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On some tridiagonal k-Toeplitz matrices: Algebraic and analytical aspects. Applications

R. Álvarez-Nodarse[a, b, *], J. Petronilho[c], N.R. Quintero[b, d]

[a] *Dpto. Análisis Matemático, Universidad de Sevilla, Apdo. 1160, 41080 Sevilla, Spain*
[b] *Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, E-18071 Granada, Spain*
[c] *Dpto. de Matemática, FCTUC, Universidade de Coimbra, Apdo. 3001-454 Coimbra, Portugal*
[d] *Dpto. Física Aplicada I, EUP, Universidad de Sevilla, Virgen de África 7, 41011 Sevilla, Spain*

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Abstract

In this paper, we use the analytic theory for 2 and 3-Toeplitz matrices to obtain the explicit expressions for the eigenvalues, eigenvectors and the spectral measure associated to the corresponding infinite matrices. As an application we consider two solvable models related with the so-called chain model. Some numerical experiments are also included.

Keywords: k-Toeplitz matrices; Jacobi matrices; Orthogonal polynomials; Chain models

1. Introduction

k-Toeplitz matrices are tridiagonal matrices of the form $A=[a_{i,j}]_{i,j=1}^{n}$ (with $n\geqslant k$) such that

$$a_{i+k,j+k}=a_{i,j} \quad (i,\, j=1,2,\ldots,n-k),$$

so that they are k-periodic along the diagonals parallel to the main diagonal [8]. When $k=1$ it reduces to a tridiagonal Toeplitz matrix.

* Corresponding address. Departamento de Análisis Matemático, Universidad de Sevilla, Apdo. 1160, 41080 Sevilla, Spain.

E-mail address: ran@us.es (R. Álvarez-Nodarse).

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The interest of the study of k-Toeplitz matrices appears to be very important not only from a theoretical point of view (in linear algebra or numerical analysis, e.g.), but also in applications. For instance, it is useful in the study of sound propagation problems (see [2,9]).

In this paper, we present a complete study of the eigenproblems for tridiagonal 2 and 3-Toeplitz matrices, including the spectral measure associated to the corresponding infinite Jacobi matrices, and then we apply the results to the study of the so called chain models in Quantum Physics. Since we hope that our discussion could be of interest both to readers working on Applied Mathematics and Orthogonal Polynomials as well as physicists, we will further develop the works [5,6,14–17] including several results on tridiagonal k-Toeplitz matrices that follow from the results in those papers but not explicitly included there. Of particular interest is the symmetric case because of its interest in the study of quantum chain models.

In fact, one of the main problems in Quantum Physics is to find the solutions of the stationary Schrödinger equation

$$\mathscr{H}|\Phi\rangle = \varepsilon|\Phi\rangle, \tag{1.1}$$

where $\mathscr{H}$ is the Hamiltonian of the system and ε is the energy corresponding to the state $|\Phi\rangle$. A usual method for solving Eq. (1.1) is to expand the unknown wave functions $|\Phi\rangle$ in the "discrete" basis (not necessarily orthogonal) $\{|\Phi_k\rangle\}_{k=1}^{\infty}$, i.e.,

$$|\Phi\rangle = \sum_{k=1}^{N} C_{Nk}|\Phi_k\rangle. \tag{1.2}$$

Substituting Eq. (1.2) in (1.1) and multiplying by $\langle\Phi_m|$ and taking into account the orthogonality of the functions $|\Phi_k\rangle$ we obtain the following linear system of equations

$$\sum_{k=1}^{N} C_{Nk}\langle\Phi_m|\mathscr{H}|\Phi_k\rangle = \varepsilon C_{Nm}. \tag{1.3}$$

If we denote the matrix elements $\langle\Phi_m|\mathscr{H}|\Phi_k\rangle$ by h_{mk} then we can rewrite (1.3) in the matrix form

$$\begin{pmatrix} h_{11} & h_{12} & \dots & h_{1N-1} & h_{1N} \\ h_{21} & h_{22} & \dots & h_{2N-1} & h_{2N} \\ h_{31} & h_{32} & \dots & h_{3N-1} & h_{3N} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ h_{N-1} & h_{N-12} & \dots & h_{N-1N-1} & h_{N-1N} \\ h_{N1} & h_{N2} & \dots & h_{NN-1} & h_{NN} \end{pmatrix} \begin{pmatrix} C_{N1} \\ C_{N2} \\ C_{N3} \\ \vdots \\ C_{N-1N} \\ C_{NN} \end{pmatrix} = \varepsilon \begin{pmatrix} C_{N1} \\ C_{N2} \\ C_{N3} \\ \vdots \\ C_{N-1N} \\ C_{NN} \end{pmatrix}. \tag{1.4}$$

In general, the computation of the eigenvalues (and also the eigenvectors) for an arbitrary matrix, as the previous one in (1.4), is very difficult since it is equivalent to the problem of finding the roots of a polynomial of degree N. Moreover, the numerical algorithms (Newton's Method, etc.) are, in general, unstable for large N. For this reason simpler models (which are easier to solve and numerically more stable and economic) have been introduced. One of these models is the so called *chain model* which has been successfully used in Solid State Physics [12], Nuclear Physics [22], and Quantum Mechanics [11], etc. In fact, any quantum model can be transformed into the corresponding *chain model* (see [10] and references therein).

In our previous paper [1] we have briefly considered the 2-periodic chain model—the *constant chain model*, i.e., when the sequences $\{a_n\}$ and $\{b_n\}$ are constants equal to a and b, respectively, has been considered in [10]—i.e., when the sequences $\{a_n\}$ and $\{b_n\}$ are periodic sequences with period 2, i.e., $\{a_n\} = \{a, b, a, b, \ldots\}$ and $\{b_n\} = \{c, d, c, d, \ldots\}$. For such models it is possible to obtain analytic formulae for the values of the energy (eigenvalues) of $\mathscr{H}$ and its corresponding wave functions. Here we will conclude the study started in [1] for the two chain model and will present the complete study of the 3-periodic chain model.

The structure of the paper is as follows. In Section 2, we give the needed mathematical background. Section 3 is devoted to some applications of the theory of tridiagonal k-Toeplitz matrices in quantum physics: concretely to the so-called chain model.

2. Mathematical background

We start with some basic results from the general theory of orthogonal polynomials (see e.g. [3]). It is known that any orthogonal polynomial sequence (OPS) $\{P_n\}_{n\geqslant 0}$ it is characterised by a three-term recurrence relation

$$xP_n(x) = \alpha_n P_{n+1}(x) + \beta_n P_n(x) + \gamma_n P_{n-1}(x), \quad n = 0, 1, 2, \ldots \tag{2.1}$$

with initial conditions $P_{-1} = 0$ and $P_0 = 1$ where $\{\alpha_n\}_{n\geqslant 0}$, $\{\beta_n\}_{n\geqslant 0}$ and $\{\gamma_n\}_{n\geqslant 1}$ are sequences of complex numbers such that $\alpha_n\gamma_{n+1} \neq 0$ for all $n \geqslant 0$, or in matrix form

$$x\mathbf{P}_n(x) = J_{n+1}\mathbf{P}_n(x) + \alpha_n P_{n+1}(x)\mathbf{e}_n, \tag{2.2}$$

where $\mathbf{P}_n(x) = [P_0(x), \ldots, P_n(x)]^{\mathrm{T}}$, $\mathbf{e}_n = [0, 0, \ldots, 0, 1]^{\mathrm{T}} \in \mathbb{R}^{n+1}$ and J_{n+1} is the tridiagonal matrix of order $n+1$

$$J_{n+1} = \begin{bmatrix} \beta_0 & \alpha_0 & 0 & 0 & \ldots & 0 & 0 \\ \gamma_1 & \beta_1 & \alpha_1 & 0 & \ldots & 0 & 0 \\ 0 & \gamma_2 & \beta_2 & \alpha_2 & \ldots & 0 & 0 \\ 0 & 0 & \gamma_3 & \beta_3 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \ldots & \beta_{n-1} & \alpha_{n-1} \\ 0 & 0 & 0 & 0 & \ldots & \gamma_n & \beta_n \end{bmatrix}.$$

If $\{x_{nj}\}_{1\leqslant j\leqslant n}$ are the zeros of the polynomial P_n, then it follows from (2.2) that each x_{nj} is an eigenvalue of the corresponding tridiagonal matrix J_n and $\mathbf{P}_{n-1}(x_{nj}) := [P_0(x_{nj}), \ldots, P_{n-1}(x_{nj})]^{\mathrm{T}}$ is a corresponding eigenvector.

When $\alpha_n = 1$ and $\gamma_n > 0$ for all $n = 1, 2, \ldots$ the (monic) polynomials $\{P_n\}_{n\geqslant 0}$ defined by the recurrence relation (2.1) arise as denominators of the approximants of the continued fraction

$$\cfrac{1}{x-\beta_0-\cfrac{\gamma_1}{x-\beta_1-\cfrac{\gamma_2}{x-\beta_2-\cdots-\cfrac{\gamma_{n-1}}{x-\beta_{n-1}-\cfrac{\gamma_n}{x-\beta_n-\ddots}}}}}$$

Under these conditions, by Favard's theorem [3], $\{P_n\}_{n\geqslant 0}$ constitutes an orthogonal polynomial sequence with respect to a positive definite moment functional, and if the moment problem associated with the continued fraction is determined, then this linear functional can be characterised by a unique distribution function, i.e., a function $\sigma : \mathbb{R} \to \mathbb{R}$ which is nondecreasing, it has infinitely many points of increase and all the moments $\int_{-\infty}^{+\infty} x^{2n}\, \mathrm{d}\sigma(x)$, $n = 0, 1, 2, \ldots,$ are finite. The numerators of the continued fraction, denoted by $\{P_n^{(1)}\}_{n\geqslant 0}$, can be given by the shifted recurrence relation

$$xP_n^{(1)}(x) = P_{n+1}^{(1)}(x) + \beta_{n+1}P_n^{(1)}(x) + \gamma_{n+1}P_{n-1}^{(1)}(x), \quad n\geqslant 0$$

with initial conditions $P_{-1}^{(1)} = 0$ and $P_0^{(1)} = 1$. This continued fraction converges to a function $F(z;\sigma)$ and the general theory of the moment problem ensures that F is analytic in the complex plane with a cut along the support of σ (i.e., the set of points of increase of σ). This fact can be summarised by Markov–Stieltjes's theorem

$$-\lim_{n\to+\infty} \frac{\mu_0 P_{n-1}^{(1)}(z)}{P_n(z)} = F(z;\sigma) := \int_{-\infty}^{+\infty} \frac{\mathrm{d}\sigma(x)}{x-z}, \quad z \in \mathbb{C}\backslash\mathrm{supp}(\sigma), \tag{2.3}$$

where $\mu_0 = \int_{-\infty}^{+\infty} \mathrm{d}\sigma(x)$ is the first moment of the distribution $\sigma(x)$ and F is its Stieltjes function. Now, the function $\sigma(x)$ can be recovered from (2.3) by applying the Stieltjes inversion formula

$$\sigma(x) - \sigma(y) = \lim_{\varepsilon\to 0^+} \frac{1}{\pi}\int_y^x \Im F(t+i\varepsilon,\sigma)\,\mathrm{d}t,$$

where it is assumed that σ is normalised in the following way

$$\sigma(-\infty) = 0, \quad \sigma(x) = \frac{\sigma(x+0)+\sigma(x-0)}{2}$$

and $\Im z$ denotes the imaginary part of z.

An important family of orthogonal polynomials are the orthonormal Chebyshev polynomials of second kind $\{U_n(x)\}_{n\geqslant 0}$ defined in terms of trigonometric polynomials in $\cos\theta$ as

$$U_n(x) = \frac{\sin(n+1)\theta}{\sin\theta}, \quad x = \cos\theta.$$

For these polynomials (2.1) takes the form

$$U_{-1} = 0, \quad U_0 = 1, \quad 2xU_n(x) = U_{n+1}(x) + U_{n-1}(x), \quad n = 0, 1, 2, \ldots .$$

They are orthonormal with respect to the distribution function

$$\mathrm{d}\sigma_U(x) = \frac{2}{\pi}\sqrt{1-x^2}\,\mathrm{d}x, \quad \operatorname{supp}(\sigma_U) = [-1,1],$$

i.e.,

$$\int_{-1}^{1} U_n(x)U_m(x)\,\mathrm{d}\sigma_U(x) = \delta_{n,m},$$

where $\delta_{n,m}$ is the Kronecker symbol: $\delta_{k,m}=1$ for $k=m$, elsewhere $\delta_{k,m}=0$. The corresponding Stieltjes function is

$$F_U(z) = \frac{-2}{z+\sqrt{z^2-1}} = -2\left(z-\sqrt{z^2-1}\right), \quad z \in \mathbb{C}\setminus[-1,1], \tag{2.4}$$

where the complex square root is such that $|z+\sqrt{z^2-1}|>1$ whenever $z \notin [-1,1]$.

The Chebychev polynomials U_n are closely related with the tridiagonal 2 and 3 Toeplitz matrices as it is shown in the next two sections.

2.1. Remarks on tridiagonal 2-Toeplitz matrices

Let B_N be the irreducible tridiagonal 2-Toeplitz matrix

$$B_N = \begin{bmatrix} a_1 & b_1 & 0 & 0 & 0 & \dots \\ c_1 & a_2 & b_2 & 0 & 0 & \dots \\ 0 & c_2 & a_1 & b_1 & 0 & \dots \\ 0 & 0 & c_1 & a_2 & b_2 & \dots \\ 0 & 0 & 0 & c_2 & a_1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \in \mathbb{R}^{(N,N)}, \quad N \in \mathbb{N}, \tag{2.5}$$

where $b_1,\ b_2,\ c_1$ and c_2 are positive numbers. Define the polynomials

$$\pi_2(x) = (x-a_1)(x-a_2)$$

and

$$P_n(x) = (b_1b_2c_1c_2)^{n/2}U_n\left(\frac{x-b_1c_1-b_2c_2}{2\sqrt{b_1b_2c_1c_2}}\right), \quad n=0,1,2,\dots,$$

where U_n is the Chebyshev polynomial of second kind.

The following theorem holds

Theorem 2.1 (*Gover [7] and Marcellán and Petronilho [14]*). *Let B_N, $N=1,2,3,\dots$, be the irreducible tridiagonal 2-Toeplitz matrix given by* (2.5), *where b_1, b_2, c_1, and c_2 are positive numbers. The sequence $\{S_n\}_{n\geqslant 0}$ of orthogonal polynomials associated with the matrices B_N is*

$$S_{2k}(x) = (b_1b_2)^{-k}\{P_k(\pi_2(x)) + b_2c_2P_{k-1}(\pi_2(x))\},$$

$$S_{2k+1}(x) = (b_1^{-1}(b_1b_2)^{-k}(x-a_1)P_k(\pi_2(x)), \quad k=0,1,\dots\ .$$

Then the eigenvalues $\lambda_{N,m}$ of B_N are the zeros of S_N, and the corresponding eigenvectors $\mathbf{v}_{N,m}$ are given by

$$\mathbf{v}_{N,m} = \begin{pmatrix} S_0(\lambda_{N,m}) \\ S_1(\lambda_{N,m}) \\ \vdots \\ S_{N-1}(\lambda_{N,m}) \end{pmatrix}, \quad m = 1, 2, \ldots, N.$$

In particular,[1] *the eigenvalues $\lambda_{2n+1,m}$ of B_{2n+1} ($m=1, 2, \ldots, 2n+1$) are $\lambda_{2n+1,1}=a_1$ and the solutions of the quadratic equations*

$$\pi_2(\lambda) - \left[b_1c_1 + b_2c_2 + 2\sqrt{b_1b_2c_1c_2}\cos\frac{k\pi}{n+1}\right] = 0, \quad k = 1, \ldots, n. \tag{2.6}$$

Notice that since the sequence $\{S_k\}_k$ is an orthogonal polynomial sequence corresponding to a positive definite case, then the zeros are simple and interlace, i.e., if $\{x_{k,j}\}_{j=1}^{k}$ denotes the zeros of the polynomial S_k, then

$$x_{k,j} < x_{k-1,j} < x_{k,j+1}, \quad j = 1, 2, \ldots, k-1.$$

Therefore using the values (2.6) we can obtain bounds for the eigenvalues of the corresponding matrices for the even case.

Moreover (cf. [20]; see also [15]), the Stieltjes function associated to the sequence $\{S_n\}_{n\geqslant 0}$ reads as

$$F_S(z) = \frac{1}{a_1 - z} - \frac{1}{2b_2c_2}\frac{1}{z - a_1}\left(\pi_2(z) - \beta - \sqrt{(\pi_2(z) - \beta)^2 - \alpha^2}\right), \tag{2.7}$$

where $\alpha = 2\sqrt{b_1b_2c_1c_2}$ and $\beta = b_1c_1 + b_2c_2$. Furthermore, $\{S_n\}_{n\geqslant 0}$ is orthogonal with respect to the distribution function

$$\mathrm{d}\sigma_S(x) = M\delta(x - a_1)\,\mathrm{d}x + \frac{1}{2\pi b_2c_2}\frac{1}{|x - a_1|}\sqrt{\alpha^2 - (\pi_2(x) - \beta)^2}\,\mathrm{d}x, \tag{2.8}$$

where $M = 1 - \min\{b_1c_1, b_2c_2\}/(b_2c_2)$ and which support is the union of two intervals if $M = 0$ and the union of two intervals with a singular set if $M > 0$, i.e.,

$$\mathrm{supp}(\sigma_S) = \begin{cases} \Sigma_S & \text{if } b_1c_1 \leqslant b_2c_2, \\ \Sigma_S \cup \{a_1\} & \text{if } b_1c_1 > b_2c_2, \end{cases}$$

---

[1] For the case when $b_1c_1 > b_2c_2$ the eigenvalues $\lambda_{2n,m}$ of B_{2n} ($m=1, 2, \ldots, 2n$) are the solutions of the quadratic equations

$$\pi_2(\lambda) - [b_1c_1 + b_2c_2 + 2\sqrt{b_1b_2c_1c_2}\cos\theta_{nk}] = 0, \quad k = 1, \ldots, n,$$

where θ_{nk}'s are the nonzero solutions of the trigonometric equation

$$\sqrt{b_1c_1}\sin[(n+1)\theta] + \sqrt{b_2c_2}\sin(n\theta) = 0, \quad (0 < \theta < \pi).$$

.

where $\Sigma_S = [\frac{a_1+a_2}{2} - s,\ \frac{a_1+a_2}{2} - r] \cup [\frac{a_1+a_2}{2} + r,\ \frac{a_1+a_2}{2} + s]$ and

$$r = \sqrt{|\sqrt{b_1c_1} - \sqrt{b_2c_2}|^2 + \left|\frac{a_1-a_2}{2}\right|^2}, \quad s = \sqrt{|\sqrt{b_1c_1} + \sqrt{b_2c_2}|^2 + \left|\frac{a_1-a_2}{2}\right|^2}.$$

2.2. Remarks on tridiagonal 3-Toeplitz matrices

Let us now consider the irreducible tridiagonal 3-Toeplitz matrix

$$B_N = \begin{bmatrix} a_1 & b_1 & 0 & 0 & 0 & 0 & 0 & \dots \\ c_1 & a_2 & b_2 & 0 & 0 & 0 & 0 & \dots \\ 0 & c_2 & a_3 & b_3 & 0 & 0 & 0 & \dots \\ 0 & 0 & c_3 & a_1 & b_1 & 0 & 0 & \dots \\ 0 & 0 & 0 & c_1 & a_2 & b_2 & 0 & \dots \\ 0 & 0 & 0 & 0 & c_2 & a_3 & b_3 & \dots \\ 0 & 0 & 0 & 0 & 0 & c_3 & a_1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \in \mathbb{R}^{(N,N)}, \quad N \in \mathbb{N}. \tag{2.9}$$

Define

$$P_n(x) = (b_1b_2b_3c_1c_2c_3)^{n/2} U_n\left(\frac{x - b_1c_1 - b_2c_2 - b_3c_3}{2\sqrt{b_1b_2b_3c_1c_2c_3}}\right), \quad n = 0, 1, 2, \dots .$$

Let ξ_1 and ξ_2 be the zeros of the quadratic polynomial

$$(x-a_1)(x-a_2) - b_1c_1 \tag{2.10}$$

and define the polynomial

$$\begin{aligned} \pi_3(x) := {} & (x-a_1)(x-a_2)(x-a_3) - (b_1c_1 + b_2c_2 + b_3c_3)(x-a_3) \\ & + b_2c_2(a_1-a_3) + b_3c_3(a_2-a_3) + b_1c_1 + b_2c_2 + b_3c_3. \end{aligned} \tag{2.11}$$

In this case we have the following

Theorem 2.2 (*Marcellán and Petronilho [16]*). *Let B_N, $N = 1, 2, 3 \dots$, be the irreducible tridiagonal* 3-*Toeplitz matrix given by* (2.9), *where b_1, b_2, b_3, c_1, c_2 and c_3 are positive numbers. The sequence $\{S_n\}_{n \geqslant 0}$ of orthogonal polynomials associated with the matrices B_N* is

$$S_{3k}(x) = (b_1b_2b_3)^{-k}\{P_k(\pi_3(x)) + b_3c_3(x-a_2)P_{k-1}(\pi_3(x))\},$$

$$S_{3k+1}(x) = b_1^{-1}(b_1b_2b_3)^{-k}\{(x-a_1)P_k(\pi_3(x)) + b_1c_1b_3c_3P_{k-1}(\pi_3(x))\},$$

$$S_{3k+2}(x) = (b_1b_2)^{-1}(b_1b_2b_3)^{-k}(x-\xi_1)(x-\xi_2)P_k(\pi_3(x)), \quad k = 0, 1, \dots,$$

where ξ_1 and ξ_2 are the roots of the polynomial (2.10) *and π_3 is the polynomial given by* (2.11). *Then the eigenvalues $\lambda_{N,m}$ of B_N are the zeros of S_N, and the corresponding eigenvectors $\mathbf{v}_{N,m}$ are given by*

$$\mathbf{v}_{N,m} = \begin{pmatrix} S_0(\lambda_{N,m}) \\ S_1(\lambda_{N,m}) \\ \vdots \\ S_{N-1}(\lambda_{N,m}) \end{pmatrix}, \quad m = 1, 2, \ldots, N.$$

In particular, when $N = 3n+2$, the eigenvalues $\lambda_{3n+2,m}$ of B_{3n+2} ($m = 1, 2, \ldots, 3n+2$) are $\lambda_{3n+2,1} = \xi_1$, $\lambda_{3n+2,2} = \xi_2$ and the solutions of the cubic equations

$$\pi_3(\lambda) - \left[b_1c_1 + b_2c_2 + b_3c_3 + 2\sqrt{b_1b_2b_3c_1c_2c_3}\cos\frac{k\pi}{n+1}\right] = 0, \quad k = 1, \ldots, n. \tag{2.12}$$

As in the previous case, we can use the values (2.12) to give bounds for the eigenvalues of the corresponding matrices in the $N = 3n$ and $N = 3n+1$ cases.

In this case [17] the Stieltjes function associated to the sequence $\{S_n\}_{n\geqslant 0}$ is

$$\begin{aligned} F_S(z) = {} & \frac{\xi_2 - a_1}{\xi_2 - \xi_1}\frac{1}{\xi_1 - z} + \frac{a_1 - \xi_1}{\xi_2 - \xi_1}\frac{1}{\xi_2 - z} \\ & - \frac{1}{2b_1c_1b_3c_3}\frac{(a_1 - \xi_1)(a_1 - \xi_2)}{(z - \xi_1)(z - \xi_2)}\left(\pi_3(z) - \beta - \sqrt{(\pi_3(z) - \beta)^2 - \alpha^2}\right), \end{aligned} \tag{2.13}$$

where $\alpha = 2\sqrt{b_1b_2b_3c_1c_2c_3}$ and $\beta = b_1c_1 + b_2c_2 + b_3c_3$. In (2.13) the square root is such that $|z - \beta + \sqrt{(z-\beta)^2 - \alpha^2}| > \alpha$ whenever $z \notin [\beta - \alpha, \beta + \alpha]$. Moreover, $\{S_n\}_{n\geqslant 0}$ is orthogonal with respect to the distribution function

$$\begin{aligned} \mathrm{d}\sigma_S(x) = {} & M_1\delta(x - \xi_1)\,\mathrm{d}x + M_2\delta(x - \xi_2)\,\mathrm{d}x \\ & - \frac{1}{2\pi b_1c_1b_3c_3}\frac{(a_1 - \xi_1)(a_1 - \xi_2)}{|(x - \xi_1)(x - \xi_2)|}\sqrt{\alpha^2 - (\pi_3(x) - \beta)^2}\,\mathrm{d}x, \end{aligned}$$

which support is contained in the union of the three intervals $\Sigma_S = \pi_3^{-1}([\beta - \alpha, \beta + \alpha])$ (see Fig. 1) with two possible mass points at ξ_1 and ξ_2, i.e.,

$$\operatorname{supp}(\sigma_S) = \begin{cases} \Sigma_S & \text{if } M_1 = 0, M_2 = 0, \\ \Sigma_S \cup \{\xi_2\} & \text{if } M_1 = 0, M_2 > 0, \\ \Sigma_S \cup \{\xi_1\} & \text{if } M_1 > 0, M_2 = 0, \\ \Sigma_S \cup \{\xi_1, \xi_2\} & \text{if } M_1 > 0, M_2 > 0, \end{cases}$$

where

$$M_1 = -\frac{a_1 - \xi_2}{\xi_1 - \xi_2}\left[1 - \frac{b_2c_2(\xi_1 - a_1)}{\alpha}F_U\left(\frac{\pi_3(\xi_1) - \beta}{\alpha}\right)\right]$$

and

$$M_2 = \frac{\xi_1 - a_1}{\xi_1 - \xi_2}\left[1 - \frac{b_2c_2(\xi_2 - a_1)}{\alpha}F_U\left(\frac{\pi_3(\xi_2) - \beta}{\alpha}\right)\right].$$

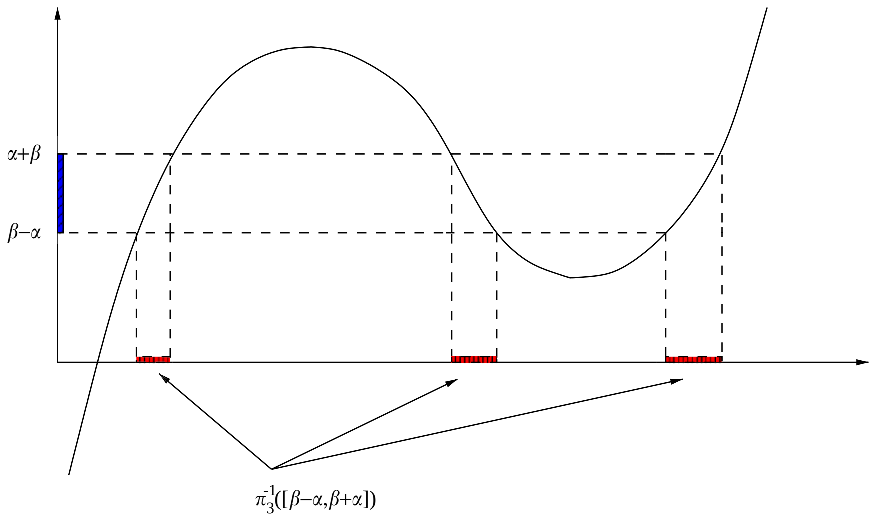

Fig. 1. The polynomial mapping $[\beta-\alpha, \beta+\alpha] \mapsto \pi_3^{-1}([\beta-\alpha, \beta+\alpha])$.

If we now take into account the identity

$$4[(\pi_3(\xi_1)-\beta)^2-\alpha^2] = [(b_3c_3-b_2c_2)\Delta + (a_1-a_2)(b_3c_3+b_2c_2)]^2,$$

where $\Delta = \sqrt{(a_1-a_2)^2+4b_1c_1}$ as well as the right choice of the branch of the square root in the definition of F_U (2.4) we find

$$M_1 = \frac{\max\{0, (b_3c_3-b_2c_2)\Delta + (a_1-a_2)(b_3c_3+b_2c_2)\}}{2b_3c_3\Delta} \geqslant 0,$$
$$M_2 = \frac{\max\{0, (b_3c_3-b_2c_2)\Delta - (a_1-a_2)(b_3c_3+b_2c_2)\}}{2b_3c_3\Delta} \geqslant 0. \tag{2.14}$$

A simple inspection of the values of M_1 and M_2 leads to the following four cases:

1. $b_3c_3 \geqslant b_2c_2$ and $a_1 \geqslant a_2$. In this case

- $M_1 = 0$ iff $a_1 = a_2$ and $b_3c_3 = b_2c_2$,
- $M_2 = 0$ iff $b_3c_3 \leqslant b_2c_2 + |a_1-a_2|(b_3c_3+b_2c_2)\Delta^{-1}$.

2. $b_3c_3 \geqslant b_2c_2$ and $a_1 \leqslant a_2$. Then

- $M_1 = 0$ iff $b_3c_3 \leqslant b_2c_2 + |a_1-a_2|(b_3c_3+b_2c_2)\Delta^{-1}$,
- $M_2 = 0$ iff $a_1 = a_2$ and $b_3c_3 = b_2c_2$.

3. $b_3c_3 \leqslant b_2c_2$ and $a_1 \geqslant a_2$. Then

- $M_1 = 0$ iff $b_3c_3 \leqslant b_2c_2 - |a_1-a_2|(b_3c_3+b_2c_2)\Delta^{-1}$,
- In this case always $M_2 = 0$.

4. $b_3c_3 \leqslant b_2c_2$ and $a_1 \leqslant a_2$.

- In this case always $M_1 = 0$,
- $M_2 = 0$ iff $b_3c_3 \leqslant b_2c_2 - |a_1 - a_2|(b_3c_3 + b_2c_2)\Delta^{-1}$.

2.3. Some remarks on a matrix theoretic approach

Here we want to emphasize another approach to the problem concerning the study of the spectral properties (eigenvalues, eigenvectors and asymptotic (limit) spectral measure) of the sequences of matrices defined by (2.5) and (2.9), based on recent results by Serra Capizzano, Fasino, Kuijlaars and Tilli (cf. [4,13,18,19]). To simplify we will consider the case when the order N of the matrix B_N in (2.5) is even. Then B_N is the block Toeplitz matrix

$$B_N = \begin{bmatrix} A_0 & A_{-1} & & & \\ A_1 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & A_{-1} \\ & & & A_1 & A_0 \end{bmatrix}$$

generated by the 2×2 matrix valued polynomial

$$\mathbf{f}_2(x) := A_0 + A_1 \mathrm{e}^{\mathrm{i}x} + A_{-1}\mathrm{e}^{-\mathrm{i}x}$$

with

$$A_0 := \begin{bmatrix} a_1 & b_1 \\ c_1 & a_2 \end{bmatrix}, \quad A_1 := \begin{bmatrix} 0 & 0 \\ b_2 & 0 \end{bmatrix}, \quad A_{-1} := \begin{bmatrix} 0 & c_2 \\ 0 & 0 \end{bmatrix}.$$

Since, in general, $\mathbf{f}_2(x)$ is not hermitian then not very much can be said on the eigenvalues. However, according to Theorem 2.1 the conditions $b_1c_1 > 0$ and $b_2c_2 > 0$ hold, and so it is well-known that, under such conditions, B_N is similar (via diagonal transformations) to the block Toeplitz matrix $\hat{B}_N$ generated by the 2×2 matrix valued polynomial

$$\hat{\mathbf{f}}_2(x) := \hat{A}_0 + \hat{A}_1 \mathrm{e}^{\mathrm{i}x} + \hat{A}_{-1}\mathrm{e}^{-\mathrm{i}x}$$

with

$$\hat{A}_0 := \begin{bmatrix} a_1 & \sqrt{b_1c_1} \\ \sqrt{b_1c_1} & a_2 \end{bmatrix}, \quad \hat{A}_1 := \begin{bmatrix} 0 & 0 \\ \sqrt{b_2c_2} & 0 \end{bmatrix}, \quad \hat{A}_{-1} := \begin{bmatrix} 0 & \sqrt{b_2c_2} \\ 0 & 0 \end{bmatrix}.$$

Similar considerations remains true for the generalized case of a tridiagonal k-Toeplitz matrix (see Eq. (2.1) in [4]). Now, the limit distribution is described in Theorems 2.1 and 2.2 in [4]. In our specific case the spectra of the matrix B_N distributes as the eigenvalues of $\hat{\mathbf{f}}_2(x)$, which are

$$\lambda_{\pm}(x) := \frac{a_1 + a_2}{2} \pm \sqrt{\left(\frac{a_1 - a_2}{2}\right)^2 + b_1c_1 + b_2c_2 + 2\sqrt{b_1c_1b_2c_2}\cos x}.$$

More precisely, it follows from Theorem 2.2 in [4] that, with possible exception of at most a denumerable set of point masses, the support of the measure of orthogonality for the orthogonal polynomials corresponding to B_N is contained in the set

$$\mathscr{S} := [\lambda_1^-, \lambda_1^+] \cup [\lambda_2^-, \lambda_2^+]$$

(and the zeros of the orthogonal polynomials are dense in this set), where

$$\begin{aligned} \lambda_1^- &:= \min\{\lambda_-(0), \lambda_-(\pi)\}, & \lambda_1^+ &:= \max\{\lambda_-(0), \lambda_-(\pi)\}, \\ \lambda_2^- &:= \min\{\lambda_+(0), \lambda_+(\pi)\}, & \lambda_2^+ &:= \max\{\lambda_+(0), \lambda_+(\pi)\}. \end{aligned}$$

Therefore, since

$$\lambda_\pm(0) = \frac{a_1 + a_2}{2} \pm \sqrt{\left(\frac{a_1 - a_2}{2}\right)^2 + \left(\sqrt{b_1 c_1} + \sqrt{b_2 c_2}\right)^2}$$

and

$$\lambda_\pm(\pi) = \frac{a_1 + a_2}{2} \pm \sqrt{\left(\frac{a_1 - a_2}{2}\right)^2 + \left(\sqrt{b_1 c_1} - \sqrt{b_2 c_2}\right)^2},$$

we see that $\mathscr{S}$ is the same union of two intervals given in the end of Section 2.1. Also, the limit spectral measure follows from asymptotic spectral theory of Toeplitz matrices.

We remark that the spectral distribution holds for odd N as well since constant rank corrections do not modify the asymptotic spectral distribution. Further, the results in [4] are true for every k-Toeplitz matrix sequences (and so, in particular, for $k = 2$ and $k = 3$), as well as for variable recurrence coefficients (see also [13]) and in the multidimensional case (cf. also [18,19]). On the other hand, our results in Theorems 2.1 and 2.2 gives more precise information on the localization of the zeros.

As a final remark, we would like to point out that in the present paper the theory of orthogonal polynomials is used for giving spectral information, while in [4,13] the idea is exactly the opposite since matrix theoretic tools are used for deducing information on the zeros of orthogonal polynomials.

3. Applications: the chain model

Here we will resume some important properties of the chain model. For a more detailed study we refer to the nice paper by Haydock [10].

Definition 3.1 (*Haydocle [10]*). The Chain Model is a quantum model determined by a sequence of orthonormal orbits (states) $\{\mathbf{u}_0, \mathbf{u}_1, \ldots\}$ and two sets of real parameters $\{a_1, a_2, \ldots\}$ and $\{b_1, b_2, \ldots\}$, which describe the action of the Hamiltonian $\mathbf{H}$ on the orbitals by a symmetric three-term recurrence relation of the form

$$\mathbf{H}\mathbf{u}_n = b_{n+1}\mathbf{u}_{n+1} + a_n \mathbf{u}_n + b_n \mathbf{u}_{n-1}. \tag{3.1}$$

The sequence $\{\mathbf{u}_0, \mathbf{u}_1, \ldots\}$ may be finite or infinite. In the first case we need to take the orbitals $\mathbf{u}_{-1}$ and $\mathbf{u}_{N+1}$ equal to zero. Moreover, in [10] it has been shown that this model is equivalent to expressing the matrix **H** by using an appropriate basis as a Jacobi (tridiagonal symmetric) matrix

$$\mathbf{H}=\begin{pmatrix} a_0 & b_1 & 0 & 0 & \dots \\ b_1 & a_1 & b_2 & 0 & \dots \\ 0 & b_2 & a_2 & b_3 & \dots \\ 0 & 0 & b_3 & a_3 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{3.2}$$

In the following we will suppose that the solution $\mathbf{u}$ of the Schrödinger equation (1.1) can be written as a linear combination of the states $\mathbf{u}_0, \mathbf{u}_1, \mathbf{u}_2, \dots$, i.e.,

$$\mathbf{u}=\sum_{k=0}^{\infty} C_k \mathbf{u}_k. \tag{3.3}$$

For this model it is possible to obtain analytic formulae for the so-called general diagonal Green function $G_0(\varepsilon)$. In [10,12] it is shown that $G_0(\varepsilon)$ for the chain model (3.1) is related to the continued fraction

$$G_0(\varepsilon)=\cfrac{1}{\varepsilon-a_0-\cfrac{b_1^2}{\varepsilon-a_1-\cfrac{b_2^2}{\varepsilon-a_2-\cdots-\cfrac{b_n^2}{\varepsilon-a_n-\ddots}}}}, \quad \varepsilon\in\mathbb{C} \tag{3.4}$$

For the finite chain model, this continued fraction reduces to the ratio of two polynomials which conforms the well known Padé approximants of order n of the infinite continued fraction. This and some other results concerning the calculation of the Green function will be considered in detail in the next section. Of particular interest are the function $G_0(\varepsilon)$—the real part of $G_0(\varepsilon)$ describes the response of the system to be driven at a given energy—and $n_0(\varepsilon)=-\lim_{\varepsilon\to 0}\frac{1}{\pi}\Im(G_0(\varepsilon+i\varepsilon))$—is the local density of the initial state—(see [11] for more details).

In the case of the infinite chain, it is possible to obtain an analytic expression for the Green function $G_0(\varepsilon)$ (3.4). In this case, using Rational Approximation Theory [21], we obtain that the continued fraction (3.4) converges to the Stieltjes function associated with the measure of orthogonality of the polynomial sequence $\{S_n\}_{n\geqslant 0}$, i.e., $G_0(\varepsilon)=F_S(\varepsilon)$. Moreover, we can obtain the local density $n_0(\varepsilon)$ which coincides with the corresponding measure of orthogonality $d\sigma_S(\varepsilon)$.

3.1. The 2-periodic chain model

We will suppose that the sequences of *coupling constants* $\{a_n\}$ and $\{b_n\}$ are periodic sequences with period 2, i.e., $\{a_n\}=\{a,b,a,b,\dots\}$ and $\{b_n\}=\{c,d,c,d,\dots\}$. Then the matrix (3.2) becomes

$$\mathbf{H}=\begin{pmatrix} a & c & 0 & 0 & 0 & \dots \\ c & b & d & 0 & 0 & \dots \\ 0 & d & a & c & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

3.1.1. The eigenvalues and eigenstates of the 2-periodic chain

In order to obtain the eigenvalues and eigenstates of the 2-periodic chain we use (3.3). Then, (1.1) can be rewritten in the form

$$\begin{pmatrix} a & c & 0 & 0 & 0 & \dots \\ c & b & d & 0 & 0 & \dots \\ 0 & d & a & c & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \vdots \end{pmatrix} = \varepsilon \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \vdots \end{pmatrix}, \tag{3.5}$$

where C_k are the coefficients in the linear combination (3.3), and ε is the corresponding eigenvalue of the matrix Hamiltonian **H**. Here, it is important to remark that we need to consider finite or infinite chains. The explicit solution of this eigenvalue problem for the finite chain with $N = 2n + 1$ states is given by Theorem 2.1.

In this case, we have $a_1 = a$, $a_2 = b$, $b_1 = c_1 = c$ and $b_2 = c_2 = d$ and then the eigenvalues of (3.5) are the following

$$\varepsilon_0 = a, \quad \varepsilon_{\pm k} = \frac{a+b}{2} \pm \sqrt{\frac{(a-b)^2}{4} + c^2 + d^2 + 2cd\cos\left(\frac{k\pi}{n+1}\right)}, \tag{3.6}$$

where $k = 1, 2, \dots, n$. Moreover, the corresponding eigenvectors are

$$\mathbf{v}_\ell = \begin{pmatrix} S_0(\varepsilon_\ell) \\ S_1(\varepsilon_\ell) \\ \vdots \\ S_{2n}(\varepsilon_\ell) \end{pmatrix}, \quad \ell = 0, \pm 1, \pm 2, \dots, \pm n, \tag{3.7}$$

where

$$S_{2k}(\varepsilon) = (cd)^{-k}\{P_k((\varepsilon-a)(\varepsilon-b)) + d^2 P_{k-1}((\varepsilon-a)(\varepsilon-b))\},$$
$$S_{2k+1}(\varepsilon) = c^{-1}(cd)^{-k}(x-a)P_k((\varepsilon-a)(\varepsilon-b)), \quad k = 0, 1, \dots$$

and $P_n(x) = (cd)^n U_n\left(\frac{x-c^2-d^2}{2cd}\right)$.

For the particular case when $a = b$ and $c = d$ Eq. (3.6) gives $\varepsilon_0 = a$, $\varepsilon_{\pm k} = a \pm 2c\cos\left(\frac{k\pi}{2n+2}\right)$ for $k = 1, 2, \dots, n$, which is in agreement with [11].

3.1.2. The Green function and the local density $n_0(\varepsilon)$

Using (2.7) the following expression for the Green function follows

$$G_0(\varepsilon) = \frac{1}{2d^2(a-\varepsilon)}\left(2 + \varphi_2(\varepsilon) - \sqrt{\varphi_2^2(\varepsilon) - (2cd)^2}\right),$$

where $\varphi_2(\varepsilon) = (\varepsilon-a)(\varepsilon-b) - c^2 - d^2$. To obtain the local density $n_0(\varepsilon)$, we use the distribution function (2.8)

$$n_0(\varepsilon) = \left(1 - \frac{\min(c^2, d^2)}{d^2}\right)\delta(\varepsilon - a) + \frac{1}{2\pi d^2}\frac{1}{|\varepsilon - a|}\sqrt{(2cd)^2 - \varphi_2^2(\varepsilon)}, \tag{3.8}$$

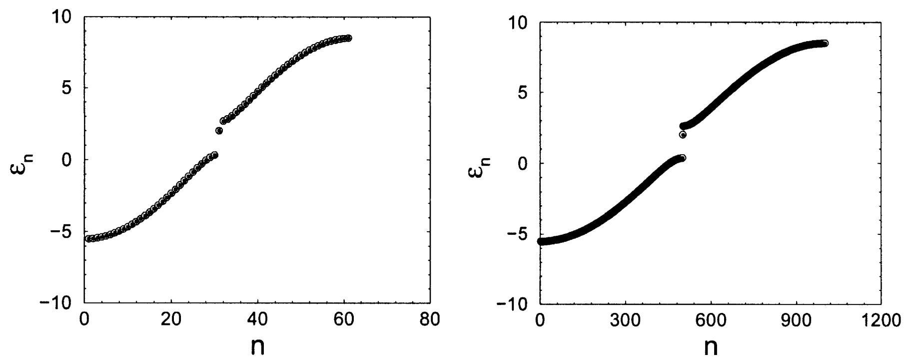

Fig. 2. The eigenvalues of the 2-chain model for $a=2$, $b=1$, $c=4$ and $d=3$.

that is located in the union of the following two intervals

$$\left[\frac{a+b}{2}-\tau_+,\frac{a+b}{2}-\tau_-\right]\cup\left[\frac{a+b}{2}+\tau_-,\frac{a+b}{2}+\tau_+\right]$$

with a possible mass point at $\varepsilon=a$, where $\tau_\pm=\frac{1}{2}\sqrt{(b-a)^2+4(c\pm d)^2}$.

3.1.3. *Some numerical experiments*

In this section, we will show some numerical results corresponding to the case of 2-Toeplitz matrix. To check the validity of the analytic formulas we have computed numerically the eigenvalues of the matrix (3.5) using MATLAB and compare them with the analytic values given, for the case $N=2n+1$ by (3.6). The corresponding analytic expressions for the eigenvectors can be obtained from (3.7). For the case $N=2n$ we can use the bounds $\varepsilon_{2n+1,j}<\varepsilon_{2n,j}<\varepsilon_{2n+1,j+1}$, $j=1,2,\ldots,2n$.

In Fig. 2 we show the eigenvalues of the 2-Toeplitz symmetric $N\times N$ matrix, $N=2n+1$ for $a=2$, $b=1$, $c=4$ and $d=3$. We show the numerical eigenvalues (stars) and the analytical ones (open circles) for $n=30$ (left panel) and $n=500$ (right panel). With this choice of parameters the density function n_0 of the initial state, represented in Fig. 4 (left panel), has not any mass point at $\varepsilon=1$ (see (3.8)), i.e., it is an absolute continuous function supported on two disjoint intervals.

In Fig. 3 we show the eigenvalues of the 2-Toeplitz symmetric $N\times N$ matrix, $N=2n+1$ for $a=2$, $b=1$, $c=3$ and $d=4$. We show the numerical eigenvalues (stars) and the analytical ones (open circles) for $n=30$ (left panel) and $n=500$ (right panel). With this choice of the parameters the density function n_0 of the initial state has a mass point $M=7/16$ at $\varepsilon=1$, i.e., it has an absolute continuous part supported on two disjoint intervals, represented in Fig. 4 (right panel), plus a delta Dirac mass at $x=1$.

Here we have shown only the case of $N=2n+1$ matrices for which always one has an isolate eigenvalue $\varepsilon_1=a$. For the case of matrices of order $N=2n$ we have not this isolated eigenvalue. Also notice that the spectrum of **H** has two branches.

3.2. *The 3-periodic chain model*

Let now suppose that the sequences of *coupling constants* $\{a_n\}$ and $\{b_n\}$ are periodic sequences with period 3, i.e., $\{a_n\}=\{a,b,c,a,b,c,\ldots\}$ and $\{b_n\}=\{d,e,f,d,e,f,\ldots\}$. Then the matrix (3.2) becomes

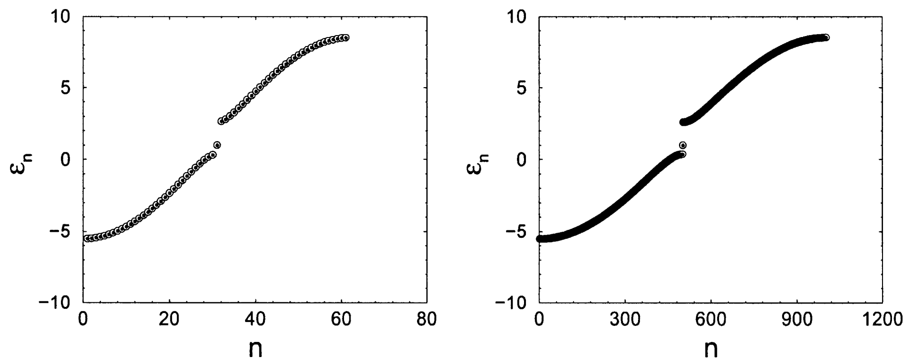

Fig. 3. The eigenvalues of the 2-chain model for $a = 1$, $b = 2$, $c = 3$ and $d = 4$.

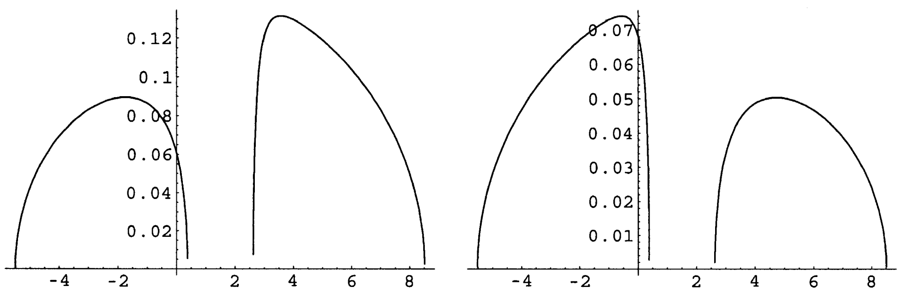

Fig. 4. The density function $n_0(\varepsilon)$ of the 2-chain model for $a = 2$, $b = 1$, $c = 4$ and $d = 3$ (left) and $a = 1$, $b = 2$, $c = 4$ and $d = 3$ (right).

$$
\mathbf{H} = \begin{bmatrix} a & d & 0 & 0 & 0 & 0 & 0 & \cdots \\ d & b & e & 0 & 0 & 0 & 0 & \cdots \\ 0 & e & c & f & 0 & 0 & 0 & \cdots \\ 0 & 0 & f & a & d & 0 & 0 & \cdots \\ 0 & 0 & 0 & d & b & e & 0 & \cdots \\ 0 & 0 & 0 & 0 & e & c & f & \cdots \\ 0 & 0 & 0 & 0 & 0 & f & a & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}.
$$

3.2.1. *The eigenvalues and eigenstates of the 3-periodic chain*

Again we will suppose that the solution $\mathbf{u}$ of the Schrödinger equation (1.1) can be written as (3.3), thus (1.1) takes the form

$$
\begin{pmatrix} a & d & 0 & 0 & 0 & \cdots \\ d & b & e & 0 & 0 & \cdots \\ 0 & e & c & f & 0 & \cdots \\ 0 & 0 & f & a & d & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ \vdots \end{pmatrix} = \varepsilon \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ \vdots \end{pmatrix}, \tag{3.9}
$$

where C_k are the coefficients in the linear combination (3.3), and ε is the corresponding eigenvalue of the matrix Hamiltonian **H**. In this case we use Theorem 2.2 which gives an explicit expression for the eigenvalue problem in the case of $N=3n+2$.

In this case, we have $a_1=a, a_2=b, a_3=c, b_1=c_1=d, b_2=c_2=e$, and $b_3=c_3=f$ and then the eigenvalues of (3.9) are the solutions $\varepsilon_{i,k},\ i=1,2,3,\ k=1,2,\dots,n$, of the polynomial equations

$$\begin{aligned} &x^3-(a+b+c)x^2+(ab+ac+bc-d^2-e^2-f^2)x \\ &\quad +cd^2+ae^2+bf^2-abc+2def\ \cos\left(\frac{k\pi}{n+1}\right)=0 \end{aligned} \tag{3.10}$$

and

$$\varepsilon_{3n+1}=\frac{a+b-\sqrt{(a-b)^2+4d^2}}{2},\quad \varepsilon_{3n+2}=\frac{a+b+\sqrt{(a-b)^2+4d^2}}{2}.$$

The corresponding eigenvectors are

$$\mathbf{v}=\begin{pmatrix} S_0(\varepsilon_\ell) \\ S_1(\varepsilon_\ell) \\ \vdots \\ S_{3n+1}(\varepsilon_\ell)\end{pmatrix},\quad \ell\in\{(i,k),3n+1,3n+2\,|\,i=1,2,3,\ k=1,\dots,n\}, \tag{3.11}$$

where

$$\begin{aligned} &S_{3k}(x)=(def)^{-k}\{P_k(\pi_3(x))+f^2(x-b)P_{k-1}(\pi_3(x))\}, \\ &S_{3k+1}(x)=d^{-1}(def)^{-k}\{(x-a)P_k(\pi_3(x))+d^2f^2P_{k-1}(\pi_3(x))\}, \\ &S_{3k+2}(x)=(de)^{-1}(def)^{-k}(x-\xi_1)(x-\xi_2)P_k(\pi_3(x)),\quad k=0,1,\dots, \end{aligned}$$

being

$$P_n(x)=(def)^nU_n\left(\frac{x-d^2-e^2-f^2}{2def}\right)$$

and

$$\begin{aligned} \pi_3(x)=&\,d^2+e^2+f^2+(a-c)e^2+(b-c)f^2 \\ &-(d^2+e^2+f^2)(x-c)+(x-a)(x-b)(x-c). \end{aligned} \tag{3.12}$$

The particular case $a=b=c$ and $d=e=f$ gives $\varepsilon_{1,k}=a+2d\cos\left(\frac{k\pi}{3n+3}\right)$,

$$\varepsilon_{2,k}=a-2d\cos\left(\frac{(n+1-k)\pi}{3n+3}\right),\quad \varepsilon_{3,k}=a+2d\cos\left(\frac{(n+1+k)\pi}{3n+3}\right),$$

for $k=1,2,\dots,n$, $\varepsilon_{3n+1}=a-d$, $\varepsilon_{3n+2}=a+d$, that is in agreement with [10].

3.2.2. The Green function and the local density $n_0(\varepsilon)$

Using (2.13) the following expression for the Green function follows

$$G_0(\varepsilon)=\frac{1}{(\varepsilon-a)(\varepsilon-b)-d^2}\left(b-\varepsilon+\frac{1}{2f^2}\left(\varphi_3(\varepsilon)-\sqrt{\varphi_3^2(\varepsilon)-(2def)^2}\right)\right),$$

where $\varphi_3(\varepsilon)=\pi_3(\varepsilon)-d^2-e^2-f^2$. To obtain the local density $n_0(\varepsilon)$, we use the distribution function (3.13)

$$n_0(\varepsilon)=M_1\delta(\varepsilon-\xi_1)+M_2\delta(\varepsilon-\xi_2)+\frac{\sqrt{(2def)^2-\varphi_3^2(\varepsilon)}}{2f^2\pi\,|(\varepsilon-a)(\varepsilon-b)-d^2|}, \tag{3.13}$$

where

$$\xi_1=\frac{a+b+\sqrt{(a-b)^2+4d^2}}{2}, \quad \xi_2=\frac{a+b-\sqrt{(a-b)^2+4d^2}}{2}, \tag{3.14}$$

which support is contained in the union of the three intervals defined by $\pi_3^{-1}([d^2+e^2+f^2-2def, d^2+e^2+f^2+2def])$, where π_3 is the polynomial defined in (3.12), and two possible mass points M_1 and M_2 (see (2.14))

$$M_1=\frac{\max\{0,\,(f^2-e^2)\sqrt{(a-b)^2+4d^2}+(a-b)(f^2+e^2)\}}{2\sqrt{(a-b)^2+4d^2}\,f^2},$$
$$M_2=\frac{\max\{0,\,(f^2-e^2)\sqrt{(a-b)^2+4d^2}-(a-b)(f^2+e^2)\}}{2\sqrt{(a-b)^2+4d^2}\,f^2},$$

located at $\varepsilon=\xi_1$ and $\varepsilon=\xi_2$, respectively. Moreover, the following four situations are possible (see Section 2.2):

1. $f\geqslant e$ and $a\geqslant b$. In this case $M_1=0$ iff $a=b$ and $f=e$, and $M_2=0$ iff $f^2\leqslant e^2+\frac{|a-b|(f^2+e^2)}{\sqrt{(a-b)^2+4d^2}}$.
2. $f\geqslant e$ and $a\leqslant b$. Then $M_1=0$ iff $f^2\leqslant e^2+\frac{|a-b|(f^2+e^2)}{\sqrt{(a-b)^2+4d^2}}$, and $M_2=0$ iff $a=b$ and $f=e$.
3. $f\leqslant e$ and $a\geqslant b$. Then $M_1=0$ iff $f^2\leqslant e^2-\frac{|a-b|(f^2+e^2)}{\sqrt{(a-b)^2+4d^2}}$. In this case always $M_2=0$.
4. $f\leqslant e$ and $a\leqslant b$. With this choice always $M_1=0$, and $M_2=0$ iff $f^2\leqslant e^2-\frac{|a-b|(f^2+e^2)}{\sqrt{(a-b)^2+4d^2}}$.

3.2.3. *Some numerical experiments*

In this section, we will present some numerical experiments related to the three periodic chain model. As in the previous case we represent with stars $*$ the values obtained by using the analytic expression (3.10) and with circles $\circ$ the values obtained numerically. The eigenvectors can be easily obtained using (3.11).

In Fig. 5 we show the eigenvalues of the three 3-Toeplitz symmetric $N\times N$ matrix, $N=3n+2$ with $a=2$, $b=1$, $c=3$, $d=4$, $e=2$ and $f=3$ for $n=20$ (left panel) and for $n=300$ (right panel). In Fig. 7 (left panel) we represent the absolute continuous part of the density function n_0 of the initial state. This case corresponds to the situation 1 discussed above for which we have two mass points

$$M_1=\frac{25+\sqrt{65}}{90}, \quad M_2=\frac{25-\sqrt{65}}{90}$$

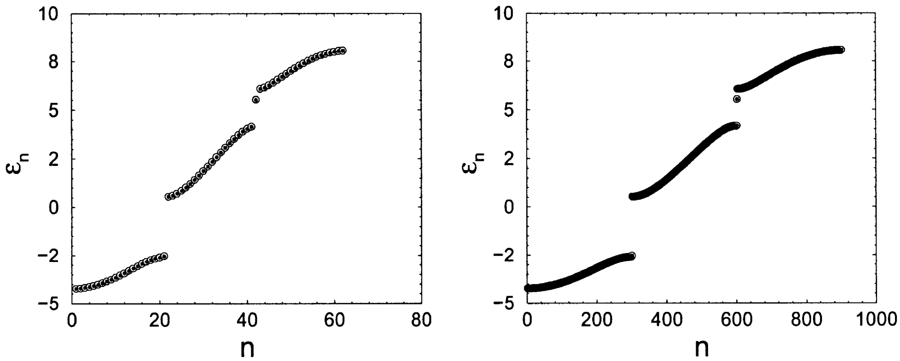

Fig. 5. The 3-chain model with $a=2$, $b=1$, $c=3$, $d=4$, $e=2$ and $f=3$.

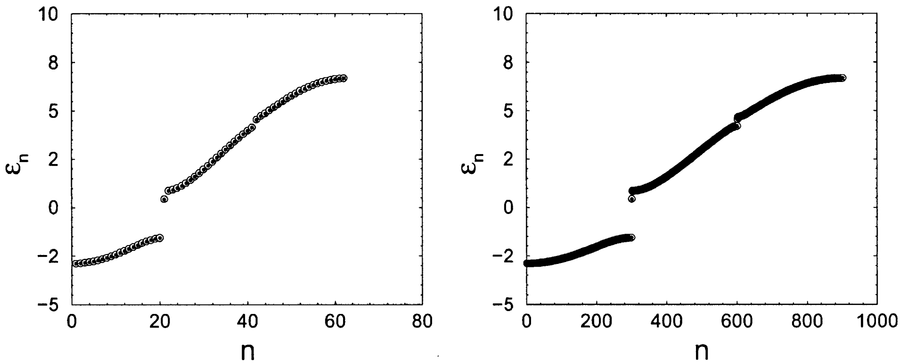

Fig. 6. The 3-chain model for $a=3$, $b=2$, $c=1$, $d=2$, $e=3$ and $f=2$.

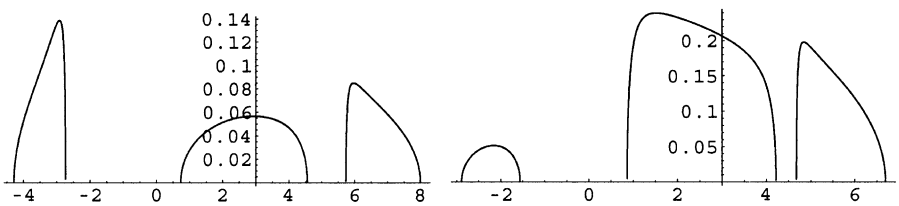

Fig. 7. The function $n_0(\varepsilon)$ of the 3-periodic chain model with $a=2, b=1, c=3, d=4, e=2$ and $f=3$ (left) and $a=2, b=1, c=3, d=4, e=2$ and $f=3$ (right).

at $\xi_1 = \frac{3+\sqrt{65}}{2}$ and $\xi_2 = \frac{3-\sqrt{65}}{2}$, respectively (see (3.14)). In this case n_0 is supported in three disjoint intervals plus two isolated points at ξ_1 and ξ_2.

In Fig. 6 we show the eigenvalues of the 3-Toeplitz symmetric $N \times N$ matrix, $N = 3n+2$ with $a=3$, $b=2$, $c=1$, $d=2$, $e=3$ and $f=2$ for $n=20$ (left panel) and for $n=300$ (right panel). In Fig. 7 (right panel) we represent the absolute continuous part of the density function n_0 of the initial state. This case corresponds to the situation 3 discussed above for which $M_1 = 0$ and $M_2 = 0$, i.e., there is no mass points, so the support of n_0 are three disjoint intervals.

Programs: For the numerical simulations presented here we have used the commercial program MATLAB. The used source code can be obtained by request via e-mail to niurka@euler.us.es or ran@us.es

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