ab, \sigma(ab) = (ab)a, S_1 = \{X_1, Y\}$$
. Then

$$\Sigma_1(X_1) = X_1 Y \qquad \Sigma_1(Y) = X_1.$$

The fixed point of Σ_1 is $X_1 Y X_1 X_1 Y \dots$ which is the Fibonacci chain over S_1 . Because

$$M_{\tau} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$$

one has $v = (\mu + 1)/\mu = \mu$ for $\mu = (1 + \sqrt{5})/2$.

Example 4.
$$m = 2, C(F_2, a) = \{aba, baa\}$$
. Here
 $\sigma^3(aba) = (aba)(aba)(baa)(baa)b$ $\sigma^3(baa) = (aba)(aba)(aba)(baa)b$.
 $S_2 = \{X_1, X_2, Y\}$. Then
 $\Sigma_2(X_1) = X_1X_1X_2X_2Y$ $\Sigma_2(X_2) = X_1X_1X_1X_2Y$ $\Sigma_2(Y) = X_1$
 $M_{\Sigma_2} = \begin{pmatrix} 2 & 3 & 1 \\ 2 & 1 & 0 \\ 1 & 1 & 0 \end{pmatrix}$
 $W = \Sigma_2(W) = X_1X_1X_2X_2YX_1X_1X_2X_2YX_1X_1X_1....$

Now we fix a block $A_k \in C(F_{2n})$ and replace each X_j $(1 \leq j \leq \ell_{2n})$ by X in theorem 1.

Corollary. Let the substitution rule Ξ_{2n} : $\{X, Y\} \rightarrow \{X, Y\}^*$ be defined by

$$\Xi_{2n}(X) = X^{\ell_{2n}} Y \qquad \Xi_{2n}(Y) = X \,.$$

If Z is the unique fixed point of Ξ_{2n} , and $\psi : \{X, Y\}^* \to \{a, b\}^*$ is defined by $\psi(X) = A_k, \psi(Y) = b$, then $\psi(Z_1)\psi(Z_2)\dots$ yields a partitioning of F_{∞} equal to the one obtained from the periodic approximation algorithm where one replaces each conjugate of F_{2n} by A_k . Moreover,

$$M_{\Xi_{2n}} = \begin{pmatrix} \ell_{2n} & 1\\ 1 & 0 \end{pmatrix} . \tag{23}$$

We only have considered here the case m even. It is easy to show that the conclusion is in general true.

Example 5. Take n = 1, then $C(F_{2n}) = \{aba, baa, aab\}$.

Then $Z = X^4 Y X^4 Y X^4 Y X^5 Y \dots$ and e.g. for k = 2, F_{∞} is approximated by $(baa)^4 b (baa)^4 b (baa)^4 b (baa)^5 b \dots$

3. Superspace embedding

The embedding of the quasiperiodic Fibonacci chain consists of atomic surfaces along a path on a two-dimensional lattice Σ generated by two vectors e_a and e_b . The points $i + j\tau$, with $\tau = (\sqrt{5} - 1)/2$, on the chain correspond to the point $ie_a + je_b$ on the lattice. The path is bounded around the eigenspace of the highest eigenvalue ($\tau + 1$) of the substitution matrix. The closure of the projection of the path on the eigenspace of the other eigenvalue $(-\tau)$ is a connected interval, called atomic surface. The approximant corresponding to a periodic repetition of the word F_m is bounded around the line through $f_{m-1}e_a + f_{m-2}e_b$ and the origin. This means that one needs more than local reordering in going from the quasiperiodic structure to its approximant. The transformation remains local if one introduces an extra b(in case $f_{m-2}/f_{m-1} < \tau$, i.e. if m is even) or a (if m is odd) as a defect in the periodic chain. The density of these defects is governed by the requirement that the frequencies of a and b in the defective periodic chain are the same as for the Fibonacci chain. The defect is introduced if the atomic surface at $i(f_{m-1}e_a + f_{m-2}e_b)$ does not intersect the physical space (the eigenspace of the highest eigenvalue). By the corollary to theorem 1 this chain with defects is exactly $F_{\infty} = \psi(Z)$ and can be obtained by our algorithm in section 2 and, therefore, by the substitution $A \to A^{\ell_{2n}} B, B \to A$.

For m even one considers blocks A identical to F_m and B identical to b. Then the ratio μ of the frequencies of letters a and b is given by

$$\mu = \tau + 1 = \frac{a_N}{b_N} = \frac{f_{m-1}A_N}{f_{m-2}A_N + B_N}$$
(24)

and this implies for the ratio of frequencies of blocks A and B

$$\nu = \frac{A_N}{B_N} = \frac{\tau}{f_{m-1} - (\tau+1)f_{m-2}} = \frac{1}{\tau f_{m-1} - f_{m-2}}.$$
(25)

This is the highest eigenvalue of the matrix (23)

$$M = \begin{pmatrix} \ell_m & 1\\ 1 & 0 \end{pmatrix} . \tag{26}$$

The embedding of the chain of A's and B's is given by a path on a two-dimensional lattice $\tilde{\Sigma}$ generated by e_A and e_B . The physical space is the eigenspace of the largest eigenvalue $\lambda = \nu$, i.e. $\lambda e_A + e_B$.

The basis transformation from e_a, e_b to e_A, e_B is given by

$$T = \begin{pmatrix} f_{m-1} & 0\\ f_{m-2} & 1 \end{pmatrix}$$
(27)

which means that the lattice $\tilde{\Sigma}$ is a superlattice for Σ with index f_{m-1} . Inside the unit cell of $\tilde{\Sigma}$ there are f_{m-1} atomic surfaces, which in principle have different lengths (figure 1). The vertex at position r has lattice coordinates

$$\xi_{1} = \operatorname{Frac}\left[\frac{r}{2\tau - 1} \left(\frac{1}{f_{m-1}}\right)\right]$$
(28)

$$\xi_2 = \operatorname{Frac}\left[\frac{r}{2\tau - 1} \left(\tau - \frac{f_{m-2}}{f_m}\right)\right]$$
(29)



Figure 1. The superspace embeddings for the cases m = 2, 3 and m = 4, where A is replaced by, respectively, *aba, abaab* and *abaababa*, and B by b, a and b, respectively. There are respectively 3, 5 and 8 atomic surfaces, but these combine to, respectively 2, 2 and 5 atomic surfaces of length greater than unity. The circles indicate the positions r_i inside the unit cell.

with respect to a basis of lattice $\tilde{\Sigma}$. These points fall on the atomic surfaces in the unit cell. For *m* odd the block *B* is *a* and

$$\nu = \frac{A_N}{B_N} = \frac{1}{(\tau+1)f_{m-2} - f_{m-1}} = \frac{1}{\tau f_{m-2} - f_{m-3}} \,.$$

Therefore, the matrix M is the same as for the even value m-1. The matrix T becomes

$$T = \begin{pmatrix} f_{m-1} & 1\\ f_{m-2} & 0 \end{pmatrix}$$
(30)

which implies that the index is f_{m-2} , the same as for the even value m - 1. Consequently for the approximants with defects with units F_{2n} as well as for those with units F_{2n+1} one has f_{2n-1} atomic surfaces in the unit cell. This can be seen as a modulation of the original quasiperiodic structure. Therefore, such ordered defects in the periodic chain which give the chain the same incommensurability as the Fibonacci chain can be compared with discommensurations in incommensurate crystal phases. These discommensurations are just inserted structure units which make the periodic chain quasiperiodic (or incommensurate). In superspace this corresponds to a commensurate modulation of the *n*-dimensional embedding. The index of the superlattice does not depend on the letter order in the substitution, but the modulation function does (figure 2).

4. Fourier transform

The Fourier transform of a quasiperiodic system of rank n and dimension d, the intersection of an *n*-dimensional periodic system consisting of (n - d)-dimensional flat objects parallel to the additional space with the d-dimensional physical space is given by

$$F(H) = \frac{1}{\Omega} \sum_{j=1}^{s} e^{iHr_j} \int_{\Omega_j} e^{iH_{t}t} dt$$
(31)

where Ω_j is the atomic surface at position r_j , $\Omega = \sum_j \Omega_j$, s the number of atomic surfaces in the unit cell and H_I the additional component of the reciprocal lattice vector (H, H_I) that projects on the H in the Fourier module.



Figure 2. Two examples of superspace embeddings with different letter order. Left: the blocks are formed by *abaab* and *a*, there are 2 atomic surfaces per unit cell, one $[1 - \sqrt{5}, 1]$ with respect to (0, 0) and one $[-(1 + \sqrt{5})/2, (5 - \sqrt{5})/2]$ with respect to $(\frac{1}{2}\frac{1}{2})$. Right: for blocks *aaabb* and *a*, with also 2 atomic surfaces, here of length $2 + \sqrt{5}$ and 1, respectively. In both cases the total length of the atomic surfaces is $3 + \sqrt{5}$, which corresponds to an average vertex distance of $(\sqrt{5} - 2)$ times the average distance of the Fibonacci chain $((3\sqrt{5} - 5)/2)$. The variation in the second case is larger than in the first one. Broken lines enclose the unit cell which is represented in figure 1 by a square.

As we have seen, the number of atomic surfaces in the unit cell is f_{m-1} for *m* even and f_{m-2} for *m* odd. They can be obtained from the lattice corresponding to the substitution rule, i.e. the lattice generated by

$$e_A = K(1, -\alpha) \qquad e_B = K(\alpha, 1) \tag{32}$$

where K is the lattice constant, and $\alpha = \lambda^{-1}$ for λ the eigenvalue of matrix (26) bigger than unity. For m even the first basis vector is replaced by the path corresponding to the word F_m , i.e. a path from the origin to $e_A = f_{m-1}e_a + f_{m-2}e_b$. If the atomic surfaces in 0 and e_A intersect the physical space, so should the atomic surfaces along this path. Therefore they extend from $-\alpha$ to $1-\alpha$, and $|\Omega_j| = 1$ for all j. In addition there is the atomic surface of length α in the origin corresponding to the points which are the left vertices of intervals of length $K\alpha$. Sometimes, these atomic surfaces may touch each other in such a way that there are atomic surfaces of length greater than unity. This means that the $f_m - 1$ surfaces of length 1 and the one with length $1+\alpha$ combine to the f_{m-1} atomic surfaces mentioned in the previous section. The latter are of different length (figure 1). Finally the lattice constant K is chosen in such a way that the lengths of the intervals become 1 and τ .

$$K = a_n \ell_a + b_n \ell_b = a_n + b_n \tau \,. \tag{33}$$

Then the Fourier transform has Fourier module

$$H = \frac{2\pi}{K(1+\alpha^2)} [h_1 + h_2 \alpha] \qquad h_1, h_2 \in \mathbb{Z}$$
(34)

and is given by

$$F(H) = \frac{1}{f_n + \alpha} \left[\sum_{j=1}^{f_n} e^{iHr_j} \int_{-\alpha}^{1-\alpha} e^{iH_l t} dt + \int_{1-\alpha}^{1} e^{iH_l t} dt \right]$$
(35)

where

$$H_{i} = \frac{2\pi}{K(1+\alpha^{2})} [-h_{1}\alpha + h_{2}]$$
(36)

and

$$r_i = a_{jn} + b_{jn}\tau \,. \tag{37}$$

Here the coefficients are found as follows. If A is replaced by $w = x_1 x_2 \dots x_{f_n}$, the prefixes $\epsilon, x_1, x_1 x_2, \dots$ (i.e. $S_j(w)$) contain $a_j = |S_j(w)|_a$ a's and $b_j = |S_j(w)|_b$ b's. The Fourier module of the periodic chain with defects contains as submodule the Fourier module of the Fibonacci chain. Therefore, the chain with defects can be considered as a (commensurately) modulated Fibonacci chain.

When the lengths of the intervals are not 1 and τ , but arbitrary ℓ_a and ℓ_b the expression (31) for the Fourier transform can be generalized. The atomic surfaces are generally not parallel to the additional space, but stay mutually parallel to a line $x = \beta t$ ($t \in \mathbb{R}$) such that

$$\ell_a = K(1 + \alpha\beta) \qquad \ell_b = K(\alpha - \beta). \tag{38}$$

The formula (31) then becomes

$$F(H) = \frac{1}{\Omega} \sum_{j=1}^{s} e^{iHr_j} \int_{\Omega_j} e^{iH_l t + i\beta t} dt.$$
(39)

5. Concluding remarks

We have considered the properties of an infinite word created from a quasiperiodic word like the infinite Fibonacci one by replacing letters by words. In this way one may obtain words with different frequencies and different rank. The frequencies are related by a fractional linear transformation. The rank may even become infinite if the fractional linear transformation is singular. Otherwise the rank remains the same.

A locally rearranged Fibonacci word (i.e. with the same frequencies) consisting of a quasiperiodic sequence of words can be obtained from a chain resulting from a substitution rule by replacing the letters in the latter by words. In this way the rearranged chain can be considered as a modulated Fibonacci chain with discommensurations. The rank remains two and the Fibonacci Fourier module is a submodule of that of the modulated chain. In other words the modulation is commensurate with respect to the quasiperiodic Fibonacci chain.

For the example of the Fibonacci chain we have shown that a quasiperiodic chain may be transformed to a chain that consists of pieces of one of the periodic approximants and discommensurations. The transformation occurs via finite phason hopping.

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