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The measure of the orthogonal polynomials related to Fibonacci chains: the periodic case*

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Abstract. The spectral measure for the two families of orthogonal polynomial systems related to periodic chains with N-particle elementary unit and nearest-neighbour harmonic interaction is computed using two different methods. The interest is in the orthogonal polynomials related to Fibonacci chains in the periodic approximation. The relation of the measure to appropriately defined Green's functions is established.

1. Introduction

Two associated families of orthogonal polynomial systems govern longitudinal time-stationary vibrations of linear chains with nearest-neighbour harmonic interaction (springs κ_n, masses m_n).

These polynomials are defined by three-term recurrence relations appropriate for orthogonal polynomials [1]. In the case of a mono-atomic chain (mass m_0) with uniform coupling (strength κ) they are deformations of Chebyshev's $S_n(2(1-x)) \equiv U_n(1-x)$ polynomials of the second kind. $x \equiv \omega^2/2\omega_0^2$, with $\omega_0^2 = \kappa/m_0$, is a normalized frequency-squared.

Our interest is in Fibonacci chains which have uniform coupling ($\kappa_n = \kappa$) and two masses (mass ratio $r \equiv m_1/m_0$) distributed at site number $n = 1, 2, \ldots$ in accordance with the binary sequence $1, 0, 1, 1, 0, 1, 0, \ldots$. This quasi-periodic sequence is generated by the Fibonacci substitution rule $1 \to 1, 0$ and $0 \to 1$. Such chains have been considered as simple models for special binary alloys [2]. The same structure is encountered in the problem of the phonon spectrum of a one-dimensional Fibonacci quasicrystal [3]. In this case the associated orthogonal polynomial systems are denoted by $\{S_n^{(r)}(x)\}$ and $\{\hat{S}_n^{(r)}(x)\}$ [4]. Up to now their spectral measures (or moment functionals) have not been determined. From rigorous results on the Fibonacci Hamiltonian in the context of the one-dimensional Schrödinger equation one expects that this measure is of the singular continuous type supported by a Cantor set of zero Lebesgue measure [5].

As an approximation to the quasiperiodic problem we identify in this work the spectral measure for *periodic* Fibonacci chains with an elementary unit consisting of N masses following the pattern of the first N entries of the above given binary sequence. The measures for general N-periodic orthogonal polynomial systems $\{\mathcal{S}_n(x)\}$ and $\{\hat{\mathcal{S}}_n(x)\}$, defined by

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three-term recursion relations with N-periodic coefficients, can be found using two different methods.

The first method employs the Bloch–Floquet solutions for these periodic chains and is based on the evaluation of a (judiciously chosen) complex contour integral. This is a special application of a general method available for orthogonal polynomials with asymptotically periodic coefficients in the recursion relation [6]. For our purpose only the strictly periodic case is of interest. With this restriction a similar procedure is discussed in [7]. The *second method* uses the fact that the continued fraction associated with orthogonal polynomials is the Stieltjes transform [8] of the spectral measure [1, 9]. For periodic systems this continued fraction can be determined as fixed-point of a certain Möbius transformation, and the measure is then obtained *via* the Perron–Stieltjes inversion formula (see e.g. [8, 10, 11]).

It turns out that the support of the absolutely continuous part of the measure (the weight function) is, for fixed N-periodic chain parameters κ_n, m_n, given by N, in general disjoint, x-intervals (bands). These are determined from the generalized Chebyshev polynomials of the first kind $\mathcal{T}_N(x)$, the so-called trace polynomials, by the condition $|\mathcal{T}_N(x)| \leqslant 1$. These bands coincide with the support of the spectral density (or density of states) of infinite chains. The weight function is, however, not given by the density of states. In general, a discrete point measure (Dirac δ-function measure) is also present. Each gap between the N intervals which support the continuous measure may contribute one point (which may lie on one of the band boundaries).

In the case of Fibonacci chains the limit $N \to \infty$ is supposed to correspond to the chains based on the quasi-periodic binary Fibonacci sequence. At present this limit is beyond our control.

The connection of the absolutely continuous part of the $\mathcal{S}$ and $\hat{\mathcal{S}}$ measures to the inverse of the imaginary part of the diagonal input Green's functions for the periodic problem is given in an extra section. The differential spectral density (or differential density of states) is recovered, as usual, from the imaginary part of the average over the elementary N-unit of the diagonal (or local) Green's functions.

In order to familiarize the reader with our notation we start with the dynamical equations for the displacements $q_n(t) = q_n\ \exp(\mathrm{i}\omega t)$ at site number n

$$q_{n+1} - 2\left(\frac{1+k_n}{2} - \frac{\omega_0^2}{\omega_n^2}x\right)q_n + k_n\ q_{n-1} = 0 \qquad n \in \mathbf{Z} \tag{1.1}$$

with $\omega_n^2 \equiv \kappa_n/m_n$, $k_n \equiv \kappa_{n-1}/\kappa_n$ and the normalized frequency-squared $x \equiv \omega^2/(2\omega_0^2)$. The spring between site number n and $n+1$ has strength κ_n. m_n is the mass at site number n.

This recursion relation can be rewritten in terms of standard associated polynomials with the help of the transfer matrix method. The displacements are then given by (cf [4] equations (2.8) and (2.10))

$$q_{n+1}(x) = \mathcal{S}_n(x)\ q_1(x) - \hat{\mathcal{S}}_{n-1}(x) \qquad q_0(x) \qquad n \in \mathbf{N} \tag{1.2}$$

with arbitrary inputs $q_1(x), q_0(x)$.* This expression is obtained from the transfer matrix M_n

$$\begin{pmatrix} q_{n+1} \\ q_n \end{pmatrix} = M_n \begin{pmatrix} q_1 \\ q_0 \end{pmatrix} \qquad M_n := R_n R_{n-1} \cdots R_1 \tag{1.3a}$$

$$R_n := \begin{pmatrix} Y(n) - k_n \\ 1 \quad\quad 0 \end{pmatrix} \qquad Y_n(x) :=\ 2\left(\frac{1+k_n}{2} - \frac{\omega_0^2}{\omega_n^2}x\right) \tag{1.3b}$$

* We do not consider negative site numbers here. See [4b] for the negative n case.

and the result

$$M_n = \begin{pmatrix} \mathcal{S}_n - \hat{\mathcal{S}}_{n-1} \\ \mathcal{S}_{n-1} - \hat{\mathcal{S}}_{n-2} \end{pmatrix} \tag{1.4}$$

where the polynomials $\mathcal{S}_n$ and $\hat{\mathcal{S}}_n$ are defined by the following three-term recurrence relation corresponding to $M_n = R_n M_{n-1}$ with input $M_1 = R_1$:

$$\mathcal{S}_n = Y_n(x)\mathcal{S}_{n-1} - k_n\mathcal{S}_{n-2} \qquad \mathcal{S}_{-1} = 0 \qquad \mathcal{S}_0 = 1 \tag{1.5a}$$

$$\hat{\mathcal{S}}_n = Y_{n+1}(x)\hat{\mathcal{S}}_{n-1} - k_{n+1}\hat{\mathcal{S}}_{n-2} \qquad \hat{\mathcal{S}}_{-1} = 0 \qquad \hat{\mathcal{S}}_0 = k_1\,. \tag{1.5b}$$

In the case of a *mono-atomic* chain ($m_n = m$) with equal springs ($k_n = 1$) the normalized eigenfrequencies-squared of a finite chain with N atoms and fixed boundary conditions ($q_0 = 0 = q_{N+1}$) are given by the zeros of $\mathcal{S}_N(x) \equiv S_N(2(1-x)) = U_N(1-x)$, where U_N are Chebyshev's polynomials of the second kind. These zeros are

$$x_k \equiv x_k^{(N)} = 1 - \cos\frac{\pi k}{N+1} = 2\sin^2\frac{\pi k}{2(N+1)} \qquad k = 1, 2, \ldots, N\,. \tag{1.6}$$

The displacements for the kth mode are $q_{n+1} = S_n(2(1-x_k))q_1$, for $n = 1, 2, \ldots, N$, with arbitrary, k-dependent input q_1.

For an *infinite* mono-atomic chain one finds one frequency-squared band from the condition $|T_N(1-x)| \leqslant 1$, where $T_N(x)$ are Chebyshev's polynomials of the first kind. The number N of atoms in the unit cell is irrelevant because due to double zeros of $T_N(1-x) + (-1)^{k+1}$ for $x = \xi_k^{(N-1)}$, $k = 1, 2, \ldots, N-1$, the $N-1$ gaps degenerate. The x-band is, independently of N, $B = [0, 2]$. In this case $\mathcal{S}_n(x) = \hat{\mathcal{S}}_n(x) = S_n(2(1-x))$, which are orthogonal on the interval $[0, 2]$ with weight function

$$w^{(1)}(x) = \frac{2}{\pi}\sqrt{x(2-x)}\,. \tag{1.7}$$

Therefore there is no discrete part of the measure present in this mono-atomic case.

The general formula for the differential spectral density per particle (also called differential *density of states*) for an infinite chain with a unit of N atoms repeated periodically is determined from the generalized Chebyshev polynomials of the first kind, $\mathcal{T}_N(x) = \frac{1}{2}\big(\mathcal{S}_N(x) - \hat{\mathcal{S}}_{N-2}(x)\big)$. These are the trace polynomials $\frac{1}{2}\,\mathrm{tr}\,M_N$ (see equation (2.4) and cf [4], equation (3.11))

$$\mathcal{G}_N(x) = \frac{1}{N\pi}\frac{(-1)^k\,\mathcal{T}_N'(x)}{\sqrt{1-(\mathcal{T}_N(x))^2}} \tag{1.8}$$

for x in one of the N bands B_k, $k = 1, 2, \ldots, N$, which are determined by $|\mathcal{T}_N(x)| < 1$ and ordered with increasing x. Otherwise the density vanishes.
In the mono-atomic case this becomes

$$G_N(x) = G(x) = \frac{1}{\pi}\frac{1}{\sqrt{x(2-x)}} \tag{1.9}$$

for $x \in [0, 2]$, and it is zero otherwise. The N independence is due to the identities involving ordinary Chebyshev polynomials: $1 - (T_N(1-x))^2 = x(2-x)(S_{N-1}(2(1-x))^2$ for $x \in [0, 2]$ and $N \in \mathbf{N}$, as well as

$$N S_{N-1}(2(1-x)) = -T_N'(1-x)\,. \tag{1.10}$$

Equation (1.8) is, by accident, the weight function for Chebyshev's $T_N(1-x)$ polynomials (for $N = 0$; for other N the weight is twice this). In the general case the trace polynomials $\{\mathcal{T}_n(x)\}$ are no longer orthogonal (see [4], p 5402).

Quasiperiodic Fibonacci chains are obtained as special case with $k_n \equiv 1$, $\omega_0^2/\omega_n^2 = r^{h(n)}$, with the mass ratio $r \equiv m_1/m_0$ and the quasiperiodic binary Fibonacci sequence

$$h(n) = \lfloor (n+1)/\varphi \rfloor - \lfloor n/\varphi \rfloor \qquad n \in \mathbf{N}_0\,. \tag{1.11}$$

In this case we use for the polynomials $\mathcal{S}_n$ and $\hat{\mathcal{S}}_n$ the notation $\{S_n^{(r)}(x)\}$ and $\{\hat{S}_n^{(r)}\}$.

2. Bloch–Floquet solutions and the measure

In this section we describe the computation of the measure with respect to which the polynomial system $\{\mathcal{S}_n(x)\}$ defined in (1.5*a*) is orthogonal, following the general method valid for the N-periodic case (more generally for the asymptotically periodic case) described in detail in [6], ch 2. The measure for the associated polynomials $\{\hat{\mathcal{S}}_n(x)\}$ defined in (1.5*b*) is obtained in the same way. This method rests on the properties of the Bloch–Floquet solutions for the N-periodic problem. Directly connected to these solutions is a map $w(x)$ of the complex plane which enters the definition of a judiciously chosen complex contour integral. This integral is evaluated in two different ways (i) and (ii). The result will be the orthogonality relation and the measure can be read off. First, however, the necessary information on the Bloch–Floquet solutions will be given.

The starting point is the recursion formula for the monic orthogonal polynomial systems (indicated by a tilde) which describe N-periodic chains with $\kappa_{n+N} = \kappa_n$ and $m_{n+N} = m_n$†,

$$\tilde{\mathcal{S}}_n(x) = (x - c_n)\,\tilde{\mathcal{S}}_{n-1}(x) - d_n\,\tilde{\mathcal{S}}_{n-2}(x) \qquad \tilde{\mathcal{S}}_{-1} = 0 \qquad \tilde{\mathcal{S}}_0 = 1 \tag{2.1a}$$

with

$$c_n := \frac{1+k_n}{2}\,\frac{\omega_n^2}{\omega_0^2} \qquad d_n := \frac{k_n}{4}\,\frac{\omega_n^2}{\omega_0^2}\,\frac{\omega_{n-1}^2}{\omega_0^2}\,. \tag{2.1b}$$

The first-associated monic polynomials $\{\tilde{\hat{\mathcal{S}}}_n(x)\}$ satisfy (2.1*a*) with shifted coefficients $\hat{c}_n := c_{n+1}$, $\hat{d}_n := d_{n+1}$ and the input $\tilde{\hat{\mathcal{S}}}_{-1} = 0$, and $\tilde{\hat{\mathcal{S}}}_0 = k_1$.

Orthogonality with positive-definite moment functional is guaranteed for all $N \in \mathbf{N}$ by Favard's theorem, because $d_n > 0$ and the c_n are real.

The relation between the polynomials (1.5) and the monic ones is given by ($n \geqslant 1$)

$$\mathcal{S}_n(x) = (-2)^n \prod_{i=1}^{n} \frac{\omega_0^2}{\omega_i^2}\,\tilde{\mathcal{S}}_n(x) \qquad \hat{\mathcal{S}}_n(x) = (-2)^n k_1 \prod_{i=2}^{n+1} \frac{\omega_0^2}{\omega_i^2}\;\tilde{\hat{\mathcal{S}}}_n(x)\,. \tag{2.2}$$

For the Fibonacci chains with $\kappa_n \equiv \kappa$ one uses the N-periodic binary sequence $h^{(N)}(n)$ obtained by repetition of the first N entries of the quasiperiodic sequence $\{h(n)\}$ of (1.11). The original polynomials $\{S_n^{(r)}(x)\}$ and $\{\hat{S}_n^{(r)}(x)\}$ for quasiperiodic Fibonacci chains, are then obtained in the limit $N \to \infty$, keeping always $n \leqslant N$.

† All quantities depend on the chosen period N, $\vec{\omega}^2 \equiv (\omega_0^2, \omega_1^2, \ldots, \omega_{N-1}^2)$ and $\vec{k} \equiv (k_1, k_2, \ldots, k_N)$ with $\kappa_0 = \kappa_N$. In the sequel this dependence will be suppressed.

In the N-periodic case the transfer matrix M_N of the elementary unit satisfies: Det $M_N = \kappa_0/\kappa_N = +1$. From this and $M_{n+N} = M_n M_N$ one derives, using (1.4)

$$\mathcal{S}_{n+2N}(x) = 2\ \mathcal{T}_N(x)\ \mathcal{S}_{n+N}(x) - \mathcal{S}_n(x) \tag{2.3a}$$

$$\hat{\mathcal{S}}_{n+2N-1}(x) = 2\ \mathcal{T}_N(x)\ \hat{\mathcal{S}}_{n+N-1}(x) - \hat{\mathcal{S}}_{n-1}(x) \tag{2.3b}$$

with the trace polynomials

$$\mathcal{T}_N(x) := \tfrac{1}{2}\,\mathrm{tr}\, M_N = \tfrac{1}{2}(\mathcal{S}_N(x) - \hat{\mathcal{S}}_{N-2}(x))\,. \tag{2.4}$$

In the *Fibonacci case* we use the N-periodic binary sequence $\{h_N(n)\}$ obtained from (1.11) by taking $h_N(n) = h(n)$ for $n = 1, 2, \ldots, N$ and defining $h_N(n+N) = h_N(n)$. In this case the polynomials $\mathcal{S}_N$, $\hat{\mathcal{S}}_{N-2}$, hence $\mathcal{T}_N$, coincide with the corresponding quasiperiodic ones. (2.3) implies for the general solution for the displacements (1.2)

$$q_{n+2N+1}(x) = 2\ \mathcal{T}_N(x)\ q_{n+N+1}(x) - q_{n+1}(x)\,. \tag{2.5}$$

The two independent Bloch–Floquet solutions are, for arbitrary input $q_0(x)$ and $q_1(x)$,

$$q_{n,\pm}(x) := q_{n+N}(x) - \lambda_{N,\pm}(x)\ q_n(x) \tag{2.6a}$$

with

$$\lambda_{N,\pm}(x) := \mathcal{T}_N(x) \pm \sqrt{(\mathcal{T}_N(x))^2 - 1} \tag{2.6b}$$

which are the two eigenvalues of M_N. With this definition the periodicity condition (2.5) yields $q_{n+N,\pm}(x) = \lambda_{N,\mp}(x)\, q_{n,\pm}(x)$. $\lambda_{N,\mp}(x) = \exp \mathrm{i}\beta_{N,\mp}(x)$ for x values in any of the N intervals (bands) B_k , $k = 1, 2, \ldots, N$, defined by†

$$|\mathcal{T}_N(x)| \leqslant 1 \tag{2.7}$$

which is necessary for harmonic vibrations. Therefore,

$$q_{n,\pm}(x) = (\lambda_{N,\mp}(x))^{n/N} \phi_n(x) \qquad n \in \mathbf{N}_0 \tag{2.8}$$

with periodic $\phi_{n+N}(x) = \phi_n(x)$, proving that (2.6*a*) defines the Bloch–Floquet solutions. The integrated spectral density (or integrated density of states) is a continuous function given by appropriate branches of the Bloch–Floquet phase $\beta_N(x) = \cos^{-1} \mathcal{T}_N(x)$ for band values x and constant pieces in the $N-1$ gaps between the bands. The differential spectral density (or differential density of states) equation (1.7) follows from this after differentiation.

In order to compute the measure with respect to which the polynomials $\{\mathcal{S}_n(x)\}$ are orthogonal one considers (see [6]) the following map for $x \in \mathbf{C}$:

$$w(x) = \left(\lambda_N(x)\right)^{1/N} \tag{2.9}$$

with the sign of the square-root in (2.6*b*) chosen such that for real $x \in B_k$, $k = 1, \ldots, N$, $\lambda_N(x)$ runs along the unit circle from $+1$ to -1 for odd numbered bands and from -1 to

† From equation (1.5) one finds $\mathcal{S}_n(0) = 1 + \kappa_0 \sum_{i=1}^{n} 1/\kappa_i$, $\hat{\mathcal{S}}_n(0) = k_1 + \kappa_0 \sum_{i=2}^{n+1} 1/\kappa_i$. Therefore, in the N-periodic case $\mathcal{T}_N(0) = 1$ holds for all chains ($\kappa_0 = \kappa_N$). For the proof of the reality of the zeros of $\mathcal{T}_N(x) \mp 1$ see [6], lemma 2.2.

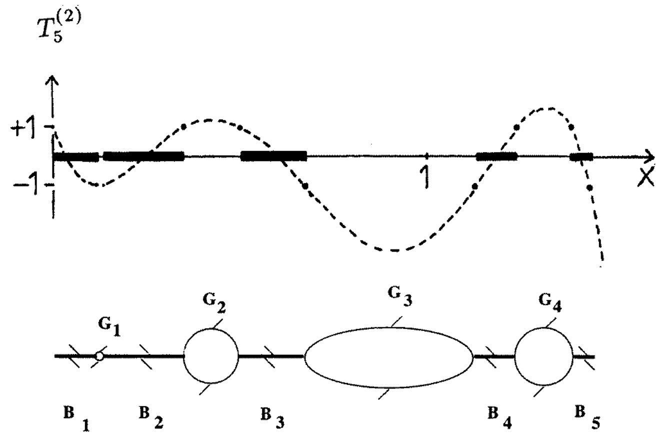

Figure 1. A sketch of the bands and gaps for the Fibonacci $N = 5, r = 2$ chain $(AABAAB)^{\infty}$. A closed path in the x-plane is indicated.

$+1$ for even numbered ones. This requires the sign $(-1)^{k+1}$ for $x \in B_k$. $\lambda_N(x)$ is real for x in the gaps G_k, $k = 1, \ldots, N-1$, and we choose the sign of the square-root as $(-1)^k$ such that $|\lambda_N(x)| > 1$ holds. $x \in (x_{\max}, \infty)$, with the maximal band value $x_{\max}$, is taken as gap G_N with the sign choice $(-1)^N$. Such a sign choice produces for $\omega(x)$ of (2.9) a path like the one shown for the Fibonacci chain example $N = 5, r = 2$ in figure 2, if x runs along the real axis from 0 to $x_{\max}$. Finally, in the $z = 1/w(x)$ plane a closed contour is obtained if x runs also backwards from $x_{\max}$ to $x = 0$. This contour is shown for the example in figure 3. The starting point is at $z = +1$. In figures 2 (resp. 3) the $B_k^{'}$ (resp. $B_k^{''}$) and $G_k^{'}$ (resp. $G_k^{''}$) labels indicate the images of the bands B_k and gaps G_k under the map $w(x)$ of (2.9) (resp. $z = 1/w(x)$). That the map w is of importance is clear from the Bloch–Floquet solution (2.8).

For the computation of the measure for the polynomials $\{S_n(x)\}$ it was found in [6] that one should consider the z-plane contour integral for $m, n = 0, 1, 2, \ldots,$

$$I \equiv I_{m,n} := -\frac{1}{2\pi \mathrm{i}} \int_{\Gamma} \frac{\mathcal{S}_m(g(z))\; q_{n+1,\pm}(g(z))}{\mathcal{S}_{N-1}(g(z))} g'(z)\,\mathrm{d}z \qquad (2.11)$$

with g the inverse map to $z(x) = 1/w(x)$, namely $x = g(z)$ and the Bloch–Floquet solution $q_{n+1,\pm}(x)$ defined by (2.6a) and (1.2) with the choice $q_1 = 1$ and $q_0 = 0$. The sign is chosen as described above in the definition of $w(x)$. In addition, for $x_{\max} < x \leqslant +\infty$ the sign choice is $(-)^N$. The contour Γ (with negative orientation) is the union $\Gamma = \Gamma_{B''} \cup \Gamma_{G''}$ with

$$\Gamma_{B''} := \left\{ z \mid z = \exp \mathrm{i}\theta, \theta \neq \pm \frac{\pi}{N} k,\;\; k = 1, 2, \ldots, N-1 \right\} \qquad (2.12)$$

and $\Gamma_{G''}$ are the $2(N-1)$ closed curves around the images $G_k^{''}$ of the gaps G_k. For the Fibonacci chain example with $N = 5, r = 2$ see figures 1 and 3.

For later use note that because $q_{n+1,\pm}(x)$ satisfies the same recursion relation as $\mathcal{S}_n(x)$ one finds, after comparison of the $n = -1$ and $n = 0$ inputs on both sides (remember $q_0 = 0$)

$$q_{n+1,\pm}(x_i)/q_{1,\pm}(x_i) = \mathcal{S}_n(x_i) \qquad (2.13)$$

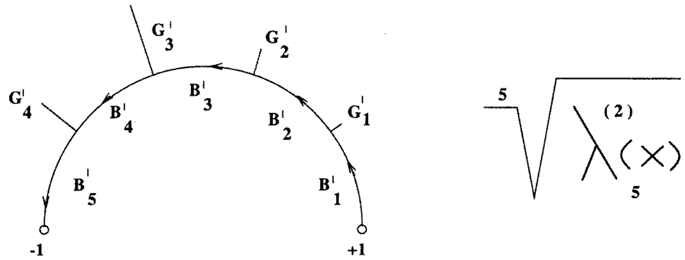

Figure 2. The map $w(x)$ of the bands and gaps in the $N = 5, r = 2$ Fibonacci case.

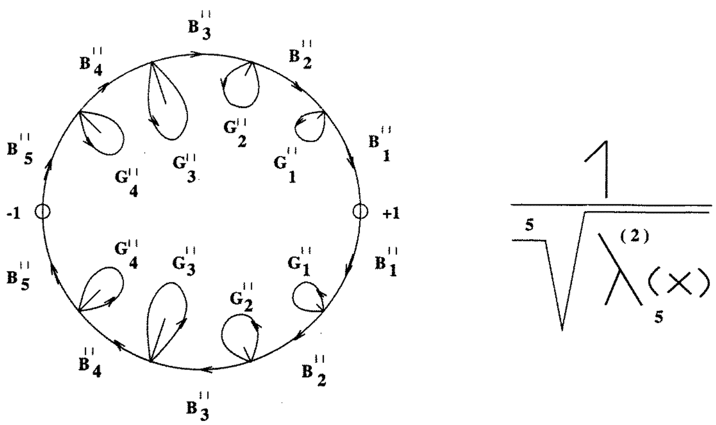

Figure 3. The map $z(x) = 1/w(x)$ in the $N = 5, r = 2$ Fibonacci case. The contour Γ is indicated.

with the zeros x_i, $i = 1, 2, \ldots, N-1$, of $\mathcal{S}_{N-1}$. The contour integral is computed in two ways (i) adding the $\Gamma_{B''}$ and $\Gamma_{G''}$ contribution, both transformed to the x-plane, and (ii) evaluating the z-plane contour integral with the help of the residue theorem.

In the *first step* of (i) one computes the $\Gamma_{B''}$ contribution using, for $x \in B_k$ with sign choice $(-1)^{k+1}$,

$$q_{n+1,\pm}(x) = q_{n+1,\mp}(x) + (1/\lambda_{N,\pm}(x) - \lambda_{N,\pm}(x))\ \mathcal{S}_n(x) \tag{2.14}$$

following from (2.6*a*), and with the choice $q_1 = 1$, $q_0 = 0$ in (1.2) one has $q_{n+1} = \mathcal{S}_n$. After some rewriting one finds (see appendix A1 for details)

$$I_B = -\frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{B''_-}} \frac{(1/\lambda_N(x) - \lambda_N(x))\ \mathcal{S}_m(x)\mathcal{S}_n(x)}{\mathcal{S}_{N-1}(x)}\ g'(z)\,\mathrm{d}z \tag{2.15}$$

with $x = g(z)$ and B''_- denoting the lower half of the punctured unit circle in the z-plane. This can be restated in the x-plane (see figure 1 for the Fibonacci case $N = 5, r = 2$):

$$I_B = \frac{1}{\pi} \int_B \frac{\mathcal{S}_m(x)\ \mathcal{S}_n(x)(-1)^{k+1}\sqrt{1 - (\mathcal{T}_N(x))^2}}{\mathcal{S}_{N-1}(x)}\,\mathrm{d}x\,. \tag{2.16}$$

The second step of the computation (i) is that along $\Gamma_{G''}$. This integral is again evaluated in x-space, such that the $N-1$ (positively oriented) closed contours around the gaps G_k

are picked up (cf figure 1 for the $N = 5$, $r = 2$ Fibonacci case). $\mathcal{S}_{N-1}(x)$ has a simple zero in each of the $N-1$ gaps. This follows from orthogonality and a lemma (Geronimus *et al* lemma 2.2, p 46 in [6]) about the interlacing of the zeros of $\mathcal{T}_N \mp 1$, which are real, and $\mathcal{S}_{N-1}$ (and $\hat{\mathcal{S}}_{N-1}$). Note, that $\mathcal{S}_{N-1}$ zeros may occur at one of the band boundaries, coinciding then with zeros of $\mathcal{T}_N - 1$ or $\mathcal{T}_N = 1$. The residue theorem now yields with the help of (2.13)

$$I_G = -\int \mathrm{d}x \left(\sum_{k=1}^{N-1} \delta(x - x_k) \frac{q_{1,(-)^k}(x)}{\mathcal{S}'_{N-1}(x)} \right) \mathcal{S}_m(x)\, \mathcal{S}_n(x) \tag{2.17}$$

with the zeros $x_k \equiv \xi_k^{(N-1)}$ of $\mathcal{S}_{N-1}$.

Computation (ii) of (2.11) is done in the z-plane using the residue theorem. The only possible pole inside Γ, coming from $g'(z)$, occurs for $x \to \infty$, i.e. $z = 0$. The zeros of $\mathcal{S}_{N-1}$ are outside of Γ. Therefore only the large-x behaviour of the integrand is of interest.

For large x the $\mathcal{S}$-polynomials behave like (see equation (2.2))

$$\mathcal{S}_m(x) \sim (-2)^m \prod_{i=1}^{m} \frac{\omega_0^2}{\omega_i^2}\; x^m . \tag{2.18}$$

The asymptotics of $q_{n+1,(-)^N}(x)$ cannot be found from its definition (2.6*a*) directly. Following [6], it is found from the formula, based on (2.6*a*) and (2.5)

$$q_{n+1,+}(x)\, q_{n+1,-}(x) = (q_{n+1+N}(x))^2 - q_{n+2N+1}(x)\, q_{n+1}(x) . \tag{2.19}$$

The right-hand side can be rewritten, using the mth *associated* polynomials $\mathcal{S}_n^{(m)}$ defined by

$$\mathcal{S}_n^{(m)}(x) = Y_{n+m}(x)\, \mathcal{S}_{n-1}^{(m)}(x) - k_{n+m}\, \mathcal{S}_{n-2}^{(m)}(x) \tag{2.20}$$

with inputs $\mathcal{S}_{-1}^{(m)} = 0$ and $\mathcal{S}_0^{(m)} = \prod_{i=1}^{m} k_i$ for $m \in \mathbf{N}$ and $\mathcal{S}_0^{(0)} = \mathcal{S}_0 = 1$. Because $\mathcal{S}_{n-m}^{(m)}$ satisfies the recursion relation of q_{n+1}, with the two independent solutions q_{n+1} and q_{n+1+N}, with Wronskian $q_{n+1}\, q_{n+N} - q_{n+1+N}\, q_n$ satisfying

$$W(q_{n+1}, q_{n+1+N}) / \prod_{i=1}^{n} k_i = W(q_1, q_{N+1}) = q_1 q_N - q_0 q_{N+1} \tag{2.21}$$

one finds (for general q_1 and q_0)

$$\mathcal{S}_{n-m}^{(m)}(x) = \frac{1}{W(q_1, q_{N+1})} \left\{ q_{m+N}(x)\; q_{n+1}(x) - q_m(x)\; q_{n+1+N}(x) \right\} . \tag{2.22}$$

Letting $n \to n + N$ and $m \to n + 1$, one obtains the right-hand side of (2.19):

$$q_{n+1,+}(x)\; q_{n+1,-}(x) = W(q_1, q_{N+1})\, \mathcal{S}_{N-1}^{(n+1)}(x) . \tag{2.23}$$

The asymptotic form of $q_{n+1,(-)^N}$ can now be inferred from the one of $q_{n+1,-(-)^N}$ which follows without difficulty from (2.6*a*)†. For $q_1 = 1$, $q_0 = 0$ one finds that the leading term for large x is

$$\frac{q_{n+1,(-)^N}(x)}{\mathcal{S}_{N-1}(x)} \sim \prod_{j=1}^{n+1} k_j \Bigg/ \left((-2)^{n+1} \prod_{i=1}^{n+1} \frac{\omega_0^2}{\omega_i^2}\, x^{n+1} \right) . \tag{2.24}$$

† The leading coefficient of $\mathcal{S}_{N-1}^{(n+1)}(x)$ is, for $n \in \mathbf{N_0}$, $(-2)^{N-1} \prod_{j=1}^{n+1} k_j\; \prod_{i=n+2}^{n+N} \omega_0^2/\omega_i^2$.

The residue theorem can now be applied to the contour integral (2.11) in the z-plane. $g'(z) \sim -C/z^2$ for small z due to $g(z) = x$ and $z = 1/w(x) \sim C/x$ for large x. The capacity C drops out in the calculation of the residue for $z = 0$. The result is

$$I_{m,n} = +\frac{1}{2}\frac{\omega_{n+1}^2}{\omega_0^2}\prod_{j=1}^{n+1} k_j \;\delta_{n,m} \,. \tag{2.25}$$

Combining both ways of calculation (i) and (ii) one ends up with the normalized measure $\mathrm{d}\sigma$ for the ortho *normal* polynomials with $s_0 = 1$

$$s_n(x) := (-1)^n \sqrt{\frac{\omega_1^2}{\omega_{n+1}^2}\frac{k_1}{\prod_{j=1}^{n+1} k_j}}\; \mathcal{S}_n(x) \tag{2.26}$$

where the factor $(-1)^n$ has been inserted to guarantee positive leading coefficient.

$$\int s_m(x)\; s_n(x)\,\mathrm{d}\sigma(x) = \delta_{m,n} \qquad m, n \in \mathbf{N_0} \tag{2.27}$$

where

$$\mathrm{d}\sigma(x) = w(x)\,\mathrm{d}x - \sum_{k=1}^{N-1}\delta(x - \xi_k^{(N-1)})\,\frac{2}{k_1}\frac{\omega_0^2}{\omega_1^2}\frac{q_{1,(-)^k}(x)}{\mathcal{S}'_{N-1}(x)}\,\mathrm{d}x \tag{2.28a}$$

$$w(x) = \frac{1}{\pi}\frac{2}{k_1}\frac{\omega_0^2}{\omega_1^2}\frac{(-1)^{k+1}\sqrt{1-(\mathcal{T}_N(x))^2}}{\mathcal{S}_{N-1}(x)} \qquad x \in B_k \qquad k = 1, 2, \ldots, N \tag{2.28b}$$

$$q_{1,(-)^k}(x) = \mathcal{S}_N(x) - \lambda_{N,(-)^k}(x) \qquad k = 1, 2, \ldots, N-1 \tag{2.28c}$$

$$\lambda_{N,(-)^k}(x) = \mathcal{T}_N(x) + (-1)^k\sqrt{(\mathcal{T}_N(x))^2 - 1} \qquad x \in G_k \,. \tag{2.28d}$$

The absolutely continuous part of the measure, $w(x)\,\mathrm{d}x$, vanishes outside the N bands $B = \cup B_k$. It is non-negative because the sign of $\mathcal{S}_{N-1}$ in band B_k is $(-1)^{k+1}$, due to the fact that $\mathcal{S}_{N-1}(0) \geqslant +2$ and the interlacing property of its zeros with the one of $\mathcal{T}_N \mp 1$. The Dirac-measure lives on the $N-1$ zeros $\xi_k^{(N-1)}$ of $\mathcal{S}_{N-1}$. The fact that also this measure is non-negative will be discussed in section 4.

A similar computation can be performed in order to find the measure for the associated orthogonal polynomial system $\{\hat{\mathcal{S}}_n\}$ of (2.2*b*). One puts in (2.1) $q_1 = 0$ and $q_0 = -1$. In the integral (2.11) one uses $\hat{\mathcal{S}}$ instead of $\mathcal{S}$ and replaces $q_{n+1,\pm}$ by $q_{n+2,\pm} := \hat{\mathcal{S}}_{n+N} - \lambda_{N,\pm}\,\hat{\mathcal{S}}_n$. In place of (2.13) one uses here $q_{n+2,\pm}(\hat{x}_i)/q_{2,\pm}(\hat{x}_i) = \hat{\mathcal{S}}_n(\hat{x}_i)/k_1$ with the zeros $\hat{x}_i$ of $\hat{\mathcal{S}}_{N-1}$. The normalized measure for the ortho*normal* polynomials with positive leading coefficient and $\hat{s}_0 = 1$

$$\hat{s}_n(x) = (-1)^n\frac{1}{k_1}\sqrt{\frac{\omega_2^2}{\omega_{n+2}^2}\frac{k_1 k_2}{\prod_{j=1}^{n+2} k_j}}\; \hat{\mathcal{S}}_n(x) \tag{2.29}$$

is then

$$\mathrm{d}\hat{\sigma}(x) = \hat{w}(x)\,\mathrm{d}x - \sum_{k=1}^{N-1}\delta(x - \hat{\xi}_k^{(N-1)})\,2\frac{\omega_0^2}{\omega_2^2}\frac{k_1}{k_2}\frac{q_{2,(-)^k}(x)/k_1}{\hat{\mathcal{S}}'_{N-1}(x)}\,\mathrm{d}x \tag{2.30a}$$

$$\hat{w}(x) = \frac{2}{\pi}\frac{\omega_0^2}{\omega_2^2}\frac{k_1}{k_2}\frac{(-1)^{k+1}\sqrt{1-(\mathcal{T}_N(x))^2}}{\hat{S}_{N-1}(x)} \qquad x \in B_k \qquad k = 1, 2, \ldots, N \tag{2.30b}$$

$$q_{2,(-)^k}(x) = \hat{\mathcal{S}}_N(x) - k_1\,\lambda_{N,(-)^k}(x) \qquad x \in G_k \qquad k = 1, 2, \ldots, N-1 \tag{2.30c}$$

where $\lambda_{N,(-)^k}$ is given in (2.28*d*) and $\hat{\xi}_k^{(N-1)}$ are the zeros of $\hat{\mathcal{S}}_{N-1}(x)$.

3. Continued fraction, Stieltjes inversion formula and the measure

The second method to compute the measure for orthogonal polynomials with periodic recursion formula coefficients relies on the fact that the continued fraction accompanying this recursion formula is the Stieltjes transform [8] of the orthogonality measure [1b, 9]. In the periodic case the continued fraction can be given explicitly, and the measure is then determined with the help of the Perron–Stieltjes inversion formula [10, 11].

The continued fraction which belongs to the recursion formulae for the (not necessarily N-periodic) associated orthogonal polynomials $\{\mathcal{S}_n(x)\}$ and $\{\hat{\mathcal{S}}_n(x)\}$ (see equations (1.5*a*) and (1.5*b*)) is

$$-\frac{k_1\omega_1^2}{2\omega_0^2}\chi(x) = \frac{k_1 \quad |}{|\ Y_1(x)} - \frac{k_2 \quad |}{|\ Y_2(x)} - \cdots - \frac{k_n \quad |}{|\ Y_n(x)} - \cdots \tag{3.1}$$

where $Y_n(x))$ is given by (1.3*b*). The factor $-k_1\omega_1^2/2\omega_0^2$ has been introduced for later convenience. The nth approximation to this continued fraction is for $n \geqslant 1$†

$$-\frac{k_1\omega_1^2}{2\omega_0^2}\chi_n(x) = \frac{k_1 \quad |}{|\quad Y_1(x)} - \frac{k_2 \quad |}{|\quad Y_2(x)} - \cdots - \frac{k_n \quad |}{|\ Y_n(x)} = \frac{\hat{\mathcal{S}}_{n-1}(x)}{\mathcal{S}_n(x)} \tag{3.2}$$

which follows by induction, using the recursion formulae. If the continued fraction converges $\chi(x) := \lim_{n\to\infty}\chi_n(x)$. A fundamental theorem (see e.g. [9], theorem 2.4, or [1b], p 90) states that $\chi(x)$ is the Stieltjes transform of the measure

$$\chi(x) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}\sigma(t)}{x-t} \qquad x \notin \mathrm{supp}(\mathrm{d}\sigma)\,. \tag{3.3}$$

Here $\mathrm{d}\sigma$ is the real, positive and normalized measure for the orthogonal $\mathcal{S}$-polynomials (1.5*a*) (cf [9], equations (2.1)–(2.5))

$$\int \mathcal{S}_n(x)\,\mathcal{S}_m(x)\,\mathrm{d}\sigma(x) = \frac{\omega_{n+1}^2}{\omega_1^2 k_1}\prod_{j=1}^{n+1} k_j\,\delta_{n,m} = \frac{m_1}{m_{n+1}}\delta_{n,m} \qquad m, n \in \mathbf{N}_0\,. \tag{3.4}$$

The Perron–Stieltjes inversion formula (see e.g. [9, 10]) for a real measure of bounded variation is

$$\sigma(t_2) - \sigma(t_1) = -\frac{1}{\pi}\lim_{\eta\to+0}\int_{t_1}^{t_2} \mathrm{Im}\,\chi(t+\mathrm{i}\eta)\,\mathrm{d}t \tag{3.5}$$

with $\sigma(t_k) := \frac{1}{2}(\sigma(t_k+0)+\sigma(t_k-0))$ for $k = 1, 2$. $\bar{\chi}(x) = \chi(\bar{x})$ for $x \in \mathbf{C}$ and χ is analytic for non-real x.

† The nth approximation to the continued J-fraction is for $n \geqslant 1$ (see equations (2.1) and (2.2))

$$\frac{k_1 \quad |}{|x-c_1} - \frac{d_2 \quad |}{|x-c_2} - \cdots - \frac{d_n \quad |}{|x-c_n} = \chi_n(x) = \frac{\tilde{\hat{\mathcal{S}}}_{n-1}(x)}{\tilde{\mathcal{S}}_n(x)}\,.$$

In the *N-periodic case* $\chi(x)$ can be calculated explicitly as follows (cf [7]). Consider, for fixed x, N and parameters k_n, ω_n^2, the map in the complex z-plane

$$J_N(x;z) \equiv z' = \frac{k_1 \quad |}{| \; Y_1(x)} - \frac{k_2 \quad |}{| \; Y_2(x)} - \cdots - \frac{k_N \qquad |}{| \quad Y_N(x) - z} \tag{3.6}$$

with $Y_n(x)$ given in (1.3*b*). By induction, with the help of the recursion formulae, one finds

$$J_N(x;z) = \frac{\hat{\mathcal{S}}_{N-2}(x)\; z - \hat{\mathcal{S}}_{N-1}(x)}{\mathcal{S}_{N-1}(x)\; z - \mathcal{S}_N(x)} \tag{3.7}$$

which is for real x a $SL(2,\mathbf{R})$ Möbius transformation due to

$$1 = \mathrm{Det}\; M_N(x) = -\mathcal{S}_N(x)\,\hat{\mathcal{S}}_{N-2}(x) + \mathcal{S}_{N-1}(x)\,\hat{\mathcal{S}}_{N-1}(x)\,. \tag{3.8}$$

Because of N-periodicity $-k_1\omega_1^2\chi(x)/2\omega_0^2$ is a fixed point of the map (3.6), and can be computed from (3.7) as

$$-\frac{k_1\omega_1^2}{2\omega_0^2}\chi_{N,\pm}(x) = \left\{\tfrac{1}{2}(\mathcal{S}_N(x) + \hat{\mathcal{S}}_{N-2}(x)) \mp \sqrt{(\mathcal{T}_N(x))^2 - 1}\right\}/\mathcal{S}_{N-1}(x) \tag{3.9}$$

where (3.8) was used, and $\mathcal{T}_N(x)$ is given in (2.4). For $|\mathcal{T}_N(x)| < 1$, which determines N bands B_k, $k = 1, 2, \ldots, N$, $\chi_{N,\pm}(x)$ becomes complex. For the gaps between the N bands, G_k, $k = 1, 2, \ldots, N-1$, it is real. See figure 1 for the Fibonacci case $N = 5, r = 2$. Introducing $\lambda_{N,\pm}(x)$ given in (2.6*b*), this is rewritten as

$$-\frac{k_1\omega_1^2}{2\omega_0^2}\chi_{N,\pm}(x) = \left\{\mathcal{S}_N(x) - \lambda_{N,\pm}(x)\right\}/\mathcal{S}_{N-1}(x)\,. \tag{3.10}$$

$\chi_{N,(-)^N}(x)$ is for large x proportional to $1/x$†. The sign choice for x values in the bands and gaps will be given below.

The measure can now be determined from the inversion formula (3.5). The absolutely continuous part of the spectral measure, $\mathrm{d}\sigma_{ac}(x) = w(x)\,\mathrm{d}x$, is found from

$$w(x) = \frac{\mathrm{d}}{\mathrm{d}x}\sigma_{ac}(x) = -\frac{1}{\pi}\lim_{\eta\to+0}\mathrm{Im}\,\chi(x + \mathrm{i}\eta) < \infty\,. \tag{3.11}$$

$\chi(x) \equiv \chi_N(x)$ has to be defined such that $\bar{\chi}(x) = \chi(\bar{x})$ holds for complex x. This single-valued function is called $\chi(x)$. $w(x)$ lives therefore on the bands B_k and coincides with (2.28*b*), after the sign of the square-root (i.e. of the Riemann sheet) has been chosen such that $w(x)$ is non-negative. See section 4 for the proof that the sign choice in (2.28*b*) leads to positive w.

The discrete part of the spectral measure (sum of Dirac δ-functions) originates from the simple poles of $\chi(x)$ with their residues determining the height of the jumps of the measure

$$\mathrm{d}\sigma_{\mathrm{Dirac}}(x) = -\frac{2}{k_1}\frac{\omega_0^2}{\omega_1^2}\sum_{k=1}^{N-1}\delta(x - \xi_k^{(N-1)})\;\frac{\mathcal{S}_N(x) - \lambda_N(x)}{\mathcal{S}'_{N-1}(x)}\,\mathrm{d}x \tag{3.12}$$

† The x-asymptotics cannot be found from (3.10). One uses $(\mathcal{S}_N - \lambda_{N,(-)^N})/\mathcal{S}_{N-1} = \hat{\mathcal{S}}_{N-1}/(\mathcal{S}_N - \lambda_{N,(-)^{N+1}})$ which is identity (2.23) with $q_0 = 0$, $q_1 = 1$, equations (2.6*a*) and (1.2).

where the sign of the square-root in $\lambda_N(x)$ of (2.6*b*) has been chosen as $(-1)^k$ for $x \in G_k$, like in the calculation leading to (2.28*c*). This choice will be seen in the next section to produce positive jumps in $\sigma(x)$ at the zeros $\xi_k^{(N-1)}$ of $\mathcal{S}_{N-1}$. For finite N and parameters $\{k_n\}, \{\omega_n^2\}$ there are no other singularities of $\chi(x)$ which could contribute to the singular part of the measure (cf [12], ch XIII, p 140).

The measure for the orthogonal $\{\hat{\mathcal{S}}_n(x)\}$ polynomials can be calculated in a similar fashion by taking into account also their first associated polynomials $\{S_n^{(2)}(x)\}$, defined in (2.20). Note that because of the cyclic property of the trace and N-periodicity one has

$$\hat{\mathcal{T}}_N(x) := (\hat{\mathcal{S}}_N(x) - \mathcal{S}_{N-2}^{(2)}(x))/2 = \tfrac{1}{2}\,\mathrm{tr}\,\hat{M}_N = k_1 \mathcal{T}_N(x) \tag{3.13}$$

with $\hat{M}_N := R_{N+1} R_N \cdots R_2$. More details are found in appendix A.2.

We have thus reproduced the results of the previous section.

4. General remarks and Fibonacci chain examples

We first state a simple conclusion concerning the discrete measure (3.12), which will show its non-negativity. With the mentioned sign choice the numerator of the kth term can be rewritten, with (2.6*b*), (2.4), and (3.8), like

$$\mathcal{S}_N - \lambda_N = \tfrac{1}{2}\big(\mathcal{S}_N + \hat{\mathcal{S}}_{N-2}\big) + \ (-1)^{k+1}\sqrt{\big(\tfrac{1}{2}(\mathcal{S}_N + \hat{\mathcal{S}}_{N-2})\big)^2 - \mathcal{S}_{N-1}\hat{\mathcal{S}}_{N-1}}\,. \tag{4.1}$$

Evaluated at the zero $x_k \equiv \xi_k^{(N-1)}$ of $\mathcal{S}_{N-1}$ this becomes

$$(\mathcal{S}_N - \lambda_N)|_{x_k} = \begin{cases} \Theta\big(-(\mathcal{S}_N + \hat{\mathcal{S}}_{N-2})|_{x_k}\big)\ (\mathcal{S}_N + \hat{\mathcal{S}}_{N-2})|_{x_k} & \text{for} \quad k \text{ even} \\ \Theta\big((\mathcal{S}_N + \hat{\mathcal{S}}_{N-2})|_{x_k}\big)\ (\mathcal{S}_N + \hat{\mathcal{S}}_{N-2})|_{x_k} & \text{for} \quad k \text{ odd} \end{cases} \tag{4.2}$$

with the step function $\Theta(x)$. Due to (3.8) $(\mathcal{S}_N + \hat{\mathcal{S}}_{N-2})|_{x_k} = \big((\mathcal{S}_N(x_k))^2 - 1\big)/\mathcal{S}_N(x_k)$. The final result for the discrete measure is

$$\mathrm{d}\sigma_{\mathrm{Dirac}}^{(N,r)}(x) = \frac{2}{k_1}\frac{\omega_0^2}{\omega_1^2}\sum_{k=1}^{N-1}\delta(x - \xi_k^{(N-1)})\ \Theta\big((-)^{k+1}(\mathcal{S}_N(x) + \hat{\mathcal{S}}_{N-2}(x))\big)\frac{\mathcal{S}_N(x) + \hat{\mathcal{S}}_{N-2}(x)}{-\mathcal{S}_{N-1}'}\,\mathrm{d}x \tag{4.3}$$

which is always non-negative because the signum of $\mathcal{S}_{N-1}'(\xi_k^{(N-1)})$ is $(-1)^k$.

Two remarks are in order.

(i) There will be no contribution to the discrete measure from those zeros of $\mathcal{S}_{N-1}$ which satisfy $\mathcal{T}_N(\xi_k^{(N-1)}) = \pm 1$. In this event the zero of $\mathcal{S}_{N-1}$ coincides with one of the band boundaries, and from the definition of $\mathcal{T}_N$ and (3.8) one finds $\mathcal{S}_N(\xi_k^{(N-1)}) = -\hat{\mathcal{S}}_{N-2}(\xi_k^{(N-1)}) = \pm 1$.

(ii) A comment on band degeneracy. A gap G_k will disappear whenever $\mathcal{T}_N + (-1)^{k+1}$ has a double zero at, say, x_k. Because the zero $\xi_k^{(N-1)}$ of $\mathcal{S}_{N-1}$ lies in the gap or on one of the adjacent band boundaries one has $x_k = \xi_k^{(N-1)}$. For the same reason the kth zero of $\hat{\mathcal{S}}_{N-1}$ is then also x_k. Due to (3.8) $\hat{\mathcal{S}}_{N-2}(x_k) = -1/\mathcal{S}_N(x_k)$, and therefore $\mathcal{S}_N(x_k) + 1/\mathcal{S}_N(x_k) = 2(-1)^k$ (definition of $\mathcal{T}_N$). Thus $\mathcal{S}_N(x_k) = (-1)^k = -\hat{\mathcal{S}}_{N-2}(x_k)$, and there will be no contribution to the discrete part (4.3) of the measure from such disappearing gaps G_k†.

Next, we consider some examples of Fibonacci chains.

In the N-periodic Fibonacci case $k_n \equiv 1$ and $Y_n(x) = 2(1-r^{h_N(n)}x)$, with the N-periodic binary sequence $\{h_N(n)\}$ obtained by continuing the first N entries of $\{h(n)\}$ given by (1.11) periodically. All polynomials will now depend on N and the mass ratio $r \equiv m_1/m_0$. We shall use non-script symbols for these polynomials and the N, r labels will be clear from the context.

(a) First we check the *mono-atomic case* $r = 1$. The results have already been given in the introduction. Remark (ii) applies for all $N - 1$ disappearing gaps.

(b) Put $N = 2$, $r \equiv m_A/m_B \neq 1$, *i.e. AB-chains*. We first show that there is no discrete part (4.3) of the measure. Here remark (i) applies. The zero of $S_1(x)= 2(1 - rx)$ (see [4a]) is $x_1 = 1/r$, and because

$$T_2(x) = 2rx^2 - 2(1+r)x + 1 \qquad S_2(x) = 4rx^2 - 4(1+r)x + 3 \tag{4.4}$$

one has $S_2(1/r) = T_2(1/r) = -1 = -\hat{S}_0$‡. The weight function is given by

$$w(x) = \frac{2r}{\pi}\sqrt{-x\left(x-\frac{1}{r}\right)(x-1)\left(x-1-\frac{1}{r}\right)}\Bigg/\left|x-\frac{1}{r}\right| \tag{4.5}$$

for x in any of the two bands

$$r \geqslant 1: \quad B_1 = \left[0, \frac{1}{r}\right] \qquad B_2 = \left[1, 1+\frac{1}{r}\right] \tag{4.6a}$$

$$r \leqslant 1: \quad B_1 = [0, 1] \qquad B_2 = \left[\frac{1}{r}, 1+\frac{1}{r}\right]. \tag{4.6b}$$

The weight function (2.30) for the associated polynomials $\{\hat{S}_n(x)\}$ is found to be

$$\hat{w} = \frac{1}{r}\frac{|x-1/r|}{|x-1|}\; w(x) \tag{4.7}$$

for x in the bands (4.6) and zero otherwise.

(c) Put $N = 3$, $r \equiv m_A/m_B \neq 1$, i.e. infinite *ABA-chains*. Now the discrete measure is present because zeros of S_2 satisfy $2rx_\mp = 1 + r \mp \sqrt{(r-1)^2 + r}$ and $S_3(x_\mp) + \hat{S}_1(x_\mp) = 2(r-1)x_\mp \neq 0$. Therefore

$$\mathrm{d}\sigma_{\mathrm{Dirac}} = \frac{4r}{\sqrt{(r-1)^2 + r}}\begin{cases}(r-1)\; x_-\; \delta(x-x_-)\,\mathrm{d}x & \text{for } r > 1\\ (1-r)\; x_+\; \delta(x-x_+)\,\mathrm{d}x & \text{for } 0 < r < 1\,.\end{cases} \tag{4.8}$$

The bands are, depending on sign$(1 - r)$,

$$r \geqslant 1: \quad B_1 = \left[0, \frac{1}{2r}\right] \qquad B_2 = \left[\frac{1}{2r}b_-(r), \frac{3}{2r}\right] \qquad B_3 = \left[\frac{2r+1}{2r}, \frac{1}{2r}b_+(r)\right] \tag{4.9a}$$

$$r \leqslant 1: \quad B_1 = \left[0, \frac{1}{2r}b_-(r)\right] \qquad B_2 = \left[\frac{1}{2r}, \frac{2r+1}{2r}\right] \qquad B_3 = \left[\frac{3}{2r}, \frac{1}{2r}b_+(r)\right] \tag{4.9b}$$

† In the N-periodic Fibonacci case an example is N=6 ($(ABA)^2$ chains) where one finds double zeros of $\mathcal{T}_6 + 1$ at the zeros of $\mathcal{T}_3$ for $k = 1, 3, 5$.

‡ This is an example where a zero of $\mathcal{S}_{N-1}$ coincides with a band boundary without having band degeneracy (no double zero of $\mathcal{T}_N \mp 1$). It seems to be a counterexample to one part of the statement found in [6], lemma 2.2, top of p 47 (the 'if' part).

with $b_\pm(r) \equiv r + \frac{3}{2} \pm \sqrt{r^2 - r + \frac{9}{4}}$.

The weight function (2.28*b*) becomes for $x \in B_k$, $k = 1, 2, 3$,

$$w(x) = \frac{2}{\pi} r^2 \times \frac{\sqrt{-x(x-(2r+1/2r))(x-(3/2r))(x-(1/2r))(x-(1/2r)b_+(r))(x-(1/2r)b_+(r))}}{(-1)^{k+1}(x-(1/2r)d_-(r))(x-(1/2r)d_+(r))} \tag{4.10}$$

with $d_\pm(r) \equiv 1 + r \pm \sqrt{r^2 - r + 1}$.

(d) Put $N = 4, r \equiv m_A/m_B \neq 1$, i.e. *ABAA-chains*. There is no contribution to the discrete measure because one finds (see [4a]) for the zeros of S_3, *viz* $x_1 = 1/r$, $2rx_\pm = 1 + r \pm \sqrt{r^2 + 1}$, $S_4(x_k)+\hat{S}_2(x_k)=0$ for $k = 1, \pm$. Like in the $N = 3$ case one can give the bands and the weight function explicitly.

5. Green's functions and the measure†

The purpose of this section is twofold: (i) to define the Green's functions of the general N-periodic problem which satisfy specific boundary conditions appropriate to the use of the Bloch–Floquet solutions encountered in section 2. (ii) To find the orthogonality measures computed in this work from these Green's functions. We shall also give the relation of the differential spectral density (or differential density of states) equation (1.8) to theses Green's functions which turns out to be the standard one. This should clarify the difference between the absolutely continuous part of the measure and the spectral density.

The Green's functions $\mathcal{G}_{n,m}(x)$ for the N-periodic problem are defined for $n, m \in \mathbf{N_0}$ by‡

$$Y_{n+1}(x)\,\mathcal{G}_{n,m}(x) - \mathcal{G}_{n+1,m}(x) - k_{n+1}\,\mathcal{G}_{n-1,m}(x) = \delta_{n,m}\,. \tag{5.1}$$

The Y-coefficient is defined in (1.3*b*). The inputs are $\mathcal{G}_{-1,m}(x)$ and $\mathcal{G}_{0,m}(x)$. The Green's functions with the proper boundary conditions turn out to be the ones constructed from the Bloch–Floquet solutions (2.6). This solution is of the type

$$\mathcal{G}_{n,m}(x) = a_m(x)\, q_{\max(n,m)+1,(-1)^k}(x)\, q_{\min(n,m)+1,(-1)^{k+1}}(x)\,. \tag{5.2}$$

The sign choice pertains to gap G_k, for which $q_{n+1,(-1)^k} \to 0$ for $x \in G_k$ and $n \to \infty$ (see equation (2.8)). The coefficient a_m is found from (5.1) putting $n = m$ and using the recursion formula for the $q_{n,\pm}$. For general input q_1 and q_0 one finds with the Wronskian (2.21)

$$\prod_{i=1}^{m+1} k_i \mathcal{G}_{n,m}(x) = \frac{1}{W(q_1, q_{N+1})\,(\lambda_{N,(-1)^k}(x) - \lambda_{N,(-1)^{k+1}}(x))} \times q_{\max(n,m)+1,(-1)^k}(x)\, q_{\min(n,m)+1,(-1)^{k+1}}(x)\,. \tag{5.3}$$

† This section is inspired by a paragraph found in [7] for periodic problems.

‡ The dependence on N, $\{k_n\}$, $\{\omega_n^2\}$ is suppressed. For the monic polynomials (2.1) one uses $(x - c_{n+1})\,\tilde{\mathcal{G}}_{n,m}(x) - d_{n+1}\,\tilde{\mathcal{G}}_{n-1,m}(x) - \tilde{\mathcal{G}}_{n+1,m}(x) = \delta_{n,m}$. The relation $(\prod_{i=1}^{n} \frac{\omega_0^2}{\omega_i^2})\,\tilde{\mathcal{G}}_{n,m} = (-2)^{m-n+1}(\prod_{i=1}^{m+1} \frac{\omega_0^2}{\omega_i^2})\,\mathcal{G}_{n,m}$ holds.

This is the Bloch–Floquet Green's function vanishing for x-values in gaps for $n \to \infty$ with fixed m and *vice versa*.

Our interest is in the diagonal Green's functions $\mathcal{G}_{n,n}(x)$ which are in fact q_0 and q_1 independent. This is due to identity (2.23) which shows that the Wronskian drops out. The final result can be written in terms of the mth associated polynomials $\{\mathcal{S}_n^{(m)}(x)\}$ defined in (2.20) like

$$\left(\prod_{i=1}^{n+1} k_i\right) \mathcal{G}_{n,n}(x) = \mathcal{S}_{N-1}^{(n+1)}(x) \Big/ \left(2\sqrt{\left(\mathcal{T}_N(x)\right)^2 - 1}\right). \tag{5.4}$$

The sign of the square root depends on the gap and band number. For the kth gap, G_k, it is $(-1)^k$, for the kth band, B_k it is $(-1)^{k+1}$ in accordance with the remarks found in section 2. In particular, one has for the input quantities

$$\mathcal{G}_{-1,-1}(x) = \frac{1}{2}\mathcal{S}_{N-1}(x) \Big/ \sqrt{\left(\mathcal{T}_N(x)\right)^2 - 1} \tag{5.5a}$$

$$\mathcal{G}_{0,0}(x) = \frac{1}{2k_1}\hat{\mathcal{S}}_{N-1}(x) \Big/ \sqrt{\left(\mathcal{T}_N(x)\right)^2 - 1}\,. \tag{5.5b}$$

The imaginary part of these input Green's functions are inversely related to the weight functions computed in this paper. For $x \in B_k$, $k = 1, 2, \ldots, N$, one finds

$$\operatorname{Im} \mathcal{G}_{-1,-1}(x) := \lim_{\eta \to 0_+} \operatorname{Im} \mathcal{G}_{-1,-1}(x + \mathrm{i}\eta) = \tfrac{1}{2}(-1)^k \mathcal{S}_{N-1}(x) \Big/ \sqrt{1 - \left(\mathcal{T}_N(x)\right)^2}\,. \tag{5.6}$$

In the gaps the imaginary part is zero. This shows that the absolutely continuous part of the $\{\mathcal{S}_n(x)\}$ measure (the weight function), which lives on the bands, is essentially the negative inverse of the imaginary part of the $\mathcal{G}_{-1,-1}$ Green's function.

$$-\operatorname{Im} \mathcal{G}_{-1,-1}(x) = \omega_0^2 / (\pi \omega_1^2 w(x)) \tag{5.7}$$

with (2.28b) and x in the bands. Similarly

$$-\operatorname{Im} \mathcal{G}_{0,0}(x) = \omega_0^2 / (\pi \omega_2^2 k_2 \hat{w}(x)) \tag{5.8}$$

with (2.30b). The average over the elementary N-unit of the chain for the diagonal Green's functions $\tilde{\mathcal{G}}_{n,n}(x)$, belonging to the monic polynomials $\{\tilde{\mathcal{S}}_n(x)\}$, can be computed with the help of the Christoffel–Darboux identities for the Bloch–Floquet solutions (2.6). These identities follow from the recursion formula (cf [1]), and they are (remember that $k_1 k_2 \ldots k_N = 1$ in the N-periodic case)

$$\begin{aligned} -2\sum_{n=0}^{N-1} \frac{\omega_0^2}{\omega_{n+1}^2 \prod_{i=1}^{n+1} k_i}\, q_{n+1,+}(x)\, q_{n+1,-}(x) \\ = q_{N,+}(x)\, q'_{N+1,-}(x) - q_{N+1,+}(x)\, q'_{N,-}(x) + q_{1,+}(x)\, q'_{0,-}(x) - q_{0,+}(x)\, q'_{1,-}(x)\,. \end{aligned} \tag{5.9}$$

There is an alternative version of this identity where the derivative acts on the left factor and an overall minus sign appears. This happens because the confluent Christoffel–Darboux identity implies

$$q_{N,+}(x)\, q_{N,-}(x) - q_{N,+}(x)\, q_{N+1,-}(x) - q_{1,+}(x)\, q_{0,-}(x) + q_{0,+}(x)\, q_{1,-}(x) \equiv 0 \tag{5.10}$$

which is in fact the Wronskian identity analogous to (2.21) for $W(q_{N+1,+}, q_{N+1,-})$. The connection between $\tilde{\mathcal{G}}_{n,n}(x)$, for the monic case, and $\mathcal{G}_{n,n}(x)$ is

$$\tilde{\mathcal{G}}_{n,n}(x) = -2\frac{\omega_0^2}{\omega_{n+1}^2}\,\mathcal{G}_{n,n}(x)\,. \tag{5.11}$$

Using equations (5.4) and (2.23) for the $(n+1)$th associated polynomials, identity (5.9), and the definitions (2.6) with (1.2), a lengthy calculation shows that for general inputs $q_0(x)$ and $q_1(x)$

$$\sum_{n=0}^{N-1} \tilde{\mathcal{G}}_{n,n}(x) = \mathcal{T}_N{}'(x)/\sqrt{\left(\mathcal{T}_N(x)\right)^2 - 1} \tag{5.12}$$

with the sign convention for gaps and bands mentioned earlier. Therefore, the imaginary part produces the differential spectral density (or differential density of states) known from the differentiation of the Bloch–Floquet phase:

$$\frac{1}{\pi}\lim_{\eta\to 0_+} \operatorname{Im}\frac{1}{N}\sum_{n=0}^{N-1} \tilde{\mathcal{G}}_{n,n}(x+\mathrm{i}\eta) = \mathcal{G}_N(x) \tag{5.13}$$

given by (1.8) for x values in the bands and zero otherwise. This result corroborates the choice of the Bloch–Floquet Green's functions. As a by-product we find from (5.12), (5.11) and (5.4) the identity

$$\sum_{n=0}^{N-1} \frac{\omega_0^2}{\omega_{n+1}^2\prod_{i=1}^{n+1} k_i}\,\mathcal{S}_{N-1}^{(n+1)}(x) = -\mathcal{T}_N{}'(x) \tag{5.14}$$

for the N-periodic case of the general associated polynomials (2.20) which collapses to the well known identity (1.10) for Chebyshev polynomials for the mono-atomic case.

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Appendix

A.1. Derivation of equation (2.14) (cf [6])

In the z-plane I_B is given by (2.11) with $\Gamma = \Gamma_{B''}$ defined by (2.12). The sign choice of $q_{n+1,\pm}$ depends on the band B_k, $k = 1, 2, \ldots, N$, where it is $(-1)^{k+1}$. $q_0 = 0$ and $q_1 = 1$ in (2.6*a*) with (1.2). The relation (2.14) with the appropriate sign choice for $\lambda_N(x) = \lambda_{N,(-1)^{k+1}}(x)$ is used in order to rewrite $q_{n+1,\pm}$ of (2.11). The piece with $q_{n+1,\mp}$ is, after a change of variable, seen to be the negative of the original integral I_B with the relevant $q_{n+1,\pm}$ choice for $x \in B_k$. The same change of variable is used to rewrite the second piece coming from (2.14) as twice the integral over only half of the contour, namely over $\Gamma_{B''_-}$ in the lower half of the z-plane.

A.2. Continued fractions for the $\{\hat{\mathcal{S}}_n\}$ measure calculation

The $\{\hat{\mathcal{S}}_n(x)\}$ recursion relation is given by (1.5*b*). Their first associated polynomials are $\{\mathcal{S}_n^{(2)}(x)\}$ defined by (2.20). The normalized measure $\mathrm{d}\hat{\sigma}$ obeys

$$\int \hat{\mathcal{S}}_n(x)\, \hat{\mathcal{S}}_m(x)\, \mathrm{d}\hat{\sigma}(x) = \frac{k_1}{k_2} \prod_{j=1}^{n+2} k_j \frac{\omega_{n+2}^2}{\omega_2^2} \delta_{n,m} = k_1^2 \frac{m_2}{m_{n+2}} \delta_{n,m} \qquad m, n \in \mathbf{N_0}\,. \tag{A.1}$$

The continued fraction $\hat{\chi}(x)$ which is related to this measure like in (3.3) has approximants

$$\hat{\chi}_n(x) = \frac{\tilde{\mathcal{S}}_{n-1}^{(2)}(x)}{\tilde{\mathcal{S}}_n^1(x)} = -\frac{2\omega_0^2}{k_2\omega_2^2}\left(\frac{k_2 \quad |}{|\quad Y_2(x)} - \frac{k_3 \quad |}{|\quad Y_3(x)} - \cdots - \frac{k_{n+1} \quad |}{|\quad Y_{n+1}(x)} - \cdots \right). \tag{A.2}$$

The tilde quantities are monic polynomials. $\mathcal{S}_n^{(1)} \equiv \hat{\mathcal{S}}_n$. The corresponding Möbius transformation is

$$\hat{J}_N(x; z) \equiv z' = \frac{k_2 \quad |}{|\ Y_2(x)} - \frac{k_3 \quad |}{|\ Y_3(x)} - \cdots - \frac{k_{N+1} \qquad |}{|\quad Y_{N+1}(x) - z} = \frac{\mathcal{S}_{N-2}^{(2)}(x)\ z - \mathcal{S}_{N-1}^{(2)}(x)}{\hat{\mathcal{S}}_{N-1}(x)\ z - \hat{\mathcal{S}}_N(x)}\,. \tag{A.3}$$

The fixed point solution can be written like

$$-\frac{k_2\omega_2^2}{2\omega_0^2}\hat{\chi}_{N,\pm}(x) = \left\{\hat{\mathcal{S}}_N(x) - k_1\lambda_{N,\pm}(x)\right\}/\hat{\mathcal{S}}_{N-1}(x) \tag{A.4}$$

where $\hat{\lambda}_{N,\pm} := \hat{\mathcal{T}}_N(x) \pm \sqrt{(\hat{\mathcal{T}}_N)^2 - k_1^2} = k_1\lambda_{N,\pm}$ was used which follows from (3.13) and (2.6*b*). The measure $\mathrm{d}\hat{\sigma}$ is then computed like in (3.5) from $\hat{\chi}$. With the definition (2.29) of the $\{\hat{s}_n\}$ polynomials one finds $\int \mathrm{d}\hat{\sigma}\ \hat{s}_n(x)\hat{s}_m(x) = \delta_{n,m}$ with $\mathrm{d}\hat{\sigma}$ given in (2.30).

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