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FIBONACCI CHAIN POLYNOMIALS: IDENTITIES FROM SELF-SIMILARITY

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Abstract

Fibonacci chains are special diatomic, harmonic chains with uniform nearest neighbour interaction and two kinds of atoms (mass-ratio r) arranged according to the self-similar binary Fibonacci sequence $ABAABABA\dots$, which is obtained by repeated substitution of $A \rightarrow AB$ and $B \rightarrow A$.

The implications of the self-similarity of this sequence for the associated orthogonal polynomial systems which govern these Fibonacci chains with fixed mass-ratio r are studied.

1 Introduction

Fibonacci chains are linear diatomic chains with nearest neighbour harmonic interaction of uniform strength κ and the two masses (ratio $r = m_1/m_0$) follow the pattern of the binary sequence $\{h(n)\}_1^\infty$ obtained by repeated substitutions σ in the following way.

$$\sigma(1) = 10 \quad , \quad \sigma(0) = 1 \quad , \quad (1)$$

starting with 0. By definition $\sigma(uv) = \sigma(u)\sigma(v)$ for any two strings u and v . $\sigma^n(0) \equiv H_n$ is a string of length $|H_n| = F_{n+1}$, where $F_n = F_{n-1} + F_{n-2}$, $n = 2, 3, \dots$, $F_0 = 0$, $F_1 = 1$ are the Fibonacci numbers. $h(n)$ is defined to be the n 'th entry of the half-infinite string $H_\infty := \lim_{n \rightarrow \infty} H_n$. E.g. $H_5 = \sigma^5(0) = 10110101$, $h(1) = 1$, $h(2) = 0$, etc. (1) is called the Fibonacci substitution rule, and the masses of the half-infinite chain are taken to be

$$m_n = m_{h(n)} \quad , \quad n = 1, 2, \dots \quad (2)$$

This sequence $\{h(n)\}_1^\infty$ is self-similar because the string H_∞ satisfies $\sigma(H_\infty) = H_\infty$. Aperiodicity follows from this invariance, or fixed point, property. (This sequence is in fact also quasiperiodic, but this does not concern us here.)

Chains of this type have been considered as models of binary alloys [1]. For instance, one may consider chains with an elementary unit determined by the first N members of the $\{h(n)\}$ sequence and repeat it periodically, using certain boundary conditions. This then corresponds to $(AB)^\infty$ chains for $N = 2$, $(ABA)^\infty$ chains for $N = 3$, etc.

The dual of such chains (with equal masses but two spring constants κ_0 and κ_1 following the pattern of the Fibonacci substitution sequence) are related to one-dimensional quasicrystals [2]. One can also make contact to artificially manufactured superlattices [3]. Originally such Fibonacci chains were considered as models for the study of the regime in between periodic and random structures.[4, 5].

The purpose of this work is to write down the identities which are satisfied by the characteristic polynomials of these Fibonacci chains due to the self-similarity of the substitution sequence $\{h(n)\}$ which determines the pattern of the masses of the oscillators. These identities will be expressed in terms of the 2×2 transfer matrices M_n which are unimodular and real. The matrix elements are given by the characteristic polynomials $\{S_n^{(r)}(x)\}$, where r is the mass-ratio of the two types of atoms and x is a normalized frequency squared ($x \equiv \omega^2/2\omega_0^2$, $\omega_0^2 = \kappa/m_0$). The zeros of $S_N^{(r)}(x)$ determine the eigenfrequencies of finite Fibonacci chains with N atoms and both ends fixed. One also encounters so-called first associated polynomials $\{\hat{S}_N^{(r)}(x)\}$. They correspond to a right shift by one unit in the substitution sequence. Hence, the zeros of $\hat{S}_N^{(r)}(x)$ produce the eigenfrequencies of chains with masses $m_{h(2)} = m_0, \dots, m_{h(N+1)}$. Both r -families of polynomials generalize Chebyshev's $\{S_n(y)\}$ polynomials ($S_{-1} = 0$, $S_0 = 1$, $S_n = yS_{n-1} - S_{n-2}$) to two variables with the identification

$$S_n^{(1)}(x) = \hat{S}_n^{(1)}(x) = S_n(2(1-x)). \quad (3)$$

They constitute, for fixed mass-ratio r , systems of orthogonal polynomials and have been studied in some detail in refs.[6, 7, 8, 9].

2 Fibonacci Chain Polynomials

For the Fibonacci chains $(\kappa, m_{h(n)})$ defined in *section 1* the equation of motion for longitudinal, time-stationary vibrations $q_n(t) = q_n \exp(i\omega t)$ are

$$q_{n+1} + q_{n-1} - Y(n)q_n = 0, \quad n = 1, 2, \dots \quad (4)$$

with

$$Y(n) \equiv 2(1 - \omega^2/(2\omega_n^2)), \quad \omega_n^2 \equiv \kappa/m_{h(n)}. \quad (5)$$

We use the two variables $r \equiv m_1/m_0$ and $x \equiv \omega^2/(2\omega_0^2)$. We put $Y(n) = Y$ if $h(n) = 1$ and $Y(n) = y$ if $h(n) = 0$. Hence

$$Y = 2(1 - rx), \quad y = 2(1 - x). \quad (6)$$

The equations of motion are rewritten with the help of the $SL(2, \mathbb{R})$ transfer matrix R_n :

$$\begin{pmatrix} q_{n+1} \\ q_n \end{pmatrix} = R_n \begin{pmatrix} q_n \\ q_{n-1} \end{pmatrix} := \begin{pmatrix} Y(n) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} q_n \\ q_{n-1} \end{pmatrix}. \quad (7)$$

R_n is either R_1 or R_0 depending on the $Y(n)$ value, *i.e.* $R_n = R_{h(n)}$. For the half-sided infinite chains considered here iteration leads to

$$\begin{pmatrix} q_{n+1} \\ q_n \end{pmatrix} = R_n R_{n-1} \cdots R_1 \begin{pmatrix} q_1 \\ q_0 \end{pmatrix} =: M_n \begin{pmatrix} q_1 \\ q_0 \end{pmatrix}, \quad (8)$$

with the inputs q_1 and q_0 (the mass at site number 0 is irrelevant). M_n is real and unimodular. The recursion $M_n = R_n M_{n-1}$ with input $M_1 = R_1$ leads to

$$M_n = \begin{pmatrix} S_n & -\hat{S}_{n-1} \\ S_{n-1} & -\hat{S}_{n-2} \end{pmatrix}, \quad (9)$$

where the recursion formulae for the generalized two-variable Chebyshev polynomials are

$$S_n = Y(n)S_{n-1} - S_{n-2}, \quad S_{-1} = 0, \quad S_0 = 1, \quad (10)$$

$$\hat{S}_n = Y(n+1)\hat{S}_{n-1} - \hat{S}_{n-2}, \quad \hat{S}_{-1} = 0, \quad \hat{S}_0 = 1. \quad (11)$$

These polynomials generate certain combinatorial numbers [10]. The meaning of these numbers can be understood if one uses the intimate connection of the Fibonacci substitution sequence with Wythoff's A and B sequences

$$A(n) = n + \sum_{k=1}^{n-1} h(k), \quad B(n) = n + A(n). \quad (12)$$

These sequences $\{A(n)\}_1^\infty$ and $\{B(n)\}_1^\infty$ cover the positive integers in a complementary way: every number $N > 0$ is either an A - or a B -number. For an A -number n (i.e. $n = A(m)$ for some m) $h(n) = 1$, and for a B -number n (i.e. $n = B(m)$ for some m) $h(n) = 0$. Wythoff's sequences are a special case of Beatty sequences: $A(n) = \lfloor n\varphi \rfloor$, $B(n) = \lfloor n\varphi^2 \rfloor$, with $\varphi^2 = \varphi + 1$, $\varphi > 0$, the golden mean.

The characteristic polynomials $\{S_n^{(r)}(x)\}$, obtained from $\{S_n(Y, y)\}$ by replacement of Y and y according to eq.(6), constitute, for fixed mass-ratio r , a system of orthogonal polynomials. $\{\hat{S}_n^{(r)}(x)\}$ are the first-associated orthogonal polynomials.

3 Self-Similarity Identities

The string, or 'word', H_∞ defined in section 1 is invariant under the inverse substitution σ^{-1} , with $\sigma^{-1}(1) = 0$, $\sigma^{-1}(0) = 1$. This is equivalent to the self-similarity of the sequence $\{h(n)\}_1^\infty$ which is shown in the FIG.

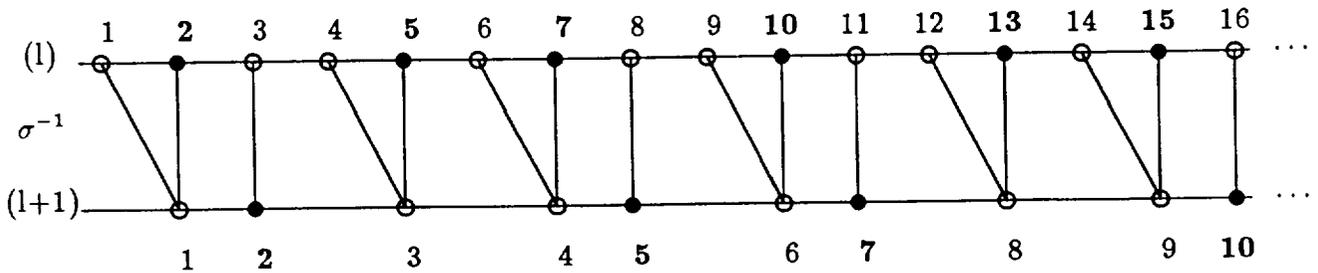


FIG. Self-similarity of the sequence $\{h(n)\}_1^\infty$. Circles stand for the value 1 (A -numbers n), and disks stand for the value 0 (B -numbers n). $\sigma^{-1}(10) = 1$, $\sigma^{-1}(1) = 0$. Level (l) is mapped to level $(l+1)$ by σ^{-1} .

The upper level, called (l) in the FIG., shows the numbers marked as A - and B -numbers. The $h(n)$ value is 1 or 0, denoted by a circle or disk, respectively. When the substitution σ^{-1} is applied one reaches the next higher level, called $(l+1)$ in the FIG., on which the same sequence is reproduced. Let the position of the n 's number at level (l) be $x_n^{(l)}$ for $l = 0, 1, \dots$. Level $l = 0$ is assumed to correspond to the original sequence. Then one finds for $p \in N_0 \equiv N \cup \{0\}$

$$x_{A(p)}^{(l+1)} = x_{B(p)}^{(l)} , \quad (13)$$

$$x_{B(p)}^{(l+1)} = x_{AB(p)}^{(l)} , \quad (14)$$

where $AB(p)$ stands for the composition $A(B(p))$ of Wythoff's sequences. *E.g.* The number $A(4) = 6$ at level $(l+1)$ occurs in the FIG. at the same position as $B(4) = 10$ at level (l) , or $B(2) = 5$ at level $(l+1)$ corresponds to $AB(2) = A(5) = 8$ at level (l) .

Iteration, depending on the parity of the level number, leads to

$$x_{A(p)}^{(2k+1)} = x_{B^{k+1}(p)}^{(0)} , \quad x_{A(p)}^{(2k)} = x_{AB^k(p)}^{(0)} , \quad (15)$$

$$x_{B(p)}^{(2k+1)} = x_{AB^{k+1}(p)}^{(0)} , \quad x_{B(p)}^{(2k)} = x_{B^{k+1}(p)}^{(0)} . \quad (16)$$

Consider the level $(l+1)$ transfer matrix

$$M_n^{(l+1)} = R_{h(n)}^{(l+1)} \dots R_{h(1)}^{(l+1)} , \quad (17)$$

satisfying the recursion relation

$$R_1^{(l+1)} = R_0^{(l)} R_1^{(l)} , \quad R_0^{(0)} \equiv R_0 = \begin{pmatrix} y & -1 \\ 1 & 0 \end{pmatrix} , \quad (18)$$

$$R_0^{(l+1)} = R_1^{(l)} , \quad R_1^{(0)} \equiv R_1 = \begin{pmatrix} Y & -1 \\ 1 & 0 \end{pmatrix} . \quad (19)$$

Iteration leads , with $M_n \equiv M_n^{(0)}$, to

$$R_1^{(l+1)} = M_{F_{(l+3)}} , \quad R_0^{(l+1)} = M_{F_{(l+2)}} , \quad (20)$$

with the Fibonacci numbers F_n .

Due to (15) and (16) one has

$$M_{A(p)}^{(2k+1)} = M_{B^{k+1}(p)} , \quad M_{A(p)}^{(2k)} = M_{AB^k(p)} , \quad (21)$$

$$M_{B(p)}^{(2k+1)} = M_{AB^{k+1}(p)} , \quad M_{B(p)}^{(2k)} = M_{B^{k+1}(p)} . \quad (22)$$

The recursion at each level is

$$M_n^{(l+1)} = R_{h(n)}^{(l+1)} M_{n-1}^{(l+1)} , \quad M_1^{(l+1)} = R_1^{(l+1)} . \quad (23)$$

Combining iteration and recursion, in a systematic way, leads to transfer matrix identities for level (0) , *i.e.* for the original matrices M_n of eq. (8). One finds altogether six families of such

identities, depending on the parity of the level one starts with and the specification of the index. These identities are, for $m \in \mathbb{N}$ and $k \in \mathbb{N}$,

$$\begin{aligned}
(I) \quad & M_{B^{k+1}(m)} = M_{F_{2k+1}} M_{AB^k A(m)} , \\
(IIa) \quad & M_{B^k A(A(m)+1)} = M_{F_{2k+1}} M_{B^{k+1}(m)} , \\
(IIb) \quad & M_{B^k A(B(m)+1)} = M_{F_{2k+1}} M_{AB^{k+1}(m)} , \\
(III) \quad & M_{AB^k(m)} = M_{F_{2k}} M_{B^k A(m)} , \\
(IVa) \quad & M_{AB^k A(A(m)+1)} = M_{F_{2(k+1)}} M_{AB^{k+1}(m)} , \\
(IVb) \quad & M_{AB^k A(B(m)+1)} = M_{F_{2(k+1)}} M_{B^{k+2}(m)} .
\end{aligned} \tag{24}$$

(I), (IIa), (IIb) and (III) result from odd levels $l = 2k + 1$, with n put $AB(m)$, $AA(A(m) + 1)$, $AA(B(m) + 1$ and $B(m)$, respectively. (III), (IVa) and (IVb) result from even levels $l = 2k$, with n put $B(m)$, $A(A(m) + 1)$ and $A(B(m) + 1)$, respectively.

E.g. (I) and (III) produce for $m = 1$, due to $A(1) = 1$, $B^{k+1}(1) = F_{2k+3}$ and $AB^k(1) = F_{2(k+1)}$, identities which are the well-known recursion formula for transfer matrices with neighbouring Fibonacci number indices

$$M_{F_{n+1}} = M_{F_{n-1}} M_{F_n} . \tag{25}$$

Not all eqs.(24) are independent. *E.g.* if one puts $m = B(p) + 1$ in (I), replaces k by $k + 1$ and combines it with eqs. (IVb), with $k \rightarrow k - 1$ and $m \rightarrow p$, one finds eqs. (IIa), due to the identity $B(p) + 1 = A(A(p) + 1)$ and eq.(25) for even n . However, eqs.(IIa) provide identities for $M_{B^k A(p)}$ which complement those obtained from eqs. (IIb).

It is possible to combine (I) of eq.(24) with (III) specialized to $m \rightarrow A(m)$ and use (I) again with $k \rightarrow k - 1$ and $m \rightarrow A^2(m)$. Continuing this process one finds for $k \in \mathbb{N}$ and $m \in \mathbb{N}$

$$\begin{aligned}
(I') \quad & M_{B^{k+1}(m)} = M_{F_{2k+1}} M_{F_{2k}} \cdots M_{F_2} M_{BA^{2k}(m)} \\
(III') \quad & M_{AB^k(m)} = M_{F_{2k}} M_{F_{2k-1}} \cdots M_{F_2} M_{BA^{2k-1}(m)}
\end{aligned} \tag{26}$$

(I) and (III) in (24) can be replaced by both eqs. (26), and the other eqs. of (24) can be rewritten using (26).

The sum of the indices of the transfer matrices on the *r.h.s.* of eqs.(24) and (26) have to match the index of the *l.h.s.* This fact produces families of identities among iterated Wythoff A and B sequences. A detailed investigation of these Wythoff composites identities will be given elsewhere. All of these identities can be rederived as corollaries of a new theorem relating two seemingly different unique number systems: the Wythoff- and the Zeckendorf- (or Fibonacci-) representations.

The transfer matrix identities (24) are equivalent to those for their matrix elements, *i.e.* the characteristic polynomials $\{S_n(Y, y)\}$ and $\{\hat{S}_n(Y, y)\}$. In order to derive them one rewrites the indices of all matrix elements as Wythoff composites. Consider, for example, (I). For the elements of $M_{B^{k+1}(m)}$ one employs the simple identities $B^{k+1}(m) - 1 = B(B^k(m)) - 1 = A^2 B^k(m)$ and $B^{k+1}(m) - 2 = ABAB^{k-1}(m)$. The last identity can be proved for $m = A(p)$ and $m = B(p)$ separately. On the *r.h.s.* of (I) one rewrites the indices of the matrix elements with the help of the identities $F_{2k+1} = B^k(1)$, $F_{2k+1} - 1 = A^2 B^{k-1}(1)$, $F_{2k+1} - 2 = ABAB^{k-2}(1)$ for $k = 2, 3, \dots$, and $F_3 - 2 = 0$. Moreover, $AB^k A(m) - 1 = BAB^{k-1} A(m)$, $AB^k A(m) - 2 = A^3 B^{k-1} A(m)$.

Finally, (I) decomposes into the following four sets of eqs.

$$\begin{aligned}
(I, (1, 1)) \quad S_{B^{k+1}(m)} &= S_{B^{k(1)}} S_{AB^k A(m)} - \hat{S}_{A^2 B^{k-1}(1)} S_{BAB^{k-1} A(m)} , \\
(I, (1, 2)) \quad \hat{S}_{A^2 B^k(m)} &= S_{B^{k(1)}} \hat{S}_{BAB^{k-1} A(m)} - \hat{S}_{A^2 B^{k-1}(1)} \hat{S}_{A^3 B^{k-1} A(m)} , \\
(I, (2, 1)) \quad S_{A^2 B^k(m)} &= S_{A^2 B^{k-1}(1)} S_{AB^k A(m)} - \hat{S}_{ABAB^{k-2}(1)} S_{BAB^{k-1} A(m)} , \\
(I, (2, 2)) \quad \hat{S}_{ABAB^{k-1}(m)} &= S_{A^2 B^{k-1}(1)} \hat{S}_{BAB^{k-1} A(m)} - \hat{S}_{ABAB^{k-2}(1)} \hat{S}_{A^3 B^{k-1} A(m)} .
\end{aligned} \tag{27}$$

The last two sets of eqs. hold only for $k = 2, 3, \dots$. For $k = 1$ one has

$$\begin{aligned}
S_{A^2 B(m)} &= Y S_{ABA(m)} - S_{BAA(m)} , \\
\hat{S}_{ABA(m)} &= Y \hat{S}_{BAA(m)} - \hat{S}_{A^4(m)} .
\end{aligned} \tag{28}$$

The other eqs. in (24) decompose in a similar way. The arguments of the polynomials is always (Y, y) , which can be replaced using eq.(6).

This concludes the derivation of the self-similarity eqs. for the Fibonacci chain polynomials. It is clear that further work is needed in order to extract from this gamut of eqs. information pertaining to chain properties, like structure of spectra and displacements.

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