©1997 M. Alfaro et al. (Eds.) Proceedings of the
International Workshop on Orthogonal Polynomials
in Mathematical Physics. Leganés, 24-26 June, 1996.

ON SOME POLYNOMIAL MAPPINGS FOR MEASURES. APPLICATIONS.

R.Alvarez-Nodarse, F.Marcellán and J.Petronilho

Abstract

Let $\{P_n\}_{n\geq 0}$ be a given system of monic orthogonal polynomials, π_k and θ_m two fixed monic polynomials of degrees k and m $(0 \leq m \leq k-1)$, respectively, and $\{Q_n\}_{n\geq 0}$ a simple set of monic polynomials such that $Q_{kn+m}(x) = \theta_m(x)P_n(\pi_k(x))$, for all $n = 0, 1, 2, \ldots$. The cases when $T(x)$ is a polynomial of degree 2 or 3 is considered. We find necessary and sufficient conditions in order that $\{Q_n\}_{n\geq 0}$ be a system of orthogonal polynomials and give the relation between the moment functionals associated with the orthogonal systems $\{P_n\}_{n\geq 0}$ and $\{Q_n\}_{n\geq 0}$. In particular, we characterize the positive definite case. Some applications to the solution of the eigenvalue problem for a tridiagonal 2 or 3-Toeplitz matrix, as well as to a quantum physics model are given.

Key words and Phrases: Orthogonal Polynomials, Recurrence coefficients, Polynomial mappings, Toeplitz matrices.

1 Introduction and preliminaries

Let us propose the general problem:

P. *Let $\{P_n\}_{n\geq 0}$ be a given system of monic orthogonal polynomials, π_k and θ_m two fixed monic polynomials of degrees k and m $(0 \leq m \leq k-1)$, respectively, and $\{Q_n\}_{n\geq 0}$ a simple set (i.e.,* deg $Q_n = n$ *for all $n = 0, 1, 2, \ldots$) of monic polynomials such that*

$$Q_{kn+m}(x) = \theta_m(x)P_n(\pi_k(x))$$

for all $n = 0, 1, 2, \ldots$. Find necessary and sufficient conditions in order that $\{Q_n\}_{n\geq 0}$ be a system of orthogonal polynomials. Under such conditions, what is the relation between the moment functionals associated with the orthogonal systems $\{P_n\}_{n\geq 0}$ and $\{Q_n\}_{n\geq 0}$? In particular, to characterize the positive definite case.

In this paper we present the solution of this problem for the cases $k = 2, 3$ and for the corresponding possible choices of m. The proof of the results presented here can be found in [18], [19] and [20]. The previous problem was solved by T.S.Chihara in [5] for the case $k = 2, m = 0$, when $\pi_2(x) \equiv x^2$, the initial sequence, $\{P_n\}_{n\geq 0}$, is a symmetric MOPS, and requiring that $\{Q_n\}_{n\geq 0}$ is also a symmetric MOPS (see also [31]). For $k = 3, m = 0$, it was partially solved in [2] and [21]. In fact, in [2], P.Barrucand and D.Dickinson considered this problem under the assumption that $\{P_n\}_{n\geq 0}$ is a symmetric orthogonal polynomial system and π_3 a general odd polynomial of degree 3, and requiring that $\{Q_n\}_{n\geq 0}$ is also a symmetric orthogonal polynomial system; on the other hand, in [21], F.Marcellán and G.Sansigre studied the case $\pi_3(x) \equiv x^3$ without any restriction on $\{P_n\}_{n\geq 0}$ or $\{Q_n\}_{n\geq 0}$. Nevertheless, in these contributions, only sufficient conditions were found and the relations between the functionals were not studied. For the positive definite case, a general approach to the case $m = 0$ (for any k) was provided by Geronimo and Van Assche [10]. In fact, these authors proved that given a sequence $\{p_n\}_{n\geq 0}$ of polynomials orthonormal with respect to some positive measure μ_0 supported on the bounded interval $[-1, 1]$ and a polynomial $T(x)$ of fixed degree $k \geq 2$ with distinct zeros and such that $|T(y_i)| \geq 1$, where y_i $(i = 1, 2, \ldots, k-1)$ are the zeros of T', then there always exists a positive measure μ and a sequence of polynomials $\{q_n\}_{n\geq 0}$ orthonormal with respect to μ such that $q_{kn}(x) = p_n(T(x))$ for all $n = 0, 1, 2, \ldots$. We also refer to the contributions by M.H.Ismail [15], M.H.Ismail, J.Charris and S.Monsalve [4] in connection with sieved orthogonal polynomials, as well as several papers by F.Peherstorfer [27], [28], related to orthogonality on several intervals and the paper by Geronimo and Van Assche [9] where the orthogonal polynomials with asymptotically periodic recurrence coefficients were considered.

We recall the definition of an orthogonal polynomial system (OPS). If $\mathbf{u}$ is a linear functional on $\mathbb{P}$ (the space of all polynomials with complex coefficients) and $\{P_n\}_{n\geq 0}$ a sequence of polynomials, $\{P_n\}_{n\geq 0}$ is said to be orthogonal with respect to $\mathbf{u}$ if it is a simple set and $\langle \mathbf{u}, P_nP_m\rangle = k_n\delta_{nm}$, for all $n = 0,1,2,\ldots$, where $\{k_n\}_{n\geq 0}$ is a sequence of nonzero complex numbers. In such a situation the functional $\mathbf{u}$ is said to be regular or quasi-definite (cf. [5, page 16]). In this paper we will consider monic orthogonal polynomial systems (MOPS). All MOPS are characterized by a three-term recurrence relation of the form

$$xP_n(x) = P_{n+1}(x) + \beta_nP_n(x) + \gamma_nP_{n-1}(x)\,, \quad n\geq 1, \quad P_0 = 1\,, \quad P_1(x) = x-\beta_0, \tag{1}$$

where $\{\beta_n\}_{n\geq 0}$ and $\{\gamma_n\}_{n\geq 1}$ are sequences of complex numbers, with $\gamma_n \neq 0$ for all $n\geq 1$. As usual, we denote by $\{P_n^{(1)}\}_{n\geq 0}$, $\{P_n^*(c;.)\}_{n\geq 0}$ (with $c\in\mathbb{C}$, and $P_n(c)\neq 0$ for all $n\geq 0$) and $\{P_n^\lambda\}_{n\geq 0}$ ($\lambda\in\mathbb{C}$), respectively, the sequence of the polynomials of the first kind associated with $\{P_n\}_{n\geq 0}$ [5, p.86], the sequence of monic kernel polynomials of K-parameter c associated with $\{P_n\}_{n\geq 0}$ [5, p.35] and the co-recursive sequence of $\{P_n\}_{n\geq 0}$ for the modification λ [6]. Explicitely, for the kernel polynomials we have

$$P_n^*(c;x) = \frac{1}{x-c}\left[P_{n+1}(x) - \frac{P_{n+1}(c)}{P_n(c)}P_n(x)\right]. \tag{2}$$

The associated polynomials are defined by

$$P_n^{(1)} = \frac{1}{\langle \mathbf{u},1\rangle}\left\langle \mathbf{u}_y, \frac{P_{n+1}(x)-P_{n+1}(y)}{x-y}\right\rangle, \tag{3}$$

where $\mathbf{u}_y$ means that $\mathbf{u}$ acts on the variable y. Finally, the co-recursive polynomials are given by

$$P_n^\lambda(x) = P_n(x) - \lambda P_{n-1}^{(1)}(x). \tag{4}$$

The following notation will be used

$$D_n^{\lambda,\mu}(x,y) = \frac{1}{y-x}\begin{vmatrix} P_n^\lambda(x) & P_{n+1}^\lambda(x) \\ P_n^\mu(y) & P_{n+1}^\mu(y)\end{vmatrix} \quad \text{if} \quad x\neq y\,.$$

The co-recursive polynomials are important in order to establish the regularity conditions for a linear functional associated with an inverse polynomial modification of a regular (quasi-definite) functional. In fact, if $\mathbf{u}$ is regular, for fixed $\lambda, c\in\mathbb{C}$ and with $\mathbf{u}(\lambda,c)$ defined by the distributional equation $(x-c)\mathbf{u}(\lambda,c) = -\lambda\mathbf{u}$, i.e., $\mathbf{u}(\lambda,c) = u_0\delta_c - \lambda(x-c)^{-1}\mathbf{u}$, where δ_c represents the Dirac measure at the point c and $(x-c)^{-1}\mathbf{u}$ is the linear functional defined by $\langle (x-c)^{-1}\mathbf{u}, f\rangle = \langle \mathbf{u}, [f(x)-f(c)]/(x-c)\rangle$, then $\mathbf{u}(\lambda,c)$ is regular if and only if $\lambda\neq 0$ and $P_n^\lambda(c)\neq 0$ for all $n = 0,1,2,\ldots$. Under such conditions the corresponding MOPS, $\{P_n(.;\lambda,c)\}_{n\geq 0}$, is given by (see [22])

$$P_n(x;\lambda,c) = P_n(x) - \frac{P_n^\lambda(c)}{P_{n-1}^\lambda(c)}P_{n-1}(x) \quad , \quad n\geq 0\,.$$

We recall the definition of the Stieltjes formal series, $S_{\mathbf{u}}(z)$, corresponding to a given functional $\mathbf{u}$,

$$S_{\mathbf{u}}(z) = -\sum_{n\geq 0}\frac{u_n}{z^{n+1}}\,,$$

where $u_n = \langle \mathbf{u}, x^n \rangle$ is the moment of order n of $\mathbf{u}$.

In the previous results we have considered "formal orthogonality", in the sense that the orthogonal polynomials $\{P_n\}_{n\geq 0}$ are related to a numerical sequence $u_n = \langle \mathbf{u}, x^n \rangle$, $n = 0, 1, 2, \ldots$, ignoring whether these numbers are actual moments of some weight or distribution function on some support or not. In order to determine under what conditions this can occur, we must analyze when a regular linear functional $\mathbf{u}$ is positive definite, i.e., $\langle \mathbf{u}, f \rangle > 0$ for all $f \in \mathbb{P}$ such that $f(x) \geq 0$, $\forall x \in \mathbb{R}$ and $f \not\equiv 0$. In fact, a sequence of orthogonal polynomials $\{P_n\}_{n\geq 0}$ with respect to some linear functional $\mathbf{u}$ is said to be orthogonal in the positive definite sense if $\mathbf{u}$ is positive definite. By a representation theorem [5, Chapter II], $\mathbf{u}$ is positive definite if and only if it admits an integral representation, in terms of the Stieltjes integral, of the form $\langle \mathbf{u}, \pi \rangle = \int_{-\infty}^{+\infty} \pi(x) d\sigma(x)$, for every polynomial π , where σ is a distribution function, i.e., a function $\sigma : \mathbb{R} \to \mathbb{R}$ which is nondecreasing, has infinitely many points of increase and such that all the moments $\int_{-\infty}^{+\infty} x^{2n} d\sigma(x)$ $(n = 0, 1, 2, \ldots)$ are finite. For a given distribution function σ, we denote the corresponding Stieltjes function by $F(.;\sigma)$,

$$F(z;\sigma) = \int_{-\infty}^{+\infty} \frac{d\sigma(t)}{t - z} \,. \tag{5}$$

The structure of the paper is the following. In Section 2 we give the characterizations for the above problem in the cases $k = 2, m = 0, 1$ and $k = 3, m = 0, 2$. The solution for the case $k = 3, m = 1$ is very similar and we omit it. As an application of our results, in Section 3 we give the solution for the eigenproblem for a tridiagonal 2 and 3-Toeplitz matrix. We mention that the problem for a tridiagonal 2-Toeplitz matrix has been solved by M.J.Gover [11] (see also [18]). Finally, in Section 4 we analyze a particular case of the so called *Chain Model* [13] which is an exactly solvable quantum model.

2 Results.

Theorem 1 *(case $k = 2, m = 0$) Let $\{P_n\}_{n\geq 0}$ be a system of monic orthogonal polynomials and $\{Q_n\}_{n\geq 0}$ a simple set of monic polynomials such that*

$$Q_1(x) = x - b \,, \quad Q_{2n}(x) = P_n(\pi_2(x)) \,, \quad n = 0, 1, 2, \ldots$$

where $\pi_2(x)$ is a (monic) polynomial of degree 2 and $b \in \mathbb{C}$. Without loss of generality, write $\pi_2(x) = (x - a)(x - b) + c$. Then, $\{Q_n\}_{n\geq 0}$ is a MOPS if and only if

$$P_n(c) \neq 0 \,, \quad Q_{2n+1}(x) = (x - b) P_n^*(c; \pi_2(x)) \,, \quad n = 0, 1, 2, \ldots \,.$$

Under such conditions, if $\{P_n\}_{n\geq 0}$ satisfies the three-term recurrence relation (1), then the coefficients $\tilde{\beta}_n$ and $\tilde{\gamma}_n$, for the corresponding three-term recurrence relation satisfied by $\{Q_n\}_{n\geq 0}$, are given by

$$\tilde{\beta}_{2n} = b \,, \quad \tilde{\beta}_{2n+1} = a \,, \quad \tilde{\gamma}_{2n+1} = -\frac{P_{n+1}(c)}{P_n(c)} \,, \quad \tilde{\gamma}_{2n+2} = -\gamma_{n+1} \frac{P_n(c)}{P_{n+1}(c)}$$

for all $n = 0, 1, 2, \ldots$. Moreover, if $\{P_n\}_{n\geq 0}$ is a MOPS with respect to the linear functional $\mathbf{u}$, then $\{Q_n\}_{n\geq 0}$ is a MOPS with respect to the linear functional $\mathbf{v}$ defined on the basis $\{\pi_2^n, (x - b)\pi_2^n\}_{n\geq 0}$ of $\mathbb{P}$ by

$$\langle \mathbf{v}, \pi_2^n(x) \rangle = \langle \mathbf{u}, x^n \rangle \,, \quad \langle \mathbf{v}, (x - b)\pi_2^n(x) \rangle = 0 \,, \quad n = 0, 1, 2, \ldots \,.$$

Corollary 1 *Under the hypothesis of Theorem 1 the following expressions hold*

$$Q_{2n-1}^{(1)}(x) = (x - a) P_{n-1}^{(1)}(\pi_2(x)) \,, \quad n = 0, 1, 2, \ldots \quad S_{\mathbf{v}}(z) = (z - a) S_{\mathbf{u}}(\pi_2(z)) \,.$$

Corollary 2 *Under the hypothesis of Theorem 1, assume that b is a real number, π_2 a real polynomial and $\{P_n\}_{n\geq 0}$ a MOPS in the positive definite sense, orthogonal with respect to some uniquely determined distribution function σ and let $[\xi,\eta]$ be the corresponding true interval of orthogonality [5]. Then, $\{Q_n\}_{n\geq 0}$ is a MOPS with respect to a positive definite linear functional if and only if*

$$c \leq \xi\,, \quad Q_{2n+1}(x) = (x-b)P_n^*(c;\pi_2(x))$$

hold for all $n=0,1,2,\ldots$. Under these conditions, $\{Q_n\}_{n\geq 0}$ is orthogonal with respect to the uniquely determined distribution function $\widetilde{\sigma}$ defined by

$$\mathrm{d}\widetilde{\sigma}(x) = |x-a|\frac{\mathrm{d}\sigma(\pi_2(x))}{\pi_2'(x)} \quad , \quad r \leq |x - \tfrac{a+b}{2}| \leq s\,,$$

where $r=(\xi+\Delta/4)^{1/2}$ and $s=(\eta+\Delta/4)^{1/2}$, with $\Delta=(b-a)^2-4c$.

Theorem 2 *(case $k=2, m=1$) Let $\{P_n\}_{n\geq 0}$ be a system of monic orthogonal polynomials and $\{Q_n\}_{n\geq 0}$ a simple set of monic polynomials such that*

$$Q_2(a) = \lambda\,, \quad Q_{2n+1}(x) = (x-a)P_n(\pi_2(x))\,, \quad n=0,1,2,\ldots$$

where $\pi_2(x)$ is a (monic) polynomial of degree 2 and $a,\lambda\in\mathbb{C}$. Without loss of generality, write $\pi_2(x)=(x-a)(x-b)+c$. Then, $\{Q_n\}_{n\geq 0}$ is a MOPS if and only if

$$\lambda \neq 0\,, \quad P_n^\lambda(c)\neq 0\,, \quad Q_{2n}(x) = P_n(\pi_2(x);\lambda,c)\,, \quad n=0,1,2,\ldots\,.$$

Under such conditions, if $\{P_n\}_{n\geq 0}$ satisfies the three-term recurrence relation (1), then the coefficients $\tilde{\beta}_n$ and $\tilde{\gamma}_n$ for the corresponding three-term recurrence relation satisfied by $\{Q_n\}_{n\geq 0}$ are given by

$$\tilde{\beta}_{2n} = a\,, \quad \tilde{\beta}_{2n+1} = b\,, \qquad n=0,1,2,\ldots\,,$$

$$\tilde{\gamma}_1 = -\lambda\,, \quad \tilde{\gamma}_{2n} = -\frac{P_n^\lambda(c)}{P_{n-1}^\lambda(c)}\,, \quad \tilde{\gamma}_{2n+1} = -\gamma_n\frac{P_{n-1}^\lambda(c)}{P_n^\lambda(c)}\,, \quad n=1,2,\ldots\,.$$

Moreover, if $\{P_n\}_{n\geq 0}$ is a MOPS with respect to the linear functional $\mathbf{u}$, then $\{Q_n\}_{n\geq 0}$ is a MOPS with respect to the linear functional $\mathbf{v}$ defined by

$$\langle \mathbf{v}, \pi_2^n(x)\rangle = \langle \mathbf{u}(\lambda,c), x^n\rangle\,, \quad \langle \mathbf{v}, (x-a)\pi_2^n(x)\rangle = 0\,, \quad n=0,1,2\ldots\,.$$

Corollary 3 *Under the hypothesis of Theorem 1, the following expressions hold*

$$Q_{2n-1}^{(1)}(x) = (x-b){P_{n-1}}^{(1)}(\pi_2(x);\lambda,c)\,, \quad n=1,2,\ldots\,, \quad S_{\mathbf{v}}(z) = (z-b)S_{\mathbf{u}(\lambda,\mathbf{c})}(\pi_2(z)).$$

Corollary 4 *Under the hypothesis of Theorem 2, assume that a,λ are real numbers, π_2 a real polynomial and $\{P_n\}_{n\geq 0}$ a MOPS in the positive definite sense, orthogonal with respect to some uniquely determined distribution function σ and let $[\xi,\eta]$ be the corresponding true interval of orthogonality [5]. Further, assume either that $c\leq \xi+\lambda$, or*

$$c \leq \xi\,, \quad -\infty < \lim_{n\to+\infty}\frac{P_n(\xi)}{P_{n-1}^{(1)}(\xi)} \equiv A \leq \lambda \leq B \equiv \lim_{n\to+\infty}\frac{P_n(\eta)}{P_{n-1}^{(1)}(\eta)} \tag{6}$$

(with $B\equiv\infty$ if $\eta=+\infty$) holds. Then, $\{Q_n\}_{n\geq 0}$ is a MOPS with respect to a positive definite linear functional if and only if $\lambda<0$ and $Q_{2n}(x)=P_n(\pi_2(x);\lambda,c)$, holds for all $n=0,1,2,\ldots$. Under these conditions, $\{Q_n\}_{n\geq 0}$ is orthogonal with respect to the uniquely determined distribution function $\widetilde{\sigma}$ given by

$$\mathrm{d}\widetilde{\sigma}(x) = M\delta_a(x) - \frac{\lambda}{|x-a|}\frac{\mathrm{d}\sigma(\pi_2(x))}{\pi_2'(x)} \quad , \quad M := u_0 + \lambda F(c;\sigma) \geq 0\,,$$

whith either $\mathrm{supp}\,(\mathrm{d}\sigma) \subset \pi_2^{-1}([\xi+\lambda,\eta])\cup\{a\}$ *if $c\leq\xi+\lambda$, or* $\mathrm{supp}\,(\mathrm{d}\sigma)\subset\pi_2^{-1}([\xi,\eta])\cup\{a\}$ *if* (6) *holds.*

Theorem 3 *(case $k=3, m=0$) Let $\{P_n\}_{n\geq 0}$ be a system of monic orthogonal polynomials and $\{Q_n\}_{n\geq 0}$ a simple set of monic polynomials such that*

$$Q_1(0) = -\beta\,, \quad Q_2(\beta) = -\gamma\,, \quad Q_{3n}(x) = P_n(\pi_3(x))\,, \quad n = 0,1,2,\ldots \tag{7}$$

where $\pi_3(x)$ is a (monic) polynomial of degree 3 and $\beta, \gamma \in \mathbb{C}$. Consider the polynomial

$$\rho(x) = \gamma + [\pi_3(x) - \pi_3(\beta)]/(x-\beta)\,.$$

Let a_1 and a_2 be the zeros of ρ and put $c_1 = \pi_3(a_1)$, $c_2 = \pi_3(a_2)$. Then, for a fixed pair (β,γ), $\{Q_n\}_{n\geq 0}$ is a MOPS if and only if

$$\gamma \neq 0\,, \quad P_n(c_1) \neq 0\,, \quad P_n(c_2) \neq 0\,, \quad P_n^*(c_1;c_2) \neq 0\,,$$

$$Q_{3n+1}(x) = \frac{1}{\rho(x)}\left[P_{n+1}(\pi_3(x)) + \gamma \frac{P_n^*(c_1;c_2)}{P_n(c_2)}\left(x - a_2 - \frac{1}{\gamma}\frac{P_{n+1}(c_2)}{P_n^*(c_1;c_2)}\right) P_n(\pi_3(x))\right],$$

$$Q_{3n+2}(x) = \frac{1}{\rho(x)}\left[\left(x - a_1 + \frac{1}{\gamma}\frac{P_{n+1}(c_2)}{P_n^*(c_1;c_2)}\right) P_{n+1}(\pi_3(x)) - \frac{1}{\gamma}\frac{P_{n+1}(c_1)P_{n+1}(c_2)}{P_n(c_1)P_n^*(c_1;c_2)} P_n(\pi_3(x))\right]$$

hold for all $n = 0,1,2,\ldots$. In such conditions, if $\{P_n\}_{n\geq 0}$ satisfies the three-term recurrence relation (1), then the coefficients $\tilde\beta_n$ and $\tilde\gamma_n$ for the corresponding three-term recurrence relation satisfied by $\{Q_n\}_{n\geq 0}$ are given by

$$\tilde\beta_{3n} = \beta\,, \quad \tilde\beta_{3n+1} = a_1 - \frac{1}{\gamma}\frac{P_{n+1}(c_2)}{P_n^*(c_1;c_2)}\,, \quad \tilde\beta_{3n+2} = a_2 + \frac{1}{\gamma}\frac{P_{n+1}(c_2)}{P_n^*(c_1;c_2)}\,,$$

$$\tilde\gamma_{3n} = -\gamma\,\gamma_n\,\frac{P_{n-1}(c_1)P_{n-1}^*(c_1;c_2)}{P_n(c_1)P_n(c_2)}\,, \quad \tilde\gamma_{3n+1} = \gamma\,\frac{P_n^*(c_1;c_2)}{P_n(c_2)}\,, \quad \tilde\gamma_{3n+2} = -\frac{1}{\gamma^2}\frac{P_{n+1}(c_1)P_{n+1}(c_2)}{P_n^*(c_1;c_2)P_n^*(c_2;c_1)}\,.$$

Finally, denote by $\mathbf{u}$ the moment functional such that $\{P_n\}_{n\geq 0}$ is the corresponding MOPS. Let $\{A_n\}_{n\geq 0}$ be the basis of $\mathbb{P}$ defined by

$$A_{3n}(x) = \pi_3^n(x)\,, \quad A_{3n+1}(x) = (x-\beta)\pi_3^n(x)\,, \quad A_{3n+2}(x) = (x^2 - \beta x - \gamma)\pi_3^n(x)$$

for $n = 0,1,2,\ldots$. Then, under the above conditions, $\{Q_n\}_{n\geq 0}$ is a MOPS associated with the moment linear functional $\mathbf{v}$ defined on the basis $\{A_n\}_{n\geq 0}$ by

$$\langle \mathbf{v}, A_{3n}(x)\rangle = \langle \mathbf{u}, x^n\rangle\,, \quad \langle \mathbf{v}, A_{3n+1}(x)\rangle = 0\,, \quad \langle \mathbf{v}, A_{3n+2}(x)\rangle = 0, \quad n = 0,1,2,\ldots\,.$$

Corollary 5 *Under the hypothesis of Theorem 3 the following expression hold*

$$Q_{3n+2}^{(1)}(x) = \rho(x) P_n{}^{(1)}(\pi_3(x)), \quad n = 0,1,2,\ldots\,, \quad S_{\mathbf{v}}(z) = \rho(z) S_{\mathbf{u}}(\pi_3(z))\,.$$

Corollary 6 *Under the hypothesis of Theorem 3, assume further that β,γ are real numbers, π_3 a real polynomial and $\{P_n\}_{n\geq 0}$ a MOPS in the positive definite sense, orthogonal with respect to some distribution function σ and let $[\xi,\eta]$ be the corresponding true interval of orthogonality [5] of $\{P_n\}_{n\geq 0}$. Then, $\{Q_n\}_{n\geq 0}$ is a MOPS with respect to a positive definite linear functional if and only if a_1 and a_2 are real (we assume, without loss of generality, that $a_1 \leq a_2$) and the following two conditions hold*

(i) $\gamma > 0 \quad , \quad c_2 \leq \xi \quad , \quad \eta \leq c_1\,;$

(ii) *$Q_{3n+1}(x)$ and $Q_{3n+2}(x)$ are defined as in Theorem 3 for $n = 0,1,2,\ldots$.*

Under these conditions, $\{Q_n\}_{n\geq 0}$ is orthogonal with respect to the uniquely determined distribution function $\tilde\sigma$ given by

$$\mathrm{d}\tilde\sigma(x) = |\rho(x)|\,\frac{\mathrm{d}\sigma(\pi_3(x))}{\pi_3'(x)} \quad , \quad x \in \pi_3^{-1}([\xi,\eta])\,.$$

Remark 1 *Conditions* (i) *imply that in order to guarantee the existence of sequences* $\{Q_n\}_{n\geq 0}$, *satisfying* (7) *and orthogonal in the positive definite sense, we must start with sequences* $\{P_n\}_{n\geq 0}$ *(orthogonal in the positive definite sense) such that the corresponding true interval of orthogonality,* $[\xi,\eta]$, *is bounded, and such that the condition* $c_1 \neq c_2$ *holds (or, equivalently,* $a_1 \neq a_2$*).*

Remark 2 *The results of the corollaries 2 and 6 agree with those of Geronimo and Van Assche [10], for the particular cases* $k = 2, 3$. *Notice that, in [10] the authors imposed, a priori, the restrictions "supp*$(\mathrm{d}\sigma)$ *compact" and "*$|\pi_k(y_i)| \geq 1$ *on the zeros* y_i *of* π_k' $(i = 1, 2)$*", which in our case correspond to the condition* $\pi_k(y_i) \notin]\xi,\eta[$. *For the case* $k = 3$, *it follows from Remark 1 that the condition "supp*$(\mathrm{d}\sigma)$ *compact" is necessary for the orthogonality of* $\{Q_n\}_{n\geq 0}$. *Furthermore (also for* $k = 3$*), assuming (without loss of generality) that* $y_1 < y_2$, *since at these points* $\pi_3(y)$ *attains its extremal values, we have* $\pi_3(y_1) \leq \pi_3(a_2) = c_2 \leq \xi < \eta \leq c_1 = \pi_3(a_1) \leq \pi_3(y_2)$, *hence again* $\pi_3(y_i) \notin]\xi,\eta[$ *must hold necessarily for the orthogonality of* $\{Q_n\}_{n\geq 0}$.

Remark 3 *In [21] it was pointed out that "there does not exist a pair of orthogonal polynomial sets* $\{P_n\}_{n\geq 0}$ *and* $\{Q_n\}_{n\geq 0}$ *associated with positive definite symmetric functionals such that* $Q_{3n}(x) = P_n(x^3)$*". We can generalize this observation, removing the restriction about the symmetry of the functionals, since for any choice of the pair* (β,γ), *with* $\gamma > 0$, *the polynomial* $\rho(x) = \gamma + (x^3 - \beta^3)/(x-\beta) \equiv x^2 + \beta x + \beta^2 + \gamma$ *has no real zeros.*

Theorem 4 *(case* $k = 3, m = 2$*) Let* $\{P_n\}_{n\geq 0}$*be a MOPS and* $\{Q_n\}_{n\geq 0}$ *a simple set of monic polynomials such that*

$$Q_{3n+2}(x) = (x-a)(x-b)P_n(\pi_3(x)), \quad n = 0, 1, 2, \ldots$$

where a *and* b *are fixed complex numbers and* $\pi_3(x)$ *is a monic polynomial of degree 3. Without loss of generality, write*

$$Q_1(x) = x - \alpha, \quad xQ_2(x) = Q_3(x) + \beta Q_2(x) + \gamma Q_1(x)$$

and put $c = \pi_3(a)$, $d = \pi_3(b)$, $\lambda = -\gamma(a-\alpha)$ *and* $\mu = -\gamma(b-\alpha)$. *Assume that* $c \neq d$. *Then, for a fixed pair* (α,γ), $\{Q_n\}_{n\geq 0}$ *is a MOPS if and only if*

$$\gamma \neq 0, \quad \beta = -\left[a + b + \pi_3''(0)/2\right], \quad P_n^{\lambda}(c) \neq 0, \quad P_n^{\mu}(d) \neq 0, \quad D_n^{\lambda,\mu}(c,d) \neq 0,$$

$$Q_{3n+3}(x) = P_{n+1}(\pi_3(x)) + \frac{d_n^{\lambda,\mu}(c,d)}{P_n^{\lambda}(c)P_n^{\mu}(d)}\left(x - a - \frac{P_{n+1}^{\lambda}(c)P_n^{\mu}(d)}{d_n^{\lambda,\mu}(c,d)}\right)P_n(\pi_3(x)),$$

$$Q_{3n+4}(x) = \left(x - b + \frac{P_{n+1}^{\lambda}(c)P_n^{\mu}(d)}{d_n^{\lambda,\mu}(c,d)}\right)P_{n+1}(\pi_3(x)) - \frac{P_{n+1}^{\lambda}(c)P_{n+1}^{\mu}(d)}{d_n^{\lambda,\mu}(c,d)}P_n(\pi_3(x))$$

hold for all $n = 0, 1, 2, \ldots$ *where* $d_n^{\lambda,\mu}(c,d) = \dfrac{d-c}{a-b}D_n^{\lambda,\mu}(c,d)$. *Under such conditions, if* $\{P_n\}_{n\geq 0}$ *satisfies the three-term recurrence relation (1), then the coefficients* $\widetilde{\beta}_n$ *and* $\widetilde{\gamma}_n$ *for the corresponding three-term recurrence relation satisfied by* $\{Q_n\}_{n\geq 0}$ *are given by*

$$\widetilde{\beta}_0 = \alpha, \quad \widetilde{\beta}_1 = a + b - \alpha,$$

$$\widetilde{\beta}_{3n+2} = \beta, \quad \widetilde{\beta}_{3n+3} = b - \frac{P_{n+1}^{\lambda}(c)P_n^{\mu}(d)}{d_n^{\lambda,\mu}(c,d)}, \quad \widetilde{\beta}_{3n+4} = a + \frac{P_{n+1}^{\lambda}(c)P_n^{\mu}(d)}{d_n^{\lambda,\mu}(c,d)}, \quad n = 0, 1, 2, \ldots$$

$$\widetilde{\gamma}_1 = -\lambda\mu/\gamma^2, \quad \widetilde{\gamma}_2 = \gamma$$

$$\widetilde{\gamma}_{3n} = \frac{d^{\lambda,\mu}_{n-1}(c,d)}{P^{\lambda}_{n-1}(c)P^{\mu}_{n-1}(d)}\,, \quad \widetilde{\gamma}_{3n+2} = -\gamma_n \frac{d^{\lambda,\mu}_{n-1}(c,d)}{P^{\lambda}_{n}(c)P^{\mu}_{n}(d)}\,, \quad \widetilde{\gamma}_{3n+1} = -\frac{P^{\lambda}_{n-1}(c)P^{\mu}_{n-1}(d)P^{\lambda}_{n}(c)P^{\mu}_{n}(d)}{\left(d^{\lambda,\mu}_{n-1}(c,d)\right)^2},$$

for $n = 0,1,2,...$ Furthermore, assume that $\{P_n\}_{n\geq 0}$ is a MOPS associated with the moment functional $\mathbf{u}$. Consider the basis $\{C_n\}_{n\geq 0}$ of $\mathbb{P}$ such that

$$\begin{aligned} &C_0(x) = 1\,, \quad C_{3n+1}(x) = (x-b)\pi_3^n(x)\,, \\ &C_{3n+2}(x) = (x-a)(x-b)\pi_3^n(x)\,, \quad C_{3n+3}(x) = (x-a)(x-b)^2\pi_3^n(x), \end{aligned}$$

for $n = 0,1,2,\ldots$. Then, under the conditions above, $\{Q_n\}_{n\geq 0}$ is a MOPS associated with the linear functional $\mathbf{v}$ defined by ($n = 0,1,2,\ldots$)

$$\langle \mathbf{v}, C_0(x)\rangle = u_0\,, \quad \langle \mathbf{v}, C_{3n+1}(x)\rangle = \tfrac{\mu}{\gamma}\langle \mathbf{u}(\lambda,c), x^n\rangle\,, \langle \mathbf{v}, C_{3n+2}(x)\rangle = 0\,, \quad \langle \mathbf{v}, C_{3n+3}(x)\rangle = 0.$$

Corollary 7 *Under the hypothesis of Theorem 4, the following expressions hold*

$$Q^{(1)}_{3n+1}(x) = (x-a-b+\alpha)\,P_n(\pi_3(x)) - \frac{\lambda\mu}{\gamma}\,P^{(1)}_{n-1}(\pi_3(x)), \quad n = 0,1,2,\ldots$$

$$S_{\mathbf{v}}(z) = -\frac{u_0(z-a-b+\alpha) + (\lambda\mu/\gamma)S_{\mathbf{u}}(\pi_3(z))}{(z-a)(z-b)}\,.$$

Corollary 8 *Under the hypothesis of Theorem 4, assume further that α,γ,a,b are real numbers, π_3 a real polynomial and $\{P_n\}_{n\geq 0}$ a MOPS in the positive definite sense, orthogonal with respect to some distribution function σ, and let $[\xi,\eta]$ be the corresponding true interval of orthogonality [5], which we assume to be bounded. Without loss of generality, suppose that $a > b$ and assume that one of the two sets of conditions hold, either $c \leq \xi+\lambda\,, \quad \eta+\mu \leq d\,,$ or*

$$c \leq \xi\,, \quad d \geq \eta\,, \quad -\infty < \lim_{n\to+\infty}\frac{P_n(\xi)}{P^{(1)}_{n-1}(\xi)} \equiv A \leq \lambda,\mu \leq B \equiv \lim_{n\to+\infty}\frac{P_n(\eta)}{P^{(1)}_{n-1}(\eta)}\,. \tag{8}$$

Then, for each fixed pair (α,γ), $\{Q_n\}_{n\geq 0}$ is a MOPS in the positive definite sense if and only if the following two conditions hold

(i) $\gamma > 0 \quad , \quad \lambda < 0 < \mu \quad , \quad \beta = -[a+b+\pi_3''(0)/2]$;
(ii) *$Q_{3n+3}(x)$ and $Q_{3n+4}(x)$ are defined as in Theorem 4 for $n = 0,1,2,\ldots$.*

Under these conditions, $\{Q_n\}_{n\geq 0}$ is orthogonal with respect to a uniquely determined distribution function $\widetilde{\sigma}$ such that

$$d\widetilde{\sigma}(x) = M\delta_a(x) + N\delta_b(x) - \frac{\lambda\mu/\gamma}{|(x-a)(x-b)|}\frac{d\sigma(\pi_3(x))}{\pi_3'(x)}\quad ,$$

where

$$M = \frac{\mu/\gamma}{a-b}\,[u_0 + \lambda F(c;\sigma)] \geq 0\,, \quad N = -\frac{\lambda/\gamma}{a-b}\,[u_0 + \mu F(d;\sigma)] \geq 0\,.$$

Furthermore, either $\operatorname{supp}(\mathrm{d}\sigma) \subset \pi_2^{-1}([\xi+\lambda, \eta+\mu]) \cup \{a,b\}$ if $c \leq \xi+\lambda\,, \quad \eta+\mu \leq d\,,$ or $\operatorname{supp}(\mathrm{d}\sigma) \subset \pi_2^{-1}([\xi,\eta]) \cup \{a,b\}$ if (8) holds.

Remark 4 *In the previous Corollary, we can assume, without loss of generality, that $a > b$ (not $a \geq b$) because if $a = b$ then Q_{3n+2} would have a double zero and so $\{Q_n\}_{n\geq 0}$ couldn't be orthogonal in the positive definite sense.*

Remark 5 *As a consequence of Corollaries 1, 3, 5 and 7, we can state that if $\{P_n\}_{n\geq 0}$ is a semiclassical MOPS (in any of the problems), then $\{Q_n\}_{n\geq 0}$ is also a semiclassical MOPS (for information about this class of orthogonal polynomials, see, e.g., [23]).*

3 Applications

First of all, let us point out some well known results of the general theory of orthogonal polynomials. As we said before, the orthogonal polynomial sequence (OPS) $\{P_n\}_{n\geq 0}$ can be characterized by the three term recurrence relation (1) satisfied by the polynomials $P_n(x)$ (which are not necessarily monic) [5]

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

with initial conditions $P_{-1} = 0$ and $P_0 = 1$ (we take this last as a normalization condition) where $\{\alpha_n\}_{n\geq 0}$, $\{\beta_n\}_{n\geq 0}$ and $\{\gamma_n\}_{n\geq 1}$ are sequences of complex numbers such that $\alpha_n \gamma_{n+1} \neq 0$ for $n \geq 0$. In matrix form, this can be written as $x\,\mathbf{P}_n = J_{n+1}\mathbf{P}_n + \alpha_n P_{n+1}(x)\mathbf{e}_n$, where J_{n+1} is a tridiagonal matrix of order $n+1$, $\mathbf{P}_n$ is the polynomial vector $[P_0(x), ..., P_n(x)]^T$ and $\mathbf{e}_n$ is the vector $[0, 0, ..., 0, 1]^T \in \mathbb{R}^{n+1}$. Explicitly the matrix form is given by

$$x\begin{bmatrix} P_0(x) \\ P_1(x) \\ P_2(x) \\ \vdots \\ P_{n-1}(x) \\ P_n(x) \end{bmatrix} = \begin{bmatrix} \beta_0 & \alpha_0 & 0 & 0 & \dots & 0 & 0 \\ \gamma_1 & \beta_1 & \alpha_1 & 0 & \dots & 0 & 0 \\ 0 & \gamma_2 & \beta_2 & \alpha_2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \beta_{n-1} & \alpha_{n-1} \\ 0 & 0 & 0 & 0 & \dots & \gamma_n & \beta_n \end{bmatrix} \begin{bmatrix} P_0(x) \\ P_1(x) \\ P_2(x) \\ \vdots \\ P_{n-1}(x) \\ P_n(x) \end{bmatrix} + \alpha_n P_{n+1}(x) \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix}. \quad (9)$$

If we denote by $\{x_{nj}\}_{1\leq j\leq n}$ the zeros of the polynomial P_n, then from (9) we conclude that each x_{nj} is an eigenvalue of the corresponding tridiagonal matrix of order n and $[P_0(x_{nj}), ..., P_{n-1}(x_{nj})]^T$ is the associated eigenvector.

When $\alpha_n = 1$ and $\gamma_n > 0$ for all $n = 1, 2, \ldots$ the (monic) polynomials $\{P_n\}_{n\geq 0}$ defined by the recurrence relation (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 [5], $\{P_n\}_{n\geq 0}$ 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 characterized by some 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 $\int_{-\infty}^{+\infty} x^{2n} d\sigma(x)$, $n = 0, 1, 2, \ldots$, are finite. The numerators of the continued fraction, denoted by $\{P_n^{(1)}\}_{n\geq 0}$, can be given by the shifted recurrence relation

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

with initial conditions $P_{-1}^{(1)} = 0$ and $P_0^{(1)} = 1$. This continued fraction converges to a function $F(z)$ 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 summarized by Markov-Stieltjes's theorem

$$-\lim_{n\to+\infty} \frac{\mu_0 P_{n-1}^{(1)}(z)}{P_n(z)} = F(z) \equiv \int_{-\infty}^{+\infty} \frac{d\sigma(x)}{x-z}, \quad z \in \mathbb{C}\backslash\mathrm{supp}(\sigma) \quad , \qquad (10)$$

where $\mu_0 = \int_{-\infty}^{+\infty} d\sigma(x)$ is the first moment of the distribution $\sigma(x)$ and F is the Stieltjes function of the distribution function σ, defined according to (5). Now, the function $\sigma(x)$ can be recovered from (10) by applying the Stieltjes inversion formula

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

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

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

3.1 The Chebyshev polynomials of the second kind.

In this paper we will consider the monic Chebyshev polynomials of second kind $\{U_n(x)\}_{n \geq 0}$. They satisfy the three-term recurrence relation

$$U_{-1} = 0 \quad , \quad U_0 = 1 \quad , \quad xU_n(x) = U_{n+1}(x) + \frac{1}{4} U_{n-1}(x), \quad n = 0, 1, 2, \ldots \,.$$

They can also be expressed in terms of trigonometric polynomials in $\cos\theta$ as

$$U_n(x) = 2^{-n} \frac{\sin(n+1)\theta}{\sin\theta}, \quad x = \cos\theta.$$

They are orthogonal with respect to the distribution function

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

The corresponding Stieltjes function is [30, page 176]

$$F_U(z) = \frac{-2}{z + \sqrt{z^2 - 1}} = -2(z - \sqrt{z^2 - 1}) \quad , \quad z \in \mathbb{C} \backslash [-1, 1]$$

where the square root is such that $|z + \sqrt{z^2 - 1}| > 1$ whenever $z \notin [-1, 1]$. Finally, we point out the second order differential equation satisfied by U_n,

$$(1 - x^2) U_n''(x) - 3x U_n'(x) + n(n+2) U_n(x) = 0, \quad n = 0, 1, 2, \ldots \tag{11}$$

3.2 The eigenvalues of a tridiagonal 2-Toeplitz matrix.

Theorem 1 can be applied to the determination of the eigenvalues of a finite tridiagonal 2-Toeplitz matrix B_{n+1}, which has the general form

$$B_{n+1} = \begin{bmatrix} a_1 & b_1 & 0 & 0 & 0 & \ldots \\ c_1 & a_2 & b_2 & 0 & 0 & \ldots \\ 0 & c_2 & a_1 & b_1 & 0 & \ldots \\ 0 & 0 & c_1 & a_2 & b_2 & \ldots \\ 0 & 0 & 0 & c_2 & a_1 & \ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \in \mathbb{C}^{(n+1, n+1)} \tag{12}$$

where we assume that b_1, b_2, c_1 and c_2 are positive numbers. The eigenvalues and eigenvectors of such a matrix were computed by M.J.C.Gover [11] and a different proof, using arguments from the Theory of Orthogonal Polynomials was provided by Marcellán and Petronilho [18] .

Theorem 5 *The eigenvalues of the tridiagonal 2-Toeplitz matrix* B_{2n+1} *defined by* (12) *are* a_1 *and the solutions of the quadratic equations*

$$(\lambda - a_1)(\lambda - a_2) - \left[b_1c_1 + b_2c_2 + 2\sqrt{b_1b_2c_1c_2}\cos\frac{k\pi}{n+1}\right] = 0 \ , \ k = 1, \ldots, n \ ,$$

and the eigenvalues of B_{2n} *are the solutions of the quadratic equations*

$$(\lambda - a_1)(\lambda - a_2) - \left[b_1c_1 + b_2c_2 + 2\sqrt{b_1b_2c_1c_2}\cos\theta_{nk}\right] = 0 \ , \ k = 1, \ldots, n \ ,$$

where θ_{nk}*'s are the nonzero solutions of the trigonometric equation* $\sqrt{b_1c_1}\sin[(n+1)\theta] + \sqrt{b_2c_2}\sin(n\theta) = 0 \quad (0 < \theta < \pi)$. ■

Since $b_i > 0$ and $c_i > 0$ for $i = 1, 2$ then there exists an OPS, $\{S_n\}_{n\geq 0}$, such that B_n is the corresponding tridiagonal matrix of order n. Let $\{Q_n\}_{n\geq 0}$ be the corresponding monic OPS. Then

$$Q_{2n}(x) = (b_1b_2)^n S_{2n}(x), \qquad Q_{2n+1}(x) = b_1(b_1b_2)^n S_{2n+1}(x).$$

Moreover, according to the results in [18] , $\{Q_n\}_{n\geq 0}$ can be obtained by a quadratic polynomial mapping on a linear transformation of the monic Chebyshev polynomials of second kind. In fact, putting

$$T(x) = (x - a_1)(x - a_2), \quad \alpha = 2\sqrt{b_1b_2c_1c_2}, \quad \beta = b_1c_1 + b_2c_2,$$

we have $Q_{2n+1}(x) = (x - a_1)P_n(T(x))$, $Q_{2n}(x) = R_n(T(x))$, where $P_n(x) = \alpha^n U_n\left(\frac{x-\beta}{\alpha}\right)$, $R_n(x) = P_n(x) + b_2c_2P_{n-1}(x)$, for all $n = 0, 1, 2, \ldots$. Notice that P_n is orthogonal with respect to the distribution function

$$\sigma_P(x) = \sigma_U\left(\frac{x-\beta}{\alpha}\right), \quad \mathrm{supp}(\sigma_P) = [\beta - \alpha, \beta + \alpha] \ , \ \text{so that } d\sigma_P(x) = \frac{2}{\pi\alpha^2}\sqrt{\alpha^2 - (x-\beta)^2}\, dx \ .$$

From [18] the polynomials of the first kind of the sequence $\{Q_n\}_{n\geq 0}$ are $Q^{(1)}_{2n-1}(x) = (x - a_2)R^{(1)}_{n-1}(T(x))$, $Q^{(1)}_{2n}(x) = P^{(1)}_n(T(x))$, the Stieltjes function of $\{Q_n\}_{n\geq 0}$ being

$$F_Q(z) = \frac{M}{a_1 - z} + \frac{b_1c_1}{z - a_1}[F_P(T(z)) - F_P(0)] \quad , \tag{13}$$

where F_P denotes the Stieltjes function associated with σ_P, $M = \mu_0 - b_1c_1F_P(0)$ and μ_0 is the first moment of σ_P. Clearly, $\mu_0 = \int_{\beta-\alpha}^{\beta+\alpha} d\sigma_P(x) = 1$. Furthermore,

$$F_P(z) = \frac{1}{\alpha}F_U\left(\frac{z-\beta}{\alpha}\right) = \frac{-2}{\alpha^2}\left(z - \beta - \sqrt{(z-\beta)^2 - \alpha^2}\right) \ ,$$

where the square root is such that $|z - \beta + \sqrt{(z-\beta)^2 - \alpha^2}| > \alpha$ whenever $z \notin [\beta - \alpha, \beta + \alpha]$. Since $0 \notin [\beta - \alpha, \beta + \alpha]$ for $b_1c_1 \neq b_2c_2$ (this is no a restriction, because the case $b_1c_1 = b_2c_2$ corresponds to constant values along the diagonal of the corresponding tridiagonal matrix), elementary computations give $F_P(0) = \min\{b_1c_1, b_2c_2\}/b_1c_1b_2c_2$, hence $M = 1 - \dfrac{\min\{b_1c_1, b_2c_2\}}{b_2c_2}$. It turns out from (13) that the Stieltjes function of $\{Q_n\}_{n\geq 0}$ reads as

$$F_Q(z) = \frac{M}{a_1 - z} - \frac{1/b_2c_2\alpha}{z - a_1}\left[\frac{1}{2}\left(T(z) - \beta - \sqrt{(T(z)-\beta)^2 - \alpha^2}\right) + \min\{b_1c_1, b_2c_2\}\right] \ . \tag{14}$$

From this we find (see [18]) that $\{Q_n\}_{n\geq 0}$ is orthogonal with respect to the distribution function

$$d\sigma_Q(x) \;=\; M\delta(x - a_1) + \frac{1}{2\pi\, b_2c_2}\frac{1}{|x - a_1|}\sqrt{4b_1b_2c_1c_2 - (T(x) - b_1c_1 - b_2c_2)^2}\, dx \quad ,$$

the support being the union of two intervals if $M = 0$ and the union of two intervals with a singular point if $M > 0$: either

$$\operatorname{supp}(\sigma_Q) = \begin{cases} T^{-1}(\operatorname{supp}(\sigma_P)) & \text{if} \quad b_1c_1 \le b_2c_2 \\ \\ T^{-1}(\operatorname{supp}(\sigma_P)) \cup \{a_1\} & \text{if} \quad b_1c_1 > b_2c_2 \end{cases} .$$

We notice that

$$T^{-1}(\operatorname{supp}(\sigma_P)) = T^{-1}([\beta-\alpha, \beta+\alpha]) = [\frac{a_1+a_2}{2} - s, \frac{a_1+a_2}{2} - r] \cup [\frac{a_1+a_2}{2} + r, \frac{a_1+a_2}{2} + s] \,,$$

$$\text{where } r = \left(\left|\sqrt{b_1c_1} - \sqrt{b_2c_2}\right|^2 + \left|\frac{a_1-a_2}{2}\right|^2 \right)^{1/2}, \quad s = \left(\left|\sqrt{b_1c_1} + \sqrt{b_2c_2}\right|^2 + \left|\frac{a_1-a_2}{2}\right|^2 \right)^{1/2}.$$

3.3 The eigenvalues of a tridiagonal 3-Toeplitz matrix.

Theorem 4 can be applied to the determination of the eigenvalues of a finite tridiagonal 3-Toeplitz matrix, which has the general form

$$B_{n+1} = \begin{bmatrix} a_1 & b_1 & 0 & 0 & 0 & 0 & 0 & \cdots \\ c_1 & a_2 & b_2 & 0 & 0 & 0 & 0 & \cdots \\ 0 & c_2 & a_3 & b_3 & 0 & 0 & 0 & \cdots \\ 0 & 0 & c_3 & a_1 & b_1 & 0 & 0 & \cdots \\ 0 & 0 & 0 & c_1 & a_2 & b_2 & 0 & \cdots \\ 0 & 0 & 0 & 0 & c_2 & a_3 & b_3 & \cdots \\ 0 & 0 & 0 & 0 & 0 & c_3 & a_1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \in \mathbf{C}^{(n+1,n+1)}$$

Again, we assume that B_{n+1} is irreducible, i.e., $b_ic_i \neq 0$ $(i = 1,2,3)$. Given B_{n+1}, define a sequence of monic polynomials $\{P_n\}_{n\ge 0}$ by

$$P_n(x) = \left(2\sqrt{b_1b_2b_3c_1c_2c_3}\right)^n \hat{U}_n\left(\frac{x - b_1c_1 - b_2c_2 - b_3c_3}{2\sqrt{b_1b_2b_3c_1c_2c_3}}\right), \quad n \ge 0 \,.$$

Now, define a polynomial π_3 as

$$\begin{aligned} \pi_3(x) = (x-a_1)(x-a_2)(x-a_3) - (b_1c_1 + b_2c_2 + b_3c_3)(x-a_3) + \\ + b_1c_1 + b_2c_2 + b_3c_3 - b_2c_2(a_3-a_1) - b_3c_3(a_3-a_2)\,, \end{aligned}$$

and denote by a and b the roots of the quadratic equation $(x-a_1)(x-a_2) - b_1c_1 = 0$. Thus, using Theorem 4, it can be shown that the eigenvalues of B_n are the zeros of a MOPS $\{Q_n\}_{n\ge 0}$ such that

$$\begin{aligned} Q_{3n}(x) &= P_n(\pi_3(x)) + b_3c_3(x-a_2)P_{n-1}(\pi_3(x)) \\ Q_{3n+1}(x) &= (x-a_1)P_n(\pi_3(x)) + b_1c_1b_3c_3P_{n-1}(\pi_3(x)) \\ Q_{3n+2}(x) &= (x-a)(x-b)P_n(\pi_3(x)) \end{aligned}$$

(the parameters for the corresponding three-term recurrence relation are $\tilde{\beta}_{3n} = a_1$, $\tilde{\beta}_{3n+1} = a_2$, $\beta_{3n+2} = a_3$, $\tilde{\gamma}_{3n+1} = b_1c_1$, $\tilde{\gamma}_{3n+2} = b_2c_2$ and $\tilde{\gamma}_{3n+3} = b_3c_3$). In particular, the eigenvalues of B_{3n+2} are a , b and the roots of the cubic equations

$$\pi_3(x) = b_1c_1 + b_2c_2 + b_3c_3 + 2\sqrt{b_1b_2b_3c_1c_2c_3}\cos\frac{k\pi}{n+1}, \quad k = 1, \ldots, n \,.$$

4 The Chain Model.

The Chain Model has been applied in several areas of Modern Physics: Solid State Physics [12], Nuclear Physics [32], Quantum Mechanics [14], etc. In this section we will describe the General Chain Model. For more details see [13]-[14] and references contained therein.

4.1 Physical Motivation.

It is well known the importance of the eigenvalue problem for symmetric matrices since many quantum systems can be described using such kind of matrices (see [26, Chapter 2, Section 6], and also [25]).

In general, the computation of the eigenvalues (and also the eigenvectors) for an arbitrary matrix is very difficult since it is equivalent to the problem of finding the roots of a polynomial of degree n and it is not posible to obtain, for an arbitrary polynomial, an analytic expressions. Moreover, the numerical algorithms (Newton's Method, etc) are, in general, unstable for large n. For this reason, in several areas of Modern Physics simpler models have been introduced, the so called *Chain Models* (see [12], [32], [13] and references contained therein). The Chain Model is, in general, easier to solve and numerically it is more stable and economic. The reason is that such a model is connected with Jacobi (tridiagonal symmetric) matrices which have a lot of *good* properties [24].

The physical interest of the Chain model consists in the fact that any quantum model can be transformed into the corresponding *Chain Model*. The main physical idea of the model is that in order to find the local density of a given state it is sufficient to consider the neighboring states. This means that the local density depends strongly on the neighboring states while the more distant ones have smaller effect. The solution of this problem is the determination of linear combinations of the local states such that the system pass through each state as it diffuses away from the local initial state. The local density for a basis state $|\Phi_0\rangle$ is determined by the sequence of *orthogonal states*(orbits) $|\Psi_n\rangle$ where $|\Psi_0>\equiv|\Phi_0>$. The orthogonal states (orbits) $|\Psi_n>$ must satisfy the time independent Schrödinger equation

$$\mathcal{H}|\Psi_n>=b_{n+1}|\Psi_{n+1}>+a_n|\Psi_n>+b_n|\Psi_{n-1}>, \tag{15}$$

where $\mathcal{H}$ is the Hamiltonian of the model. Here the parameters a_n, b_n describe the coupling of each orthogonal state with itself and its neighbors. In [13] has been considered the *constant chain model* corresponding to the special cases when the sequences $\{a_n\}$ and $\{b_n\}$ are constants equal to a and b, respectively. Here we will consider a generalization of the constant model: The 2-Periodic Chain Model corresponding to it where the sequences $\{a_n\}$ and $\{b_n\}$ are periodic sequences with period 2, i.e., $\{a_n\}=\{a,b,a,b,\cdots\}$ and $\{b_n\}=\{c,d,c,d,\cdots\}$. For such a model it is possible to obtain analytic formulas for the values of the energy (eigenvalues) of $\mathcal{H}$ and the corresponding wave functions.

4.2 Notation.

Before define the Chain Model let us introduce some notation. Assume that the set of wave functions $\{|\Phi_k>\}_{k\geq 0}$ is a basis of our space of states not necessarily orthogonal in the sense that the inner product $<\Phi_m|\Phi_n>\equiv\displaystyle\int\overline{\Phi_m}\Phi_n\,d\tau$ could be different from zero for $m\neq n$. In the following, we will suppose that any state $|u>$ of the system can be represented as a linear combination of the basis $\{|\Phi_k>\}_{k\geq 0}$, i.e., $|u>=\sum_{k=0}^{\infty}u_k|\Phi_k>$ and we will represent it by the infinite column vector $\mathbf{u}$ with coordinates u_k. The action of the Hamiltonian $\mathcal{H}$ (15) on a basis state $|\Phi_n>$ is represented, in general, by the Hamiltonian matrix $\mathbf{H}$ defined by means of the parameters $\mathbf{H}_{mn}$ in such a way that

$$\mathcal{H}|\Phi_n>=\sum_{m=0}^{\infty}\mathbf{H}_{mn}|\Phi_m> . \tag{16}$$

The $\mathbf{H}_{mn}$ are, in general, different from the matrix elements of the Hamiltonian $\mathcal{H}_{mn}$ defined by $\mathcal{H}_{mn}=<\Phi_m|\mathcal{H}|\Phi_n>$. The matrix elements $\mathcal{H}_{mn}$ of the Hamiltonian constitute a self-adjoint matrix (Hermitian), i.e., $\overline{\mathcal{H}^T_{mn}}=\mathcal{H}_{mn}$. Here, by A^T we denote the transpose of a matrix A and by $\overline{A}$ the complex conjugate of A. We also need the overlap matrix $\mathbf{S}$ defined by the matrix elements $\mathbf{S}_{mn}=<\Phi_m|\Phi_n>$, which is also a self-adjoint matrix. The elements $\mathcal{H}_{mn}$ and $\mathbf{H}_{mn}$ are related to each other by the expression

$$\mathcal{H}_{mn}=[\mathbf{SH}]_{mn} \tag{17}$$

In some cases, it is known $\mathbf{S}$ and $[\mathcal{H}_{mn}]$. Then, for $\mathcal{H}$ the following formula holds $\mathbf{H}=\mathbf{S}^{-1}[\mathcal{H}_{mn}]$. Using the above notation the time independent Schrödinger equation can be written in the matrix form

$$\mathbf{H}\mathbf{u}_\alpha=\varepsilon_\alpha\mathbf{u}_\alpha, \tag{18}$$

where α is an index containing all quantum numbers.

4.3 The Chain Model.

Definition 4.1 *The Chain Model is a quantum model determined by a sequence of orthonormal orbits (states)* $\{\mathbf{u}_0,\mathbf{u}_1,\cdots\}$ *and two sets of real parameters* $\{a_1,a_2,\cdots\}$ *and* $\{b_1,b_2,\cdots\}$*, which describe the action of the Hamiltonian* $\mathbf{H}$ *on the orbitals by a symmetric three-term recurrence relation of the form*

$$\mathbf{H}\mathbf{u}_n=b_{n+1}\mathbf{u}_{n+1}+a_n\mathbf{u}_n+b_n\mathbf{u}_{n-1}. \tag{19}$$

The sequence $\{\mathbf{u}_0,\mathbf{u}_1,\cdots\}$ *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. The overlap of the states* $\{\mathbf{u}_n\}$ *is defined in terms of the matrix* $\mathbf{S}$ *by formula* $\mathbf{u}_n^+\mathbf{S}\mathbf{u}_m=\delta_{nm}$*, where* $a^+\equiv\overline{a}^T$ *and* $\delta_{km}=1$ *for* $k=m$*, elsewhere* $\delta_{km}=0$*. This model is equivalent to expressing the matrix of* $\mathbf{H}$ *as a Jacobi (tridiagonal symmetric) matrix [13]*

$$\mathbf{H}=\begin{pmatrix} a_0 & b_1 & 0 & 0 & \dots \\ b_1 & a_1 & b_2 & 0 & \dots \\ 0 & b_2 & a_2 & b_3 & \dots \\ 0 & 0 & b_3 & a_3 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{20}$$

The chain model can be interpreted as follows: Given a system in the initial state $\mathbf{u}_0$ it can go from $\mathbf{u}_0$ to a new state $\mathbf{u}_1$ which can represent a linear combination of the physical (real) states neighboring $\mathbf{u}_0$. Similarly, having reached $\mathbf{u}_1$, the system can go back to the previous state $\mathbf{u}_0$ or go on to another state $\mathbf{u}_2$, etc. In other words, the behaviour of the system is most influenced by the nearer preceding or succeeding states and less influenced by the more distant ones. This is the mathematical expression of the physical concept of local environment [13]. In the following, we will suppose that the states are ordered by the sequence $\{\mathbf{u}_0,\mathbf{u}_1,\mathbf{u}_2,\cdots\}$ where $\mathbf{u}_0$ is the initial state and the others $\mathbf{u}_k$, $k\geq 1$ are the succeeding states. We will say that a state $\mathbf{u}_k$ is even or odd if $k=2n$ or $k=2n+1$, $n=0,1,2,\cdots$, respectively.

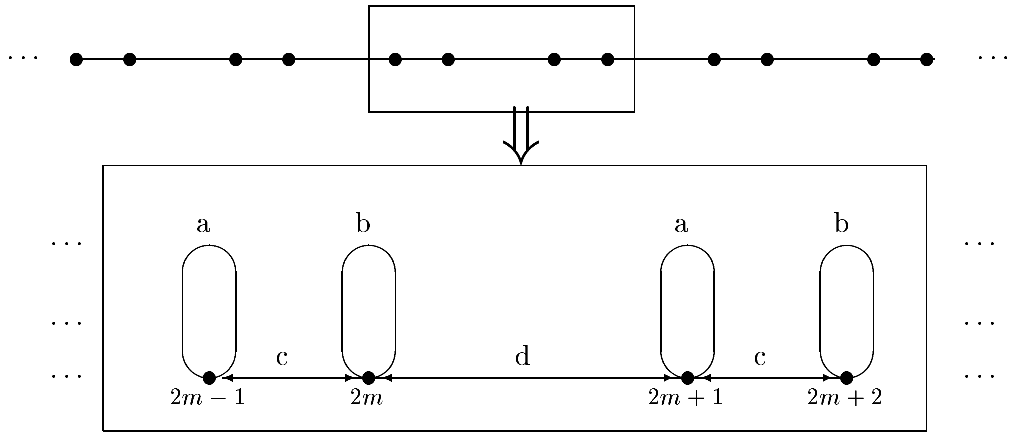

Figure 1: Scheme of the 2-Periodic Chain Model.

4.4 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., $\{a_n\} = \{a, b, a, b, \cdots\}$ and $\{b_n\} = \{c, d, c, d, \cdots\}$. Then the matrix (20) becomes

$$\mathbf{H} = \begin{pmatrix} a & c & 0 & 0 & 0 & \dots \\ c & b & d & 0 & 0 & \dots \\ 0 & d & a & c & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{21}$$

These coupling constants are defined in such a way that the interaction between different states leads us to a Hamiltonian $\mathcal{H}$ with the following properties ($|u_k> \equiv \mathbf{u}_k$)

$$\begin{aligned} h_{mm} &=< u_m|\mathbf{H}|u_m >= \begin{cases} a & \text{if } m \text{ is even} \\ \\ b & \text{if } m \text{ is odd} \end{cases} \\ h_{mn} &=< u_m|\mathbf{H}|u_n >= \begin{cases} c & \text{for } m = 2n-1,\ k = 2n \\ \\ d & \text{for } m = 2n,\ k = 2n+1 \end{cases} \end{aligned} \tag{22}$$

Notice that the order of the interaction and the parity is crucial, i.e., even and odd states have a different behavior. This can be interpreted as follows: the coupling between even or odd states is equal to a and b, respectively and not necessarily equal. The coupling between an even state and its preceding or its succeeding is equal to c or d, respectively and not necessarily equal. Analogously, for the coupling between odd states and their neighbors, we have coupling d or c, respectively, when it is coupled with the preceding or the succeeding state. The scheme represented in Figure 1 can be useful to understand this 2-Periodic Chain Model.

4.5 The Eigenvalues and Eigenstates of the 2-Periodic Chain.

In order to obtain the eigenvalues and eigenstates of the 2-Periodic Chain we will suppose that the solution $\mathbf{u}$ of the Schrödinger equation (18) can be written as a linear combination of the states $\{\mathbf{u}_0, \mathbf{u}_1, \mathbf{u}_2, \cdots\}$, i.e.,

$$\mathbf{u} = \sum_{k=0}^{\infty} C_k \mathbf{u}_k. \tag{23}$$

Then, (18) can be rewritten in the form

$$\begin{pmatrix} a & c & 0 & 0 & 0 & \dots \\ c & b & d & 0 & 0 & \dots \\ 0 & d & a & c & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \vdots \end{pmatrix} = \varepsilon \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \vdots \end{pmatrix}, \tag{24}$$

where C_k are the coefficients in the linear combination (23), and ε is the corresponding eigenvalue of the matrix Hamiltonian $\mathbf{H}$. Here, it is important to remark that we need to consider finite or infinite chains. The solution of this eigenvalue problem for the finite chain is given by theorem 5, which leads us to the following two cases:

4.5.1 Case of $N = 2n+1$ states in the Chain.

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 ε of (24) are the following

$$\varepsilon_0 = a, \quad \varepsilon_{\pm k} = \frac{a+b}{2} \pm \sqrt{\frac{(a-b)^2}{4} + c^2 + d^2 + 2cd\cos\tfrac{k\pi}{n+1}}\,, \quad k = 1, 2, ..., n \tag{25}$$

The particular case $a = b$ and $c = d$ gives us $\varepsilon_0 = a$, $\varepsilon_{\pm k} = a \pm 2c\cos\frac{k\pi}{2(n+1)}$ para $k = 1, 2, ..., n$.

4.5.2 Case of $N = 2n$ states in the Chain.

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 ε of (24) are the following

$$\varepsilon_{\pm k} = \frac{a+b}{2} \pm \sqrt{\frac{(a-b)^2}{4} + c^2 + d^2 + 2cd\cos\theta_{Nk}}, \quad k = 1, 2, ..., n \tag{26}$$

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

$$c\sin[(n+1)\theta] + d\sin(n\theta) = 0 \quad .$$

The particular case $a = b$ and $c = d$ gives us the values $\varepsilon_{\pm k} = a \pm 2c\cos\frac{k\pi}{2n+1}$.

4.6 The Green Function $G_0(\varepsilon)$.

For this model it is possible to obtain analytic formulas for the general diagonal Green function $G_0(\varepsilon) \equiv G_{00}(\varepsilon)$. The Green function (usually called the *projected density of states*) $G_{nm}(\varepsilon)$ between two states $\mathbf{u}_n$ and $\mathbf{u}_m$ is formally defined by $G_{nm}(\varepsilon) = \mathbf{u}_n^+ \mathbf{S}(\varepsilon - \mathbf{H})^{-1}\mathbf{u}_m$. The quantity $G_{nn}(\varepsilon)$ is the density of states in energy with each state weighted by its projection on the atomic orbital $\mathbf{u}_n$. In [13], [12] it is shown that the Green function of the initial state $\mathbf{u}_0$ $G_0(\varepsilon)$ for the Chain Model (19) is related to the continued fraction

$$G_0(\varepsilon) = \cfrac{1}{\varepsilon - a_0 - \cfrac{b_1^2}{\varepsilon - a_1 - \cfrac{b_2^2}{\varepsilon - a_2 - \ddots}}}, \quad \varepsilon \in \mathbb{C}. \tag{27}$$

For the finite Chain Model, this continued fraction reduces to the ratio of two polynomials which conforms the well known Padé Approximant 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. Here we want to remark that the real part of $G_0(\varepsilon)$ describes the response of the system to be driven at a given energy, i.e., the resistence to excitation different from the eigenenergies, although the $n_0(\varepsilon) = -\lim_{\epsilon\to 0} \frac{1}{\pi} Im\,(G_0(\varepsilon + i\epsilon))$ is the local density of the initial state. In [14], it has been shown the relation of this quantity $n_0(\varepsilon)$ and the electron density in multielectron systems and also in Quantum Mechanics.

4.7 The infinite chain.

In the case of the infinite chain, it is possible to obtain an analytic expression for the Green function $G_0(\varepsilon)$ (27). In this case, using Rational Approximation Theory [33], we obtain that the continued fraction (27) converges to the Stieltjes function associated with the measure of orthogonality of the polynomial sequence $\{Q_n\}_{n\geq 0}$, i.e., $G_0(\varepsilon) = F_Q(\varepsilon)$. In this case, we can obtain the local density $n_0(\varepsilon)$ which coincides with the corresponding measure of orthogonality $d\sigma_Q(\varepsilon)$ (see formula (14)).

4.8 The semiclassical approximation to the density of the distribution of the eigenvalues and their moments.

Here, we will apply the semiclassical or WKB approximation [1], [35], [36] to obtain the density of the distribution $\rho_n(\varepsilon)$ of the eigenvalues of the 2-periodic Hamiltonian (24) and use the method developed by Dehesa [7] to obtain their moments μ_r around the origin, i.e., we will calculate the quantities

$$\rho_n(\varepsilon) = \frac{1}{n}\sum_{i=1}^{n} \delta(\varepsilon - \varepsilon_{n,i}), \quad \mu_r = \frac{1}{n} y_r = \frac{1}{n}\sum_{i=1}^{n} \varepsilon_{n,i}^r \quad , \tag{28}$$

where $\varepsilon_{n,i}$, $i = 1, 2, ..., n$, are the eigenvalues of the matrix (21). To obtain the WKB-density (and its moments), we will use the fact that the eigenvalues of the matrix B_m (21) coincide with the zeros of the polynomial Q_m associated with the (infinite) Jacobi matrix polynomial sequence $\{Q_k\}_{k\geq 0}$. For odd matrices, i.e., when B_{2n+1}, the corresponding polynomials are quadratic mappings of the Chebyshev ones. In the even case we will have the co-recursive polynomials R_n. In both cases, it is possible to find the second order differential equation that those polynomials satisfy, and then, we can use the semiclassical or WKB approximation which allows us to obtain an analytic expression for the density $\rho_n(\varepsilon)$.

First of all we point out that, since we are working with a Jacobi matrix, all its eigenvalues are real, simple and located in the interior of the convex hull of the interval of orthogonality of the associated orthogonal polynomials. This is a necessary condition in order to apply both algorithms.

Now, let us analyze the so-called semiclassical or WKB approximation (see [1],[35] and references contained therein). Denoting the zeros of a polynomial $\tilde{P}_n(x)$ by $\{x_{n,k}\}_{k=1}^n$, we can define its distribution function $\rho_n(x)$ and their moments around the origin μ_r as

$$\rho_n(x) = \frac{1}{n}\sum_{k=1}^{n} \delta(x - x_{n,k}), \quad \mu_r = \frac{1}{n} y_r = \frac{1}{n}\sum_{i=1}^{n} x_{n,i}^r. \tag{29}$$

We will follow the method presented in [35] in order to obtain the WKB density of zeros, which is an approximate expression for the density of zeros of solutions of any second order linear differential equation with polynomial coefficients (SODE)

$$p(x)y''(x) + q(x)y'(x) + r(x)y(x) = 0. \tag{30}$$

The main result is established in the following

Theorem 6 *[1], [35] Let $S(x)$ and $\epsilon(x)$ be the functions*

$$S(x) = \frac{1}{4p(x)^2}\{2p(x)(2r(x) - q'(x)) + q(x)(2p'(x) - q(x))\}, \tag{31}$$

$$\epsilon(x) = \frac{1}{4[S(x)]^2}\left\{\frac{5[S'(x)]^2}{4[S(x)]} - S''(x)\right\} = \frac{\tilde{P}(x,n)}{\tilde{Q}(x,n)}, \tag{32}$$

where $\tilde{P}(x,n)$ and $\tilde{Q}(x,n)$ are polynomials in x as well as in n. If the condition $\epsilon(x) << 1$ holds, then, the semiclassical or WKB density of zeros of the solutions of (30) is given by

$$\rho_{WKB}(x) = \frac{1}{\pi}\sqrt{S(x)}, \quad x \in I \subseteq \mathbb{R}, \tag{33}$$

in every interval I where the function $S(x)$ is positive. ■

In order to study the moments of the distribution of eigenvalues of our 2-periodic matrix we will use a general method presented in [7] for the moments of low order μ_r of the distribution of zeros (29). Dehesa [7] has obtained a general formula to find these quantities. We will apply these formulas to obtain the general expression for the moments μ_1 μ_2 and μ_3. If we have a tridiagonal symmetric matrix J_n where $\alpha_n \equiv \gamma_{n+1}$, then the first three moments of its eigenvalue distribution are given by the formulas

$$\mu_1 = \frac{1}{n}\sum_{k=0}^{n-1}\beta_k, \quad \mu_2 = \frac{1}{n}\sum_{k=0}^{n-1}\beta_k^2 + 2\sum_{k=0}^{n-2}\alpha_k^2, \quad \mu_3 = \frac{1}{n}\sum_{k=0}^{n-1}\beta_k^3 + 3\sum_{k=0}^{n-2}\alpha_k^2(\beta_k + \beta_{k+1}). \tag{34}$$

Let us to apply the Theorem above to calculate the distribution of eigenvalues of our symmetric Hamiltonian matrix (24). Here we wish to point out that in the odd case the corresponding polynomials are $Q_{2n+1}(\varepsilon) = (\varepsilon - a_1)P_n(T(\varepsilon))$, so we can consider only the distribution of zeros of P_n, since for any $n = 1, 2, ...$, $\varepsilon = a$ is always a zero of the polynomial and thus an eigenenergy. Furthermore, $P_n(T(\varepsilon))$ is a quadratic modification of the Chebyshev polynomials $U_n(\varepsilon)$ and then the SODE follows from the classical ones (11) simply making the change of variables $\varepsilon \leftrightarrow T(\varepsilon)$. In fact we deduce that the polynomial $P_n(T(\varepsilon))$ satisfies a SODE (30) with the coefficients

$$\begin{aligned}
p(\varepsilon) = {} & \left(4\,c^2\,d^2 - \left(-\left(a\,b\right) + c^2 + d^2 + a\,\varepsilon + b\,\varepsilon - \varepsilon^2\right)^2\right), \\
q(\varepsilon) = {} & 3\left(-a - b + 2\,\varepsilon\right)\,\left(-\left(a\,b\right) + c^2 + d^2 + a\,\varepsilon + b\,\varepsilon - \varepsilon^2\right) - \\
& -2\,\left(4\,c^2\,d^2 - \left(-\left(a\,b\right) + c^2 + d^2 + a\,\varepsilon + b\,\varepsilon - \varepsilon^2\right)^2\right), \\
r(\varepsilon) = {} & n\,\left(2 + n\right)\,\left(-a - b + 2\,\varepsilon\right)^2.
\end{aligned} \tag{35}$$

For the even case the situation is more complicated since we need to calculate the SODE for the co-recursive polynomials $R_n(T(\varepsilon))$. Using the symbolic program *Mathematica* [34], as well as the package *PowerSeries* developed by Koepf [16], we obtain for the co-recursive polynomials $R_n(\varepsilon)$ a SODE (30) with coefficients

$$\begin{aligned}
p(\varepsilon) &= \left(1 + n + c^4\,n + c^2\,\varepsilon + 2\,c^2\,n\,\varepsilon\right)\,\left(-1 + \varepsilon^2\right), \\
q(\varepsilon) &= c^2 + 2\,c^2\,n + 3\,\varepsilon + 3\,n\,\varepsilon + 3\,c^4\,n\,\varepsilon + 2\,c^2\,\varepsilon^2 + 4\,c^2\,n\,\varepsilon^2, \\
r(\varepsilon) &= -2\,n + c^4\,n - 3\,n^2 - n^3 - c^4\,n^3 - c^2\,n\,\varepsilon - 3\,c^2\,n^2\,\varepsilon - 2\,c^2\,n^3\,\varepsilon.
\end{aligned} \tag{36}$$

Making the change of variables $\varepsilon \leftrightarrow T(\varepsilon)$ $(T(\varepsilon) = (\varepsilon - a)(\varepsilon - b))$ in the previous SODE, we find the following SODE for the polynomials $Q_{2n}(\varepsilon)$

$$\tilde{p}(\varepsilon)Q''_{2n}(\varepsilon) + \tilde{q}(\varepsilon)Q'_{2n}(\varepsilon) + \tilde{r}(\varepsilon)Q_{2n}(\varepsilon) = 0,$$

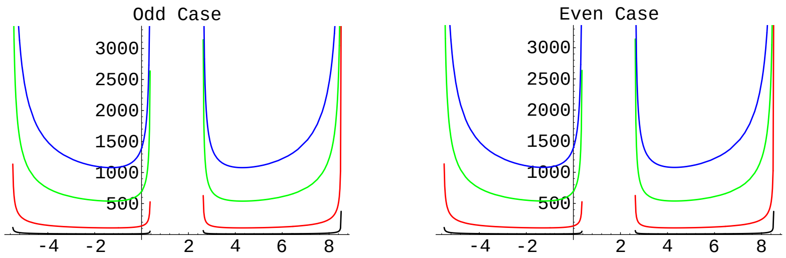

Figure 2: WKB Density of the Distribution of the eigenvalues of the Hamiltonian matrix **H**.

where the coefficients are given by

$$\begin{array}{ll} \tilde{p}(\varepsilon) = 4c^2d^2T''(\varepsilon)p\left(\frac{T(\varepsilon)-a^2-b^2}{2cd}\right), & \tilde{r}(\varepsilon) = T'(\varepsilon)^3 r\left(\frac{T(\varepsilon)-a^2-b^2}{2cd}\right), \\ \tilde{q}(\varepsilon) = 2cdT'(\varepsilon)^2 q\left(\frac{T(\varepsilon)-a^2-b^2}{2cd}\right) - 8c^2d^2p\left(\frac{T(\varepsilon)-a^2-b^2}{2cd}\right). & \end{array} \tag{37}$$

Substituting (35), (37) in (33) we can find the WKB density of the eigenvalues of the Hamiltonian matrix **H** (21). A straightforward calculation shows us that the conditions of Theorem 6 are satisfied if n large enough. The expression for the $\rho^{WKB}(x)$, in both cases, is large and we will only show the typical behaviour of the WKB density (see Figure 2). As we can see in Figure 2 we have that all eigenvalues are located inside the support of the measure, except one, equal to a in the odd case. In the picture, the values $a = 1$, $b = 2$, $c = 3$ and $d = 4$ are used (from top to bottom $n = 10000, 5000, 1000, 100$). Notice that, if we look for the above picture, the eigenvalues of the matrix **H** (the zeros of the corresponding orthogonal polynomials) are concentrated in the union of two intervals (with constitute the support of their orthogonality measure).

To calculate the moments μ_r, we will use formula (34). Then we find, for the odd case, the expressions

$$\mu_1 = \frac{a+b}{2} + \frac{a-b}{2n+1}, \quad \mu_2 = \frac{a^2+b^2}{2} + c^2 + d^2 + \frac{a^2-b^2-c^2-d^2}{2n+1},$$

$$\mu_3 = \frac{a^3+b^3}{2}\frac{3}{2}(a+b)(c^2+d^2) + \frac{a^3-b^3-3(a+b)(c^2+d^2)}{2n+1}.$$

Analogously, for the even case, we have

$$\mu_1 = \frac{a+b}{2}, \quad \mu_2 = \frac{a^2+b^2}{2} + c^2 + d^2 - \frac{d^2}{2m},$$

$$\mu_3 = \frac{a^3+b^3}{2}\frac{3}{2}(a+b)(c^2+d^2) + \frac{(a+b)(2c^2+d^2)}{2n}.$$

Finally, in both cases, we have the following asymptotic formulas

$$\mu_1 \sim \frac{a+b}{2}, \quad \mu_2 \sim \frac{a^2+b^2}{2} + c^2 + d^2, \quad \mu_3 \sim \frac{a^3+b^3}{2}\frac{3}{2}(a+b)(c^2+d^2).$$

The dependence of the central moments via a modification of one of the interaction parameters a, b, c or d can be studied by using formulas obtained in [17]. Analogous calculations can be done for 3-periodic Chain models. For this case computations are in progress.

ACKNOWLEDGEMENTS This work was finished during a stay of the first author in the Departamento de Matemática da Faculdade de Ciências e Tecnologia da Universidade de Coimbra. The research of the first two authors was partially supported by Dirección General de Investigación Científica y Técnica (DGICYT) of SPAIN under grant PB 93-0228-C02-01. The research of the third author was supported by the grant BD976 from Junta Nacional de Investigação Científica e Tecnológica (JNICT) of PORTUGAL.

References

[1] E.R. Arriola, A. Zarzo and J.S. Dehesa: *Spectral Properties of the biconfluent Heun differential equation.* J.Comput. Appl. Math. **37**, (1991), 161-169.

[2] P. Barrucand and D. Dickinson: *On Cubic Transformations of Orthogonal Polynomials.* Proc. Amer. Math. Soc. **17**, (1966), 810-814.

[3] E. Buendía, S. J. Dehesa and F. J. Gálvez: *The distribution of the zeros of the polynomial eigenfunction of ordinary differential operators of arbitrary order.* In ORTHOGONAL POLYNOMIALS AND THEIR APPLICATIONS. M.Alfaro et al. Eds. Lecture Notes in Mathematics. **Vol. 1329**, Springer-Verlag, Berlin, 1988, 222-235.

[4] J. Charris, M. H. Ismail and S. Monsalve: *On Sieved Orthogonal Polynomials, X: General Blocks of Recurrence Relations.* Pacific J. of Math. **163**(2), (1994), 237-267.

[5] T. S. Chihara: AN INTRODUCTION TO ORTHOGONAL POLYNOMIALS. Gordon and Breach. New York. 1978.

[6] T. S. Chihara: *On Co-recursive Orthogonal Polynomials.* Proc. Amer. Math. Soc. **8**, (1957), 899-905.

[7] J. S. Dehesa: *On the conditions for a Hamiltonian matrix to have an eigenvalue density with some prescribed characteristic.* J. Comput. Appl. Math. **2**, (1976), 249-254.

[8] J. S. Dehesa: *The eigenvalue density of rational Jacobi matrices. II.* Linear Alg. and its Appl. **33**, (1980), 41-55.

[9] J.S. Geronimo and W. Van Assche: *Orthogonal Polynomials with Asymptotically Periodic Recurrence Coefficients.* J. Approx. Theory **46**, (1986), 251-283.

[10] J. Geronimo and W. Van Assche: *Orthogonal Polynomials on Several Intervals via a Polynomial Mapping* Trans. Amer. Math. Soc. **308**(2), (1988), 559-581.

[11] M. J. C. Gover: *The Eigenproblem of a Tridiagonal 2-Toeplitz Matrix.* Linear Alg. and Its Applic. **197-198**, (1994), 63-78.

[12] R. Haydock, V. Heine and M.J. Kelly: *Electronic structure based on the local atomic environment for tight-binding bands:II* J. Phys. C**8**, (1975), 2591-2604.

[13] R. Haydock: *Recursive Solution of Schrödinger's Equation.*SOLID STATE PHYSICS **35**. (1980). 215-294.

[14] R. Haydock: *The Recursion Method and the Schrödinger's Equation.* In ORTHOGONAL POLYNOMIALS: THEORY AND PRACTICE. P. Nevai Ed. NATO ASI Series C, **Vol. 294**, (Kluwer Acad. Publ., Dordrecht, 1990), 217-228.

[15] M. H. Ismail: *On Sieved Orthogonal Polynomials, III: Orthogonality on Several Intervals.* Trans. Amer. Math. Soc. **249**(1), (1986), 89-111.

[16] W. Koepf: *A Package on Formal Power Series.* Mathematica Journal. **4** (2), (1994) 62-69.

[17] F. Marcellán, J.S. Dehesa and A. Ronveaux: *On Orthogonal Polynomial with perturbed recurrence relations* J. Comput. Appl. Math. **30**, (1990), 203-212.

[18] F. Marcellán and J. Petronilho: *Eigenproblems for Tridiagonal 2-Toeplitz Matrices and Quadratic Polynomial Mappings.* Linear Alg. and Its Applic. (1996). To appear.

[19] F. Marcellán and J. Petronilho: *Orthogonal Polynomials and Quadratic Transformations.* (1996). Submmitted.

[20] F.Marcellán and J.Petronilho: *Orthogonal Polynomials and Cubic Polynomial Mappings.* (1996). Submmitted.

[21] F.Marcellán and G.Sansigre: *Orthogonal Polynomials and Cubic Transformations.* J. Comput. App. Math. **49**, (1993), 161-168.

[22] P.Maroni: *Sur la Suite de Polynômes Orthogonaux Associée à la Forme* $\mathbf{u} = \delta_c + \lambda(x-c)^{-1}\mathcal{L}$. Periodica Mathematica Hungarica. **21**(3), (1990), 223-248.

[23] P.Maroni: *Une Théorie Algébrique des Polynômes Orthogonaux. Application aux Polynômes Orthogonaux Semi-Classiques.* in ORTHOGONAL POLYNOMIALS AND THEIR APPLICATIONS, (C.Brezinski, L.Gori, A.Ronveaux eds.), Proc. Erice (1990), IMACS. Ann. Comp. Appl. Math. **50**, (1991), 95-130.

[24] M. Marcus and H. Minc: A SURVEY OF MATRIX THEORY AND MATRIX INEQUALITIES. Dover, New York, (1992).

[25] A Messiah: MÉCANIQUE QUANTIQUE. Dunod, Paris, (1959).

[26] J. von Neummann: FUNDAMENTOS MATEMÁTICOS DE LA MÉCANICA CUÁNTICA. C.S.I.C., Madrid, (1991).

[27] F.Peherstorfer: *On Bernstein-Szegö Orthogonal Polynomials on Several Intervals.* SIAM J. Math. Anal. **21**, (1990), 461-482.

[28] F.Peherstorfer: *On Bernstein-Szegö Orthogonal Polynomials on Several Intervals II.* J. Approx. Theory. **64**, (1991), 123-161.

[29] J. Riordan: AN INTRODUCTION TO COMBINATORIAL ANALYSIS. Wiley, New York, (1958).

[30] W. Van Assche: ASYMPTOTICS FOR ORTHOGONAL POLYNOMIALS. Lecture Notes in Mathematics **Vol. 1265**. Springer-Verlag, Berlin, (1987).

[31] W. Van Assche: *Asymptotic Properties of Orthogonal Polynomials from their Recurrence Formula, I.* J. Approx. Theory **44** (1985), 258-276.

[32] R.R. Whitehead, A. Watt, B.J. Cole and D. Morrinson: *Computational Methods for Shell-Model Calculations.*Adv. Nucl. Phys.**9**, (1977), 123-173.

[33] H. S. Wall: ANALYTIC THEORY OF CONTINUED FRACTIONS. Van Nostrand-Reinhold, Princeton, New Jersey, (1948).

[34] S. Wolfram: *MATHEMATICA*. A SYSTEM FOR DOING MATHEMATICS BY COMPUTER. Addison-Wesley Publishing Co., New York, (1991).

[35] A. Zarzo and J. S. Dehesa: *Spectral Properties of solutions of hypergeometric-type differential equations.* J. Comput. Appl. Math. **50**, (1994), 613-623.

[36] A.Zarzo, J.S. Dehesa and R.J. Yañez: *Distribution of zeros of Gauss and Kummer hypergeometric functions: A semiclassical approach.* Annals Numer. math. **2**, (1995), 457-472.

RENATO ALVAREZ-NODARSE
DEPARTAMENTO DE MATEMÁTICAS, ESCUELA POLITÉCNICA SUPERIOR, UNIV. CARLOS III DE MADRID, BUTARQUE 15, 28911 LEGANÉS, MADRID, SPAIN.
E-Mail: renato@dulcinea.uc3m.es

Francisco Marcellán
Departamento de Matemáticas, Escuela Politécnica Superior, Univ. Carlos III de Madrid, Butarque 15, 28911 Leganés, Madrid, SPAIN.
E-Mail: pacomarc@ing.uc3m.es

José Petronilho
Departamento de Matemática, Faculdade de Ciências e Tecnologia, Univ. Coimbra, Apartado 3008, Coimbra, PORTUGAL.
E-Mail: josep@mat.uc.pt