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On the characteristic polynomials of Fibonacci chains

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Abstract. Special diatomic linear chains with elastic nearest-neighbour interaction and the two masses distributed according to the binary Fibonacci sequence are studied.

1. Introduction

The one-dimensional (1D) discrete Schrödinger equation with a discontinuous quasi-periodic potential of the Fibonacci type has been the subject of a large number of works following the original proposal of two groups [1a, b] in 1983. At that time the physical motivation was to study a model intermediate between the regimes of periodic and random potentials in order to gain a better understanding of the transition from extended to localized states. From the mathematical point of view this model belongs to the class of almost periodic Schrödinger operators [2a, b] which displays unusual spectral properties. In particular, it was found that for the Fibonacci Hamiltonian the support of the spectrum is a Cantor set of zero Lebesgue measure, and that the spectral measure is of the purely singular continuous type [3a, b].

Because of the similarity of this tight-binding problem for an electron on a regular chain subject to a quasi-periodic potential and the phonon problem for a quasi-periodic chain the Fibonacci model has also featured as a 1D incommensurable crystal (for a review see [4a, b]). After the experimental discovery of alloys with crystallographically forbidden symmetry in 1984 [5] and their theoretical interpretation as quasicrystals [6] the quasiperiodic binary Fibonacci sequence $1, 0, 1, 1, 0, 1, 0, 1, \ldots$ was found to determine the spacings of layers of quasicrystals in certain directions. For reviews on quasicrystals see [7a–d]. The phonon problem for a 1D Fibonacci quasicrystal [8a, b] can be transformed to the problem of a periodic chain with nearest-neighbour harmonic interaction, one spring constant and two masses M and m arranged according to the binary Fibonacci sequence [9].

In this work we consider diatomic Fibonacci chains of three types: finite chains of N particles with fixed or open boundary conditions, and infinite chains where a unit cell of N particles is repeated periodically. The characteristic polynomials of finite chains are shown to stem from two families of two-variable generalizations of Chebyshev's S_n polynomials which were introduced earlier as generating functions for certain combinatorial numbers [10]. The band structure of the infinite periodic N-chain is determined from the two-variable generalized T_N Chebyshev polynomials,

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which are also obtained from these generating functions. The two variables in the chain problem are the mass ratio $r \equiv M/m$ and the (dimensionless) frequency-squared $x \equiv \omega^2/2\omega_0^2$, where $\omega_0^2 \equiv \kappa/m$.

The dispersion relation and the spectral density for periodic Fibonacci N-chains are given in terms of these generalized T_N polynomials. In agreement with a general observation made in [11] it is found that the two-variable polynomials S_n and $\hat{S}_n$ which generalize Chebyshev's S_n polynomials are both systems of orthogonal polynomials in the variable x when r is kept fixed. The explicit form of the measure is not known except for the monoatomic case, i.e. for $r = 1$. The T_n polynomials are orthogonal in the variable x only for $r = 1$. The same statement applies to the characteristic polynomials of finite open chains.

Usually, in works based on the binary Fibonacci sequence, only systems with N being a Fibonacci number ($F_{n+2} = F_{n+1} + F_n$, $F_0 = 0$, $F_1 = 1$) are considered. This is because the transfer matrices then satisfy a simple composition law. Also, the infinite quasi-periodic system is usually taken as the limit of a periodic system by approximating the golden mean φ ($\varphi^2 = \varphi + 1$, $\varphi > 0$) by rationals $(\varphi)_m = F_{m+1}/F_m$. In this work we do not need the N restriction, and a theorem shows that the approximation of φ by rationals is, as far as the band structure is concerned, equivalent to a treatment of periodic chains with Fibonacci $N = F_{m+1}$ unit cells.

The quasi-periodicity of the binary Fibonacci sequence entails a large number of identities among the various two-variable polynomials encountered in the chain problems. They are derived in section 4 . Some of them allow one to factorize polynomials; thus eigenfrequencies or band ends can be determined by the zeros of lower-degree polynomials. In section 5 a special type of identity, known to hold for the transfer-matrix trace polynomials T_n in the monoatomic case, is examined for general r. A criterion for the persistence of this identity for diatomic Fibonacci chains is given there.

In section 6 the generating functions of the two-variable Chebyshev polynomials are considered. It is possible to derive formulae which express these polynomials in terms of ordinary one-variable ones and powers of the difference of the two variables. For the chain problem these formulae provide the basis for a perturbative treatment, the expansion parameter being the relative mass difference $\lambda \equiv 1 - r$. The band structure for periodic chains with an N-particle unit cell is computed to lowest non-trivial order in λ.

2. Fibonacci chains

Consider longitudinal time-stationary vibrations of a linear chain with nearest-neighbour harmonic interaction. The displacement $q_n(t) = q_n \exp(\mathrm{i}\omega t)$ of the nth particle (mass m_n) from its equilibrium position $x_n^0 \equiv na$ satisfies the following set of difference equations for $y_n \equiv \sqrt{m_n}q_n$, $|q_n|/a \ll 1$ [12a–c]:

$$(\alpha_n - \omega^2)y_n + \beta_n y_{n-1} + \beta_{n+1} y_{n+1} = 0 \tag{2.1}$$

where $\alpha_n \equiv (\kappa_n + \kappa_{n-1})/m_n$, $\beta_n \equiv -\kappa_{n-1}/\sqrt{m_n m_{n-1}}$, and κ_n is the spring constant between particles numbered $n+1$ and n. Fibonacci chains [9] are special diatomic chains with the two masses $M = m_1$ and $m = m_0$ (mass ratio $r \equiv M/m$) distributed along the sites according to the rule

$$m_n = m_{h(n)} \qquad h(n) := \lfloor (n+1)/\varphi \rfloor - \lfloor n/\varphi \rfloor \tag{2.2}$$

with φ the golden mean, and $\lfloor\alpha\rfloor$ the biggest integer less than or equal to the real number α. $h(n)$ is called the binary Fibonacci sequence. References are found in [10]. In the following we shall discuss Fibonacci chains with the following boundary conditions and κ_n simplifications:

(a) Finite N-particle Fibonacci chains with masses $m_{h(n)}$, $n = 1, 2, \ldots, N$, and $N+1$ equal springs $\kappa_n = \kappa$ for $n = 0, 1, \ldots, N$, and fixed boundaries:

$$q_0 = 0 = q_{N+1} \tag{2.3a}$$

(b) finite N-particle Fibonacci chains with masses $m_{h(n)}$, $n = 1, 2, \ldots, N$ and $N-1$ equal springs $\kappa_n = \kappa$, for $n = 1, 2, \ldots, N-1$ with both ends free:

$$\kappa_0 = 0 = \kappa_N \tag{2.3b}$$

(c) infinite periodic chains with unit cell of length $L = Na$ consisting of N particles with masses $m_{h(n)}$ and N equal springs $\kappa_n = \kappa$ for $n = 1, 2, \ldots, N$. This chain can be obtained from a finite one built from $2M$ such Fibonacci N-cells with periodic boundary conditions

$$q_{2MN+i} = q_i \qquad \text{for all} \quad i$$

in the limit $M \to \infty$. Mixed boundary conditions for finite chains could also be considered. For such type of chains the difference equations (2.1) reduces to

$$q_{n+1} + q_{n-1} - (2 - \omega^2/\omega_n^2)q_n = 0 \tag{2.4}$$

with $\omega_n^2 \equiv \kappa/m_n = \kappa/m_{h(n)}$. In the case of open chains (b) one has $\beta_1 y_0 = 0 = \beta_{N+1} y_{N+1}$ in (2.1), $\alpha_1 = \kappa/m_1, \alpha_N = \kappa/m_N$, and (2.4) holds only for $n = 2, 3, \ldots, N-1$ whereas the $n = 1$ and N equations become

$$\begin{aligned} q_2 &= (1 - \omega^2/\omega_1^2)q_1 \\ q_{N-1} &= (1 - \omega^2/\omega_{h(N)}^2)q_N\,. \end{aligned} \tag{2.4'}$$

The following notation will be used:

$$Y(n) \equiv 2 - \omega^2/\omega_n^2 = h(n)Y + (1 - h(n))y \tag{2.5}$$

with

$$Y \equiv 2(1 - rx) \qquad y \equiv 2(1 - x) \tag{2.6}$$

where $x \equiv \omega^2/2\omega_0^2$ is the normalized frequency squared and we recall $r \equiv m_1/m_0 = M/m$. The SL$(2, R)$ transfer matrix associated with system (2.4) is defined by

$$\begin{pmatrix} q_{n+1} \\ q_n \end{pmatrix} = R_n \begin{pmatrix} q_n \\ q_{n-1} \end{pmatrix} := \begin{pmatrix} Y(n) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} q_n \\ q_{n-1} \end{pmatrix}. \tag{2.7}$$

For the cases (a) and (c) this means

$$\begin{pmatrix} q_{n+1} \\ q_n \end{pmatrix} = R_n R_{n-1} \ldots R_1 \begin{pmatrix} q_1 \\ q_0 \end{pmatrix} =: M_n \begin{pmatrix} q_1 \\ q_0 \end{pmatrix} \tag{2.8}$$

which allows computation of q_n in terms of the inputs q_1 and q_0. In the open chain case (b) one has

$$\begin{aligned} &\begin{pmatrix} q_{n+1} \\ q_n \end{pmatrix} = M_n R_1^{-1} \begin{pmatrix} q_2 \\ q_1 \end{pmatrix} \qquad n = 2, 3, \ldots, N-1 \\ &q_2 = (Y(1) - 1) q_1 \qquad q_{N-1} = (Y(N) - 1) q_N \,. \end{aligned} \tag{2.9}$$

The Fibonacci matrix 'word' $M_n = R_n R_{n-1} \ldots R_1$ is found to be the SL(2, $\mathbf{R}$) matrix

$$M_n = \begin{pmatrix} S_n & -\hat{S}_{n-1} \\ S_{n-1} & -\hat{S}_{n-2} \end{pmatrix} \tag{2.10}$$

where the polynomials $S_n(Y, y)$ and $\hat{S}_n(Y, y)$ are defined by the following three-term recurrence relation†:

$$S_n = Y(n) S_{n-1} - S_{n-2} \qquad S_{-1} = 0 \qquad S_0 = 1 \tag{2.11a}$$

$$\hat{S}_n = Y(n+1) \hat{S}_{n-1} - \hat{S}_{n-2} \qquad \hat{S}_{-1} = 0 \qquad \hat{S}_0 = 1 \tag{2.11b}$$

with $Y(n)$ given by (2.5). These two-variable generalizations of Chebyshev's S_n polynomials were introduced in [10]. There one can also find their explicit form and the combinatorial meaning of their integer coefficients. These polynomials appear as the numerator and denominator of the nth approximation to a continued fraction, namely

$$\frac{1 \,|}{|Y(1)} - \frac{1 \,|}{|Y(2)} - \cdots - \frac{1 \,|}{|Y(n)} = \frac{\hat{S}_{n-1}}{S_n} \,. \tag{2.12}$$

For monoatomic chains ($r = 1$) $S_n = \hat{S}_n$ and both reduce to Chebyshev's ordinary polynomials [13] $S_n(y) = U_n(y/2)$, with $U_n(\cos\Theta) = \sin[(n+1)\Theta]/\sin\Theta$ provided $|y| < 2$. The trace-polynomials generalize Chebyshev's polynomials of the first kind, $T_n(\cos\Theta) = \cos\, n\Theta$, to two variables:

$$T_n\left(\frac{Y}{2}, \frac{y}{2}\right) := \frac{1}{2} \operatorname{tr}\, M_n = \frac{1}{2}[S_n(Y, y) - \hat{S}_{n-2}(Y, y)] \,. \tag{2.13}$$

Transfer matrices R_n of type (2.7) appear in other 1D models based on the binary Fibonacci sequence. We show how to adapt the variables Y and y for some of them.

First, there is the model of the 1D discrete Schrödinger equation with the quasi-periodic potential $V_n := V(n\varphi)$ at site number n of a periodic chain, where the periodically continued step function

$$V(x) := \begin{cases} V_0 & \text{if } 0 \leqslant x < 2 - \varphi \\ V_1 & \text{if } 2 - \varphi \leqslant x < 1 \end{cases} \qquad V(x+1) = V(x) \tag{2.14}$$

† If one uses the S_n recurrence formula with the inputs $S_{-1} = -1$, $S_0 = 0$, one finds $S_{n+1} = \hat{S}_n$ for $n \in N$.

is used. In this case one should replace (2.6) by

$$Y = E - V_1 \qquad y = E - V_0 \tag{2.15}$$

and the (shifted) energy E is measured in units of $\hbar^2/2ma^2$, where m is the particle mass and a the chain spacing. There exists a vast amount of literature on this Fibonacci Hamiltonian, based on [1a, b]. For more recent references with rigorous results like the proof of a Cantor-type spectrum of zero Lebesgue measure see [3a,b]. Besides this electronic tight-binding problem there is, secondly, the eigenvalue problem of the 1D Laplace operator, $(\Delta + z)\phi = 0$, discretized on a quasi-periodic chain with two bond lengths λ_0 and λ_1 following the pattern of the binary $h(n)$ sequence. This phonon problem of a 1D Fibonacci quasicrystal [8] is, by a change of the dynamical variables, brought to the above-considered Schrödinger problem on a regular chain with quasi-periodic potential $V_n = -z\lambda_{h(n)}$ and $E = 2$. Here z is the reduced eigenfrequency squared. Now (2.6) has to be replaced by

$$Y = 2(1 - x\lambda_1) \qquad y = 2(1 - x\lambda_0) \tag{2.16}$$

with $x \equiv z/2$. The transfer matrix R_n is identical to the one of the Fibonacci chains provided one puts $\lambda_0 = 1$ and $\lambda_1 = r > 1$.

3. Fibonacci chain polynomials

In this section the characteristic polynomials for the three types of diatomic chains (a), (b), and (c) defined in the last section are introduced. For the N-chain with both ends fixed, type (a), only the S_n polynomials enter the problem. Due to the $q_{N+1} = 0$ requirement one finds the eigenfrequencies from the zeros of

$$S_N^{(r)}(x) := S_N(2(1 - rx), 2(1 - x)). \tag{3.1}$$

Also, $q_{n+1} = S_n^{(r)}(x)\, q_1$ for $n = 2, 3, \ldots, N - 1$. The recurrence relation for these $S_n^{(r)}(x)$ polynomials derives from (2.11*a*):

$$S_{n+1}^{(r)}(x) - 2(1 - r^{h(n+1)}x)\; S_n^{(r)}(x) + S_{n-1}^{(r)}(x) = 0 \qquad n = 0, 1, \ldots \tag{3.2}$$

with the inputs $S_{-1}^{(r)} = 0$, $S_0^{(r)} = 1$.

Because the explicit form of the $S_n(Y, y)$ polynomials is known in terms of certain combinatorial numbers $(n; l, k)$ (see [10] for their definition) one could give such a form for the $S_n^{(r)}$ polynomials as well. It suffices to notice here that $S_n^{(r)}(0) = n + 1$ and the coefficient of x^n in $S_n^{(r)}(x)$ is $(-2)^n r^{z(n)}$, with the sequence

$$z(n) := \sum_{m=1}^{n} h(m) = \lfloor (n + 1)\varphi \rfloor - (n + 1). \tag{3.3}$$

If one rewrites recursion formula (3.2) for the monic polynomials

$$\tilde{S}_n^{(r)}(x) := (-2)^{-n} r^{-z(n)} S_n^{(r)}(x)$$

one finds the standard three-term form [14a, b]

$$\tilde{S}_n^{(r)}(x) = (x - c_n^{(r)})\tilde{S}_{n-1}^{(r)}(x) - \lambda_n^{(r)}\tilde{S}_{n-2}^{(r)}(x) \qquad n = 1,2,\ldots$$
$$\tilde{S}_{-1}^{(r)} = 0 \qquad \tilde{S}_0^{(r)} = 1 \tag{3.4}$$

with

$$c_n^{(r)} \equiv r^{-h(n)} \qquad \lambda_n^{(r)} \equiv \tfrac{1}{4} r^{-[1+k(n-1)]} \tfrac{1}{4} c_n^{(r)} c_{n-1}^{(r)}$$

where $k(n) := h(n) - [1 - h(n+1)]$. This shows that for any $r > 0$ the $S_n^{(r)}(x)$ satisfy the necessary and sufficient conditions [14a, b] for an orthogonal polynomial system. Moreover, for any $r > 0$

$$s_n^{(r)}(x) := r^{h(n+1)/2} S_n^{(r)}(x) \tag{3.5}$$

constitute a system of ortho*normal* polynomials with respect to some positive-definite moment functional (or measure). Up to now we only know the weight function and the interval for the monoatomic case, i.e. for $r = 1$. The $S_n^{(1)}(x) = S_n[2(1-x)] = U_n(1-x)$ are orthonormal polynomials in the interval $[0, 2]$ with weight function $w(x) = 2\sqrt{x(2-x)}/\pi$. The zeros of $S_{n-1}^{(1)}(x)$ are [13]

$$\xi_k^{(n-1)} = 1 - \cos\frac{\pi k}{n} \qquad k = 1,2,\ldots,n-1\,. \tag{3.6}$$

The first few $S_n^{(r)}(x)$ polynomials are listed in table 1.

Table 1. $S_n^{(r)}(x)$, $S_{-1}^{(r)} = 0$, $S_0^{(r)} = 1$.

n	$S_n^{(r)}(x)$
1	$2(1 - xr)$
2	$4rx^2 - 4(1+r)x + 3$
3	$-8r^2x^3 + 8r(r+2)x^2 - 4(2+3r)x + 4$
4	$16r^3x^4 - 16r^2(3+r)x^3 + 4r(11+10r)x^2 - 4(3+7r)x + 5$
5	$2[-16r^3x^5 + 16r^2(2r+3)x^4 - 4r(4r^2+21r+11)x^3+$ $+4(9r^2+16r+3)x^2 - (22r+13)x + 3]$
6	$64r^4x^6 - 128r^3(r+2)x^5 + 16r^2(4r^2+28r+23)x^4+$ $-32r(6r^2+17r+7)x^3 + 8(24r^2+33r+6)x^2 - 8(9r+5)x + 7$
...	...

For the *open* N-*chain* of type (b) the solution (2.9) can be written as†

$$q_n = \left[S_{n-1}^{(r)}(x) - \hat{S}_{n-2}^{(r)}(x)\right] q_1 \qquad n = 2,3,\ldots,N \tag{3.7}$$

† The $\hat{S}_n^r(x)$ recurrence relation becomes with (2.11*b*), (2.5) and (2.6)

$$\hat{S}_{n+1}^{(r)}(x) - 2(1 - r^{h(n+2)}x)\hat{S}_n^{(r)}(x) + \hat{S}_{n-1}^{(r)}(x) = 0$$
$$\hat{S}_{-1}^{(r)} = 0 \qquad \hat{S}_0^{(r)} = 1.$$

and the subsidiary condition (assuming $q_1 \neq 0$)

$$[Y(N)-1]\left(S_{N-1}^{(r)} - \hat{S}_{N-2}^{(r)}\right) = S_{N-2}^{(r)} - \hat{S}_{N-3}^{(r)} \tag{3.8}$$

results from the two possible ways to express q_{N-1} in terms of q_1†.

With the help of recursion relations (2.11) this condition reads

$$B_N^{(r)}(x) \equiv S_N^{(r)}(x) - S_{N-1}^{(r)}(x) - \left[\hat{S}_{N-1}^{(r)}(x) - \hat{S}_{N-2}^{(r)}(x)\right] = 0\,. \tag{3.8'}$$

This polynomial equation of order N has a trivial solution $x = 0$ because $\hat{S}_N^{(r)}(0) = S_N^{(r)}(0) = N + 1$. It describes the translational mode of the open N-chain with a uniform displacement $q_n = q_1 \neq 0,\ \ n = 1, 2, \ldots, N$. We are interested in the non-trivial solutions of (3.8′), the internal vibrational modes. If one defines

$$B_N^{(r)}(x) =: -2x\ P_{N-1}^{(r)}(x) \tag{3.9}$$

these internal $N - 1$ modes are given by the zeros of $P_{N-1}^{(r)}(x)$. Only for $r = 1$ do the $P_n^{(r)}(x)$ constitute a system of orthogonal polynomials‡. The first few of these polynomials are listed in table 2.

Table 2. $P_n^{(r)}(x)$, $P_{-1}^{(r)} = 0$, $P_0^{(r)} = r$.

n	$P_n^{(r)}(x)$
1	$-2rx + r + 1$
2	$4r^2x^2 - 4r(1+r)x + 2r + 1$
3	$-8r^3x^3 + 8r^2(2+r)x^2 - 4r(2+3r)x + 1 + 3r$
4	$16r^3x^4 - 8r^2(3r+5)x^3 + 4r(2r^2+12r+7)x^2$ $-2(3r+1)(2r+3)x + 3r + 2$
5	$2[-16r^4x^5 + 16r^3(2r+3)x^4 - 16r^2(r^2+5r+3)x^3$ $+4r(8r^2+15r+5)x^2 - (4r+1)(4r+3)x + 2r + 1]$
6	$64r^4x^6 - 32r^3(5r+7)x^5 + 16r^2(8r^2+30r+17)x^4$ $-8r(4r^3+40r^2+59r+17)x^3 + 8(8r^3+30r^2+22r+3)x^2$ $-4(8r^2+15r+5)x + 3 + 4r$
...	...

† The coefficient of x^n in $\hat{S}_n^{(r)}(x)$ is $(-2)^n r^{\hat{z}(n)}$, where $\hat{z}(n) \equiv z(n+1) - 1$. The monic $\bar{\hat{S}}_n^{(r)}$ polynomials satisfy (3.4) with $c_n^{(r)} \to \hat{c}_n^{(r)} = r^{-h(n+1)}$, $\lambda_n^{(r)} \to \hat{\lambda}_n^{(r)} = \frac{1}{4} r^{-1-k(n)} > 0$. Therefore, $\hat{s}_n^{(r)}(x) := r^{h(n+2)/2}\hat{S}_n^{(r)}(x)$ defines a set of orthonormal polynomials.

‡ For $n = 0, 1, \ldots$ one has

$$P_{n+1}^{(r)}(x) = 2(1 - r^{h(n+2)}x)P_n^{(r)}(x) - P_{n-1}^{(r)}(x)$$
$$+ (r-1)\mu(n+2)[S_n^{(r)}(x) - \hat{S}_{n-1}^{(r)}(x)] \qquad P_{-1}^{(r)} = 0 \qquad P_0^{(r)} = r$$

with $\mu(n+2) := h(n+2) - h(n+1)$.

For periodic chains with an *N-particle Fibonacci unit cell* (type (c)) the band structure is determined by the trace of the unit cell's transfer matrix M_N (see e.g. [15], chapter 3.4). M_N satisfies $M_N^2 - (\mathrm{tr}\, M_N)M_N + 1 = 0$. With (2.13) its eigenvalues are therefore ($\lambda_+\lambda_- = 1$)

$$\lambda_\pm = T_N \pm \sqrt{T_N^2 - 1} \tag{3.10}$$

with $T_N \equiv T_N(Y/2, y/2)$ and Y, y given in (2.6). Vibrations occur for those x-intervals (bands) satisfying $|T_N^{(r)}(x)| < 1$. In this case $\lambda \equiv \lambda_+ = \bar{\lambda}_- = \exp \mathrm{i}\beta$, with real $\beta^{(N,r)}(x) = \cos^{-1} T_N^{(r)}(x)$ which is the integrated spectral function. The differential spectral density (per particle) is then

$$G_N^{(r)}(\hat{x}) = \left|\frac{\mathrm{d}}{\mathrm{d}x} T_N^{(r)}(X(N,r)\hat{x})\right| X(N,r)/N\pi\sqrt{1 - [T_N^{(r)}(X(N,r)\hat{x})]^2} \tag{3.11}$$

for $\hat{x} \equiv x/X(N,r)$ out of any of the N bands whose maximal x value is $X(N,r)$. For $r = 1$ one recovers the (N-independent) spectral density of a monoatomic chain $G_N^{(1)}(\hat{x}) = 1/\pi\sqrt{\hat{x}(1-\hat{x})}$. This is due to the identity $(\mathrm{d}/\mathrm{d}x)T_n^{(1)}(x) = -nS_{n-1}^{(1)}(x)$. The band gaps are found from the condition $|T_N^{(r)}(x)| > 1$, and the boundaries of the N bands are the solutions of

$$T_N^{(r)}(x) \equiv T_N(1 - rx, 1 - x) = \pm 1\,. \tag{3.12}$$

The explicit form of these polynomials in terms of certain combinatorial numbers, defined in [10] can be given. We shall, however, not quote this result here. (2.13) shows that the leading coefficient of $T_n^{(r)}$ is $(-1)^n 2^{n-1} r^{z(n)}$ for $n = 1, 2, \ldots$. The first few polynomials are listed in table 3. Only for $r = 1$ do they form a set of orthogonal polynomials†.

The $T_n^{(1)}(x) = T_n(1-x)$ are orthonormal in the interval [0, 2] with weight function $w(x) = 2/\pi\sqrt{x(2-x)}$ for $n \in \mathbb{N}$‡.

We remark that in the literature on quasi-periodic problems of the Fibonacci type one usually considers the mth rational approximation to the golden mean, $(\varphi)_m := F_{m+1}/F_m$, $m = 1, 2, \ldots$, with the Fibonacci numbers F_m. In this case the binary sequence

$$h^{(m)}(n) := \lfloor (n+1)F_m/F_{m+1} \rfloor - \lfloor nF_m/F_{m+1} \rfloor \tag{3.13}$$

† Namely

$$T_{n+1}^{(r)}(x) = 2(1 - r^{h(n+1)}x)T_n^{(r)}(x) - T_{n-1}^{(r)}(x) + (1-r)x\mu(n+1)\hat{S}_{n-2}^{(r)}(x)$$
$$n = 1, 2, \ldots$$
$$T_0^{(r)}(x) = 1 \qquad T_1^{(r)}(x) = 1 - rx\,.$$

‡ For $N = 2$ (3.11) reproduces the spectral density of the AB-chain (see e.g. [15], figure 1.6). For $N = 3$ a comparison with figure 1 of [16] has been made. There the abscissa label should read $(\omega/\omega_{L_2})^2$ which is $x/2$ in our notation for the $AAB \simeq ABA$ chain with $r = \frac{1}{2}$. We have also checked figures 2–5 of this reference.

Table 3. $T_n^{(r)}(x)$.

n	$T_n^{(r)}(x)$
0	1
1	$-rx+1$
2	$2rx^2-2(1+r)x+1$
3	$-4r^2x^3+4r(r+2)x^2-3(1+2r)x+1$
4	$8r^3x^4-8r^2(3+r)x^3+20r(r+1)x^2-4(1+3r)x+1$
5	$-16r^3x^5+16r^2(3+2r)x^4-4r(4r^2+20r+11)x^3$ $+4(8r^2+14r+3)x^2-5(3r+2)x+1$
6	$32r^4x^6-64r^3(2+r)x^5+16r^2(2r^2+14r+11)x^4$ $-32r(3r^2+8r+3)x^3+2(44r^2+52r+9)x^2-12(2r+1)x+1$
...	...

becomes periodic with period F_{m+1}. The unit cell's transfer matrix is then $M^{(m)}_{Fm+1}$ defined like in (2.8) but with $h(n)$ in (2.5) replaced by $h^{(m)}(n)$. These matrices differ, in general, from M_{Fm+1}, but one can prove the following:

$$T^{(m)}_{F_{m+1}} = T_{F_{m+1}} \qquad m = 1, 2, \dots . \tag{3.14}$$

This result follows immediately from

$$\{h^{(m)}(n)\}_{n=1}^{Fm+1} \bigcirc \{h(n)\}_{n=1}^{Fm+1} \tag{3.15}$$

where $\bigcirc$ means cyclic equivalence. For example, if $m = 3$ one has $\{1, 1, 0\} \bigcirc \{1, 0, 1\}$, and for $m = 1, 2, 4$ both sequences are identical. In fact, the identity holds for all even m. For odd $m \neq 1$ a cyclic rearrangement is necessary. The proof of (3.15) will not be reproduced here. It is found in the preprint version of this work. Due to the identities (3.14) the band structure of type-(c) Fibonacci chains coincides with the one of periodic chains based on the sequence $h^{(m)}(n)$ with $n \in \mathbf{Z}$ and $m \in \mathbf{N}$ if one specializes $N = F_{m+1}$.

4. Identities from quasiperiodicity

One of the distinguished properties of the binary Fibonacci sequence $h(n)$ (2.2) is (see e.g. [3a])

$$\forall k \geqslant 4 : h(n + F_k) = h(n) \qquad 1 \leqslant n \leqslant F_k . \tag{4.1}$$

The same quasiperiodicity law is obeyed by the $Y(n)$ sequence defined in (2.5). An immediate consequence of (4.1) is the matrix identity

$$\forall k \geqslant 4 : M_{2F_k} = (M_{F_k})^2 \tag{4.2}$$

where M_n was defined in (2.8). This, together with the det $M_n = 1$ condition and the T_n polynomials (2.13), is equivalent to the following four identities, valid for all

$k = 4, 5, \dots$:

$$S_{2F_k} = 2T_{F_k} S_{F_k} - 1 \tag{4.3a}$$

$$\hat{S}_{2F_k-2} = 2T_{F_k} \hat{S}_{F_k-2} + 1 \tag{4.3b}$$

$$\hat{S}_{2F_k-1} = 2T_{F_k} \hat{S}_{F_k-1} \tag{4.3c}$$

$$S_{2F_k-1} = 2T_{F_k} S_{F_k-1} \tag{4.3d}$$

where the arguments of the S and $\hat{S}$ polynomials are Y,y and those of the T polynomials are $Y/2$, $y/2$. The last two identities can be used to factorize certain S_n and $\hat{S}_n$ polynomials. (4.3*b*, *d*) are also valid for $k = 2, 3$. Quasiperiodicity (4.1) also implies

$$\forall k \geqslant 4 \qquad n = 1, 2, \dots, F_k : S_{n+F_k} = Y(n) S_{n+F_k-1} - S_{n+F_k-2} \tag{4.4a}$$

$$\forall k \geqslant 4 \qquad n = 0, 1, \dots, F_k - 1 : \hat{S}_{n+F_k} = Y(n+1) \hat{S}_{n+F_k-1} - \hat{S}_{n+F_k-2} \,. \tag{4.4b}$$

Putting $n = F_k$ in (4.4*a*), using (4.3*a*) and (4.3*d*), yields for $k \geqslant 4$

$$S_{2F_k-2} = T_{F_k} S_{F_k-2} + 1 \,. \tag{4.5}$$

Putting $n = F_k - 1$ in (4.4*a*) produces for $k \geqslant 4$

$$S_{2F_k-3} = 2T_{F_k} S_{F_k-3} + Y(F_k - 1) \,. \tag{4.6}$$

This can be continued for $n = F_k - j$, $j = 0, 1, \dots, F_k - 1$. One finds for $k \geqslant 4$

$$S_{2F_k-j} = 2T_{F_k} S_{F_k-j} + S^{\{k\}}_{j-2} \tag{4.7}$$

where the 'retro'-polynomials $S^{\{k\}}_n$ satisfy

$$\begin{aligned} &S^{\{k\}}_n = Y(F_k - n) S^{\{k\}}_{n-1} - S^{\{k\}}_{n-2} \qquad n = 1, 2, \dots \\ &S^{\{k\}}_{-1} = 0 \qquad S^{\{k\}}_0 = 1 \end{aligned} \tag{4.8}$$

which shows that they are, for each $k \geqslant 4$, also two-variable generalizations of Chebyshev's S_n polynomials. For (4.7) one only needs $S^{\{k\}}_n$ for $n = 1, 2, \dots, F_k - 3$. We give an example for $k = 5$, $S^{\{5\}}_1 = Y = S_1$, $S^{\{5\}}_2 = Y^2 - 1$. Thus

$$\begin{aligned} S_{10} &= 2T_5\, S_5 - 1 \\ S_9 &= 2T_5\, S_4 \\ S_8 &= 2T_5\, S_3 + 1 \\ S_7 &= 2T_5\, S_2 + S_1 \\ S_6 &= 2T_5\, S_1 + (Y^2 - 1) \,. \end{aligned} \tag{4.9}$$

Similarly, one derives from (4.4*b*), together with the inputs (4.3*b*) and (4.3*c*), the following family of identities:

$$k \geqslant 4 \qquad j = 1,2,\ldots,F_k : \hat{S}_{2F_k-j} = 2T_{F_k}\hat{S}_{F_k-j} + \hat{S}_{j-2}^{\{k\}} \tag{4.10}$$

with the 'retro' $\hat{S}_n^{\{k\}}$ polynomials defined by

$$\begin{aligned} &\hat{S}_n^{\{k\}} = Y(F_k - n + 1)\hat{S}_{n-1}^{\{k\}} - \hat{S}_{n-2}^{\{k\}} \\ &\hat{S}_{-1}^{\{k\}} = 0 \qquad \hat{S}_0^{\{k\}} = 1\,. \end{aligned} \tag{4.11}$$

Only the ones with $n = 1,2,\ldots,F_k - 2$ are needed in (4.10) for given $k \geqslant 4$. (4.11) defines more two-variable generalized $S_n(y)$ polynomials.

From (4.7) and (4.10) the following identities among the T_ns result:

$$k \geqslant 4 \qquad j = 0,1,\ldots,F_k - 2 : 2T_{F_k}2T_{(F_k-j)} = 2(T_{2F_k-j} + T_j) - (Y - y)R_{j-1}^{\{k\}} \tag{4.12}$$

with the 'excess'-polynomials

$$R_{j-1}^{\{k\}} := \hat{s}_{j-1}^{\{k\}} + s_{j-3}^{\{k\}} \tag{4.13}$$

defined by

One should remember that the arguments of all polynomials are Y, y except for the T_ns whose arguments are $Y/2$, $y/2$. For vanishing excess-polynomials R the identities (4.12) are of the type

$$2T_n\ 2T_m = 2(T_{n+m} + T_{|n-m|}) \tag{4.15}$$

well known for the one-variable T_n polynomials (trigonometric identities). This is, for instance, the case for $j = 0$, when $R_{-1}^{\{k\}} = 0$ for all $k \geqslant 4$. Thus

$$T_{2F_k} + 1 = 2(T_{F_k})^2 \tag{4.16}$$

which can be rewritten as

$$T_{2F_k} - 1 = 2(T_{F_k} - 1)(T_{F_k} + 1)\,. \tag{4.16$'$}$$

These two equations show that $N = 2F_k$ chains of type (c) for $k = 4,5,\ldots$ have a band degeneracy. Indeed, the F_k zeros of T_{F_k} are double (-1) values of T_{2F_k}. Thus F_k gaps shrink to a point, and the $2F_k$ values $(+1)$ of T_{2F_k} coincide with the edges of the F_k bands of the $N = F_k$ chain of type (c). Therefore the band structure for $N = 6,10,16,\ldots$ chains is the same as the one for $N = 3,5,8,\ldots$ chains, respectively. In each case the unit cell is doubled, describing the same chain.

For $j = 1$ one has

$$R_0^{\{k\}} = \hat{s}_0^{\{k\}} = \begin{cases} 0 & \text{for } k = 2i \qquad i \geqslant 2 \\ 1 & \text{for } k = 2i+1 \qquad i \geqslant 2 \end{cases}$$

due to the fact that $h(F_{2i})=1$, $h(F_{2i+1})=0$. Therefore,

$$i=1,2,\dots\ :2T_{F_{2i}}\ 2T_{F_{2i}-1}=2(T_{2F_{2i}-1}+T_1)\,. \tag{4.17}$$

For $i=1$ this is trivial. For odd $k\geqslant 4$ there is an excess of $-(Y-y)$.

For $j=2$ one finds

$$k\geqslant 4:2T_{F_k}\ 2T_{F_k-2}=2(T_{2F_k-2}+T_2) \tag{4.18}$$

due to the fact that F_k can never be the bigger member of an A-pair (see [10] for the definition).

The analysis of three consecutive $\{h(n)\}$ members, the last one being $h(F_k)$, shows that also for $j=3$ no excess polynomial is present, i.e.

$$k\geqslant 4\ :\ 2T_{F_k}2T_{F_k-3}=2(T_{2F_k-3}+T_3)\,. \tag{4.19}$$

For higher j the analysis becomes more involved. All the above derived identities hold for all Y,y, therefore especially for chains with substitution (2.6).

Identities for the open $N+1$ chain polynomials $P_N^{(r)}$ follow from the results (4.7) and (4.10). One has

$$k\geqslant 4,\ j=0,1,\dots,F_k-2\ :\ P^{(r)}_{2F_k-j-1}(x)=2T^{(r)}_{F_k}(x)\ P^{(r)}_{F_k-j-1}(x)+p^{(r)\{k\}}_{j-1}(x) \tag{4.20}$$

with the definition

$$(-2x)p^{(r)\{k\}}_{j-1}(x):=(S^{\{k\}}_{j-2}-S^{\{k\}}_{j-1}-\hat{S}^{\{k\}}_{j-1}+\hat{S}^{\{k\}}_{j})\| \tag{4.21}$$

where $\|$ signals substitution of Y,y according to (2.6). For $j=0$ one finds $p^{(r)\{k\}}_{-1}=0$, which shows that the eigenfrequencies of the $2F_k-1$ internal vibrations of the open $N=2F_k$ chain are for $k=4,5,\dots$ given by those of the $N=F_k$ chain and the zeros of $T^{(r)}_{F_k}$.

5. Identities from logotomy

In the seminal works [1a, b] the identities

$$k\geqslant 5\ :\ T_{F_k}=2T_{F_{(k-1)}}\ T_{F_{(k-2)}}-T_{F_{(k-3)}} \tag{5.1}$$

were used as recursion relations for the Fibonacci-numbered trace polynomials. This is a special case of a more general class of identities which can be inferred from the basic formulae valid for any $\mathrm{SL}(2,\boldsymbol{R})$ matrices A,P,Q (cf [3a]):

$$\operatorname{tr}A=\operatorname{tr}A^{-1} \tag{5.2a}$$

$$\tfrac{1}{2}\operatorname{tr}(PQ)+\tfrac{1}{2}\operatorname{tr}(PQ^{-1})=2\left(\tfrac{1}{2}\operatorname{tr}\ P\right)\left(\tfrac{1}{2}\operatorname{tr}\ Q\right). \tag{5.2b}$$

In fact, (5.2*a*) follows from (5.2*b*) by putting $P=\mathbf{1}$. Observe the symmetry $P\leftrightarrow Q$. Consider the matrix-'word' M_n defined in (2.8) for $n\geqslant 1$ over the two matrix 'alphabet' R_0 and R_1, given in (2.7), and put $M_0=\mathbf{1}$. The word M_{n+m} is cut into two pieces $M_{n+m}=W_nM_m$ or $M_{n+m}=W_mM_n$, where W_n is a word of length n. The identity (4.15), which reduces to a simple trigonometric identity in the one-variable case $Y=y$, also remains valid in the two-variable case whenever one of the following conditions is satisfied:

Condition 1.

$$M_{n+m} = W_n M_m \qquad n \geqslant m \geqslant 0$$
$$W_n \bigcirc M_n \tag{5.3a}$$
$$W_n (M_m)^{-1} \bigcirc M_{n-m}$$

Condition 2.

$$M_{n+m} = W_m M_n \qquad n \geqslant m \geqslant 0$$
$$W_m \bigcirc M_m \tag{5.3b}$$
$$M_n (W_m)^{-1} \bigcirc M_{n-m} \, .$$

The symbol $\bigcirc$ stands for cyclic equivalence. Note that $(M_m)^{-1}$ or $(W_m)^{-1}$ are no words in the sense defined above. In order that the last conditions in (5.3*a*, *b*) be satisfied it is necessary that all R_0^{-1} and R_1^{-1} matrices are eaten up by corresponding R_0 and R_1 matrices. The proof is a simple consequence of identity (5.2b). For the first condition put $P = W_n$, $Q = M_m$, and for the second one $P = W_m$, $Q = M_n$ with $\mathrm{tr}\ PQ^{-1} = \mathrm{tr}\ QP^{-1}$. We give three examples. *First* consider the case $m = n$. Both conditions need $W_n = M_n$. Therefore, (4.15) holds whenever $M_{2n} = (M_n)^2$. From the quasiperiodicity of the $\{h(n)\}$ sequence this happens exactly for $n = F_k$ for $k \geqslant 4$. Thus we recover identity (4.16); *secondly* consider $M_{F_k} = M_{F_{k-2}} M_{F_{k-1}}$ which holds for $k = 2$, and $\geqslant 4$, and check (5.3*b*):

$$M_{F_{k-1}} (M_{F_{k-2}})^{-1} = M_{F_{k-3}} M_{F_{k-2}} (M_{F_{k-2}})^{-1} = M_{F_{k-3}} = M_{(F_{k-1} - F_{k-2})}$$

for $k = 3$ or $\geqslant 5$. This is how the original identities (5.1) are proved. As a *third example* take $n = 6$ and $m = 2$ and check condition (5.3*b*). $M_8 = W_2 M_6$ and $W_2 = R_1 R_0 \bigcirc R_0 R_1 = M_2$; $M_6 (W_2)^{-1} = R_1 R_0 R_1^2 R_0 R_1 R_0^{-1} R_1^{-1} \bigcirc R_1^2 R_0 R_1 = M_4$, and therefore

$$T_6 T_2 - \tfrac{1}{2}(T_8 + T_4) = 0 \tag{5.4}$$

which is not covered by the identities given in the last section. This is, in fact, a special case of

$$2T_n\ T_2 - (T_{n+2} + T_{n-2}) = 0 \tag{5.5}$$

valid if $n + 1$ or n is of the form $B(B(p)) + 1$ for some $p \in \mathbb{N}$, where the Wythoff sequence is defined by $B(n) = \lfloor n\varphi^2 \rfloor$ (see e.g. [10]). The first values are $n = 5, 6, 13, 14, 18, 19, \ldots$.

We close this section with the quantity which was used in the original works [1a, b] as an 'invariant' under recursion formula (5.1). We use the form given in [3a]:

$$\begin{aligned}
\lambda^2 &\equiv \tfrac{1}{4} \mathrm{tr}\, M_{F_{n+1}} M_{F_n} M_{F_{n+1}}^{-1} M_{F_n}^{-1} - \tfrac{1}{2} \\
&= \tfrac{1}{8} \mathrm{tr}\, [M_{F_n}, M_{F_{n+1}}]^2 = \tfrac{1}{4} \mathrm{tr}(M_{F_n} [M_{F_{n+1}}, M_{F_{n+2}}]) \\
&= T_{F_{n+2}}^2 + T_{F_{n+1}}^2 + T_{F_n}^2 - 2T_{F_{n+2}} T_{F_{n+1}} T_{F_n} = \tfrac{1}{4}(Y - y)^2 \, .
\end{aligned} \tag{5.6}$$

This shows the n-independence of λ^2 for all $n \geqslant 2$. (5.2*b*) and the composition law $M_{F_{n+1}} = M_{F_{n-1}} M_{F_n}$ for $n \geqslant 3$ were used. (5.1) and the quasiperiodicity identity (4.16) allows one to rewrite λ^2 as

$$\lambda^2 = -T_{F_{n+3}}\ T_{F_n} + \tfrac{1}{2}(T_{2F_{n+2}} + T_{2F_{n+1}}) = \tfrac{1}{4}(Y - y)^2 \tag{5.7}$$

for $n \geqslant 3$ which can also be obtained *via* (4.12) for $k = n + 3$, $j = 2F_{n+1}$.

6. Generating functions for S_n and $\hat{S}_n$ polynomials; $S_n(Y,y)$ and $\hat{S}_n(Y,y)$ in terms of $\{S_k\}$

We first define the generating function for the $S_n(Y,y)$ polynomials

$$G(z;Y,y) := \sum_{n=0}^{\infty} S_n(Y,y) z^n . \tag{6.1}$$

The recurrence relation (2.11a) yields

$$G(z;Y,y) = \{1 + (Y-y) z G_{(A-1)}(z;Y,y)\}/(1 - yz + z^2) \tag{6.2}$$

where the generating function for a subsequence of the S_ns is introduced, namely

$$G_{(A-1)}(z;Y,y) := \sum_{n=0}^{\infty} h(n+1) S_n(Y,y) z^n = \sum_{l=1}^{\infty} S_{A(l)-1}(Y,y) z^{A(l)-1} . \tag{6.3}$$

In the last step we used a property of $\{h(n)\}$, namely $h(n) = 1$ iff $n = A(l)$ for $l \in \mathbf{N}$, where A-numbers are defined by $A(l) := \lfloor l\varphi \rfloor$ (see [10] for details on Wythoff numbers $A(l)$ and references). Therefore, $G_{(A-1)}$ generates S_k for $k = 0, 2, 3, 5, 7, 8, \ldots$. As a check we put in (6.2) $Y = y$ to obtain

$$G(z;y) = (1 - yz + z^2)^{-1} = \sum_{n=0}^{\infty} S_n(y) z^n \tag{6.4}$$

the well known generating function for Chebyshev's $S_n(y)$ polynomials. Due to identities for Wythoff sequences (see e.g. [10], equation (2.5)) one can also write

$$G_{(A-1)}(z;Y,y) = G_B(z;Y,y) + G_{AB}(z;Y,y) \tag{6.5}$$

where G_B generates all S_k with $k = B(m) := m + A(m)$ for $m \in \mathbf{N}_0$, i.e. $k = 0, 2, 5, 7, \ldots$, and G_{AB} generates all S_k with $k = A(B(m))$ for $m \in \mathbf{N}$, i.e. $k = 3, 8, 11, 16, \ldots$. Indeed, $A(l) - 1$ is either of the form $A(A(m)+1) - 1 = B(m)$ with $m \in \mathbf{N}_0$, or of the form $A(B(m)+1) - 1 = AB(m)$ with $m \in \mathbf{N}$. This holds because the natural numbers decompose into two disjoint and exhaustive sets, the A- and B-numbers. Because $G = G_A + G_B = G_{AA} + G_{AB} + G_B$ where we include, by convention, 0 as a B-number, (6.5) can be written as $G_{(A-1)} = G - G_{AA}$. Due to $G_{AA} = G_{(B-1)}$ one may then replace (6.2) by

$$G(z;Y,y) = \{1 - (Y-y) z G_{(B-1)}(z;Y,y)\} G(z;Y) . \tag{6.5'}$$

In a similar way one derives from (2.11b) the result

$$\hat{G}(z;Y,y) = \{1 + (Y-y) z \hat{G}_{(A-2)}(z;Y,y)\} G(z;y) \tag{6.6}$$

for the generating functions

$$\hat{G}(z;Y,y) := \sum_{n=0}^{\infty} \hat{S}_n(Y,y) z^n \tag{6.7}$$

$$\hat{G}_{(A-2)}(z;Y,y) := \sum_{n=0}^{\infty} h(n+2) \hat{S}_n(Y,y) z^n = \sum_{l=2}^{\infty} \hat{S}_{A(l)-2}(Y,y) z^{A(l)-2} . \tag{6.8}$$

We continue with formulae which express the two-variable Chebyshev polynomials $S_n(Y, y)$ and $\hat{S}_n(Y, y)$ in terms of ordinary Chebyshev polynomials $S_k(y)$ and powers of $Y - y$. They can be derived from (6.2) (respectively (6.6)). We skip all details and only quote the result which involves $z(n)$ which counts the number of (positive) A-numbers less or equal to n. It is given by (3.3) as $z(n) = A(n+1) - (n+1)$.

For $n = (0,)\ 1, 2, \ldots$ one finds

$$S_n(Y, y) = S_n(y) + \sum_{k=1}^{z(n)} (Y - y)^k s_{n,k}(y) \tag{6.9a}$$

$$s_{n,k}(y) \equiv \sum_{l_1=k}^{z(n)} S_{n-A(l_1)}(y) \sum_{l_2=k-1\geqslant 1}^{l_1-1} S_{A(l_1)-A(l_2)-1}(y) \sum_{l_3=k-2\geqslant 1}^{l_2-1} S_{A(l_2)-A(l_3)-1}(y) \cdots$$
$$\times \cdots \sum_{l_k=1}^{l_{k-1}-1} S_{A(l_{k-1})-A(l_k)-1}(y) S_{A(l_k)-1}(y) . \tag{6.9b}$$

For $k = 1$ one has to put $l_0 - 1 = z(n)$ and $A(l_0) = n + 1$ in $s_{n,1}(y)$. The formula for $\hat{S}_n(Y, y)$ is

$$\hat{S}_n(Y, y) = S_n(y) + \sum_{k=1}^{z(n+1)-1} (Y - y)^k \hat{s}_{n,k}(y) \tag{6.10a}$$

$$\hat{s}_{n,k}(y) \equiv \sum_{l_0=k+1}^{z(n+1)} S_{n+1-A(l_0)}(y) \left(\prod_{j=1}^{k-1} \sum_{l_j=k-j+1\geqslant 2}^{l_{j-1}-1} S_{A(l_{j-1})-1-A(l_j)}(y) \right)$$
$$\times S_{A(l_{k-1})-2}(y) . \tag{6.10b}$$

For $k = 1$ the product should be replaced by 1. For $n = 0, 1$ only the first term of (6.10a) is present. We next quote the results for the T_n polynomials (2.13). Their generating function is related to those of the S and $\hat{S}$ polynomials:

$$G_T(z; Y, y) := \sum_{n=0}^{\infty} T_n\left(\frac{Y}{2}, \frac{y}{2}\right) z^n = \frac{1}{2}[1 + G(z; Y, y) - z^2 \hat{G}(z; Y, y)] . \tag{6.11}$$

Using (6.10) and (6.11) one finds

$$T_n\left(\frac{Y}{2}, \frac{y}{2}\right) = T_n\left(\frac{y}{2}\right) + \sum_{m=1}^{z(n)} (Y - y)^m t_{n,m}(y) \tag{6.12a}$$

$$t_{n,m}(y) \equiv \tfrac{1}{2}[s_{n,m}(y) - \hat{s}_{n-2,m}(y)] . \tag{6.12b}$$

In the appendix the results for $n = 0(1)6$ are listed.

This polynomial expansion in powers of $Y - y$ has an interesting application in the case of Fibonacci chains of type (c). For small relative mass difference $\mu \equiv 1 - M/m$ one can compute the $2N$ band boundaries in lowest non-trivial order. Details will be published elsewhere. We quote the result which is given in terms of the quantities $f(N,k)$, $k=1,2,\dots,N-1$ defined by

$$f(N,k) := \sum_{l=2}^{z(N)} \sin^2\left((A(l)-1)\frac{\pi k}{N}\right) + h(N) \sum_{l=2}^{z(N)-1} \sin^2\left(A(l)\frac{\pi k}{N}\right)$$

$$+ \sum_{l=3}^{z(N-1)} \sum_{m=2}^{l-1} \sin^2\left([A(l)-A(m)]\frac{\pi k}{N}\right). \tag{6.13}$$

and

$$W(N,k) \equiv_+ \sqrt{1-4f(N,k)/z^2(N)}. \tag{6.14}$$

Up to first order (indicated by the tilde) in $\mu \equiv 1-r$, the band boundaries of periodic chains with an N-particle unit cell are are given by

$$\tilde{\eta}_{k,\pm}^{(N,r)} = \xi_k^{(N-1)}\left(1+\mu\ \frac{z(N)}{N}[1 \pm W(N,k)]\right). \tag{6.15}$$

for $k=1,2,\dots,N-1$, $\eta_0^{(N,r)}=0$ and the maximal band value

$$\tilde{\eta}_N^{(N,r)} = 2\left(1+\mu\ \frac{z(N)}{N}\right). \tag{6.16}$$

ξ_k^{N-1} are the zeros of $S_{N-1}[2(1-x)]$ given by (3.6).

Observe that $f(N,k)$ obeys

$$f(N,l) = f(N,N-l) \qquad l=1,2,\dots,\left\lfloor\frac{N}{2}\right\rfloor. \tag{6.17}$$

Due to this symmetry and the fact that $\xi_l^{(N-1)} + \xi_{N-l}^{(N-1)} = 2$ for the given values of l, one finds for the total bandwidth of periodic chains with N-particle unit cell of the Fibonacci type (in units of $x=\omega^2/2\omega_0^2$ and first order in $\mu \equiv 1-r$)

$N=2m \qquad m \in \mathbf{N}$:

$$\tilde{\Delta}_{2m}^{(\mu)} = 2\left\{1-\frac{z(2m)}{2m}\left[|\mu|\left(2\sum_{k=1}^{m} W(2m,k) - W(2m,m)\right) - \mu\right]\right\} \tag{6.18a}$$

$N=2m+1 \qquad m \in \mathbf{N}$:

$$\tilde{\Delta}_{2m+1}^{(\mu)} = 2\left[1-\frac{z(2m+1)}{2m+1}\left(2|\mu|\sum_{k=1}^{m} W(2m+1,k) - \mu\right)\right]. \tag{6.18b}$$

7. Concluding remarks

(i) The spectral measure for the orthogonal polynomials $S_n^{(r)}(x)$ and the associated ones $\hat{S}_n^{(r)}(x)$ can, for fixed r, in principle, be found *via* Stieltjes' inversion formula (cf [11] and [17]) from the continued S-fraction related to the recurrence relation. Work along these lines is in progress.

(ii) The limit $N \to \infty$ for the various chains can be studied, and it is expected to recover the rigorous results for the Fibonacci Hamiltonian mentioned in the introduction.

In the application for chains with small relative mass difference the first two terms of $f(N,k)$ given by (6.13) do not contribute to $W(N,k)$ of (6.14) for $k = 1,2,\ldots,N-1$ in this limit. For the last term, the double sum $f_{\mathrm{ds}}(N,k)$, it is difficult to find a sensible estimate.

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Note added in proof. One of the referees pointed out reference [18]. There one can find an excellent summary of the method of orthogonal polynomials in connection with second-order difference equations with periodic coefficients. In the general discussion one can identify the polynomials α_n and β_n/t_0^2 with our monic $\tilde{S}_n$ and $\tilde{\hat{S}}_{n-1}$. The polynomials Θ_N are not directly related to our T_N of (2.13). We stress that the T_N polynomials (not the Θ_N) are relevant for the chain problem. Our formula (3.11) for the differential spectral density is similiar to equation (2.9) of [18]. The measure for the N-periodic orthogonal polynomials $\{S_n^{(r)}\}$ can be computed along the lines leading to (5.10) of [18]. None of the examples considered there corresponds to the Fibonacci chains.

Appendix. Some $T_n(Y/2, y/2)$ formulae

Equation (6.12) with (6.9*b*) and (6.10*b*) yields ($S_0(y) \equiv 1$)

$n = 0, z(0) = 0:$

$$T_0\left(\frac{Y}{2},\frac{y}{2}\right) = T_0\left(\frac{y}{2}\right) = 1 \tag{A1}$$

$n = 1, z(1) = 1:$

$$T_1\left(\frac{Y}{2},\frac{y}{2}\right) = T_1\left(\frac{y}{2}\right) + \frac{1}{2}(Y-y) = \frac{Y}{2} \tag{A2}$$

$n = 2, z(2) = 1:$

$$T_2\left(\frac{Y}{2},\frac{y}{2}\right) = T_2\left(\frac{y}{2}\right) + \frac{1}{2}(Y-y)S_1(y) = \frac{1}{2}Yy - 1 \tag{A3}$$

$n = 3, z(3) = 2:$

$$T_3\left(\frac{Y}{2}, \frac{y}{2}\right) = T_3\left(\frac{y}{2}\right) + (Y-y)S_2(y) + \frac{1}{2}(Y-y)^2 S_1(y) = \tfrac{1}{2}Y^2 y - \left(Y + \tfrac{1}{2}y\right) \tag{A4}$$

$n = 4, z(4) = 3:$

$$\begin{aligned} T_4\left(\frac{Y}{2}, \frac{y}{2}\right) &= T_4\left(\frac{y}{2}\right) + \frac{1}{2}(Y-y)[2S_3(y) + S_2(y)S_1(y) - S_1(y)] \\ &\quad + \tfrac{1}{2}(Y-y)^2[S_1^2(y) + 2S_2(y)] + \tfrac{1}{2}(Y-y)^3 S_1(y) \\ &= \tfrac{1}{2}Y^3 y - (Y^2 + Yy) + 1 \end{aligned} \tag{A5}$$

$n = 5, z(5) = 3:$

$$\begin{aligned} T_5\left(\frac{Y}{2}, \frac{y}{2}\right) &= T_5\left(\frac{y}{2}\right) + \frac{1}{2}(Y-y)(S_4 + S_2^2 + S_3 S_1 - S_1^2 - S_2) \\ &\quad + \tfrac{1}{2}(Y-y)^2\left(3S_2 S_1 - S_1\right) + \tfrac{1}{2}(Y-y)^3 S_1^2 \\ &= \tfrac{1}{2}Y^3 y^2 - \left(2Y^3 y + \tfrac{1}{2}Yy^2\right) + \left(\tfrac{3}{2}Y + y\right) \end{aligned} \tag{A6}$$

$n = 6, z(6) = 4:$

$$\begin{aligned} T_6\left(\frac{Y}{2}, \frac{y}{2}\right) &= T_6\left(\frac{y}{2}\right) + (Y-y)(S_5 + S_3 S_2 - S_2 S_1) \\ &\quad + \tfrac{1}{2}(Y-y)^2(2S_3 S_1 + 3S_2^2 + S_4 - S_1^2) \\ &\quad + 2(Y-y)^3 S_2 S_1 + \tfrac{1}{2}(Y-y)^4 S_1^2 \\ &= \tfrac{1}{2}Y^4 y^2 - (2Y^3 y + Y^2 y^2) + (2Yy + 2Y^2 + \tfrac{1}{2}y^2) - 1\,. \end{aligned} \tag{A7}$$

The missing S_n arguments are always y.

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