On-line supplementary material to Haydock's recursive solution of self-adjoint problems. Discrete spectrum

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The aim of the supplementary information is to supply some of intermediary steps skipped over in the main text. Equations of the main text are referred to with a number preceded by M.

I. FINITE OPS

An infinite sequence of polynomials defined by a TTRR (M6) in the case when some of the coefficients $\{\lambda_k\}$ equals zero (e.g. $\lambda_{\mathcal{N}} = 0$) is called *weakly* orthogonal polynomial system (see p. 23 of Ref. [1] or Ref. [2]). The present work suggests that it is more appropriate to view such a *weakly* orthogonal polynomial system as composed of (at least) two independent parts:

- a (at least one) *finite* sequence of polynomials defined by a TTRR (M6) with $\lambda_k > 0$ for $k < \mathcal{N}$
- an *infinite* orthogonal polynomial sequence of quotient polynomials $\{Q_k\}$ defined by a suitably modified TTRR (M6)

and to focus on each of the parts independently. Since the latter is well described, we summarize here some of the elementary results for the *finite* orthogonal polynomial sequences $\{P_k\}_{k=1}^{\mathcal{N}-1}$. The main focus is on the case when $\{c_n\}$ in a TTRR (M6) are *real* numbers.

A. Simplicity of zeros of $\{P_k\}_{k=1}^{\mathcal{N}-1}$

If the coefficients $\lambda_k > 0$ for all $k \in \mathbb{N}$ in a TTRR (M6) then the zeros of the polynomials P_k satisfying the TTRR (M6) are real and simple (Theorem I-5.2 of Ref. [1]). However, in our case $\lambda_{\mathcal{N}} = 0$ and the classical results obtained for the OPS [1] no longer apply. Nevertheless, one can prove that the zeros of the polynomials of a *finite* orthogonal polynomial sequence $\{P_k\}_{k=1}^{\mathcal{N}-1}$ satisfying a TTRR (M6) with the coefficients $\lambda_k > 0$ for all $k < \mathcal{N}$ are still *real* and *simple*.

Before proceeding any further, let us recall *Favard*'s theorem (Theorem I-4.4 of Ref. [1]). The theorem says that for given arbitrary sequences of *complex* numbers $\{c_n\}$ and $\{\lambda_n\}$ in the TTRR (M6) there always exists a *moment functional*, that is a linear functional $\mathcal{L}$ acting in the space of (complex) monic polynomials $\mathbb{C}[E]$, such that the polynomials P_n defined by the TTRR (M6) are *orthogonal* under $\mathcal{L}$:

$$\mathcal{L}(P_k\, P_l) = 0, \qquad k \neq l \in \mathbb{N}. \tag{1}$$

The functional $\mathcal{L}$ is *unique* if we impose the normalization condition $\mathcal{L}(P_0) = \mathcal{L}(1) = \mu_0$, where μ_0 is a chosen positive constant. The coefficient $\mathfrak{n}_k = \mathcal{L}(P_k^2)$ is the square of the norm of P_k that is given by Eq. (B3). The latter implies the property of the *weakly* orthogonal polynomial system that $\mathfrak{n}_k = 0$, $k \geq \mathcal{N}$, so that *all the polynomials P_k with $k \geq \mathcal{N}$ have zero norm.* From Eq. (B3) it also follows that the squared norms $\mathfrak{n}_k$ will be *positive* for $k < \mathcal{N}$ if and only if $\lambda_k > 0$ for $1 \leq k < \mathcal{N}$.

The following simple lemma obtained by Finkel et al. (cf. Lemma 3 of Ref. [2]) is of paramount importance for us:

Let $\mathcal{P}_n$ be the space of *real* polynomials of degree at most n in z. If $\lambda_k > 0$ for $k = 1, 2, \ldots, n$ and c_k is real for $k = 0, 1, \ldots, n$ in a TTRR (M6), then $\mathcal{L}$ is *positive-definite* on $\mathcal{P}_{2n}$. In other words, if $p \in \mathcal{P}_{2n}$ is a real polynomial of degree at most $2n$, $p \neq 0$ and $p(E) \geq 0$ for all $E \in \mathbb{R}$ then $\mathcal{L}(p) > 0$.

Now, given that $\mathcal{L}$ is *positive-definite* on $\mathcal{P}_{2n}$, Theorem I-5.2 of Ref. [1], i.e. the theorem that guarantees simplicity of zeros of an infinite OPS, can easily be extended to the case of *finite* OPS. Indeed, all what the proof of Theorem I-5.2 of Ref. [1] requires is that (cf. Theorem I-2.1 of Ref. [1])

- $\mathcal{L}[\pi(x) P_l(x)] = 0$ [cf. Eq. (B1)] holds for every polynomial $\pi(x)$ of degree $k < l \leq n$
- $\mathcal{L}[x^k P_k(x)] > 0$ for $k \leq n$.

However the above conditions have been for $k < \mathcal{N}$ both guaranteed by Favard's theorem (Theorem I-4.4 of Ref. [1]). Thus we have the following result:

If we have a TTRR (M6) with $\lambda_k > 0$ and c_k real for $k = 0, 1, \ldots, \mathcal{N}-1$, then the polynomials of the resulting *finite* orthogonal polynomial sequence $\{P_k\}_{k=1}^{\mathcal{N}-1}$ have *real* and *simple* zeros.

Surprisingly enough, the above result has been overlooked by Finkel et al [2]. They needed an extra assumption of the Hamiltonian H being fully algebraic to prove the simplicity of zeros (cf. arguments above their Eq. (47)).

B. Interlacing property of zeros of $\{P_k\}_{k=1}^{\mathcal{N}}$

Interlacing property of zeros of an infinite OPS follows from the identity (Eq. (I-4.13) of Ref. [1])

$$P_n'(x) P_{n-1}(x) - P_n(x) P_{n-1}'(x) > 0, \tag{2}$$

which is valid for a *positive-definite* $\mathcal{L}$. The identity is obtained as a limiting case of the *Christoffel-Darboux* identity (Theorem I-4.5 of Ref. [1])

$$\sum_{l=0}^{n-1}\frac{P_l(x)P_l(u)}{\mathfrak{n}_l}=\frac{1}{\mathfrak{n}_{n-1}}\frac{P_n(x)P_{n-1}(u)-P_n(u)P_{n-1}(x)}{x-u}. \tag{3}$$

Identity (2) combined with the simplicity of zeros is all what is needed to prove the so-called *separation* theorem for polynomial zeros (cf. Theorem I-5.3 of Ref. [1]). In the case of a *finite* OPS we need its validity only up to some critical value of $n=\mathcal{N}$. But the latter is obvious as the Christoffel-Darboux identity is a direct consequence of a TTRR (M6) with $\lambda_l>0$, and hence $\mathfrak{n}_l>0$, for $l<\mathcal{N}$.

Now one can prove that the zeros of $P_\mathcal{N}$ have to interlace the zeros of $P_{\mathcal{N}-1}$ even if the norm of $P_\mathcal{N}$ is zero. First, in contrast to $p_\mathcal{N}$ and the TTRR (M5), $P_\mathcal{N}$ is well defined by the TTRR (M6). Second, identity (2) requires the TTRR (M6) to be valid only up to $n=\mathcal{N}-1$, which is the case. The interlacing of the zeros of $P_{\mathcal{N}-1}$ and $P_\mathcal{N}$ then follows from the identity (2) for $n=\mathcal{N}$. Indeed, one has (Eq. (I-5.3) of Ref. [1])

$$\operatorname{sgn} P_n'(x_{nk})=(-1)^{n-k}, \qquad k\le n<\mathcal{N}.$$

On substituting into Eq. (2) for $n=\mathcal{N}$ and $x=x_{\mathcal{N}-1,k}$,

$$-P_\mathcal{N}(x_{\mathcal{N}-1,k})P_{\mathcal{N}-1}'(x_{\mathcal{N}-1,k})>0,$$

one finds

$$\operatorname{sgn} P_\mathcal{N}(x_{\mathcal{N}-1,k})=(-1)^{\mathcal{N}-k}.$$

Hence between any two subsequent zeros of $P_{\mathcal{N}-1}$ the polynomial $P_\mathcal{N}$ changes its sign. Given that $P_\mathcal{N}$ is monic, for sufficiently large $x>x_{\mathcal{N}-1,\mathcal{N}-1}$ one would have $\operatorname{sgn} P_\mathcal{N}(x)=1$ and $P_\mathcal{N}(x)$ will also change sign once for $x>x_{\mathcal{N}-1,\mathcal{N}-1}$. Because $P_\mathcal{N}$ cannot have more than $\mathcal{N}$ zeros, all zeros of $P_\mathcal{N}$ have to be simple.

Thus there is no typing error in the headings of the last two subsections. Sec. I A establishes simplicity of zeros of $\{P_k\}_{k=1}^{\mathcal{N}-1}$ resulting from the *positive-definiteness* of $\mathcal{L}$ on $\mathcal{P}_{2n}$. Sec. I B adds $P_\mathcal{N}$ to the earlier set thanks to the *Christoffel-Darboux* identity (3).

We have seen that the normalized $p_\mathcal{N}$ is not defined because of $\mathfrak{n}_\mathcal{N}\equiv 0$. This prohibits among others arriving at (B4) from (M6). Nevertheless, with monic not normalized $P_\mathcal{N}$ being well defined by the TTRR (M6), the latter provides a justification for considering the zeros of the l.h.s. of Eq. (M7) as the zeros of $P_\mathcal{N}$.

C. Explicit expression for $d\nu_P(E)=w(E)dE$

It is known from *Boas*'s theorem [3] (Theorems II-6.3-4 of Ref. [1]) that there is a (not necessarily unique) function of bounded variation ν such that

$$\mathcal{L}(p)=\int_{-\infty}^{\infty}p(E)\,d\nu(E) \tag{4}$$

for an arbitrary polynomial p. Orthogonality relations (M3) can be then expressed as

$$\mathcal{L}(p_n):=\int p_n(E)d\nu_P(E)=\delta_{n0}. \tag{5}$$

An integral equation for $w(E)$ in $d\nu_P(E)=w(E)dE$ is obtained as follows [2, 4]. Multiplying relation (M2) by $d\nu_P(E)$, taking the integral over E and using (5), one obtains for an arbitrary eigenvector $|E\rangle\in\mathcal{V}_\mathcal{N}$ of the Hamiltonian H

$$\int |E\rangle\,d\nu_P(E)=\mathbf{e}_0. \tag{6}$$

The basis element $\mathbf{e}_0$, or the *cyclic* vector of H, can be obviously represented as a linear combination of eigenvectors of the Hamiltonian H corresponding to exactly calculable energy levels in $\mathcal{V}_\mathcal{N}$, or to the zeros of $P_\mathcal{N}(x)$,

$$\mathbf{e}_0=\sum_{k=0}^{\mathcal{N}-1}w_k|E_k\rangle. \tag{7}$$

Substituting (7) into (6) one obtains with $d\nu_P(E)=w(E)dE$

$$\int |E\rangle\,w(E)dE=\sum_{k=0}^{\mathcal{N}-1}w_k|E_k\rangle. \tag{8}$$

This is equation first obtained by Krajewska, Ushveridze, and Walczak [4] and later rigorously analyzed by Finkel et al [2].

It was heuristically argued by Krajewska et al [4] that $w(E)$ solving Eq. (8) is given by (cf. Eq. (5.6) of Ref. [4]; Eq. (49) of Ref. [2])

$$w(E)=\sum_{k=0}^{\mathcal{N}-1}w_k\,\delta(E-E_k). \tag{9}$$

Indeed, the *discrete* Stieltjes measure $d\nu_P(E)$ defined by the function

$$\nu_P(E)=\sum_{k=0}^{\mathcal{N}-1}w_k\,\theta(E-E_k), \tag{10}$$

where $\theta(x)$ is Heaviside's step function, obviously satisfies (8).

The coefficients w_k can be found by solving a finite non-degenerate system of linear equations (cf. Eq. (5.8) of Ref. [4]; Eq. (50) of Ref. [2])

$$\sum_{l=0}^{\mathcal{N}-1}p_k(E_l)\,w_l=\delta_{k0}, \qquad k=0,1,\ldots,\mathcal{N}-1. \tag{11}$$

Because the matrix M with elements $M_{kl} := p_k(E_l)$ has orthogonal rows, the linear system (11) of $\mathcal{N}$ equations for $\mathcal{N}$ unknowns *uniquely* determines the $\mathcal{N}$ constants w_k defined by Eq. (7) [2, 4]. The coefficients w_k are in fact *positive* (cf. Sec. I D). This makes $\nu_P(E)$ a *nondecreasing* function of bounded variation.

It is not difficult to show that the orthogonality relations (1) are satisfied. Indeed, by the *uniqueness* of $\mathcal{L}$ this is equivalent to showing that $\mathcal{L}$ given through $\nu_P(E)$ of Eq. (10) satisfies the orthogonality relations (1) for $k, l < \mathcal{N}$. From the linear system (11) which determines w_k, and which derives from Eq. (5), we deduce that

$$\mathcal{L}(p_l) = \delta_{0l}, \qquad 0 \le l < \mathcal{N}. \tag{12}$$

The remaining orthogonality relations (1) then follows inductively on applying the above relations (12) to the TTRR (M5), and then continuing similarly as in the proof of *Favard*'s theorem (Theorem I-4.4 of Ref. [1]).

D. Positivity of the coefficients w_k

The *positivity* of the coefficients w_k is obvious in Haydock's approach, because $w(E)$ corresponds to the local DOS $n_0(E)$. Nevertheless it is instructive to have its independent mathematical proof, which in a general setting of finite OPS was essentially provided by Finkel et al (cf. Proposition 4 of Ref. [2]). In brief, all the coefficients w_k in Eqs. (7), (9) and (10) are *positive*, $w_k > 0$, for $0 \le k < \mathcal{N}$ if c_k is real for all $0 \le k < \mathcal{N}$ and $\lambda_k > 0$ for $1 \le k < \mathcal{N}$ in the TTRR (M6).

Proof: From Lemma 3 of Finkel et al [2] we know that $\mathcal{L}$ is *positive-definite* on $\mathcal{P}_{2(\mathcal{N}-1)}$. Apply the lemma to the polynomials $\prod_{0\le j\ne k<\mathcal{N}-1}(E-E_j)^2 \in \mathcal{P}_{2(\mathcal{N}-1)}$ for $k = 0, 1, \ldots, \mathcal{N}-1$. Then, with the moment functional (9), one has

$$\mathcal{L}(p) = w_k \prod_{0\le j\ne k<\mathcal{N}-1} (E_k - E_j)^2 > 0,$$

from which it follows that necessarily $w_k > 0$ for all $k = 0, 1, \ldots, \mathcal{N}-1$.

The *moments* of the moment functional $\mathcal{L}$ are by definition the numbers determined by Eq. (A3). In the present case of a finite OPS,

$$\mu_k = \int_{-\infty}^{\infty} E^k \, d\nu(E) = \sum_{l=0}^{\mathcal{N}-1} w_l \, E_l^k, \qquad k \in \mathbb{N}. \tag{13}$$

Because $w_k > 0$, all the moments are *real* (and positive if all eigenvalues are positive). From (13) we see that the modulus of the k-th moment μ_k diverges like the k-th power of a constant [2].

E. Uniqueness of $d\nu_P(E) = w(E)dE$

In virtue of that $\nu_P(E)$ of Eq. (10) is a non-decreasing function of bounded variation, $\nu_P(E)$ defines a *distribution function* (cf. Definition II-1.1 of of Ref. [1]). This distribution function is unique (up to an additive constant), so that the moment problem associated to the weakly orthogonal polynomial system $\{P_k\}_{k\in\mathbb{N}}$, or a finite OPS $\{P_k\}_{k=1}^{\mathcal{N}-1}$, is always *determined*. Essentially, this is due to the fact that the *spectrum*

$$\mathfrak{S}(\nu_P) = \{x \in \mathbb{R} : \nu_P(x+\delta) - \nu_P(x-\delta) > 0, \ \forall \delta > 0\}$$

of the distribution function ν_P is the *finite* set $\{E_l\}_{l=0}^{\mathcal{N}-1}$ determined by the zeros of $P_{\mathcal{N}}(x)$.

According to a well known result in the classical theory of orthogonal polynomials [1], a distribution function ν defines a positive-definite functional on $\mathbb{C}[E]$ through integration with respect to the Stieltjes measure $d\nu(E)$ if and only if the spectrum of ν is *infinite*. Since $\mathcal{L}$ is not positive-definite $[\mathcal{L}(P_{\mathcal{N}}^2) = \mathfrak{n}_{\mathcal{N}} = 0]$, any solution ν of (4) must have a *finite* spectrum, and will thus be of the form

$$\hat{\nu}(E) = \sum_{k=0}^{\tilde{n}} \tilde{w}_k \theta(E - \tilde{E}_k) + C$$

for some constant C, up to an irrelevant redefinition of ν in $\mathfrak{S}(\nu)$. If I is a compact interval containing $\mathfrak{S}(\nu)\cup\mathfrak{S}(\hat{\nu})$, then $\forall p \in \mathbb{C}[E]$

$$\mathcal{L}(p) = \int_I p(E)\, d\hat{\nu}(E) = \int_I p(E)\, d\nu(E).$$

Following the arguments of Finkel et al [2], since I is *compact*, a well known theorem (cf. Theorem II-5.7 of Ref. [1]) shows that $\hat{\nu}$ and ν may only differ by a constant at all points in which both $\hat{\nu}$ and ν are *continuous*. But this easily implies that $E_k = \tilde{E}_k$ and $w_k = \tilde{w}_k$ for $k = 0, 1, \ldots, \tilde{n} = \mathcal{N}-1$, whence $\nu = \hat{\nu} + C$, as stated. The same argument shows that the moment problem in any interval containing $[E_0, E_{\mathcal{N}-1}]$, in particular, the Stieltjes moment problem in $[E_0, \infty)$ is also determined.

II. BASIC PROPERTIES OF A GENERAL FINITE TRIDIAGONAL MATRIX J

It is expedient to see how finite OPS are linked to the properties of a general finite tridiagonal matrix J. Consider $N \times N$ *tridiagonal* matrix J which acts on a basis $\mathbf{e}_k$, $0 \le k \le N-1$ by

$$J\mathbf{e}_k = C(k+1)\mathbf{e}_{k+1} + B(k)\mathbf{e}_k + A(k-1)\mathbf{e}_{k-1}.$$

We will assume the *irreducibility* condition

$$C(s)A(s-1) \ne 0 \tag{14}$$

for $1 \le s \le N-1$ together with $C(N) = A(-1) = 0$, which means merely that that the matrix J acts in linear space of dimension N.

Following the arguments by Vinet and Zhedanov [5], find the eigenvectors $\mathbf{v}^{(k)}, 0 \le k \le N-1$, of the matrix J, i.e.

$$J\mathbf{v}^{(k)} = E_k \mathbf{v}^{(k)},$$

with some eigenvalues E_k. We assume that all eigenvalues are distinct: $E_j \neq E_k$ if $j \neq k$. Then all vectors $\mathbf{v}^{(k)}$, $0 \le k \le N-1$, are independent and we have

$$\mathbf{v}^{(k)} = \sum_{s=0}^{N-1} v_{ks}\mathbf{e}_s,$$

where $v_{ks}, 0 \le s \le N-1$, are components of the vector $\mathbf{v}^{(k)}$ in the basis $\mathbf{e}_s$. For the components we have relation [5]

$$A(s)v_{k,s+1} + B(s)v_{ks} + C(s)v_{k,s-1} = E_k v_{ks}. \qquad (15)$$

Now we can identify components v_{ks} with $P_s(E_)$, i.e. we merely put $v_{ks} = P_s(E_k)$ for all values $0 \le k, s \le N-1$. Eq. (15) is a TTRR in the s-variable. Therefore it defines a finite OPS $\{P_s\}_{s=0}^{N-1}$.

Consider *transposed* Jacobi matrix J^* defined as

$$J^*\mathbf{e}_k = A(k)\mathbf{e}_{k+1} + B(k)\mathbf{e}_k + C(k)\mathbf{e}_{k-1}$$

and corresponding eigenvalue vectors $\mathbf{v}^{*(k)}$,

$$J^*\mathbf{v}^{*(k)} = E_k\, \mathbf{v}^{*(k)}, \quad 0 \le k \le N-1.$$

The eigenvectors $\mathbf{v}^{*(k)}$ can be expanded in terms of the same basis $\mathbf{e}_s$:

$$\mathbf{v}^{*(k)} = \sum_{s=0}^{N-1} v^*_{ks}\mathbf{e}_s.$$

From elementary linear algebra it is known that in *non-degenerate* case (i.e. if $E_i \neq E_j$ for $i \neq j$) the eigenvectors $\mathbf{v}^k$ and $\mathbf{v}^{*(j)}$ are *biorthogonal*:

$$(\mathbf{v}^k, \mathbf{v}^{*(j)}) \equiv \sum_{s=0}^{N-1} v_{ks}v^*_{js} = 0 \quad \text{if} \quad k \neq j. \qquad (16)$$

(The biorthogonality property is valid for any non-symmetric matrix having all distinct eigenvalues.)

Introduce now the *diagonal* matrix M which acts on basis $\mathbf{e}_s$ as

$$M\mathbf{e}_s = \mu_s \mathbf{e}_s, \quad 0 \le s \le N-1,$$

where

$$\mu_0 = 1, \quad \mu_s = \frac{A(0)A(1)\dots A(s-1)}{C(1)C(2)\dots C(s)}, \ 1 \le s \le N-1.$$

Note that all μ_s are well defined due to irreducibility condition (14). It is elementary verified that

$$J^* = M^{-1}JM,$$

and hence

$$\mathbf{v}^{*(k)} = M^{-1}\mathbf{v}^{(k)}, \quad 0 \le k \le N-1 \qquad (17)$$

(inverse matrix M^{-1} exists due to the irreducibility condition (14)).

Relation (17) allows one to rewrite biorthogonality condition (16) in the form

$$\sum_{s=0}^{N-1} w_s v_{ks} v_{js} = 0 \quad \text{if} \quad k \neq j,$$

where

$$w_s = \mu_s^{-1} = \prod_{i=1}^{s} \frac{C(i)}{A(i-1)}. \qquad (18)$$

In terms of $P_n(x)$ this relation becomes (cf. Eq. (5.8) of Krajewska et al [4])

$$\sum_{s=0}^{N-1} w_s P_s(E_j)P_s(E_k) = 0 \quad \text{if} \quad k \neq j. \qquad (19)$$

In the symmetric Haydock's case Eq. (18) reduces to

$$w_s = \prod_{i=1}^{s} \frac{b_i}{b_i} \equiv 1.$$

Eq. (19) of Ref. [5] then becomes essentially the *dual* orthogonality relation (10.18) of Haydock [6]

$$\sum_{s=0}^{N-1} p_s(E_k)p_s(E_j) = \delta_{EE'},$$

where E_k and E_j are both eigenvalues.

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