From Standard Orthogonal Polynomials to Sobolev Orthogonal Polynomials: The Role of Semiclassical Linear Functionals

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Abstract In this contribution, we present an overview of standard orthogonal polynomials by using an algebraic approach. Discrete Darboux transformations of Jacobi matrices are studied. Next, we emphasize the role of semiclassical orthogonal polynomials as a basic background to analyze sequences of polynomials orthogonal with respect to a Sobolev inner product. Some illustrative examples are discussed. Finally, we summarize some results in multivariate Sobolev orthogonal polynomials.

Keywords Orthogonal polynomials · Discrete Darboux transformations · Semi-classical functionals · Sobolev orthogonal polynomials

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1 Introduction

The aim of this contribution is to provide a self-contained presentation of the so called Sobolev orthogonal polynomials, i.e., polynomials which are orthogonal with respect to a bilinear form involving derivatives of its inputs, defined in the linear space of polynomials with real coefficients. We start by focusing our attention on an algebraic approach to the so called standard orthogonal polynomials, which are polynomials orthogonal with respect to a linear functional, taking into account that we can associate with such polynomials a structured matrix for their moments (a Hankel matrix), a tridiagonal matrix (a Jacobi matrix reflecting the fact that the multiplication operator is symmetric with respect to the above linear functional), as well as an analytic function around infinity (the so called Stieltjes function, that is the z-transform of the sequence of moments of the linear functional), such that the denominators of the diagonal Padé approximants to such a function are the corresponding orthogonal polynomials (we refer the reader to [17] and [70] for an introduction to these topics). These three basic ingredients allow us to deal with a theory that knows an increasing interest in the last decades (see [64], [37]).

The most useful standard orthogonal polynomials appear as polynomial eigenfunctions of second-order differential operators and constitute the so called classical families—Hermite, Laguerre, Jacobi and Bessel—see [42] as well as [11]. All of them can be written in terms of hypergeometric functions and they can be characterized in several ways taking into account their hypergeometric character. Beyond the above classical orthogonal polynomials, the so-called semiclassical orthogonal polynomials constitute a wide class with an increasing interest for researchers, taking into account their connections with Painlevé equations and integrable systems [73]. They have been introduced in [69] from the point of view of holonomic equations satisfied by orthogonal polynomials associated with weight functions $w(x)$ satisfying a Pearson differential equation $(A(x)w(x))' = B(x)w(x)$, where A and B are polynomials. In the 80s, they have been intensively studied by P. Maroni and co-workers (see [59] as an excellent and stimulating survey paper). The role of semiclassical orthogonal polynomials in the study of orthogonal polynomials with respect to univariate Sobolev inner products has been emphasized when the so called coherent pairs of measures are introduced (see [63]) as well as some of their generalizations (see [22]).

The structure of the paper is the following. In Sect. 2, a basic background concerning linear functionals and the algebraic structure of the topological dual space corresponding to the linear space of polynomials with real coefficients is presented. Orthogonal polynomials with respect to linear functionals are defined and the three-term recurrence relation they satisfy constitute a key point in the analysis of their zeros. Discrete Darboux transformations for linear functionals are studied in Sect. 3 in the framework of LU and UL factorizations of Jacobi matrices (see [14]). The connection formulas between the corresponding sequences of orthogonal polynomials are studied in the framework of the linear spectral transformations of the Stieltjes functions associated with linear functionals. In Sect. 4, following [59], semiclassical linear functionals are introduced and some of their characterizations are provided. The definition of class plays a key role in order to give a classification of semiclassical orthogonal polynomials, mainly those of class zero (the classical ones) and of class one (see [10]), which will play a central role in the sequel. Thus, a constructive approach to describe families of semiclassical linear functionals is presented. In particular, every linear spectral transformation of a semiclassical linear functional is also semiclassical. On the other hand, the symmetrization process of linear functionals is also studied and the invariance of the semiclassical character of a linear functional by symmetrization is pointed out. This constitutes the core of Sect. 5. In Sect. 6, orthogonal polynomials with respect to Sobolev inner products associated with a vector of measures supported on the real line are introduced. We emphasize the case where this vector of measures is coherent, i.e., their corresponding sequences of orthogonal polynomials satisfy a simple algebraic relation. This fact allows to deal with an algorithm to generate Sobolev orthogonal polynomials associated with coherent pairs of measures. Some analytic properties of these polynomials are shown. Notice that the three-term recurrence relation that constitutes a basic tool for the standard orthogonality is lost and, as a consequence, new techniques for studying asymptotic properties of such orthogonal polynomials are needed. In Sect. 7, multivariate Sobolev orthogonal polynomials are studied and their representations in terms of semiclassical orthogonal polynomials and spherical harmonics are given. A recent survey on Sobolev orthogonal polynomials can be found in [56], both in the univariate and multivariate case. Finally, an updated list of references provides a good guideline for the readers interested in these topics.

2 Background

Recall that a linear functional $\mathbf{u}$ defined on the linear space $\mathbb{P}$ of polynomials with real coefficients is a mapping

$$\begin{aligned}\mathbf{u} :& \mathbb{P} \to \mathbb{R}\\ & p \to \langle \mathbf{u}, p\rangle\end{aligned}$$

such that for every polynomials p, q, and every real numbers α, β,

$$\langle \mathbf{u}, \alpha p + \beta q \rangle = \alpha \langle \mathbf{u}, p\rangle + \beta \langle \mathbf{u}, q\rangle.$$

In general, given a basis of polynomials $\{p_n(x)\}_{n\geq 0}$, and a sequence of real numbers $\{\mu_n\}_{n\geq 0}$, a linear functional $\mathbf{u}$ is defined by means of its action on the basis

$$\langle \mathbf{u}, p_n\rangle = \mu_n, \quad n \geq 0,$$

and extended by linearity to all polynomials. If $p_n(x) = x^n, n \geq 0$, then the real numbers $\mu_n = \langle \mathbf{u}, x^n \rangle, n \geq 0$, are called *moments* with respect to the canonical basis and we usually say that $\mathbf{u}$ is a *moment functional*. If $p_n(x) = a_n x^n +$ lower degree terms, $n \geq 0$,, $a_n \neq 0$, the real numbers $\tilde{\mu}_n = \langle \mathbf{u}, p_n \rangle, n \geq 0$, are called the *modified moments* associated with the linear functional $\mathbf{u}$.

For a linear functional $\mathbf{u}$, we define its moment matrix as the semi-infinite Hankel matrix $M = (\mu_{i+j})_{i,j=0}^{\infty}$. If we denote

$$\Delta_n = \det[(\mu_j)_{j=0}^n] = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_n \\ \mu_1 & \mu_2 & \cdots & \mu_{n+1} \\ \vdots & \vdots & \cdots & \vdots \\ \mu_n & \mu_{n+1} & \cdots & \mu_{2n} \end{vmatrix},$$

then $\mathbf{u}$ is said to be quasi-definite if $\Delta_n \neq 0$ for $n \geq 0$, and $\mathbf{u}$ is said to be positive-definite if $\Delta_n > 0$ for $n \geq 0$.

Definition 2.1 Given a linear functional $\mathbf{u}$ and a polynomial $q(x)$ we define a new linear functional $q(x)\mathbf{u}$ as

$$\langle q(x)\mathbf{u}, p \rangle = \langle \mathbf{u}, q(x)\, p(x) \rangle,$$

for every polynomial $p \in \mathbb{P}$.

Definition 2.2 Given a linear functional $\mathbf{u}$ and a polynomial $p(x) = \sum_{k=0}^{n} a_k\, x^k$, we define the polynomial $(\mathbf{u} * p)(x)$ as

$$(\mathbf{u} * p)(x) := \left\langle \mathbf{u}_y, \frac{xp(x) - yp(y)}{x - y} \right\rangle = \sum_{k=0}^{n} \left(\sum_{m=k}^{n} a_m\, \mu_{m-k} \right) x^k$$

$$= (1, x, \dots, x^n) \begin{pmatrix} \mu_0 & \dots & \mu_n \\ & \ddots & \vdots \\ & & \mu_0 \end{pmatrix} \begin{pmatrix} a_0 \\ \vdots \\ a_n \end{pmatrix}.$$

Definition 2.3 A sequence of polynomials $\{P_n(x)\}_{n\geq 0}$ is said to be a sequence of orthogonal polynomials with respect to $\mathbf{u}$ if

(i) $\deg(P_n) = n$, and
(ii) $\langle \mathbf{u}, P_n\, P_m \rangle = \delta_{n,m}\, K_n$ with $K_n \neq 0$,

where, as usual, $\delta_{n,m}$ denotes the Kronecker delta.

Theorem 2.4 (Existence and Uniqueness of Orthogonal Polynomials)

1. *If* $\mathbf{u}$ *is a quasi-definite functional, then there exists a sequence of orthogonal polynomials* $\{P_n(x)\}_{n\geq 0}$ *associated with* $\mathbf{u}$.

2. *If* $\{Q_n(x)\}_{n\geq 0}$ *is another sequence of orthogonal polynomials associated with* **u**, *then*

$$Q_n(x) = c_n\, P_n(x), \quad n \geq 0,$$

where c_n *are non zero real numbers. That is,* $\{P_n(x)\}_{n\geq 0}$ *is unique up to multiplicative scalar factors.*

Let **u** be a quasi-definite linear functional and $\{P_n(x)\}_{n\geq 0}$ a sequence of orthogonal polynomials associated with **u**. For each $n \geq 0$, let k_n denote the leading coefficient of the polynomial $P_n(x)$. The sequence of polynomials $\{\hat{P}_n(x)\}_{n\geq 0}$ with

$$\hat{P}_n(x) := k_n^{-1}\, P_n(x), \qquad n \geq 0,$$

is called a sequence of monic orthogonal polynomials associated with **u**. In particular, if **u** is positive-definite, then we can define a norm on $\mathbb{P}$ by

$$||p||_{\mathbf{u}} = \sqrt{\langle \mathbf{u}, p^2 \rangle}.$$

The sequence of polynomials $\{Q_n(x)\}_{n\geq 0}$ with

$$Q_n(x) := \frac{P_n(x)}{||P_n(x)||_{\mathbf{u}}}, \qquad n \geq 0,$$

is called the sequence of orthonormal polynomials with respect to **u**.

Using a matrix approach, we can rewrite the orthogonality as follows. If M is the Hankel moment matrix associated with a quasi-definite linear functional, then M has a unique Gauss-Borel factorization [35, p. 441] with

$$M = S^{-1} D\, S^{-t}, \tag{2.1}$$

where, as usual, the superscript t denotes the transpose, S is a non-singular lower triangular matrix with 1's in the main diagonal, $S^{-t} := (S^{-1})^t$, and D is a diagonal matrix. With this in mind, if $\chi(x)$ denotes the semi-infinite column vector $\chi(x) := (1, x, x^2, \cdots)^t$, then the sequence of monic orthogonal polynomials arranged in a column vector as $\mathbf{P} := (P_0(x), P_1(x), P_2(x), \cdots)^t$ can be written as $\mathbf{P} = S\chi(x)$. In other words, S is the matrix of change of basis from the canonical basis to the basis of monic orthogonal polynomials.

Notice also that if **u** is a positive-definite linear functional, then the entries of D in (2.1) are positive and thus the factorization of the moment matrix M is the standard Cholesky factorization. Moreover, if $\mathbf{Q} := (Q_0(x), Q_1(x), Q_2(x), \ldots)^t$ is the vector of orthonormal polynomials, then $\mathbf{Q} := \tilde{S}\chi(x)$, where $\tilde{S} = D^{-1/2}S$.

Definition 2.5 The shift matrix is the semi-infinite matrix

$$\Lambda := \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}.$$

The shift matrix satisfies the spectral property $\Lambda \chi(x) = x\,\chi(x)$. Notice also that from the symmetry of the Hankel moment matrix M, we have that $\Lambda M = M \Lambda^t$.

Theorem 2.6 (Three-Term Recurrence Relation) *Let* $\mathbf{u}$ *be a quasi-definite linear functional and let* $\{P_n(x)\}_{n\geq 0}$ *be the sequence of monic orthogonal polynomials with respect to* $\mathbf{u}$. *Then there exist two sequences of real numbers* $\{a_n\}_{n\geq 1}$ *and* $\{b_n\}_{n\geq 0}$, *with* $a_n \neq 0$ *for* $n \geq 1$, *such that*

$$\begin{aligned} &x\,P_n(x) = P_{n+1}(x) + b_n\,P_n(x) + a_n\,P_{n-1}(x), \quad n \geq 0, \\ &P_{-1}(x) = 0, \qquad P_0(x) = 1. \end{aligned} \tag{2.2}$$

Moreover,

$$b_n = \frac{\langle \mathbf{u}, x\,P_n^2\rangle}{\langle \mathbf{u}, P_n^2\rangle}, \quad n \geq 0, \qquad a_n = \frac{\langle \mathbf{u}, P_n^2\rangle}{\langle \mathbf{u}, P_{n-1}^2\rangle}, \quad n \geq 1.$$

The above three-term recurrence relation can be written in matrix form as follows

$$x\,\mathbf{P} = J_{\text{mon}}\mathbf{P}, \quad \text{where} \quad J_{\text{mon}} = \begin{pmatrix} b_0 & 1 & & \\ a_1 & b_1 & 1 & \\ & a_2 & b_2 & \ddots \\ & & \ddots & \ddots \end{pmatrix}.$$

The matrix J_{mon} is called a monic Jacobi tridiagonal matrix associated with the sequence of monic orthogonal polynomials $\{P_n(x)\}_{n\geq 0}$.

Similarly, if $\mathbf{u}$ is positive-definite, then the sequence of orthonormal polynomials satisfies a three-term recurrence relation $x\,\mathbf{Q} = J\,\mathbf{Q}$, where J is a tridiagonal semi-infinite symmetric matrix called a Jacobi matrix.

Theorem 2.7 *If* S *is the semi-infinite upper triangular matrix obtained in the Gauss-Borel factorization* (2.1)*, then*

$$J_{\text{mon}} = S\,\Lambda\,S^{-1}.$$

Similarly, if $\mathbf{u}$ *is a positive-definite linear functional and* $\tilde{S}$ *is the upper triangular matrix obtained from the Cholesky factorization of the moment matrix, then* $J = \tilde{S}\,\Lambda\,\tilde{S}^{-1}$.

Proof Let $\mathbf{P} = (P_0(x), P_1(x) \cdots)^t$ be the vector of monic orthogonal polynomials. Using the shift matrix properties, we have

$$x\,\mathbf{P} = x\,S\chi(x) = S\,\Lambda\,\chi(x) = S\,\Lambda\,S^{-1}\,(S\,\chi(x)) = S\,\Lambda\,S^{-1}\,\mathbf{P},$$

and the result follows.

If $\mathbf{u}$ is positive-definite, let $\mathbf{Q} = (Q_0(x), Q_1(x) \cdots)^t$ be the vector of orthonormal polynomials.

$$x\,\mathbf{Q} = x\,\tilde{S}\chi(x) = \tilde{S}\,\Lambda\,\chi(x) = \tilde{S}\,\Lambda\,\tilde{S}^{-1}\,(\tilde{S}\,\chi(x)) = \tilde{S}\,\Lambda\,\tilde{S}^{-1}\,\mathbf{Q},$$

and we obtain the result □

Theorem 2.8 (Favard's Theorem) *Let $\{b_n\}_{n\geq 0}$ and $\{a_n\}_{n\geq 1}$ be arbitrary sequences of real numbers with $a_n \neq 0$ for $n \geq 1$, and let $\{P_n(x)\}_{n\geq 0}$ be a sequence of monic polynomials defined by the recurrence formula*

$$\begin{aligned} &x\,P_n(x) = P_{n+1}(x) + b_n\,P_n(x) + a_n\,P_{n-1}(x), \quad n \geq 0,\\ &P_{-1}(x) = 0, \qquad P_0(x) = 1, \end{aligned}$$

then there exists a quasi-definite linear functional $\mathbf{u}$ *such that $\{P_n(x)\}_{\geq 0}$ is the sequence of monic orthogonal polynomials with respect to* $\mathbf{u}$. *Furthermore, if $\{a_n\}_{n\geq 1}$ is a sequence such that $a_n > 0$ for $n \geq 1$, then* $\mathbf{u}$ *is positive-definite.*

If $\{P_n(x)\}_{n\geq 0}$ is a sequence of monic orthogonal polynomials satisfying a three-term recurrence (2.2), we define the sequence of associated polynomials of the first kind $\{P_n^{(1)}(x)\}_{n\geq 0}$ as the sequence of polynomials that satisfy the three-term recurrence relation

$$\begin{aligned} &x\,P_n^{(1)}(x) = P_{n+1}^{(1)}(x) + b_{n+1}\,P_n^{(1)}(x) + a_{n+1}\,P_{n-1}^{(1)}(x), \quad n \geq 0,\\ &P_0^{(1)}(x) = 1, \quad P_{-1}^{(1)}(x) = 0. \end{aligned} \tag{2.3}$$

Proposition 2.9 *Let* $\mathbf{u}$ *be a quasi-definite linear functional and $\{P_n(x)\}_{n\geq 0}$ its corresponding sequence of monic orthogonal polynomials. The sequence of associated polynomials of the first kind is given by*

$$P_{n-1}^{(1)}(x) = \frac{1}{\mu_0}\left\langle \mathbf{u}_y, \frac{P_n(x) - P_n(y)}{x - y} \right\rangle, \quad n \geq 1.$$

Notice that the families of polynomials $\{P_n(x)\}_{n\geq 0}$ and $\{P_{n-1}^{(1)}(x)\}_{n\geq 0}$ are linearly independent solutions of (2.2). Thus, any other solution can be written as a linear combination of $\{P_n(x)\}_{n\geq 0}$ and $\{P_{n-1}^{(1)}(x)\}_{n\geq 0}$ with polynomial coefficients.

Definition 2.10 For each $n \geq 0$, the nth kernel polynomial is defined by

$$\mathcal{K}_n(x, y) = \sum_{j=0}^{n} \frac{P_j(x)\, P_j(y)}{\| P_j(x) \|_{\mathbf{u}}^2}. \tag{2.4}$$

Definition 2.11 Let $\mathbf{u}$ be a quasi-definite functional with moments $\{\mu_n\}_{n\geq 0}$. We define the Stieltjes function associated with $\mathbf{u}$ as the formal power series

$$\mathcal{S}(z) = \sum_{n=0}^{\infty} \frac{\mu_n}{z^{n+1}}.$$

By a linear spectral transformation of $\mathcal{S}(z)$ we mean the following transformation

$$\tilde{\mathcal{S}}(z) = \frac{A(z)\mathcal{S}(z) + B(z)}{C(z)}$$

where $A(z)$, $B(z)$, $C(z)$ are polynomials in the variable z such that

$$\tilde{\mathcal{S}}(z) = \sum_{n=0}^{\infty} \frac{\tilde{\mu}_n}{z^{n+1}}.$$

Definition 2.12 Let $\mathbf{u}$ be a linear functional and let $\{P_n(x)\}_{n\geq 0}$ be a sequence of polynomials with $\deg(P_n) = n$. We say that $\{P_n(x)\}_{n\geq 0}$ is quasi-orthogonal of order m with respect to $\mathbf{u}$ if

$$\begin{aligned} \langle \mathbf{u}, P_k\, P_n \rangle &= 0, \ m + 1 \leq |n - k|, \\ \langle \mathbf{u}, P_{n-m}\, P_n \rangle &\neq 0, \ \text{for some } n \geq m. \end{aligned}$$

The sequence of polynomials $\{P_n(x)\}_{n\geq 0}$ is said to be strictly quasi-orthogonal of order m with respect to $\mathbf{u}$ if

$$\begin{aligned} \langle \mathbf{u}, P_k\, P_n \rangle &= 0, \ m + 1 \leq |n - k|, \\ \langle \mathbf{u}, P_{n-m}\, P_n \rangle &\neq 0, \ \text{for every } n \geq m. \end{aligned}$$

3 Discrete Darboux Transformations

Several examples of perturbations of a quasi-definite linear functional $\mathbf{u}$ have been studied (see for example [14, 17, 18, 23, 31, 32, 71, 72, 76, 77]). In particular, the following three canonical cases (see [14, 76]) have attracted the interest of researchers. These transformations are known in the literature as discrete Darboux transformations.

3.1 Christoffel Transformation

Let $\mathbf{u}$ be a quasi-definite linear functional and $\{P_n(x)\}_{n\geq 0}$ a sequence of monic orthogonal polynomials associated with $\mathbf{u}$. Suppose that the linear functional $\tilde{\mathbf{u}}$ satisfies

$$\tilde{\mathbf{u}} = (x-a)\mathbf{u}, \tag{3.1}$$

with $a \in \mathbb{R}$. Then $\tilde{\mathbf{u}}$ is called a canonical Christoffel transformation of $\mathbf{u}$ (see [14]). Necessary and sufficient conditions for the functional $\tilde{\mathbf{u}}$ to be quasi-definite are given in [16, 76]. If $\tilde{\mathbf{u}}$ is also a quasi-definite functional, then its sequence of monic orthogonal polynomials $\{\tilde{P}_n(x)\}_{n\geq 0}$ satisfies the following connection formulas.

Proposition 3.1 *The sequences of monic orthogonal polynomial* $\{P_n(x)\}_{n\geq 0}$ *and* $\{\tilde{P}_n(x)\}_{n\geq 0}$ *are related by*

$$\begin{aligned} (x-a)\,\tilde{P}_n(x) &= P_{n+1}(x) + \lambda_n\, P_n(x), \quad n \geq 0, \\ P_n(x) &= \tilde{P}_n(x) + \nu_n\, \tilde{P}_{n-1}(x), \quad n \geq 1, \end{aligned} \tag{3.2}$$

with

$$\lambda_n = -\frac{P_{n+1}(a)}{P_n(a)}, \quad n \geq 0, \qquad \nu_n = \frac{\langle \mathbf{u}, P_n^2\rangle}{\lambda_{n-1}\langle \mathbf{u}, P_{n-1}^2\rangle}, \quad n \geq 1.$$

Notice that (3.2) can be written in matrix form

$$\begin{pmatrix} P_0(x) \\ P_1(x) \\ P_2(x) \\ \vdots \end{pmatrix} = \begin{pmatrix} 1 & & & \\ \nu_1 & 1 & & \\ & \nu_2 & 1 & \\ & & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \tilde{P}_0(x) \\ \tilde{P}_1(x) \\ \tilde{P}_2(x) \\ \vdots \end{pmatrix},$$

$$(x-a)\begin{pmatrix} \tilde{P}_0(x) \\ \tilde{P}_1(x) \\ \tilde{P}_2(x) \\ \vdots \end{pmatrix} = \begin{pmatrix} \lambda_0 & 1 & & \\ & \lambda_1 & 1 & \\ & & \ddots & \ddots \end{pmatrix} \begin{pmatrix} P_0(x) \\ P_1(x) \\ P_2(x) \\ \vdots \end{pmatrix}.$$

Theorem 3.2 ([14, 76]) *Let* J_{mon} *and* $\tilde{J}_{\text{mon}}$ *be the Jacobi matrices associated with* $\mathbf{u}$ *and* $\tilde{\mathbf{u}} = (x-a)\,\mathbf{u}$*, respectively. If* $J_{\text{mon}} - aI$ *can be written as*

$$J_{\text{mon}} - aI = L\,U,$$

where L is a lower bidiagonal matrix with 1's in the main diagonal and U is an upper bidiagonal matrix, then

$$\tilde{J}_{\text{mon}} - aI = UL.$$

Proof Recall that from (3.2),

$$(x-a)\,\tilde{\mathbf{P}} = U\,\mathbf{P} \quad \text{and} \quad \mathbf{P} = L\,\tilde{\mathbf{P}},$$

where $\mathbf{P} = (P_0(x), P_1(x)\cdots)^t$, $\tilde{\mathbf{P}} = (\tilde{P}_0(x), \tilde{P}_1(x)\cdots)^t$, L is a lower bidiagonal matrix with 1's in the main diagonal, and U is an upper bidiagonal matrix. Thus,

$$(x-a)\,\mathbf{P} = (x-a)\,L\,\tilde{\mathbf{P}} = L\,(x-a)\,\tilde{\mathbf{P}} = (L\,U)\,\mathbf{P},$$

and since $(x-a)\,\mathbf{P} = (J_{\text{mon}} - aI)\mathbf{P}$, it follows that

$$(J_{\text{mon}} - aI)\mathbf{P} = (L\,U)\mathbf{P}.$$

Since $\{P_n(x)\}_{n\geq 0}$ constitutes a basis of the linear space of polynomials, then $J_{\text{mon}} - aI = L\,U$. On the other hand,

$$(x-a)\,\tilde{\mathbf{P}} = U\,\mathbf{P} = (UL)\,\tilde{\mathbf{P}},$$

but, as above, this implies that $\tilde{J}_{\text{mon}} - aI = UL$. □

3.2 Geronimus Transformation

Let $\mathbf{u}$ be a quasi-definite linear functional, and introduce the linear functional $\hat{\mathbf{u}}$

$$\hat{\mathbf{u}} = (x-a)^{-1}\mathbf{u} + M\delta(x-a), \tag{3.3}$$

i.e., for every polynomial $p(x)$,

$$\langle \hat{\mathbf{u}}, p(x)\rangle = \left\langle \mathbf{u}, \frac{p(x)-p(a)}{x-a} \right\rangle + Mp(a). \tag{3.4}$$

We say that $\hat{\mathbf{u}}$ is a canonical Geronimus transformation of $\mathbf{u}$ (see [31]). Necessary and sufficient conditions for the functional $\hat{\mathbf{u}}$ to be quasi-definite are given in [23, 32, 76]. If $\hat{\mathbf{u}}$ is also a quasi-definite linear functional, then we denote by $\{\hat{P}_n(x)\}_{n\geq 0}$ its sequence of monic orthogonal polynomials.

Proposition 3.3 *The sequences of monic orthogonal polynomials* $\{P_n(x)\}_{n\geq 0}$ *and* $\{\hat{P}_n(x)\}_{n\geq 0}$ *are related by*

$$\begin{aligned} \hat{P}_n(x) &= \quad P_n(x) + \varsigma_n\, P_{n-1}(x), \quad n \geq 1, \\ (x-a)\, P_n(x) &= \quad \hat{P}_{n+1}(x) + \rho_n\, \hat{P}_n(x), \quad n \geq 0, \end{aligned} \tag{3.5}$$

where

$$\varsigma_n = -\frac{\mu_0 P_{n-1}^{(1)}(a) + M P_n(a)}{\mu_0 P_{n-2}^{(1)}(a) + M P_{n-1}(a)}, \quad n \geq 1,$$

$$\rho_n = \frac{\left(\mu_0 P_{n-2}^{(1)}(a) + M P_{n-1}(a)\right)\langle \mathbf{u}, P_n^2(x)\rangle}{\left(\mu_0 P_{n-1}^{(1)}(a) + M P_n(a)\right)\langle \mathbf{u}, P_{n-1}^2(x)\rangle}, \quad n \geq 1,$$

$$\rho_0 = \frac{\mu_0}{\hat{\mu}_0},$$

and $\{P_n^{(1)}(x)\}_{n\geq 0}$ *is the sequence of polynomials of the first kind* (2.3).

Notice that (3.5) can be written in matrix form as

$$\begin{pmatrix} \hat{P}_0(x) \\ \hat{P}_1(x) \\ \hat{P}_2(x) \\ \vdots \end{pmatrix} = \begin{pmatrix} 1 & & & \\ \varsigma_1 & 1 & & \\ & \varsigma_2 & 1 & \\ & & \ddots & \ddots \end{pmatrix} \begin{pmatrix} P_0(x) \\ P_1(x) \\ P_2(x) \\ \vdots \end{pmatrix},$$

$$(x-a)\begin{pmatrix} P_0(x) \\ P_1(x) \\ P_2(x) \\ \vdots \end{pmatrix} = \begin{pmatrix} \rho_0 & 1 & & \\ & \rho_1 & 1 & \\ & & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \hat{P}_0(x) \\ \hat{P}_1(x) \\ \hat{P}_2(x) \\ \vdots \end{pmatrix}.$$

Theorem 3.4 ([14, 76]) *Let* J_{mon} *and* $\hat{J}_{\text{mon}}$ *be the Jacobi matrices associated with* $\mathbf{u}$ *and* $\hat{\mathbf{u}}$, *respectively. If the semi-infinite matrix* $J_{\text{mon}} - aI$ *can be written as*

$$J_{\text{mon}} - aI = UL,$$

where L *is a lower bidiagonal matrix and* U *is a upper bidiagonal matrix, then*

$$\hat{J}_{\text{mon}} - aI = L\,U.$$

Proof From (3.5),

$$(x-a)\,\mathbf{P} = U\,\hat{\mathbf{P}}, \quad \text{and} \quad \hat{\mathbf{P}} = L\,\mathbf{P},$$

where, $\mathbf{P} = (P_0(x), P_1(x)\cdots)^t$, $\hat{\mathbf{P}} = (\hat{P}_0(x), \hat{P}_1(x)\cdots)^t$, L is a lower bidiagonal matrix with 1's in the main diagonal, and U is an upper bidiagonal matrix. Then,

$$(x-a)\,\mathbf{P} = U\,\hat{\mathbf{P}} = (UL)\,\mathbf{P}.$$

But $\{P_n(x)\}_{n\geq 0}$ is a basis for $\mathbb{P}$, and $(x-a)\,\mathbf{P} = (J_{\text{mon}} - aI)\,\mathbf{P}$, we get

$$J_{\text{mon}} - aI = UL.$$

Notice that this factorization depends on the choice of the free parameter $\hat{\mu}_0 \neq 0$. For a fixed $\hat{\mu}_0$,

$$(x-a)\,\hat{\mathbf{P}} = (x-a)\,L\,\mathbf{P} = L\,(x-a)\,\mathbf{P} = (L\,U)\,\hat{\mathbf{P}}.$$

As above, $\hat{J}_{\text{mon}} - aI = LU$. □

3.3 Uvarov Transformation

Let $\mathbf{u}$ be a quasi-definite linear functional and suppose that the linear functional $\check{\mathbf{u}}$ is defined by

$$\check{\mathbf{u}} = \mathbf{u} + M\delta(x-a). \tag{3.6}$$

The linear functional $\check{\mathbf{u}}$ is said to be a canonical Uvarov transformation of $\mathbf{u}$ (see [71, 72]). Necessary and sufficient conditions for the quasi-definiteness of the linear functional $\check{\mathbf{u}}$ are given in [49].

Proposition 3.5 *Suppose that $\check{\mathbf{u}}$ is quasi-definite, and let $\{\check{P}_n(x)\}_{n\geq 0}$ denote the sequence of monic orthogonal polynomials associated with $\check{\mathbf{u}}$. The sequences of polynomial $\{P_n(x)\}_{n\geq 0}$, and $\{\check{P}_n\}_{n\geq 0}$ are related by*

$$\check{P}_n(x) = P_n(x) - \frac{M P_n(a)}{1 + M\mathcal{K}_{n-1}(a,a)}\mathcal{K}_{n-1}(x,a), \quad n \geq 1,$$

where $\mathcal{K}_n(x, y)$ denotes the nth kernel polynomial defined in (2.4).

For any linear functional $\mathbf{u}$, it is straightforward to verify that if a canonical Christoffel transformation is applied to $\hat{\mathbf{u}}$ in (3.3) with the same parameter a, then we recover the original linear functional $\mathbf{u}$, that is, the canonical Christoffel transformation is the left inverse of the canonical Geronimus transformation.

However, a canonical Geronimus transformation applied to the linear functional $\tilde{\mathbf{u}}$ in (3.1) with the same parameter a, transforms $\tilde{\mathbf{u}}$ into a linear functional $\check{\mathbf{u}}$ as in (3.6), that is, a canonical Uvarov transformation. It is important to notice that the following result holds.

Theorem 3.6 ([77]) *Every linear spectral transform is a finite composition of Christoffel and Geronimus transformations.*

4 Semiclassical Linear Functionals

Let D denote the derivative operator. Given a linear functional $\mathbf{u}$, we define $D\mathbf{u}$ as

$$\langle D\mathbf{u}, p\rangle = -\langle \mathbf{u}, p'\rangle,$$

for every polynomial $p \in \mathbb{P}$. Inductively, we define

$$\langle D^n\mathbf{u}, p\rangle = (-1)^n\langle \mathbf{u}, p^{(n)}\rangle.$$

Notice that, for any polynomial $q(x)$,

$$D(q(x)\,\mathbf{u}) = q'(x)\,\mathbf{u} + q(x)\,D\mathbf{u}.$$

Definition 4.1 A quasi-definite linear functional $\mathbf{u}$ is said to be semiclassical if there exist non-zero polynomials ϕ and ψ with $\deg(\phi) =: r \geq 0$ and $\deg(\psi) =: t \geq 1$, such that $\mathbf{u}$ satisfies the Pearson equation

$$D(\phi(x)\mathbf{u}) + \psi(x)\mathbf{u} = 0. \tag{4.1}$$

In general, if $\mathbf{u}$ satisfies (4.1), then it satisfies an infinite number of Pearson equations. Indeed, for any non-zero polynomial $q(x)$, $\mathbf{u}$ satisfies

$$D(\tilde{\phi}\,\mathbf{u}) + \tilde{\psi}\,\mathbf{u} = 0,$$

where $\tilde{\phi}(x) = q(x)\,\phi(x)$ and $\tilde{\psi}(x) = q'(x)\,\phi(x) + q(x)\,\psi(x)$.

Remark 4.2 In order to avoid any incompatibility with the quasi-definite character of the semiclassical functional $\mathbf{u}$, it will be required from now on that, if

$$\phi(x) = a_r\,x^r + \cdots \quad \text{and} \quad \psi(x) = b_t\,x^t + \cdots,$$

then, for any $n = 0, 1, 2, \ldots$, if $t = r - 1$, then $n\,a_r - b_t \neq 0$. In such a case, every moment of the linear functional $\mathbf{u}$ is well defined.

This motivates the following definition.

Definition 4.3 The *class* of a semiclassical linear functional $\mathbf{u}$ is defined as

$$\mathfrak{s}(\mathbf{u}) := \min \max\{\deg(\phi) - 2,\ \deg(\psi) - 1\},$$

where the minimum is taken among all pairs of polynomials ϕ and ψ such that $\mathbf{u}$ satisfies (4.1).

Lemma 4.4 *Let* $\mathbf{u}$ *be a semiclassical functional such that*

$$D(\phi_1\mathbf{u}) + \psi_1\mathbf{u} = 0, \qquad s_1 := \max\{\deg(\phi_1) - 2, \deg(\psi_1) - 1\}, \tag{4.2}$$

$$D(\phi_2\mathbf{u}) + \psi_2\mathbf{u} = 0, \qquad s_2 := \max\{\deg(\phi_2) - 2, \deg(\psi)_2 - 1\}, \tag{4.3}$$

where $\phi_i(x)$ *and* $\psi_i(x)$*,* $i = 1, 2$*, are non-zero polynomials with* $\deg(\phi_i) \geq 0$ *and* $\deg(\psi_i) \geq 1$*. Let* $\phi(x)$ *be the greatest common divisor of* $\phi_1(x)$ *and* $\phi_2(x)$*.*

Then there exists a polynomial $\psi(x)$ *such that*

$$D(\phi\,\mathbf{u}) + \psi\,\mathbf{u} = 0, \qquad s := \max\{\deg(\phi) - 2, \deg(\psi) - 1\}.$$

Moreover, $s - \deg(\phi) = s_1 - \deg(\phi_1) = s_2 - \deg(\phi_2)$*.*

Proof From the hypothesis, there exist polynomials $\tilde{\phi}_1$ and $\tilde{\phi}_2$ such that $\phi_1 = \phi\,\tilde{\phi}_1$ and $\phi_2 = \phi\,\tilde{\phi}_2$. If ϕ_1 and ϕ_2 are coprime, then set $\phi = 1$. From (4.2) and (4.3), we obtain

$$\tilde{\phi}_2 D(\phi_1\mathbf{u}) - \tilde{\phi}_1 D(\phi_2\mathbf{u}) + (\tilde{\phi}_2\,\psi_1 - \tilde{\phi}_1\,\psi_2)\mathbf{u} = 0. \tag{4.4}$$

Observe that, for any polynomial $p \in \mathbb{P}$,

$$\begin{aligned}
\langle \tilde{\phi}_2 D(\phi_1\mathbf{u}) - \tilde{\phi}_1 D(\phi_2\mathbf{u}), p\rangle &= -\langle \mathbf{u}, \phi_1(\tilde{\phi}_2\,p)'\rangle + \langle \mathbf{u}, \phi_2\,(\tilde{\phi}_1\,p)'\rangle \\
&= \langle \mathbf{u}, (\phi_2\,\tilde{\phi}_1' - \phi_1\,\tilde{\phi}_2')\,p + (\tilde{\phi}_1\,\phi_2 - \tilde{\phi}_2\,\phi_1)\,p'\rangle \\
&= \langle \mathbf{u}, (\phi_2\,\tilde{\phi}_1' - \phi_1\,\tilde{\phi}_2')\,p + \phi\,(\tilde{\phi}_1\,\tilde{\phi}_2 - \tilde{\phi}_2\,\tilde{\phi}_1)\,p'\rangle \\
&= \langle \mathbf{u}, (\phi_2\,\tilde{\phi}_1' - \phi_1\,\tilde{\phi}_2')\,p\rangle \\
&= \langle (\phi_2\,\tilde{\phi}_1' - \phi_1\,\tilde{\phi}_2')\,\mathbf{u}, p\rangle.
\end{aligned}$$

Therefore, (4.4) becomes $(\phi_2\,\tilde{\phi}_1' - \phi_1\,\tilde{\phi}_2' + \tilde{\phi}_2\,\psi_1 - \tilde{\phi}_1\,\psi_2)\,\mathbf{u} = 0$. Since $\mathbf{u}$ is quasi-definite, then

$$\phi_2\,\tilde{\phi}_1' - \phi_1\,\tilde{\phi}_2' + \tilde{\phi}_2\,\psi_1 - \tilde{\phi}_1\,\psi_2 = 0,$$

or, equivalently, $(\tilde{\phi}_1'\,\phi + \psi_1)\tilde{\phi}_2 = (\tilde{\phi}_2'\,\phi + \psi_2)\tilde{\phi}_1$.

But $\tilde{\phi}_1$ and $\tilde{\phi}_2$ are coprime polynomials. Hence, there exists a polynomial ψ such that

$$\tilde{\phi}_1' \phi + \psi_1 = \psi \tilde{\phi}_1, \quad \tilde{\phi}_2' \phi + \psi_2 = \psi \tilde{\phi}_2. \tag{4.5}$$

Since $\phi_1 = \phi \tilde{\phi}_1$ and $\phi_2 = \phi \tilde{\phi}_2$, (4.2) and (4.3) can be written as

$$\tilde{\phi}_1 D(\phi \mathbf{u}) + (\tilde{\phi}_1' \phi + \psi_1) \mathbf{u} = 0, \quad \tilde{\phi}_2 D(\phi \mathbf{u}) + (\tilde{\phi}_2 \phi + \psi_2) \mathbf{u} = 0.$$

Using (4.5), we write

$$\tilde{\phi}_1 (D(\phi\mathbf{u}) + \psi\mathbf{u}) = 0, \quad \tilde{\phi}_2 (D(\phi\mathbf{u}) + \psi\mathbf{u}) = 0,$$

and the result follows from the Bézout identity for coprime polynomials. □

Theorem 4.5 ([59]) *For any semiclassical linear functional* $\mathbf{u}$*, the polynomials* ϕ *and* ψ *in* (4.1) *such that*

$$\mathfrak{s}(\mathbf{u}) = \max\{\deg(\phi) - 2, \deg(\psi) - 1\}$$

are unique up to a constant factor.

Proof Suppose that $\mathbf{u}$ satisfies (4.1) with ϕ_i and ψ_i, $i = 1, 2$, and suppose that $\mathfrak{s}(\mathbf{u}) = \max\{\deg(\phi_i) - 2, \deg(\psi_i) - 1\}$, $i = 1, 2$. If in Lemma 4.4 we take $s_1 = s_2$, then $s = s_1 = s_2$. But this implies that $\deg(\phi) = \deg(\phi_1) = \deg(\phi_2)$, or, equivalently, $\phi = \phi_1 = \phi_2$. Notice also that ψ is unique up to a constant factor. □

The polynomials ϕ and ψ such that $\mathfrak{s}(\mathbf{u}) = \max\{\deg(\phi) - 2, \deg(\psi) - 1\}$ are characterized in the following result.

Proposition 4.6 ([57]) *Let* $\mathbf{u}$ *be a semi-classical linear functional and let* $\phi(x)$ *and* $\psi(x)$ *be non-zero polynomials with* $\deg(\phi) =: r$ *and* $\deg(\psi) =: t$*, such that* (4.1) *holds. Let* $s := \max(r - 2, t - 1)$*. Then* $s = \mathfrak{s}(\mathbf{u})$ *if and only if*

$$\prod_{c:\,\phi(c)=0} \Big(|\psi(c) + \phi'(c)| + |\langle \mathbf{u}, \theta_c\psi + \theta_c^2\phi\rangle|\Big) > 0. \tag{4.6}$$

Here, $(\theta_c f)(x) = \dfrac{f(x) - f(c)}{x - c}$.

Proof Let c be a zero of ϕ, then there exists a polynomial $\phi_c(x)$ of degree $r - 1$ such that $\phi(x) = (x - c)\phi_c(x)$. On the other hand, since

$$\theta_c^2\phi(x) = \frac{\phi(x) - \phi(c)}{(x - c)^2} - \frac{\phi'(c)}{x - c},$$

then

$$\psi(x) + \phi_c(x) = (x - c)\psi_c(x) + r_c,$$

where

$$\psi_c(x) = \theta_c\psi(x) + \theta_c^2\phi(x), \quad r_c = \psi(c) + \phi'(c).$$

With this in mind, (4.1) can be written as $(x - c)(D(\phi_c\,\mathbf{u}) + \psi_c\,\mathbf{u}) + r_c\mathbf{u} = 0$. From here, we obtain

$$\begin{aligned} D(\phi_c\mathbf{u}) + \psi_c\mathbf{u} &= -\frac{r_c}{(x-c)}\mathbf{u} + \langle \mathbf{u}, \psi_c\rangle\, \delta(x - c) \\ &= -\frac{\psi(c) + \phi'(c)}{(x - c)}\mathbf{u} + \langle \mathbf{u}, \theta_c\psi + \theta_c^2\phi\rangle\, \delta(x - c). \end{aligned}$$

Next, we proceed to the proof of the proposition.

Suppose that $\mathfrak{s}(\mathbf{u}) = s$, $r_c = 0$ and $\langle \mathbf{u}, \psi_c\rangle = 0$ for some c such that $\phi(c) = 0$. Then $D(\phi_c\mathbf{u}) + \psi_c\mathbf{u} = 0$. But $\deg(\phi_c) = r - 1$ and $\deg(\psi_c) = t - 1$. This means that $\mathfrak{s}(\mathbf{u}) = s - 1$, which is a contradiction.

Now, suppose that (4.6) holds and that $\mathbf{u}$ is of class $\tilde{s} \leq s$, with $D(\tilde{\phi}\,\mathbf{u})+\tilde{\psi}\,\mathbf{u} = 0$. From Lemma 4.4, there exists a polynomial $\rho(x)$ such that

$$\phi(x) = \rho(x)\tilde{\phi}(x), \qquad \psi(x) = \rho(x)\tilde{\psi}(x) - \rho'(x)\tilde{\phi}(x).$$

If $\tilde{s} < s$, then necessarily $\deg(\rho) \geq 1$. Let c be a zero of $\rho(x)$ and let $\rho_c(x)$ be the polynomial such that $\rho(x) = (x - c)\,\rho_c(x)$. Then,

$$\psi(x) + \phi_c(x) = (x - c)\,\Big(\rho_c(x)\,\tilde{\psi}(x) - \rho_c'(x)\,\tilde{\phi}(x)\Big).$$

It follows that

$$r_c = 0, \qquad \psi_c(x) = \rho_c(x)\,\tilde{\psi}(x) - \rho_c'(x)\,\tilde{\phi}(x).$$

Hence,

$$\langle \mathbf{u}, \psi_c\rangle = \langle \mathbf{u}, \tilde{\psi}\,\rho_c\rangle - \langle \mathbf{u}, \rho_c'\,\tilde{\phi}\rangle = \langle D(\tilde{\phi}\,\mathbf{u}) + \tilde{\psi}\,\mathbf{u}, \rho_c\rangle = 0.$$

But this means that $\phi(c) = 0$ and

$$|\psi(c) + \phi'(c)| + |\langle \mathbf{u}, \theta_c\psi + \theta_c^2\phi\rangle| = 0,$$

which contradicts (4.6). Thus, $s = \tilde{s}$ and, by Theorem 4.5, $\tilde{\phi}$ and $\tilde{\psi}$ are multiple of ϕ and ψ, respectively, up to a constant factor. □

Proposition 4.7 ([34, 58]) *Let* **u** *be a linear functional. The following statements are equivalent.*

(1) **u** *is semiclassical.*
(2) *There exist two non-zero polynomials* ϕ *and* ψ *with* $\deg(\phi) =: r \geq 0$ *and* $\deg(\psi) =: t \geq 1$*, such that the Stieltjes function* $\mathcal{S}(z)$ *associated with* **u** *satisfies*

$$\phi(z)\,\mathcal{S}'(z) + (\psi(z) + \phi'(z))\,\mathcal{S}(z) = C(z), \tag{4.7}$$

where

$$C(z) = (\mathbf{u} * \theta_0\left(\psi + \phi'\right))(z) - (D\mathbf{u} * \theta_0\phi)(z).$$

Proof (1)⇒(2) Let **u** be a semiclassical functional of class s satisfying (4.1).

$$\phi(z) = \sum_{k=0}^{r} \frac{\phi^{(k)}(0)}{k!} z^k, \qquad \psi(z) = \sum_{m=0}^{t} \frac{\psi^{(m)}(0)}{m!} z^m,$$

we have

$$\begin{aligned} 0 = \langle D(\phi\mathbf{u}) + \psi\mathbf{u}, x^n\rangle &= -\langle \mathbf{u}, nx^{n-1}\phi(x)\rangle + \langle \mathbf{u}, x^n\psi(x)\rangle \\ &= -n\sum_{k=0}^{r} \frac{\phi^{(k)}(0)}{k!}\mu_{n+k-1} + \sum_{m=0}^{t} \frac{\psi^{(m)}(0)}{m!}\mu_{n+m}. \end{aligned}$$

Multiplying the above relation by $1/z^{n+1}$ and taking the infinite sum over n, we obtain

$$0 = -\sum_{n=0}^{\infty} n \sum_{k=0}^{r} \frac{\phi^{(k)}(0)}{k!}\frac{\mu_{n+k-1}}{z^{n+1}} + \sum_{n=0}^{\infty}\sum_{m=0}^{t} \frac{\psi^{(m)}(0)}{m!}\frac{\mu_{n+m}}{z^{n+1}}. \tag{4.8}$$

It is straightforward to verify that

$$\begin{aligned} \sum_{n=0}^{\infty}\sum_{m=0}^{t} \frac{\psi^{(m)}(0)}{m!}\frac{\mu_{n+m}}{z^{n+1}} &= \psi(z)\mathcal{S}(z) - \sum_{m=1}^{t}\sum_{n=0}^{m-1} \frac{\psi^{(m)}(0)}{m!}\mu_n z^{m-1-n} \\ &= \psi(z)\mathcal{S}(z) - (\mathbf{u} * \theta_0\psi)(z). \end{aligned}$$

On the other hand,

$$\mathcal{S}'(z) = -\sum_{n=0}^{\infty}(n+1)\frac{\mu_n}{z^{n+2}}.$$

Thus,

$$\sum_{n=0}^{\infty}\sum_{k=0}^{r} n\frac{\phi^{(k)}(0)}{k!}\frac{\mu_{n+k-1}}{z^{n+1}} = -\phi(z)\mathcal{S}'(z) - \phi'(z)\mathcal{S}(z) + \sum_{k=2}^{r}\sum_{n=0}^{k-2}\frac{\phi^{(k)}(0)}{(k-1)!}\frac{\mu_n}{z^{n-k+2}}$$
$$-\sum_{k=2}^{r}\sum_{n=0}^{k-2}(n+1)\frac{\phi^{(k)}(0)}{k!}\frac{\mu_n}{z^{n-k+2}}$$
$$= -\phi(z)\mathcal{S}'(z) - \phi'(z)\mathcal{S}(z) + (\mathbf{u} * \theta_0\phi')(z) - (D\mathbf{u} * \theta_0\phi)(z).$$

Hence, (4.7) follows from (4.8).
(2)⇒(1) Suppose that (4.7) holds for some non-zero polynomials ϕ and ψ. Since each step above is also true in the reverse direction, then (4.7) is equivalently to (4.8). But this implies that, for every $n \geq 0$,

$$0 = -\langle \mathbf{u}, n\, x^{n-1}\,\phi\rangle + \langle \mathbf{u}, x^n\,\psi\rangle = \langle D(\phi\,\mathbf{u}) + \psi\,\mathbf{u}, x^n\rangle.$$

Therefore, **u** is semiclassical. □

Proposition 4.8 ([59]) *Let* **u** *be a linear functional, and let* $\{P_n(x)\}_{n\geq 0}$ *be its sequence of monic orthogonal polynomials. The following statements are equivalent.*

(1) *The linear functional* **u** *is semiclassical of class* s.
(2) *For* $n \geq 0$*, let* $R_n(x) = \dfrac{P'_{n+1}(x)}{n+1}$. *There exists a non-zero polynomial* $\phi(x)$ *with* $\deg(\phi) = r$*, such that the sequence of monic polynomials* $\{R_n(x)\}_{n\geq 0}$ *is quasi-orthogonal of order* s *with respect to the linear functional* $\phi(x)\,\mathbf{u}$.

Proof (1)⇒(2) Let ϕ and ψ be non-zero polynomials with $\deg(\phi) =: r \geq 0$ and $\deg(\psi) =: t \geq 1$ such that **u** satisfies $D(\phi\,\mathbf{u}) + \psi\,\mathbf{u} = 0$ and $s := \max\{r-2, t-1\}$ is the class of **u**. Note that

$$\langle \phi\,\mathbf{u}, x^m P'_{n+1}\rangle = \langle \phi\,\mathbf{u}, (x^m P_{n+1})'\rangle - \langle \phi\,\mathbf{u}, m\,x^{m-1}P_{n+1}\rangle$$
$$= \langle \mathbf{u}, \left(x^m\psi - m\,x^{m-1}\phi\right)\, P_{n+1}\rangle.$$

The above implies that $\langle \phi\,\mathbf{u}, x^m P'_{n+1}\rangle = 0$ for $0 \leq m \leq n-s-1$. Moreover, from Remark 4.2, $x^m\psi(x) - m\,x^{m-1}\phi(x)$ has degree $s+m+1$ and, thus, $\langle \phi\,\mathbf{u}, x^{n-s}P'_{n+1}\rangle \neq 0$. Hence, $R_n(x)$ is quasi-orthogonal of order s.

(2)⇒(1) Suppose that there exists some non-zero polynomial ϕ with $\deg(\phi) =: r \geq 0$, such that the sequence of polynomials $\{R_n(x)\}_{n\geq 0}$ is quasi-orthogonal of order s with respect to the linear functional $\phi(x)\mathbf{u}$. Since $\left\{\frac{P_n(x)}{\|P_n\|^2}\mathbf{u}\right\}_{n\geq 0}$ is a basis of the dual space of $\mathbb{P}$, then

$$D(\phi\,\mathbf{u}) = \sum_{n=0}^{\infty} \alpha_n \frac{P_n(x)}{\|P_n\|^2}\mathbf{u},$$

where $\alpha_n = \langle D(\phi\,\mathbf{u}), P_n\rangle = -\langle \phi\,\mathbf{u}, P_n'\rangle = -n\langle \mathbf{u}, \phi\, R_{n-1}\rangle$, $n \geq 1$, $\alpha_0 = 0$.

From the quasi-orthogonality of $\{R_n(x)\}_{n\geq 0}$, $\alpha_n = 0$ when $s+2 \leq n$. Thus,

$$D(\phi\mathbf{u}) + \psi\mathbf{u} = 0, \quad \text{where} \quad \psi(x) = -\sum_{n=1}^{s+1} \alpha_n \frac{P_n(x)}{\|P_n\|^2}.$$

□

Corollary 4.9 *A linear functional* $\mathbf{u}$ *with associated sequence of monic orthogonal polynomials* $\{P_n(x)\}_{n\geq 0}$ *is semiclassical of class* s *if and only if there is a non-zero polynomial* ϕ *such that sequence of monic polynomials* $\{F_n(x)\}_{n\geq 0}$*, where* $F_n(x) = \dfrac{P_{n+m}^{(m)}(x)}{(n+1)_m}$*, is quasi-orthogonal of order* s *with respect to the linear functional* $\phi^m\,\mathbf{u}$.

Proposition 4.10 ([59]) *Let* $\mathbf{u}$ *be a linear functional and* $\{P_n(x)\}_{n\geq 0}$ *its sequence of monic orthogonal polynomials. The following statements are equivalent.*

(1) $\mathbf{u}$ *is semiclassical of class* s.
(2) *There exist a nonnegative integer number* s *and a monic polynomial* $\phi(x)$ *of degree* r *with* $0 \leq r \leq s+2$*, such that*

$$\phi(x)\, P_{n+1}'(x) = \sum_{k=n-s}^{n+r} \lambda_{n,k}\, P_k(x), \quad n \geq s, \quad \lambda_{n,n-s} \neq 0. \tag{4.9}$$

If $s \geq 1$, $r \geq 1$ *and* $\lambda_{s,0} \neq 0$*, then* s *is the class of* $\mathbf{u}$.

Proof (1)⇒(2) Suppose that $\mathbf{u}$ is of class s satisfying $D(\phi\,\mathbf{u}) + \psi\,\mathbf{u} = 0$ with $\deg(\phi) = r$. Since $\{P_n(x)\}_{n\geq 0}$ is a basis of $\mathbb{P}$, for each $n \geq 0$, there exists a set of real numbers $(\lambda_{n,k})_{k=0}^{n+r}$ such that

$$\phi(x)\, P_{n+1}'(x) = \sum_{k=0}^{r+n} \lambda_{n,k}\, P_k(x).$$

Using orthogonality,

$$\lambda_{n,k} = \frac{\langle \phi\,\mathbf{u}, P_{n+1}'\, P_k\rangle}{\langle \mathbf{u}, P_k^2\rangle} = \frac{(n+1)\langle \phi\,\mathbf{u}, R_n\, P_k\rangle}{\langle \mathbf{u}, P_k^2\rangle},$$

where, for each $n \geq 0$, $R_n(x) = \frac{P_{n+1}'(x)}{n+1}$. But $\mathbf{u}$ is semiclassical of class s, then, from Proposition 4.8, $R_n(x)$ is quasi-orthogonal of order s with respect to $\phi\,\mathbf{u}$. Therefore, $\lambda_{n,k} = 0$, when $s+1 < n-k$, and $\lambda_{n,n-s} \neq 0$.

(2)⇒(1) Assume that $\{P_n(x)\}_{n\geq 0}$ satisfies (4.9). Since $\left\{\frac{P_n(x)}{\|P_n(x)\|^2}\mathbf{u}\right\}_{n\geq 0}$ is a basis of the dual space of $\mathbb{P}$, then

$$D(\phi\mathbf{u}) = \sum_{n=0}^{\infty} \alpha_n \frac{P_n(x)}{\|P_n(x)\|^2}\mathbf{u}.$$

Using (4.9),

$$\alpha_n = \langle \mathbf{u}, \phi P_n'(x)\rangle = \sum_{k=n-s}^{n+r} \lambda_{n,k}\langle \mathbf{u}, P_k(x)\rangle = \begin{cases} 0, & n > s, \\ \lambda_{n,0}\langle \mathbf{u}, P_0\rangle, & n \leq s. \end{cases}$$

Therefore, $\mathbf{u}$ satisfies $D(\phi\,\mathbf{u}) + \psi\,\mathbf{u} = 0$ with

$$\psi(x) = -\sum_{n=0}^{s+1} \alpha_n \frac{P_n(x)}{\|P_n\|^2},$$

hence, $\mathbf{u}$ is semiclassical. Observe that if in particular $\lambda_{s,0} \neq 0$, $\mathbf{u}$ is of class s. □

Using the three-term recurrence relation (2.2), (4.9) can be written in a compact form as shown in the following result.

Theorem 4.11 ([59]) *Let* $\mathbf{u}$ *be a semiclassical functional of class s, and* $\{P_n(x)\}_{n\geq 0}$ *its associated sequence of monic orthogonal polynomials. Then there exists a non-zero polynomial* ϕ *with* $\deg(\phi) =: r \geq 0$*, such that*

$$\phi(x)P_{n+1}'(x) = \frac{C_{n+1}(x) - C_0(x)}{2}P_{n+1}(x) - D_{n+1}(x)P_n(x), \quad n \geq 0, \tag{4.10}$$

where $\{C_n(x)\}_{n\geq 0}$ *and* $\{D_n(x)\}_{n\geq 0}$ *are polynomials satisfying*

$$\begin{aligned} C_{n+1}(x) &= -C_n(x) + \frac{2D_n(x)}{a_n}(x - b_n), \quad n \geq 0, \\ C_0(x) &= -\psi(x) - \phi'(x) \end{aligned} \tag{4.11}$$

and

$$D_{n+1}(x) = -\phi(x) + \frac{a_n}{a_{n-1}}D_{n-1}(x) + \frac{D_n(x)}{a_n}(x - b_n)^2 - C_n(x)(x - b_n), \; n \geq 0,$$

$$D_0(x) = -(\mathbf{u} * \theta_0\phi)'(x) - (\mathbf{u} * \theta_0\psi)(x), \quad D_{-1}(x) = 0.$$

The above expression leads to the so-called ladder operators associated with the linear functional $\mathbf{u}$. Using (4.11) and the three-term recurrence relation (2.2), we can deduce from (4.10) that, for $n \geq 0$,

$$\phi(x)P'_{n+1}(x) = -\left(\frac{C_{n+2}(x) + C_0(x)}{2}\right) P_{n+1}(x) + \frac{D_{n+1}(x)}{a_{n+1}} P_{n+2}(x). \qquad (4.12)$$

The relations (4.10) and (4.12) are essential to deduce a second-order linear differential equation satisfied by the polynomials $\{P_n(x)\}_{n\geq 0}$ (see [34, 37, 59]), which reads

$$J(x,n)P''_{n+1}(x) + K(x,n)P'_{n+1}(x) + L(x,n)P_{n+1}(x) = 0, \quad n \geq 0,$$

where, for $n \geq 0$,

$$J(x,n) = \phi(x)D_{n+1}(x),$$

$$K(x;n) = (\phi'(x) + C_0(x))D'_{n+1}(x) - \phi(x)\, D'_{n+1}(x),$$

and

$$L(x,n) = \left(\frac{C_{n+1}(x) - C_0(x)}{2}\right) D'_{n+1}(x) - \left(\frac{C'_{n+1}(x) - C'_0(x)}{2}\right) D_{n+1}(x) - D_{n+1}(x) \sum_{k=0}^{n} \frac{D_k(x)}{a_k}.$$

Notice that the degrees of the polynomials J, K, L are at most $2s+2$, $2s+1$, and $2s$, respectively.

Theorem 4.12 ([9, 10]) *Let* **u** *be a quasi-definite linear functional and* $\{P_n(x)\}_{n\geq 0}$ *the sequence of monic orthogonal polynomials associated with* **u**. *The following statements are equivalent.*

(1) **u** *is semiclassical.*
(2) $\{P_n(x)\}_{n\geq 0}$ *satisfies the following nonlinear differential equation.*

$$\phi(x)[P_{n+1}(x)\, P_n(x)]' = \frac{D_n(x)}{a_n} P^2_{n+1}(x) - C_0(x)P_{n+1}(x)P_n(x) - D_{n+1}(x)P^2_n(x), \qquad (4.13)$$

where $D_n(x)$, $C_0(x)$ *and* a_n *are the same as in* (4.10).

Proof (1)⇒(2) Suppose that $\mathbf{u}$ is semiclassical. From (4.10), we have

$$\phi(x)[P_{n+1}(x)P_n(x)]' = P_n(x)\left(\frac{C_{n+1}(x)-C_0(x)}{2}P_{n+1}(x) - D_{n+1}(x)P_n(x)\right)$$
$$+ P_{n+1}(x)\left(\frac{C_n(x)-C_0(x)}{2}P_n(x) - D_n(x)P_{n-1}(x)\right)$$
$$= -D_{n+1}(x)P_n^2(x) + \left(\frac{C_{n+1}(x)+C_n(x)-2C_0(x)}{2}\right)P_{n+1}(x)P_n(x)$$
$$- D_n(x)P_{n+1}(x)P_{n-1}(x).$$

Now, taking into account that $P_{n-1}(x) = \frac{(x-b_n)}{a_n}P_n(x) - \frac{1}{a_n}P_{n+1}(x)$ the above relation becomes

$$\phi[P_{n+1}(x)P_n(x)]' = -D_{n+1}P_n^2(x) + \frac{D_n}{a_n}P_{n+1}^2(x)$$
$$+ \left(\frac{C_{n+1}(x)+C_n(x)-2C_0(x)}{2} - \frac{(x-b_n)}{a_n}D_n\right)P_{n+1}(x)P_n(x).$$

Using the relation (4.11), we get the result.

(2)⇒(1) Let $\mathbf{u}$ be a quasi-definite linear functional, and let $\{P_n(x)\}_{n\geq 0}$ be the sequence of monic orthogonal polynomials associated with $\mathbf{u}$.

Suppose that $\{P_n(x)\}_{n\geq 0}$ satisfies (4.13). Using the three-term recurrence relation $P_{n+1}(x) = (x-b_n)\,P_n(x) - a_n\,P_{n-1}(x)$ and (4.11), we can write (4.13) as

$$\phi(x)\,P'_{n+1}(x)P_n(x) = \left(\frac{C_{n+1}(x)+C_n(x)-2C_0(x)}{2}\right)P_{n+1}(x)P_n(x)$$
$$- D_{n+1}(x)P_n^2(x) - D_n(x)P_{n+1}(x)P_{n-1}(x) - \phi(x)P_{n+1}(x)P'_n(x). \tag{4.14}$$

Multiplying the above relation by $P_{n-1}(x)$, and replacing $\phi(x)\,P'_n(x)\,P_{n-1}(x)$ with (4.14) for $n-1$, we obtain

$$\phi(x)\,P'_{n+1}(x)\,P_{n-1}(x) = \left(\frac{C_{n+1}(x)-C_{n-1}(x)}{2}\right)P_{n+1}(x)\,P_{n-1}(x)$$
$$- D_{n+1}(x)\,P_n(x)\,P_{n-1}(x) + P_{n+1}(x)\,(D_{n-1}(x)\,P_{n-2}(x) + \phi(x)\,P'_{n-1}(x)).$$

Similarly, multiplying the above relation by $P_{n-2}(x)$, and then replacing $\phi(x)\, P'_{n-1}(x)\, P_{n-2}(x)$ by (4.14) for $n-2$, we get

$$\phi(x)\, P'_{n+1}(x)\, P_{n-2}(x) = \left(\frac{C_{n+1}(x) + C_{n-2}(x) - 2C_0(x)}{2}\right) P_{n+1}(x)\, P_{n-2}(x)$$
$$- D_{n+1}(x)\, P_n(x)\, P_{n-2}(x) - P_{n+1}(x) \left(D_{n-2}(x)\, P_{n-3}(x) + \phi(x)\, P'_{n-2}(x)\right).$$

Iterating this process, we obtain that for odd $k \leq n$,

$$\phi(x)\, P'_{n+1}(x)\, P_{n-k}(x) = \left(\frac{C_{n+1}(x) - C_{n-k}(x)}{2}\right) P_{n+1}(x) P_{n-k}(x)$$
$$-D_{n+1}(x)\, P_n(x)\, P_{n-k}(x) + P_{n+1}(x)(D_{n-k}(x)\, P_{n-(k+1)}(x) + \phi(x)\, P'_{n-k}(x)),$$

and for even $k \leq n$,

$$\phi(x)\, P'_{n+1}(x)\, P_{n-k}(x) = \left(\frac{C_{n+1}(x) + C_{n-k}(x) - 2C_0(x)}{2}\right) P_{n+1}(x)\, P_{n-k}(x)$$
$$- D_{n+1}(x)\, P_n(x)\, P_{n-k}(x) - P_{n+1}(x) \left(D_{n-k}(x)\, P_{n-(k+1)}(x) + \phi(x)\, P'_{n-k}(x)\right).$$

In either case, for n either odd or even, when $k = n$ we obtain (4.9), but this implies that **u** is semiclassical. □

Before dealing with the next result, we fix some notation. Let $\{Q_n(x)\}_{n\geq 0}$ be a basis of $\mathbb{P}$. We define the vector $\mathbf{Q} := (Q_0(x), Q_1(x), Q_2(x), \dots)^t$. Let N be the semi-infinite matrix such that $\chi'(x) = N\,\chi(x)$. Therefore,

$$N = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots \\ 1 & 0 & 0 & 0 & \dots \\ 0 & 2 & 0 & 0 & \dots \\ 0 & 0 & 3 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

We denote by $\tilde{N}$ the semi-infinite matrix such that $\mathbf{Q}' = \tilde{N}\,\mathbf{Q}$. Observe that if S is a matrix of change of basis from the monomials $\chi(x)$ to $\mathbf{Q}$, that is, $\mathbf{Q} = S\,\chi(x)$, then $\tilde{N} = S\,N\,S^{-1}$.

If $\mathbf{Q}$ is semiclassical, we write (4.9) in matrix form as $\phi(x)\,\mathbf{Q}' = F\,\mathbf{Q}$, where F is a semi-infinite band matrix. Finally, for square matrices A and B of size n, we define its commutator as $[A, B] = AB - BA$.

Proposition 4.13 *Let* $\mathbf{u}$ *be a positive-definite semiclassical functional satisfying the Pearson equation* $D(\phi\,\mathbf{u}) + \psi\,\mathbf{u} = 0$*, and let* $\{Q_n(x)\}_{n\geq 0}$ *be the sequence of orthonormal polynomials associated with* $\mathbf{u}$*. Then,*

1. $[J, F] = \phi(J)$,
2. $\tilde{N}\,\phi(J)^t + \phi(J)\,\tilde{N}^t = \psi(J)$,
3. $F + F^t = \psi(J)$,

where J *is the Jacobi matrix associated with* $\{Q_n(x)\}_{n\geq 0}$.

Remark 4.14 This is the matrix representation of the Laguerre-Freud equations satisfied by the parameters of the three-term recurrence relation of semiclassical orthonormal polynomials. As a direct consequence, you can deduce nonlinear difference equations that the coefficients of the three-term recurrence relation satisfy. They are relate to discrete Painlevé equations. Some illustrative examples appear in [73].

Proof

1. Differentiating $x\,\mathbf{Q} = J\,\mathbf{Q}$ and then multiplying by $\phi(x)$, we get

$$J\phi(x)\,\mathbf{Q}' = \phi(x)\,\mathbf{Q} + x\,\phi(x)\,\mathbf{Q}'.$$

But $\phi(x)\,\mathbf{Q}' = F\mathbf{Q}$ and $\phi(x)\mathbf{Q} = \phi(J)\mathbf{Q}$. Hence,

$$JF\mathbf{Q} = \phi(J)\mathbf{Q} + x\,F\,\mathbf{Q} = (\phi(J) + FJ)\mathbf{Q},$$

and, since $\mathbf{Q}$ is a basis, the result follows.

2. From the Pearson equation

$$\begin{aligned}0 &= \langle D(\phi\mathbf{u}), \mathbf{Q}\,\mathbf{Q}^t\rangle + \langle\psi\,\mathbf{u}, \mathbf{Q}\,\mathbf{Q}^t\rangle = -\langle\phi\,\mathbf{u}, \mathbf{Q}'\,\mathbf{Q}^t + \mathbf{Q}\,(\mathbf{Q}')^t\rangle + \langle\psi\,\mathbf{u}, \mathbf{Q}\,\mathbf{Q}^t\rangle\\ &= -\tilde{N}\langle\mathbf{u}, \phi(x)\,\mathbf{Q}\,\mathbf{Q}^t\rangle - \langle\mathbf{u}, \mathbf{Q}\,\mathbf{Q}^t\phi(x)\rangle\tilde{N}^t + \langle\mathbf{u}, \psi(x)\,\mathbf{Q}\,\mathbf{Q}^t\rangle\\ &= -\tilde{N}\phi(J)\langle\mathbf{u}, \mathbf{Q}\,\mathbf{Q}^t\rangle - \langle\mathbf{u}, \mathbf{Q}\,\mathbf{Q}^t\rangle\phi(J)^t\tilde{N}^t + \psi(J)\langle\mathbf{u}, \mathbf{Q}\,\mathbf{Q}^t\rangle.\end{aligned}$$

But $\langle\mathbf{u}, \mathbf{Q}\,\mathbf{Q}^t\rangle$ is equal to the identity matrix since $\{Q_n(x)\}_{n\geq 0}$ are orthonormal, and the result follows.

3. Similarly, from the Pearson equation

$$\begin{aligned}0 &= \langle D(\phi\mathbf{u}), \mathbf{Q}\,\mathbf{Q}^t\rangle + \langle\psi\,\mathbf{u}, \mathbf{Q}\,\mathbf{Q}^t\rangle = -\langle\phi\,\mathbf{u}, \mathbf{Q}'\,\mathbf{Q}^t + \mathbf{Q}\,(\mathbf{Q}')^t\rangle + \langle\psi\,\mathbf{u}, \mathbf{Q}\,\mathbf{Q}^t\rangle\\ &= -\langle\mathbf{u}, \phi(x)\,\mathbf{Q}'\,\mathbf{Q}^t\rangle - \langle\mathbf{u}, \mathbf{Q}\,(\mathbf{Q}')^t\phi(x)\rangle + \langle\mathbf{u}, \psi(x)\,\mathbf{Q}\,\mathbf{Q}^t\rangle\\ &= -F\langle\mathbf{u}, \mathbf{Q}\,\mathbf{Q}^t\rangle - \langle\mathbf{u}, \mathbf{Q}\,\mathbf{Q}^t\rangle F^t + \psi(J)\langle\mathbf{u}, \mathbf{Q}\,\mathbf{Q}^t\rangle,\end{aligned}$$

and the result follows. □

5 Examples of Semiclassical Orthogonal Polynomials

It is well know that the semiclassical functionals of class $s = 0$ are the classical linear functionals (Hermite, Laguerre, Jacobi, and Bessel) defined by an expression of the form

$$\langle \mathbf{u}, p \rangle = \int_E p(x) w(x) dx, \quad \forall p \in \mathbb{P},$$

where

Family	$\phi(x)$	$\psi(x)$	$w(x)$	E
Hermite	1	$2x$	e^{-x^2}	$\mathbb{R}$
Laguerre	x	$x - \alpha - 1$	$x^\alpha e^{-x}$	$(0, +\infty)$
Jacobi	$x^2 - 1$	$-(\alpha + \beta + 2)x + \beta - \alpha$	$(1-x)^\alpha (1+x)^\beta$	$(-1, 1)$
Bessel	x^2	$-2(\alpha x + 1)$	$x^\alpha e^{-2/x}$	Unit circle

The Hermite, Laguerre, and Jacobi functionals are positive-definite when $\alpha, \beta > -1$, and the Bessel functional is a quasi-definite linear functional that is not positive-definite.

If $\mathbf{u}$ is a semiclassical functional of class $s = 1$, we can distinguish two situations

$$(A)\ \deg(\psi) = 2,\ 0 \le \deg(\phi) \le 3; \qquad (\text{B})\ \deg(\psi) = 1,\ \deg(\phi) = 3.$$

S. Belmehdi [10] exposed the canonical forms of the functionals of the class 1, up to linear changes of the variable, according to the degree of $\phi(x)$ and the multiplicity of its zeros.

(A) $\deg(\psi) = 2$	
$\deg(\phi) = 0$	1
$\deg(\phi) = 1$	x
$\deg(\phi) = 2$	x^2 $x^2 - 1$
$\deg(\phi) = 3$	x^3 $x^2(x-1)$ $(x^2-1)(x-c)$

(B) $\deg(\psi) = 1$	
$\deg(\phi) = 3$	x^3 $x^2(x-1)$ $(x^2-1)(x-c)$

Example Let $\mathbf{u}$ be the linear functional defined by (see [40])

$$\langle \mathbf{u}, p \rangle = \int_0^\infty p(x)\, x^\alpha e^{-x} dx + M p(0), \quad \forall p \in \mathbb{P},$$

with $\alpha > -1$ and $M > 0$. Then $\mathbf{u}$ is a semiclassical functional of class $s = 1$ satisfying $D(\phi\,\mathbf{u}) + \psi\,\mathbf{u} = 0$ with $\phi(x) = x^2$ and $\psi(x) = x(x - \alpha - 2)$.

The sequence of polynomials orthogonal with respect to the above functional is known in the literature as Laguerre-type orthogonal polynomials (see [39, 49], among others).

Example Let $\mathbf{u}$ be the linear functional defined by (see [10])

$$\langle \mathbf{u}, p\rangle = \int_{-1}^{1} p(x)\,(x-1)^{(a+b-2)/2}(x+1)^{(b-a-2)/2}e^{ax}dx, \quad \forall p \in \mathbb{P},$$

with $b > a$. Then $\mathbf{u}$ satisfies $D(\phi\,\mathbf{u}) + \psi\,\mathbf{u} = 0$ with $\phi(x) = x^2 - 1$ and $\psi(x) = -ax^2 - bx$. The functional is semiclassical of class $s = 1$.

Example Let $\mathbf{u}$ be the linear functional defined by (see [12, 73])

$$\langle \mathbf{u}, p\rangle = \int_{0}^{\infty} p(x)\,x^{\alpha}e^{-x^2+tx}dx, \quad \forall p \in \mathbb{P},$$

with $\alpha > -1$ and $t \in \mathbb{R}$. In [12], it is shown that $\mathbf{u}$ is a semiclassical functional of class $s = 1$ satisfying $D(\phi\,\mathbf{u})+\psi\,\mathbf{u} = 0$ with $\phi(x) = x$ and $\psi(x) = 2x^2-tx-\alpha-1$.

Example Let $\mathbf{u}$ be the functional defined by (see [10])

$$\langle \mathbf{u}, p\rangle = \int_{0}^{N} p(x)\,x^{\alpha}e^{-x}dx, \quad \forall p \in \mathbb{P},$$

with $\alpha > -1$ and $N > 0$. The functional $\mathbf{u}$ is semiclassical of class $s = 1$ satisfying $D(\phi\,\mathbf{u}) + \psi\,\mathbf{u} = 0$ with $\phi(x) = (x - N)x$ and $\psi(x) = (x - \alpha)(x - N) + N - 2x$.

This functional is known in the literature as truncated gamma functional and the corresponding sequences of orthogonal polynomials are called truncated Laguerre orthogonal polynomials.

Semiclassical functionals can be constructed via discrete Darboux transformations. First, we need to prove the following theorem.

Theorem 5.1 *Let* $\mathbf{u}$ *and* $\mathbf{v}$ *be two linear functionals related by*

$$A(x)\mathbf{u} = B(x)\mathbf{v},$$

where $A(x)$ *and* $B(x)$ *are non-zero polynomials. Then* $\mathbf{u}$ *is semiclassical if and only if* $\mathbf{v}$ *is semiclassical.*

Proof Suppose that $\mathbf{u}$ is semiclassical satisfying $D(\phi_0\mathbf{u}) + \psi_0\mathbf{u} = 0$. Let $\phi_1(x) = A(x)\,B(x)\phi_0(x)$. Then,

$$\begin{aligned}\langle D(\phi_1\,\mathbf{v}), x^n\rangle =&\langle D(A\,B\,\phi_0\,\mathbf{v}), x^n\rangle = \langle D(A^2\,\phi_0\,\mathbf{u}), x^n\rangle = -\langle \phi_0\,\mathbf{u}, n\,A^2\,x^{n-1}\rangle \\ =&-\langle \phi_0\mathbf{u}, (A^2\,x^n)'\rangle + \langle \phi_0\,\mathbf{u}, (A^2)'x^n\rangle\end{aligned}$$

$$
\begin{aligned}
&=\langle A^2\,\psi_0\,\mathbf{u}, x^n\rangle - \langle 2\phi_0\,A'\,A\mathbf{u}, x^n\rangle\\
&=\langle \big(A\,\psi_0 - 2A'\,\phi_0\big)\,B\,\mathbf{v}, x^n\rangle.
\end{aligned}
$$

Therefore, $\mathbf{v}$ is semiclassical with $\psi_1(x) = \big(A(x)\psi_0(x) - 2\phi_0(x)A'(x)\big)\,B(x)$.

Similarly, if $\mathbf{v}$ is semiclassical, by interchanging the role of the functionals above, it follows that $\mathbf{u}$ is semiclassical. □

Corollary 5.2 *Any linear spectral transformation of a semiclassical functional is also a semiclassical functional.*

Remark 5.3

- For canonical Christoffel (3.1) and Geronimus (3.3) transformations, the class of the new functional depends on the location of the point a in terms of the zeros of $\phi(x)$.
- Uvarov transformations (3.6) of classical orthogonal polynomials generate semiclassical linear functionals. The so called Krall-type linear functionals appear when a Dirac measure, or mass point, is located at a zero of $\phi(x)$. The corresponding sequences of orthogonal polynomials satisfy, for some choices of the parameters (in the Laguerre case, for α a non negative integer number) higher order linear differential equations with order depending on α. It is an open problem to describe the sequences of orthogonal polynomials which are eigenfunctions of higher order differential operators. For order two (S. Bochner [11]) and four (H. L. Krall [43]), the problem has been completely solved.

Example The linear functional obtained from a Uvarov transformation of the Laguerre functional will be of class 1 if a mass point is located at $a = 0$, and will be of class 2 if a mass point is located at $a \neq 0$. See [49].

Other examples of semiclassical functionals of class 2 are also known.

Example Let $\mathbf{u}$ be the functional defined by

$$
\langle \mathbf{u}, p\rangle = \int_{\mathbb{R}} p(x)\, e^{-\frac{x^4}{4} - tx^2} dx, \quad \forall p \in \mathbb{P},
$$

where $t \in \mathbb{R}$. In this case, $\mathbf{u}$ is a semi-classical functional of class $s = 2$, with $\phi(x) = 1$ and $\psi(x) = 2tx + x^3$.

This is a particular case of the so called generalized Freud linear functionals [19, 20].

New semiclassical functionals can also be constructed through symmetrized functionals [17].

Definition 5.4 Let $\mathbf{u}$ be a linear functional. Its symmetrized functional $\mathbf{v}$ is defined by

$$
\langle \mathbf{v}, x^{2n}\rangle = \mu_n, \quad \langle \mathbf{v}, x^{2n+1}\rangle = 0, \quad n \geq 0.
$$

Given a functional with Stieltjes function $\mathcal{S}(z)$, the Stieltjes function $\tilde{\mathcal{S}}(z)$ of its symmetrized functional satisfies $\tilde{\mathcal{S}}(z) = z\mathcal{S}(z^2)$. The following holds for the semiclassical case.

Theorem 5.5 ([5]) *Let* $\mathbf{u}$ *be a semiclassical functional satisfying* $D(\phi\mathbf{u}) + \psi\mathbf{u} = 0$*, and let* $\mathcal{S}(z)$ *be its Stieltjes function, which satisfies* (4.7)

$$\phi(z)\mathcal{S}'(z) + (\psi(z) + \phi'(z))\mathcal{S}(z) = C(z).$$

The Stieltjes function $\tilde{\mathcal{S}}(z)$ *associated with the symmetrized linear functional* $\mathbf{v}$ *satisfies*

$$z\phi(z^2)\tilde{\mathcal{S}}'(z) + [2z^2(\psi(z^2) + \phi'(z^2)) + \phi(z^2)]\tilde{\mathcal{S}}(z) = 2z^3C(z^2).$$

Thus, the symmetrized functional of a semiclassical linear functional is semiclassical. The class of $\mathbf{v}$ *is either* $2s$*,* $2s+1$*, or* $2s+3$*, according to the coprimality of the polynomial coefficients in the ordinary linear differential equation satisfied by* $\tilde{\mathcal{S}}(z)$*.*

6 Analytic Properties of Orthogonal Polynomials in Sobolev Spaces

An inner product is said to be a Sobolev inner product if

$$\langle f, g\rangle_S := \int_{E_0} f(x)\, g(x)\, d\mu_0 + \sum_{k=1}^{m} \int_{E_k} f^{(k)}(x)\, g^{(k)}(x)\, d\mu_k,$$

where $(d\mu_0, \ldots, d\mu_m)$ is a vector of positive Borel measures and $E_k = \operatorname{supp} d\mu_k$, $k = 0, 1, \ldots, m$.

Using the Gram-Schmidt orthogonalization method for the canonical basis $\{x^n\}_{n\geq 0}$, one gets a sequence of monic orthogonal polynomials. Thus, the nth orthogonal polynomial is a minimal polynomial in terms of the Sobolev norm

$$||f||_S := \sqrt{\langle f, f\rangle_S}$$

among all monic polynomials of degree n.

Taking into account that $\langle x\, f, g\rangle_S \neq \langle f, x\, g\rangle_S$, these polynomials do not satisfy a three-term recurrence relation. Thus, a basic property of standard orthogonal polynomials is lost. A natural question is to compare analytic properties of these polynomials and the standard ones.

In 1947, D. C. Lewis [45] dealt with the following problem in the framework of polynomial least square approximation. Let $\alpha_0, \ldots, \alpha_p$ be monotonic, nondecreasing functions defined on $[a, b]$ and let f be a function on $[a, b]$ that satisfies certain regularity conditions. Determine a polynomial $P_n(x)$ of degree at most n that minimizes

$$\sum_{k=0}^{p} \int_a^b |f^{(k)}(x) - P_n^{(k)}(x)|^2 d\alpha_k(x).$$

Lewis did not use Sobolev orthogonal polynomials and gave a formula for the remainder term of the approximation as an integral of the Peano kernel. The first paper on Sobolev orthogonal polynomials was published by Althammer [3] in 1962, who attributed his motivation to Lewis's paper. These Sobolev orthogonal polynomials are orthogonal with respect to the inner product

$$\langle f, g \rangle_S = \int_{-1}^{1} f(x)\, g(x)\, dx + \lambda \int_{-1}^{1} f'(x)\, g'(x)\, dx, \quad \lambda > 0.$$

Observe that the first and second integral of this inner product involve the Lebesgue measure dx on $[-1, 1]$, which means that every point in $[-1, 1]$ is equally weighted.

Let $S_n(x; \lambda)$ denote the orthogonal polynomial of degree n with respect to the inner product $\langle \cdot, \cdot \rangle_S$, normalized by $S_n(1; \lambda) = 1$, and let $P_n(x)$ denote the n-th Legendre polynomial. The following properties hold for $S_n(x; \lambda)$:

1. $\langle S_n(x; \lambda)\}_{n \geq 0}$ satisfies a differential equation

$$\lambda\, S_n''(x; \lambda) - S_n(x; \lambda) = A_n\, P_{n+1}'(x) + B_n\, P_{n-1}'(x),$$

   where A_n and B_n are real numbers which are explicitly given.
2. $\{S_n(x; \lambda)\}_{n \geq 0}$ satisfies a recursive relation

$$S_n(x; \lambda) - S_{n-2}(x; \lambda) = a_n\, (P_n(x) - P_{n-2}(x)), \quad n = 1, 2, \ldots$$

3. $S_n(x; \lambda)$ has n real simple zeros in $(-1, 1)$.

For a more detailed account on the development of these results, we refer to [45, 62, 67]. The Sobolev-Legendre polynomials were also studied by Gröbner, who established a version of the Rodrigues formula in [33]. Indeed, he states that, up to a constant factor c_n,

$$S_n(x; \lambda) = c_n \frac{D^n}{1 - \lambda D^2} \left((x^2 - x)^n - \alpha_n (x^2 - x)^{n-1} \right)$$

where α_n are real numbers explicitly given in terms of λ and n.

In [3], Althammer also gave an example in which he replaced dx in the second integral in $\langle \cdot, \cdot \rangle_S$ by $w(x)dx$ with $w(x) = 10$ for $-1 \leq x < 0$ and $w(x) = 1$ for $0 \leq x \leq 1$, and made the observation that $S_2(x; \lambda)$ for this new inner product has one real zero outside of $(-1, 1)$.

In [13], Brenner considered the inner product

$$\langle f, g\rangle := \int_0^\infty f(x)\, g(x)\, e^{-x} dx + \lambda \int_0^\infty f'(x)\, g'(x)\, e^{-x} dx, \quad \lambda > 0,$$

and obtained results in a direction very similar to those of Althammer. Sobolev inner products when you replace the above weight by $x^\alpha e^{-x}$, $\alpha \geq -1$ has been studied in [51].

An important contribution in the early development of the Sobolev polynomials was made in 1972 by Schäfke and Wolf in [68], where they considered a family of inner products

$$\langle f, g\rangle_S = \sum_{j,k=0}^{\infty} \int_a^b f^{(j)}(x)\, g^{(k)}(x)\, v_{j,k}(x)\, w(x)\, dx, \tag{6.1}$$

where w and (a, b) are one of the three classical cases (Hermite, Laguerre, and Jacobi) and the functions $v_{j,k}$ are polynomials that satisfy $v_{j,k} = v_{k,j}$, $k = 0, 1, 2, \ldots$, and allow to write the inner product (6.1) as

$$\langle f, g\rangle_S = \int_a^b f(x)\, \mathcal{B}g(x)\, w(x)\, dx, \quad \text{with} \quad \mathcal{B}g := w^{-1} \sum_{j,k=0}^{\infty} (-1)^j D^j\, (w\, v_{j,k}\, D^k) g$$

by using an integration by parts. Under further restrictions on $v_{j,k}$, they are narrowed down to eight classes of Sobolev orthogonal polynomials, which they call simple generalizations of classical orthogonal polynomials.

The primary tool in the early study of Sobolev orthogonal polynomials is integration by parts. Schäfke and Wolf [68] explored when this tool is applicable and outlined potential Sobolev inner products. It is remarkable that their work appeared in such an early stage of the development of Sobolev orthogonal polynomials.

The study of Sobolev orthogonal polynomials unexpectedly became largely dormant for nearly two decades, from which it reemerged only when a new ingredient, *coherent pairs*, was introduced in [36].

6.1 Coherent Pairs of Measures and Sobolev Orthogonal Polynomials

The concept of coherent pair of measures was introduced in [36] in the framework of the study of the inner product

$$\langle f, g\rangle_\lambda = \int_a^b f(x)\, g(x)\, d\mu_0(x) + \lambda \int_a^b f'(x)\, g'(x)\, d\mu_1(x), \tag{6.2}$$

where $-\infty \le a < b \le \infty$, $\lambda \ge 0$, μ_0 and μ_1 are positive Borel measures on the real line with finite moments of all orders. Let $P_n(x; d\mu_i)$ denote the monic orthogonal polynomial of degree n with respect to $d\mu_i$, $i = 0, 1$.

Definition 6.1 The pair $\{d\mu_0,\ d\mu_1\}$ is called coherent if there exists a sequence of nonzero real numbers $\{\alpha_n\}_{n\ge1}$ such that

$$P_n(x; d\mu_1) = \frac{P'_{n+1}(x; d\mu_0)}{n+1} + \alpha_n \frac{P'_n(x; d\mu_0)}{n}, \quad n \ge 1. \tag{6.3}$$

If $[a, b] = [-c, c]$ and $d\mu_0$ and $d\mu_1$ are both symmetric, then $\{d\mu_0, d\mu_1\}$ is called a symmetrically coherent pair if

$$P_n(x; d\mu_1) = \frac{P'_{n+1}(x; d\mu_0)}{n+1} + \alpha_n \frac{P'_{n-1}(x; d\mu_0)}{n-1}, \quad n \ge 2.$$

If $d\mu_1 = d\mu_0$, the measure $d\mu_0$ is said to be self-coherent (resp. symmetrically self-coherent).

For $n = 0, 1, 2, \ldots$, let

$$M_n(\lambda) = \begin{pmatrix} \langle 1, 1\rangle_\lambda & \langle 1, x\rangle_\lambda & \cdots & \langle 1, x^n\rangle_\lambda \\ \langle x, 1\rangle_\lambda & \langle x, x\rangle_\lambda & \cdots & \langle x, x^n\rangle_\lambda \\ \dots & \dots & \ddots & \dots \\ \langle x^n, 1\rangle_\lambda & \langle x^n, x\rangle_\lambda & \cdots & \langle x^n, x^n\rangle_\lambda \end{pmatrix}.$$

Since $\det M_n(\lambda) > 0$ for all $n \ge 0$, then a sequence of monic orthogonal polynomials with respect to $\langle\cdot,\cdot\rangle_\lambda$ exists. Let $\{S_n(x; \lambda)\}_{n\ge0}$ denote the sequence of monic Sobolev orthogonal polynomials with respect to $\langle\cdot,\cdot\rangle_\lambda$. In fact, the monic orthogonal polynomials are $S_0(x; \lambda) = 1$ and, for $n \ge 1$,

$$S_n(x; \lambda) = \frac{1}{\det M_{n-1}(\lambda)} \det \left(\begin{array}{cccc|c} & & & & \langle 1, x^n\rangle_\lambda \\ & & & & \langle x, x^n\rangle_\lambda \\ & M_{n-1}(\lambda) & & & \vdots \\ & & & & \langle x^{n-1}, x^n\rangle_\lambda \\ \hline 1 & x & \cdots & x^{n-1} & x^n \end{array}\right).$$

It is easy to see that

$$T_n(x) := \lim_{\lambda\to\infty} S_n(x; \lambda)$$

is a monic polynomial of degree n which satisfies

$$T_n'(x) = n\, P_{n-1}(x; d\mu_1) \quad \text{and} \quad \int_{\mathbb{R}} T_n(x)\, d\mu_0 = 0 \quad n \geq 1. \tag{6.4}$$

Theorem 6.2 ([36]) *If* $\{d\mu_0,\ d\mu_1\}$ *is a coherent pair, then*

$$S_n(x; \lambda) + \beta_{n-1}(\lambda)\, S_{n-1}(x; \lambda) = P_n(x; d\mu_0) + \hat{\alpha}_{n-1} P_{n-1}(x; d\mu_0),\ n \geq 2, \tag{6.5}$$

where $\hat{\alpha}_{n-1} = n\, \alpha_n/(n-1)$ *and* $\beta_{n-1}(\lambda) = \hat{\alpha}_{n-1} ||P_{n-1}(x; d\mu_0)||^2_{d\mu_0}/||S_{n-1}(x; \lambda)||^2_\lambda$.

Proof According to (6.3) and (6.4), we see that

$$T_n(x) = P_n(x; d\mu_0) + \hat{\alpha}_{n-1} P_{n-1}(x; d\mu_0).$$

For $0 \leq j \leq n-2$, it follows from (6.4) that

$$\langle T_n(x), S_j(x; \lambda)\rangle_\lambda = \langle T_n(x), S_j(x; \lambda)\rangle_{d\mu_0} + n\lambda \langle P_{n-1}(x; d\mu_1), S_j'(x; \lambda)\rangle_{d\mu_1} = 0.$$

Considering the expansion of $T_n(x)$ in terms of the polynomials $S_j(x; \lambda)$, we see that

$$T_n(x) = S_n(x; \lambda) + \beta_{n-1}(\lambda)\, S_{n-1}(x; \lambda), \quad \text{where} \quad \beta_{n-1}(\lambda) = \frac{\langle T_n(x), S_{n-1}(x; \lambda)\rangle_\lambda}{||S_{n-1}(x; \lambda)||^2_\lambda}.$$

The expresion for $\beta_{n-1}(\lambda)$ follows from $\langle T_n'(x), S_{n-1}'(x; \lambda)\rangle_{d\mu_1} = 0$ as well as from the fact that both $P_{n-1}(x; d\mu_0)$ and $S_{n-1}(x; \lambda)$ are monic. □

The notion of coherent pairs can be extended to linear functionals $\{\mathbf{u}_0,\ \mathbf{u}_1\}$, if the relation (6.3) holds with $P_n(x; d\mu_i)$ replaced by $P_n(x; \mathbf{u}_i)$.

The following theorem was established in [63].

Theorem 6.3 *If* $\{d\mu_0,\ d\mu_1\}$ *is a coherent pair of measures, then at least one of them has to be classical (Laguerre, Jacobi).*

Together, [52, 63] give a complete list of coherent pairs. In the case when $\mathbf{u}_0$ and $\mathbf{u}_1$ are positive-definite linear functionals associated with measures $d\mu_0$ and $d\mu_1$, the coherent pairs are given as follows:

Laguerre Case

(1) $d\mu_0(x) = (x - \xi)x^{\alpha-1}e^{-x}dx$ and $d\mu_1(x) = x^\alpha e^{-x}dx$, where if $\xi < 0$, then $\alpha > 0$, and if $\xi = 0$ then $\alpha > -1$.

(2) $d\mu_0(x) = x^\alpha e^{-x}dx$ and $d\mu_1(x) = (x - \xi)^{-1}x^{\alpha+1}e^{-x}dx + M\,\delta(x - \xi)$, where if $\xi < 0$, $\alpha > -1$ and $M \geq 0$.

(3) $d\mu_0(x) = e^{-x}dx + M\delta(x)$ and $d\mu_1(x) = e^{-x}dx$, where $M \geq 0$.

Jacobi Case

(1) $d\mu_0(x) = |x-\xi|(1-x)^{\alpha-1}(1+x)^{\beta-1}dx$ and $d\mu_1(x) = (1-x)^{\alpha}(1+x)^{\beta}dx$, where if $|\xi| > 1$ then $\alpha > 0$ and $\beta > 0$, if $\xi = 1$ then $\alpha > -1$ and $\beta > 0$, and if $\xi = -1$ then $\alpha > 0$ and $\beta > -1$.
(2) $d\mu_0(x) = (1-x)^{\alpha}(1+x)^{\beta}dx$ and $d\mu_1(x) = |x-\xi|^{-1}(1-x)^{\alpha+1}(1+x)^{\beta+1}dx + M\delta(x-\xi)$, where $|\xi| > 1$, $\alpha > -1$ and $\beta > -1$ and $M \geq 0$.
(3) $d\mu_0(x) = (1+x)^{\beta-1}dx + M\delta(x-1)$ and $d\mu_1(x) = (1+x)^{\beta}dx$, where $\beta > 0$ and $M \geq 0$.
(4) $d\mu_0(x) = (1-x)^{\alpha-1}dx + M\delta(x+1)$ and $d\mu_1(x) = (1-x)^{\alpha}dx$, where $\alpha > 0$ and $M \geq 0$.

A similar analysis was also carried out for symmetrically coherent pairs in the work cited above. It lead to the following list of symmetrically coherent pairs.

Hermite Case

(1) $d\mu_0(x) = e^{-x^2}dx$ and $d\mu_1(x) = (x^2+\xi^2)^{-1}e^{-x^2}dx$, where $\xi \neq 0$.
(2) $d\mu_0(x) = (x^2+\xi^2)e^{-x^2}dx$ and $d\mu_1(x) = e^{-x^2}dx$, where $\xi \neq 0$.

Gegenbauer Case

(1) $d\mu_0(x) = (1-x^2)^{\alpha-1}dx$ and $d\mu_1(x) = (x^2+\xi^2)^{-1}(1-x^2)^{\alpha}dx$, where $\xi \neq 0$ and $\alpha > 0$.
(2) $d\mu_0(x) = (1-x^2)^{\alpha-1}dx$ and $d\mu_1(x) = (\xi^2-x^2)^{-1}(1-x^2)^{\alpha}dx + M\delta(x-\xi) + M\delta(x+\xi)$, where $|\xi| > 1$, $\alpha > 0$ and $M \geq 0$.
(3) $d\mu_0(x) = (x^2+\xi^2)(1-x^2)^{\alpha-1}dx$ and $d\mu_1(x) = (1-x^2)^{\alpha}dx$, where $\alpha > 0$.
(4) $d\mu_0(x) = (\xi^2-x^2)(1-x^2)^{\alpha-1}dx$ and $d\mu_1(x) = (1-x^2)^{\alpha}dx$, where $|\xi| \geq 1$ and $\alpha > 0$.
(5) $d\mu_0(x) = dx + M\delta(x-1) + M\delta(x+1)$ and $d\mu_1(x) = dx$, where $M \geq 0$.

6.1.1 Generalized Coherent Pairs

Identity (6.5) was deduced from definition (6.3) of coherent pairs. In the reverse direction, however, (6.3) does not follow from the identity (6.5), as observed in [38].

Let $\mathtt{S}_n(x)$ denote the left hand side of (6.5). Clearly $\mathtt{S}_n'$ can be expanded in terms of $\{P_k(x;d\mu_1)\}_{k\geq 0}$,

$$\mathtt{S}_n'(x) = n\,P_{n-1}(x;d\mu_1) + \sum_{k=0}^{n-2} d_{k,n}P_k(x;d\mu_1), \qquad d_{k,n} = \frac{\langle \mathtt{S}_n'(x), P_k(x;d\mu_1)\rangle_{d\mu_1}}{||P_k(x;d\mu_1)||^2_{d\mu_1}}, \qquad n \geq 1.$$

For $0 \leq j \leq n-2$, it follows directly from the definition of $\mathtt{S}_n$ that

$$\langle \mathtt{S}_n(x), P_j(x;d\mu_1)\rangle_{\lambda} = 0,$$

and it follows from (6.5) that $\langle \mathtt{S}_n(x), P_j(x; d\mu_1)\rangle_{d\mu_0} = 0$. Consequently, by the definition of $\langle\cdot,\cdot\rangle_\lambda$ we must have $\langle \mathtt{S}_n', P_j(x; d\mu_1)\rangle_{d\mu_1} = 0$ for $0 \le j \le n-2$, which implies that $d_{k,n} = 0$ if $0 \le k \le n-2$. Hence,

$$\mathtt{S}_n'(x) = P_n'(x; d\mu_0) + \hat{a}_{n-1} P_{n-1}'(x; d\mu_0) = n\, P_{n-1}(x; d\mu_1) + d_{n-2,n} P_{n-2}(x; d\mu_1).$$

Recall that $\hat{\alpha}_n = (n+1)\alpha_n/n$. Setting $\beta_{n-2} = d_{n-2,n}/n$ and shifting the index from n to $n+1$, we conclude the following relation between $\{P_n(x; d\mu_0)\}_{n\ge 0}$ and $\{P_n(x; d\mu_1)\}_{n\ge 0}$,

$$P_n(x; d\mu_1) + \beta_{n-1}\, P_{n-1}(x; d\mu_1) = \frac{P_{n+1}'(x; d\mu_0)}{n+1} + \alpha_n \frac{P_n'(x; d\mu_0)}{n}, \quad n \ge 1. \tag{6.6}$$

Thus, in the reverse direction, (6.5) leads to (6.6) instead of (6.3).

Evidently, (6.6) is a more general relation than (6.3).

Definition 6.4 The pair $\{d\mu_0, d\mu_1\}$ is called a generalized coherent pair if (6.6) holds for $n \ge 1$, and this definition extends to linear functionals $\{\mathbf{u}_0, \mathbf{u}_1\}$.

Semiclassical orthogonal polynomials of class 1 (see Sect. 5) are involved in the analysis of generalized coherent pairs. The following theorem is established in [22].

Theorem 6.5 *If* $\{\mathbf{u}_0, \mathbf{u}_1\}$ *is a generalized coherent pair, then at least one of them must be semiclassical of class at most* 1.

All generalized coherent pairs of linear functionals are listed in [22].

On the other hand, given two sequences of monic orthogonal polynomials $\{P_n(x; d\mu_0)\}_{n\ge 0}$ and $\{P_n(x; d\mu_1)\}_{n\ge 0}$, where $d\mu_0$ and $d\mu_1$ are symmetric measures, such that the following relation holds

$$P_{n+1}(x; d\mu_1) + \beta_{n-1}\, P_{n-1}(x; d\mu_1) = \frac{P_{n+2}'(x; d\mu_0)}{n+1} + \alpha_n \frac{P_n'(x; d\mu_0)}{n}, \quad n \ge 1. \tag{6.7}$$

We introduce the following

Definition 6.6 The pair $\{d\mu_0, d\mu_1\}$ is called a symmetrically generalized coherent pair if (6.7) holds for $n \ge 1$, and this definition extends to linear functionals $\{\mathbf{u}_0, \mathbf{u}_1\}$.

Some examples of symmetrically generalized coherent pairs have been studied in [21], where $\mathbf{u}_0$ is associated with the Gegenbauer weight and

$$\mathbf{u}_1 = \frac{1-x^2}{1+qx^2}\mathbf{u}_1 + M_q\left[\delta(x+1/\sqrt{-q}) + \delta(x-1/\sqrt{-q})\right], \quad q \ge -1,$$

where $M_q \ge 0$ if $-1 \le q < 0$ and $M_q = 0$ if $q \ge 0$.

More recently, in [24] the authors obtain analytic properties of Sobolev orthogonal polynomials with respect to a symmetrically generalized coherent pair $\{\mathbf{u}_0, \mathbf{u}_1\}$, where $\mathbf{u}_0$ is the linear functional associated with the Hermite weight and $\mathbf{u}_1 = \frac{x^2+a^2}{x^2+b^2}\mathbf{u}_0$.

6.2 Sobolev-Type Orthogonal Polynomials

An inner product is said to be a Sobolev-type inner product if the derivatives appear only as function evaluations on a finite discrete set. More precisely, such an inner product takes the form

$$\langle f, g\rangle_S := \int_{\mathbb{R}} f(x)\, g(x)\, d\mu_0 + \sum_{k=1}^{m} \int_{\mathbb{R}} f^{(k)}(x)\, g^{(k)}(x)\, d\mu_k, \tag{6.8}$$

where $d\mu_0$ is a positive Borel measure on an infinite subset of the real line and $d\mu_k$, $k = 1, 2, \ldots, m$, are positive Borel measures supported on finite subsets of the real line. In most cases considered below, $d\mu_k = A_k\delta(x-c)$ or $d\mu_k = A_k\delta(x-a) + B_k\delta(x-b)$, where A_k and B_k are nonnegative real numbers. Orthogonal polynomials for such an inner product are called Sobolev-type orthogonal polynomials.

The first study was carried out for the classical weight functions. The Laguerre case was studied in [40, 41] with $d\mu_0 = x^\alpha e^{-x} dx$, $\alpha > -1$, and

$$d\mu_k = M_k\delta(x), \quad k = 1, 2, \ldots, m,$$

the nth Sobolev orthogonal polynomial, S_n, is given by

$$S_n(x) = \sum_{k=0}^{\min\{n,m+1\}} (-1)^k\, A_{n,k}\, L_{n-k}^{\alpha+k}(x), \quad n \geq 1,$$

where $A_{n,k}$ are real numbers determined by a linear system of equations. The Gegenbauer case was studied in [7, 8] with $d\mu_0 = (1-x^2)^{\lambda-1/2}dx + A(\delta(x-1) + \delta(x+1))$, $\lambda > -1/2$, and $m = 1$, $d\mu_1 = B(\delta(x-1) + \delta(x+1))$; the nth Sobolev orthogonal polynomial is given by

$$S_n(x) = a_{0,n}C_n^{\lambda}(x) + a_{1,n}x\, C_{n-1}^{\lambda+1}(x) + a_{2,n}x^2\, C_{n-2}^{\lambda+2}(x), \quad n \geq 2,$$

where $a_{0,n}$, $a_{1,n}$, and $a_{2,n}$ are appropriate real numbers. In both cases, the Sobolev orthogonal polynomials satisfy higher order (greater than three) recurrence relations.

When $M_k = 0$ for $k = 1, 2, \ldots, m-1$, and $d\mu_m = M_m\,\delta(x-c)$, the inner product (6.8) becomes

$$\langle f, g\rangle_m := \int_{\mathbb{R}} f(x)\,g(x)\,d\mu_0 + M_m\, f^{(m)}(c)\,g^{(m)}(c),$$

where $c \in \mathbb{R}$ and $M_m \geq 0$.

For $i, j \in \mathbb{N}_0$, define

$$\mathcal{K}_{n-1}^{(i,j)}(x, y) := \sum_{l=0}^{n-1} \frac{P_l^{(i)}(x)\,P_l^{(j)}(y)}{||P_l||_{d\mu_0}^2}, n \geq 1.$$

It was shown in [53] that

$$S_n(x) = P_n(x) - \frac{M_m\,P_n^{(m)}(c)}{1 + M_m\,\mathcal{K}_{n-1}^{(m,m)}(c, c)} \mathcal{K}_{n-1}^{(0,m)}(x, c), n \geq 1,$$

which extends the expression for $m = 0$ by A. M. Krall in [44]. From this relation, one deduces immediately that

$$S_{n+1}(x) + \alpha_n S_n(x) = P_{n+1}(x) + \beta_n P_n(x), \quad n \geq 0,$$

where α_n and β_n are constants that can be easily determined. This shows a similar structure to (6.5) derived for the Sobolev orthogonal polynomials in the case of coherent pairs.

The Sobolev polynomials $S_n(x)$ also satisfy a higher order recurrence relation

$$(x-c)^{m+1} S_n(x) = \sum_{j=n-m-1}^{n+m+1} c_{n,j} S_j(x), n \geq 0, \tag{6.9}$$

where $c_{n,n+m+1} = 1$ and $c_{n,n-m-1} \neq 0$.

If a sequence of polynomials satisfies a three-term recurrence relation, then it is orthogonal. The precise statement is known as Favard's theorem. For higher order recurrence relations, there are two types of results in this direction, both related to Sobolev orthogonal polynomials.

The first one gives a characterization of an inner product $\langle\cdot,\cdot\rangle$ for which the corresponding sequence of orthogonal polynomials satisfy a recurrence relation (6.9), which holds if the operation of multiplication by $M_{m,c} := (x-c)^{m+1}$ is symmetric, that is, $\langle M_{m,c}\,p, q\rangle = \langle p, M_{m,c}\,q\rangle$. It was proved in [26] that if $\langle\cdot,\cdot\rangle$ is an inner product such that $M_{m,c}$ is symmetric and it communtes with the operator $M_{0,c}$, that is, $\langle M_{m,c}\,p, M_{0,c}\,q\rangle = \langle M_{0,c}\,p, M_{m,c}\,q\rangle$, then there exists a nontrivial positive Borel measure $d\mu_0$ and a real, positive semi-definite matrix A of size $m+1$, such that the inner product is of the form

$$\langle p, q\rangle = \int_{\mathbb{R}} p(x)\, q(x)\, d\mu_0 + \left(p(c), p'(c), \ldots, p^{(m)}(c)\right) A \left(q(c), q'(c), \ldots, q^{(m)}(c)\right)^t . \qquad (6.10)$$

A connection between such Sobolev orthogonal polynomials and matrix orthogonal polynomials was established in [27], by representing the higher order recurrence relation as a three-term recurrence relation with matrix coefficients for a family of matrix orthogonal polynomials defined in terms of the Sobolev orthogonal polynomials.

The second type of Favard type theorem was given in [28], where it was proved that the operator of multiplication by a polynomial h is symmetric with respect to the inner product (6.8) if and only if $d\mu_k$, $k = 1, 2, \ldots, m$, are discrete measures whose supports are related to the zeros of h and its derivatives. Consequently, higher order recurrence relations for Sobolev inner products appear only in Sobolev inner products of the second type.

6.3 Asymptotics of Sobolev Orthogonal Polynomials

For standard orthogonal polynomials, three different types of asymptotics are considered: strong asymptotics, outer ratio asymptotics, and nth root asymptotics. All three have been considered in the Sobolev setting and we summarize the most relevant results in this section.

The first work on asymptotics for Sobolev orthogonal polynomials is [54] where the authors deal with the inner product

$$\langle f, g\rangle_S = \int_{-1}^{1} f(x)\, g(x)\, d\mu_0(x) + M_1\, f'(c)\, g'(c),$$

where $c \in \mathbb{R}$, $M_1 > 0$, and the measure $d\mu_0$ belongs to the Nevai class $M(0, 1)$. Using the outer ratio asymptotics for the ordinary orthogonal polynomials $P_n(x; d\mu_0)$ and the connection formula between $P_n(x; d\mu_0)$ and the Sobolev orthogonal polynomials $S_n(x)$, it was shown that, if $c \in \mathbb{R} \setminus \operatorname{supp} \mu_0$, then

$$\lim_{n\to\infty} \frac{S_n(z)}{P_n(z, d\mu_0)} = \frac{(\Phi(z) - \Phi(c))^2}{2\,\Phi(z)\,(z - c)}, \qquad \Phi(z) := z + \sqrt{z^2 - 1},$$

locally uniformly outside the support of the measure, where $\sqrt{z^2-1} > 0$ when $z > 1$. If $c \in \operatorname{supp} \mu_0$, then

$$\lim_{n\to\infty} \frac{S_n(z)}{P_n(z; d\mu_0)} = 1$$

outside the support of the measure.

The first extension of the above results was carried out in [1] for the Sobolev inner product (6.10) with a 2×2 matrix A. Under the same conditions on the measure, it was proved that

$$\lim_{n\to\infty} \frac{S_n(z)}{P_n(z; d\mu_0)} = \left(\frac{(\Phi(z) - \Phi(c))^2}{2\,\Phi(z)\,(z-c)}\right)^r, \qquad r := \operatorname{rank} A,$$

locally uniformly outside the support of the measure.

The second extension was given in [48] for the inner product

$$\langle f, g\rangle = \int_{\mathbb{R}} f(x)\,g(x)\,d\mu_0(x) + \sum_{j=1}^{N}\sum_{k=0}^{N_j} f^{(k)}(c_j)\,L_{j,k}(g; c_j),$$

where $d\mu_0 \in M(0,1)$, $\{c_k\}_{k=1}^N \in \mathbb{R}\backslash \operatorname{supp} \mu_0$, $j = 1, \ldots, N$, and $L_{j,k}$ is an ordinary linear differential operator acting on g such that L_{j,N_j} is not identically zero for $j = 1, \ldots, N$. Assuming that the inner product is quasi-definite so that a sequence of orthogonal polynomials exists, then on every compact subset in $\mathbb{C} \setminus \operatorname{supp} d\mu_0$,

$$\lim_{n\to\infty} \frac{S_n^{(\nu)}(z)}{P_n^{(\nu)}(z, d\mu_0)} = \prod_{j=1}^{m} \left(\frac{(\Phi(z) - \Phi(c))^2}{2\,\Phi(z)\,(z-c)}\right)^{I_j},$$

where I_j is the dimension of the square matrix obtained from the matrix of coefficients of L_{j,N_j} after deleting all zero rows and columns.

On the other hand, if both the measure $d\mu_0$ and its support Δ are regular, then techniques from potential theory can be used (see [47]) to derive the nth root asymptotics of the Sobolev orthogonal polynomials,

$$\limsup_{n\to\infty} ||S_n^{(j)}||_{\Delta}^{1/n} = C(\Delta), \qquad j \geq 0,$$

where $||\cdot||_{\Delta}$ denotes the uniform norm on the support of the measure and $C(\Delta)$ is its logarithmic capacity.

When the support of the measure in the inner product (6.10) is unbounded, the analysis has been focused on the case of the Laguerre weight function. A first study [4] considered the case when $c = 0$ and A is a 2×2 diagonal matrix (see also [50] for a survey of the unbounded case). Assuming that the leading coefficients of S_n

are standardized to be $(-1)^n/n!$, the following results on the asymptotic behavior of S_n were established:

(1) (Outer relative asymptotics) $\lim_{n\to\infty} \frac{S_n(z)}{L_n^{(\alpha)}(z)} = 1$ uniformly on compact subsets of the exterior of the positive real semiaxis.
(2) (Outer relative asymptotics for scaled polynomials) $\lim_{n\to\infty} \frac{S_n(nz)}{L_n^{(\alpha)}(nz)} = 1$ uniformly on compact subsets of the exterior of $[0, 4]$.
(3) (Mehler-Heine formula) $\lim_{n\to\infty} n^{-\alpha} S_n(z/n) = z^{-\alpha/2} J_{\alpha+4}(2\sqrt{z})$ uniformly on compact subsets of the complex plane, assuming that rank $A = 2$.
(4) (Inner strong asymptotics)

$$\frac{S_n(x)}{n^{\alpha/2}} = c_3(n) e^{x/2} x^{-\alpha/2} J_{\alpha+4}\left(2\sqrt{(n-2)x}\right) + O\left(n^{-\min\{\alpha+5,3/4\}}\right)$$

on compact subsets of the positive real semiaxis, where $\lim_{n\to\infty} c_3(n) = 1$.

If the point c is a negative real number, then the following outer relative asymptotics was established in [55],

$$\lim_{n\to\infty} \frac{S_n(z)}{L_n^{(\alpha)}(z)} = \left(\frac{\sqrt{-z}-\sqrt{-c}}{\sqrt{-z}+\sqrt{-c}}\right)^r, \qquad r = \operatorname{rank} A,$$

uniformly on compact subsets of the exterior of the real positive semiaxis.

When $c = 0$ and A is a non-singular diagonal matrix of size $m + 1$, the following asymptotic properties of the Sobolev orthogonal polynomials with respect to the inner product (6.10) were obtained in [2]:

(1) (Outer relative asymptotics) For every $\nu \in \mathbb{N}$, $\lim_{n\to\infty} \frac{S_n^{(\nu)}(z)}{(L_n^{(\alpha)})^{(\nu)}(z)} = 1$ uniformly on compact subsets of the exterior of the positive real semiaxis.
(2) (Mehler-Heine formula)

$$\lim_{n\to\infty} \frac{(-1)^n}{n!} \frac{S_n(z/n)}{n^\alpha} = (-1)^{m+1} z^{-\alpha/2} J_{\alpha+2m+2}(2\sqrt{z})$$

uniformly on compact subsets of the complex plane.

6.3.1 Continuous Sobolev Inner Products

Let $\{\mu_0, \mu_1\}$ be a coherent pair of measures and supp $\mu_0 = [-1, 1]$. Then the outer relative asymptotic relation for the Sobolev orthogonal polynomials with respect to (6.10) in terms of the orthogonal polynomials $P_n(x; d\mu_1)$ is (see [61])

$$\lim_{n\to\infty} \frac{S_n(z)}{P_n(z; d\mu_1)} = \frac{2}{\Phi'(z)}, \qquad \Phi(z) := z + \sqrt{z^2 - 1},$$

where $\sqrt{z^2-1} > 0$ when $z > 1$, uniformly on compact subsets of the exterior of the interval $[-1, 1]$.

When the measures μ_0 and μ_1 are absolutely continuous and belong to the Szegő class, the above result is also true [60].

For measures of coherent pairs that have unbounded support, asymptotic properties of the corresponding Sobolev orthogonal polynomials have been extensively studied in the literature (see [50] for an overview). The outer relative asymptotics, the scaled outer asymptotics, as well as the inner strong asymptotics of such polynomials have been considered for all families of coherent pairs and symmetrically coherent pairs.

The case where both measures in (6.2) correspond to the Freud weight, that is, $d\mu_0 = d\mu_1 = e^{-x^4}dx$, was studied in [15] (see also [30]), where the connection between Sobolev and standard orthogonal polynomials is given by

$$P_n(x; d\mu) = S_n(x; \lambda) + c_{n-2}(\lambda)S_{n-2}(x; \lambda), \quad n \geq 2.$$

7 Sobolev Orthogonal Polynomials of Several Variables

In contrast with the univariate case, Sobolev orthogonal polynomials of several variables have been studied only recently. In this section, we collect some results in this direction.

7.1 Orthogonal Polynomials of Several Variables

For $x = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d$ and $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_d) \in \mathbb{N}_0^d$, the (total) degree of the monomial

$$x^\alpha := x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_d^{\alpha_d}$$

is, by definition, $|\alpha| := \alpha_1 + \alpha_2 + \cdots + \alpha_d$. Let Π_n^d denote the linear space of polynomials in d variables of total degree at most n. It is known that $\dim \Pi_n^d = \binom{n+d}{n}$. Let $\Pi^d := \bigcup_{n\geq 0} \Pi_n^d$ denote the space of all polynomials in d variables.

Let $\langle \cdot, \cdot \rangle$ be an inner product defined on $\Pi^d \times \Pi^d$. A polynomial $P \in \Pi_n^d$ is orthogonal if

$$\langle P, q \rangle = 0, \qquad \forall q \in \Pi_{n-1}^d.$$

For $n \in \mathbb{N}_0$, let $\mathcal{V}_n^d$ denote the space of orthogonal polynomials of total degree n. Then $\dim \mathcal{V}_n^d = \binom{n+d-1}{n}$. In contrast with the univariate case, the space $\mathcal{V}_n^d$ can have many different bases when $d \geq 2$. Moreover, the elements of $\mathcal{V}_n^d$ may not be mutually orthogonal.

For the structure and properties of orthogonal polynomials of several variables, we refer to [25]. We describe briefly a family of orthogonal polynomials as example.

A polynomial Y is said to be a spherical harmonic of degree n if it is a homogeneous polynomial such that $\Delta Y = 0$, where Δ is the Laplacian operator,

$$\Delta = \frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_n^2}.$$

Let $\mathcal{H}_n^d$ denote the space of spherical harmonics of degree n. It is known that

$$a_n^d := \dim \mathcal{H}_n^d = \binom{n+d-1}{n} - \binom{n+d-3}{n-2}.$$

The elements of $\mathcal{H}_n^d$ are orthogonal with respect to polynomials of degree at most $n-1$ with respect to the inner product

$$\langle f, g \rangle_{\mathbb{S}^{d-1}} := \int_{\mathbb{S}^{d-1}} f(\xi)\, g(\xi)\, d\sigma(\xi),$$

where $d\sigma$ denotes the surface measure on $\mathbb{S}^{d-1}$.

For $\mu > -1$, let $w_\mu(x) = (1 - ||x||^2)^{\mu - 1/2}$ be the weight function defined on the unit ball $\mathbb{B}^d = \{x \in \mathbb{R}^d : ||x|| \leq 1\}$, where $|| \cdot ||$ denotes the Euclidean norm in $\mathbb{R}^d$. Orthogonal polynomials with respect to w_μ can be given in several different formulations. We give one basis of $\mathcal{V}_n^d(w_\mu)$ in terms of the classical Jacobi polynomials and spherical harmonics in the spherical coordinates $x = r\xi$, where $0 < r \leq 1$ and $\xi \in \mathbb{S}^{d-1} = \{x \in \mathbb{R}^d : ||x|| = 1\}$.

For $0 \leq j \leq n/2$ and $1 \leq \nu \leq a_{n-2j}^d$, define

$$P_{j,\nu}^n(x) := P_j^{(\mu, n-2j+(d-2)/2)}(2||x||^2 - 1)\, Y_\nu^{n-2j}(x),$$

where $\{Y_\nu^{n-2j} : 1 \leq \nu \leq a_{n-2j}^d\}$ is an orthonormal basis of $\mathcal{H}_{n-2j}^d$. Then the set $\{P_{j,\ell}^n(x) : 0 \leq j \leq n/2,\ 1 \leq \ell \leq a_{n-2j}^d\}$ is a mutually orthogonal basis of $\mathcal{V}_n^d(w_\mu)$. The elements of $\mathcal{V}_n^d(w_\mu)$ are eigenfunctions of a second-order linear partial differential operator $\mathcal{D}_\mu$. More precisely, we have

$$\mathcal{D}_\mu P = -(n+d)(n+2\mu)\, P, \qquad \forall P \in \mathcal{V}_n^d(w_\mu), \tag{7.1}$$

where

$$\mathcal{D}_\mu := \Delta - \sum_{j=1}^{d} \frac{\partial}{\partial x_j} x_j \left[2\mu + \sum_{i=1}^{d} x_i \frac{\partial}{\partial x_i} \right]. \tag{7.2}$$

7.1.1 Sobolev Orthogonal Polynomials on the Unit Ball

The first work in this direction is [74] and deals with the inner product

$$\langle f, g \rangle_\Delta := \int_{\mathbb{B}^d} \Delta \Big[(1 - ||x||^2)\, f(x) \Big] \Delta \Big[(1 - ||x||^2)\, g(x) \Big] dx,$$

which arises from the numerical solution of the Poisson equation studied in [6]. The geometry of the ball and (7.3) suggest that one can look for a mutually orthogonal basis of the form

$$q_j(2||x||^2 - 1)\, Y_\nu^{n-2j}(x), \qquad Y_\nu^{n-2j} \in \mathcal{H}_{n-2j}^d, \tag{7.3}$$

where $q_j(x)$ is a polynomial of degree j in one variable. Such a basis was constructed in [74] for the space

$$\mathcal{V}_n^d(\Delta) = \mathcal{H}_n^d \bigoplus (1 - ||x||^2) \mathcal{V}_{n-2}(w_2).$$

The next inner product considered on the ball is defined by

$$\langle f, g \rangle_{-1} := \lambda \int_{\mathbb{B}^d} \nabla f(x) \cdot \nabla g(x)\, dx + \int_{\mathbb{S}^{d-1}} f(\xi)\, g(\xi)\, d\sigma(\xi),$$

where $\nabla f = (\partial_x f, \partial_y f)$ and $\lambda > 0$. An alternative way is to replace the integral over $\mathbb{S}^{d-1}$ by $f(0)\, g(0)$. A basis of the form (7.3) was constructed explicitly in [75] for the space $\mathcal{V}_n^d(\Delta)$ with respect to $\langle \cdot, \cdot \rangle_{-1}$, from which it follows that

$$\mathcal{V}_n^d(w_{-1}) = \mathcal{H}_n^d \bigoplus (1 - ||x||^2) \mathcal{V}_{n-2}(w_1). \tag{7.4}$$

The elements in $(1 - ||x||^2)\mathcal{V}_{n-2}(w_1)$ can be given in terms of the Jacobi polynomials $P_n^{(-1,b)}(x)$ of negative index, which explains the notation w_{-1}. Another interesting aspect of this case is that the polynomials in $\mathcal{V}_n^d(w_{-1})$ are eigenfunctions of the differential operator $\mathcal{D}_{-1}$, the limit case of (7.1).

For $k \in \mathbb{N}$, the operator $\mathcal{D}_{-k}$ in (7.2) makes perfect sense. The equation $\mathcal{D}_{-k} Y = \lambda_n Y$ was studied in [66], where a complete system of polynomial solutions was determined explicitly. For $k \geq 2$, however, it is not known if the solutions are

Sobolev orthogonal polynomials. Closely related to the case when $k = 2$ is the following inner product

$$\langle f, g\rangle_{-2} := \lambda \int_{\mathbb{B}^d} \Delta f(x)\, \Delta g(x)\, dx + \int_{\mathbb{S}^{d-1}} f(\xi)\, g(\xi)\, d\sigma(\xi), \qquad \lambda > 0.$$

An explicit basis for the space $\mathcal{V}_d^d(w_{-2})$ of the Sobolev polynomials with respect to $\langle \cdot, \cdot \rangle_{-2}$ was constructed in [66], from which it follows that

$$\mathcal{V}_d^d(w_{-2}) = \mathcal{H}_n^d \bigoplus (1-||x||^2)\mathcal{H}_{n-2}^d \bigoplus (1-||x||^2)^2 \mathcal{V}_{n-4}^d(w_2). \tag{7.5}$$

The elements in $(1-||x||^2)^2\mathcal{V}_{n-4}^d(w_2)$ can be given in terms of the Jacobi polynomials $P_n^{(-2,b)}$ of negative index.

It turns out that the Sobolev orthogonal polynomials for the last two cases can be used to study the spectral method for the numerical solutions of partial differential equations. This connection was established in [46], where, for $s \in \mathbb{N}$, the following inner product in the Sobolev space $W_p^s(\mathbb{B}^d)$ is defined

$$\langle f, g\rangle_{-s} := \langle \nabla^s f, \nabla^s g\rangle_{\mathbb{B}^d} + \sum_{k=0}^{\lceil \varrho/2 \rceil - 1} \lambda_k \langle \Delta^k f, \Delta^k g\rangle_{\mathbb{S}^{d-1}}.$$

Here λ_k, $k = 0, 1, \ldots, \lceil \varrho/2 \rceil - 1$, are positive real numbers, and

$$\nabla^{2m} := \Delta^m \qquad \text{and} \qquad \nabla^{2m+1} := \nabla\Delta^m, \qquad m = 1, 2, \ldots$$

For $s > 2$, the space $\mathcal{V}_n^d(w_{-s})$ associated with $\langle \cdot, \cdot \rangle_{-s}$ cannot be decomposed as in (7.4) and (7.5). Nevertheless, an explicit mutually orthogonal basis was constructed in [46]. It requires considerable effort, and the basis uses a generalization of the Jacobi polynomials $P_n^{(\alpha,\beta)}$ for $\alpha, \beta \in \mathbb{R}$ that avoids the degree reduction when $-\alpha-\beta-n \in \{0, 1, \ldots, n\}$. The main result in [46] establishes an estimate for the polynomial approximation in the Sobolev space $W_p^s(\mathbb{B}^d)$. The proof relies on the Fourier expansion with respect to the Sobolev orthogonal polynomials associated with $\langle \cdot, \cdot \rangle_{-s}$.

Another Sobolev inner product considered on the unit ball is defined by

$$\langle f, g\rangle := \int_{\mathbb{B}^d} \nabla f(x) \cdot \nabla g(x)\, W_\mu(x)\, dx + \lambda \int_{\mathbb{B}^d} f(x)\, g(x)\, W_\mu(x)\, dx,$$

which is an extension of the Sobolev inner product (6.2) of coherent pairs where $d\mu_1 = d\mu_2$ correspond to the Gegenbauer weight in one variable. A mutually orthogonal basis was constructed in [65], which has the form (7.3) where the corresponding q_j is orthogonal with respect to a rather involved Sobolev product in one variable.

7.1.2 Sobolev Orthogonal Polynomials on Product Domains

On the product domain $[a_1, b_1] \times [a_2, b_2] \subset \mathbb{R}^2$, we define the weight function

$$\varpi(x, y) = w_1(x)\, w_2(y),$$

where w_i, $i = 1, 2$, is a weight function on $[a_i, b_i]$, $i = 1, 2$. With respect to ϖ, we consider the Sobolev inner product

$$\langle f, g\rangle_S := \int_{[a,b]^2} \nabla f(x, y) \cdot \nabla g(x, y) \varpi(x, y)\, dxdy + \lambda\, f(c_1, c_2)\, g(c_1, c_2),$$

where $\lambda > 0$, and (c_1, c_2) is a fixed point in $\mathbb{R}^2$.

Two cases are considered in [29]. The first one is the product of Laguerre weights for which

$$\langle f, g\rangle_S := \int_0^\infty \int_0^\infty \nabla f(x, y) \cdot \nabla g(x, y) w_\alpha(x)\, w_\beta(y) dxdy + \lambda_k f(0, 0)\, g(0, 0),$$

where $w_\alpha(x) = x^\alpha e^{-x}$, $\alpha > -1$. The Sobolev orthogonal polynomials are related to the polynomials $Q_{j,m}^{\alpha,\beta}(x, y)$ defined by

$$Q_{j,m}^{\alpha,\beta}(x, y) := Q_{m-j}^{\alpha}(x)\, Q_j^{\beta}(y) \quad \text{with} \quad Q_n^{\alpha}(x) := \hat{L}_n^{(\alpha)}(x) + n\, \hat{L}_{n-1}^{(\alpha)}(x),$$

where $\hat{L}_n^{(\alpha)}(x)$ denotes the nth monic Laguerre polynomial. The polynomial $Q_n^{\alpha}(x)$ is monic and satisfies $\frac{d}{dx} Q_n^{\alpha}(x) = n\, \hat{L}_{n-1}^{(\alpha)}(x)$. For $0 \le k \le n$, let $S_{n-k,k}^{\alpha,\beta}(x, y) = x^{n-k} y^k + \cdots$ be the monic Sobolev orthogonal polynomial of degree n. Define the column vectors

$$\mathbb{Q}_n^{\alpha,\beta} := (Q_{0,n}^{\alpha,\beta}, \ldots, Q_{n,n}^{\alpha,\beta})^t \quad \text{and} \quad \mathbb{S}_n^{\alpha,\beta} := (S_{0,n}^{\alpha,\beta}, \ldots, S_{n,n}^{\alpha,\beta})^t.$$

It was shown in [29] that there is a matrix B_{n-1} such that

$$\mathbb{Q}_n^{\alpha,\beta} = \mathbb{S}_n^{\alpha,\beta} + B_{n-1} \mathbb{S}_{n-1}^{\alpha,\beta}.$$

Notice that the matrix B_{n-1} and the norm $\langle \mathbb{S}_n^{\alpha,\beta}, \mathbb{S}_n^{\alpha,\beta}\rangle_S$ can both be computed by one recursive algorithm.

The above construction of orthogonal bases for the product domain works if w_1 and w_2 are self-coherent, that is, are classical weights (Jacobi, Laguerre, Hermite). The case when both are Gegenbauer weight functions was given as a second example in [29].

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