

Chapter 2

Some Applications of the Sheffer A-Type 0 Orthogonal Polynomial Sequences

In this chapter, we address several of the many applications of the classical orthogonal polynomial sequences. These applications include first-order differential equations that characterize linear generating functions, additional first-order differential equations, second-order differential equations (with applications to quantum mechanics), difference equations and numerical integration (Gaussian Quadrature). We first develop each of these applications in a general context and then cover examples using specific Sheffer Sequences, i.e. the Laguerre, Hermite, Charlier, Meixner, Meixner–Pollaczek, and Krawtchouk polynomials.

2.1 Preliminaries

Throughout this chapter, we make use of each of the following definitions, terminologies and notations.

Definition 2.1. We always assume that a *set* of polynomials $\{P_n(x)\}_{n=0}^{\infty}$ is such that each $P_n(x)$ has degree exactly n , which we write as $\deg(P_n(x)) = n$.

Definition 2.2. A set of polynomials $\{Q_n(x)\}_{n=0}^{\infty}$ is *monic* if $Q_n(x) - x^n$ is of degree at most $n - 1$ or equivalently if the leading coefficient of each $Q_n(x)$ is unitary.

Definition 2.3. The set of polynomials $\{P_n(x)\}_{n=0}^{\infty}$ is *orthogonal* if it satisfies one of the two weighted inner products below:

$$\text{Continuous : } \langle P_m(x), P_n(x) \rangle = \int_{\Omega_1} P_m(x)P_n(x)w(x)dx = \alpha_n \delta_{m,n}, \quad (2.1)$$

$$\text{Discrete : } \langle P_m(x), P_n(x) \rangle = \sum_{\Omega_2} P_m(x)P_n(x)w(x) = \beta_n \delta_{m,n}, \quad (2.2)$$

where $\delta_{m,n}$ denotes the *Kronecker delta*

$$\delta_{m,n} := \begin{cases} 1 & \text{if } m = n \\ 0 & \text{if } m \neq n, \end{cases}$$

with $\Omega_1 \subseteq \mathbb{R}$, $\Omega_2 \subseteq \{0, 1, 2, \dots\}$, and $w(x) > 0$ is entitled the *weight function*. We also always assume the following *normalizations*:

$$\int_{\Omega_1} w(x) dx = 1 \quad \text{and} \quad \sum_{\Omega_2} w(x) = 1.$$

Definition 2.4 (The Three-Term Recurrence Relations). It is a necessary and sufficient condition that an orthogonal polynomial sequence $\{P_n(x)\}_{n=0}^{\infty}$ satisfies an *unrestricted three-term recurrence relation* of the form

$$P_{n+1}(x) = (A_n x + B_n)P_n(x) - C_n P_{n-1}(x), \quad A_n A_{n-1} C_n > 0, \\ \text{where } P_{-1}(x) = 0 \text{ and } P_0(x) = 1. \quad (2.3)$$

If $Q_n(x)$ represents the monic form of $P_n(x)$, then it is a necessary and sufficient condition that $\{Q_n(x)\}_{n=0}^{\infty}$ satisfies the following *monic three-term recurrence relation*

$$Q_{n+1}(x) = (x - b_n)Q_n(x) - c_n Q_{n-1}(x), \quad c_n > 0, \\ \text{where } Q_{-1}(x) = 0 \text{ and } Q_0(x) = 1. \quad (2.4)$$

We entitle the conditions $A_n A_{n-1} C_n > 0$ and $c_n > 0$ above *positivity conditions*.

Definition 2.5. We shall define a *generating function* for a polynomial sequence $\{P_n(x)\}_{n=0}^{\infty}$ as follows:

$$\sum_{\Lambda} \zeta_n P_n(x) t^n = F(x, t),$$

with $\Lambda \subseteq \{0, 1, 2, \dots\}$ and $\{\zeta_n\}_{n=0}^{\infty}$ a sequence in n that is independent of x and t . Moreover, we say that the function $F(x, t)$ *generates* the set $\{P_n(x)\}_{n=0}^{\infty}$.

Before we give our next definition, we discuss that in 1939 Sheffer [22] developed a characterization theorem that gave necessary and sufficient conditions for a polynomial sequence to be *A-Type 0* via a linear generating function. Originally, in 1934, J. Meixner published [15], wherein he essentially determined which orthogonal sets satisfy the aforementioned *A-Type 0* generating function using a different approach than Sheffer. Meixner basically used the *A-Type 0* generating function as the *definition* of the *A-Type 0* class. In this chapter, we follow Meixner's convention. We mention that the interested reader can also refer to [1] for a concise overview of Meixner's analysis.

Definition 2.6. A polynomial set $\{P_n(x)\}_{n=0}^{\infty}$ is classified as *A-Type 0* if $\{a_j\}_{j=0}^{\infty}$ and $\{h_j\}_{j=1}^{\infty}$ exist such that

$$A(t)e^{xH(t)} = \sum_{n=0}^{\infty} P_n(x)t^n,$$

$$A(t) := \sum_{n=0}^{\infty} a_n t^n, \quad a_0 = 1 \quad \text{and} \quad H(t) := \sum_{n=1}^{\infty} h_n t^n, \quad h_1 = 1.$$

The orthogonal sets that satisfy Definition 2.6, which are often simply called the *Sheffer Sequences*, are listed below as defined by their *A-Type 0* generating function.

The Laguerre Polynomials $\{L_n^{(\alpha)}(x)\}_{n=0}^{\infty}$

$$\sum_{n=0}^{\infty} L_n^{(\alpha)}(x)t^n = (1-t)^{-(\alpha+1)} \exp\left(\frac{xt}{t-1}\right).$$

The Hermite Polynomials $\{H_n(x)\}_{n=0}^{\infty}$

$$\sum_{n=0}^{\infty} \frac{1}{n!} H_n(x)t^n = \exp(2xt - t^2).$$

The Charlier Polynomials $\{C_n(x; a)\}_{n=0}^{\infty}$

$$\sum_{n=0}^{\infty} \frac{1}{n!} C_n(x; a)t^n = e^t \left(1 - \frac{t}{a}\right)^x.$$

The Meixner Polynomials $\{M(x; \beta, c)\}_{n=0}^{\infty}$

$$\sum_{n=0}^{\infty} \frac{(\beta)_n}{n!} M(x; \beta, c)t^n = \left(1 - \frac{t}{c}\right)^x (1-t)^{-(x+\beta)}.$$

The Meixner–Pollaczek Polynomials $\{P_n^{(\lambda)}(x; \phi)\}_{n=0}^{\infty}$

$$\sum_{n=0}^{\infty} P_n^{(\lambda)}(x; \phi)t^n = (1 - e^{i\phi}t)^{-\lambda+ix} (1 - e^{-i\phi}t)^{-\lambda-ix}.$$

The Krawtchouk Polynomials $\{K_n(x; p, N)\}_{n=0}^{\infty}$

$$\sum_{n=0}^N C(N, n) K_n(x; p, N)t^n = \left(1 - \frac{1-p}{p}t\right)^x (1+t)^{N-x},$$

for $x = 0, 1, 2, \dots, N$, where $C(N, n)$ denotes the binomial coefficient.

Example 2.1. We see that we can write the generating function for the Krawtchouk polynomials as

$$\sum_{n=0}^{\infty} \frac{1}{n!} K_n(x; p, N) t^n = (1+t)^N \exp \left(x \ln \left(\frac{(p-1)t+p}{p(1+t)} \right) \right)$$

from which $A(t)$ and $H(t)$ can be readily identified. Similar trivial manipulations can be made to the generating functions of the remaining five orthogonal sets to obtain the form $A(t) \exp(xH(t))$.

Now that both orthogonality and the Sheffer Sequences have been defined, we address the fact that the Laguerre, Hermite, and Meixner–Pollaczek polynomials satisfy a continuous orthogonality relation of the form (2.1), and the Charlier, Meixner, and Krawtchouk polynomials satisfy a discrete orthogonality relation of the form (2.2). For more information refer to [11] and the references therein.

Definition 2.7. We can express each of our polynomials in the *generalized hypergeometric form* $({}_rF_s)$ as seen below:

$${}_rF_s \left(\begin{matrix} a_1, \dots, a_r \\ b_1, \dots, b_s \end{matrix} \middle| z \right) = \sum_{k=0}^{\infty} \frac{(a_1, \dots, a_r)_k z^k}{(b_1, \dots, b_s)_k k!}, \quad (2.5)$$

where the *Pochhammer symbol* $(a)_k$ is defined as

$$(a)_k := a(a+1)(a+2) \cdots (a+k-1), \quad (a)_0 := 1 \quad (2.6)$$

and

$$(a_1, \dots, a_j)_k := (a_1)_k \cdots (a_j)_k.$$

The sum (2.5) terminates if one of the numerator parameters is a negative integer, e.g., if one such parameter is $-n$, then (2.5) is a finite sum on $0 \leq k \leq n$.

2.2 Differential Equations Part I: The “Inverse Method”

In this section, we demonstrate how each of the *A-Type 0* generating functions satisfy a first-order differential equation. We entitle our approach for deriving these differential equations “*the inverse method*” because of the connection our approach has to inverse problems. That is, in the study of orthogonal polynomials, the term *inverse problem* refers to the problem of obtaining the weight function of an orthogonal set by using only the corresponding recursion coefficients. For inverse problems, the generating function that is obtained via a differential equation can be viewed as a by-product. For additional examples of inverse problems, consider Chap. 5 of [12] and the references therein.

To begin, we assume that $\{P_n(x)\}_{n=0}^{\infty}$ is a polynomial set that satisfies an unrestricted three-term recurrence relation of the form (2.3). We first multiply this relation by $c_n t^n$, where c_n is a function in n that is independent of x and t ,

and sum for $n = 0, 1, 2, \dots$. Then, from the assignment $F(t; x) := \sum_{n=0}^{\infty} c_n P_n(x) t^n$, we obtain a first-order differential equation in t with x regarded as a parameter. The initial condition for this equation is $F(0; x) = 1$ via the initial condition $P_0(x) = 1$ in (2.3). The existence and uniqueness of the solution to this differential equation is ensured and the solution $F(t; x)$ will be a generating function for the set $\{P_n(x)\}_{n=0}^{\infty}$. To demonstrate the procedure, we work out all of the details for the Charlier and Laguerre polynomials and sketch the details for the Miexner–Pollaczek polynomials.

Example 2.2. To begin, we note that from examining the generating function of the Charlier polynomials, c_n as described above must be $1/n!$. The three-term recurrence relation for the Charlier polynomials can be written as

$$-x C_n(x; a) = a C_{n+1}(x; a) - (n + a) C_n(x; a) + n C_{n-1}(x; a).$$

Thus, we multiply both sides of this relation by $t^n/n!$ and sum the result for $n = 0, 1, 2, \dots$:

$$\begin{aligned} -x \sum_{n=0}^{\infty} \frac{C_n(x; a)}{n!} t^n &= a \sum_{n=0}^{\infty} \frac{C_{n+1}(x; a)}{n!} t^n - \sum_{n=1}^{\infty} \frac{C_n(x; a)}{(n-1)!} t^n \\ &\quad - a \sum_{n=0}^{\infty} \frac{C_n(x; a)}{n!} t^n + \sum_{n=1}^{\infty} \frac{C_{n-1}(x; a)}{(n-1)!} t^n. \end{aligned}$$

Next, we define $F := F(t; x, a) := \sum_{n=0}^{\infty} \frac{C_n(x; a)}{n!} t^n$ and it therefore follows that

$$\dot{F} := \frac{\partial}{\partial t} F(t; x, a) = \sum_{n=1}^{\infty} \frac{C_n(x; a)}{(n-1)!} t^{n-1}.$$

Then, we see that our relation becomes

$$\dot{F} - \left(1 + \frac{x}{t-a}\right) F = 0,$$

which is a first-order differential equation with initial condition $F(0; x, a) = 1$. A general solution is

$$F(t; x, a) = c(x; a) e^t (a-t)^x,$$

where $c(x; a)$ is an arbitrary function of x . From the initial condition, it is immediate that $c(x; a) = a^{-x}$ and thus, the unique solution turns out to be

$$F(t; x, a) = \sum_{n=0}^{\infty} \frac{C_n(x; a)}{n!} t^n = e^t \left(1 - \frac{t}{a}\right)^x,$$

which is the Sheffer *A-Type 0* generating function for the Charlier polynomials.

Example 2.3. We next consider the Laguerre polynomials, which have the following unrestricted three-term recurrence relation:

$$(n+1)L_{n+1}^{(\alpha)}(x) - (2n + \alpha + 1 - x)L_n^{(\alpha)}(x) + (n + \alpha)L_{n-1}^{(\alpha)}(x) = 0.$$

We multiply both sides of this relation by t^n ($c_n \equiv 1$) and sum for $n = 0, 1, 2, \dots$, which yields

$$\begin{aligned} \sum_{n=0}^{\infty} (n+1)L_{n+1}^{(\alpha)}(x)t^n - 2 \sum_{n=1}^{\infty} nL_n^{(\alpha)}(x)t^n - (\alpha + 1 - x) \sum_{n=0}^{\infty} L_n^{(\alpha)}(x)t^n \\ + \sum_{n=1}^{\infty} nL_{n-1}^{(\alpha)}(x)t^n + \alpha \sum_{n=0}^{\infty} L_{n-1}^{(\alpha)}(x)t^n = 0. \end{aligned}$$

We next assign $G := G(t; x) := \sum_{n=0}^{\infty} L_n^{(\alpha)}(x)t^n$ and recall that $L_{-1}^{(\alpha)}(x) = 0$, which gives

$$\dot{G} - 2t\dot{G} - (\alpha + 1 - x)G + \sum_{n=2}^{\infty} nL_{n-1}^{(\alpha)}(x)t^n + \alpha tG = 0.$$

We also observe that

$$\sum_{n=1}^{\infty} nL_{n-1}^{(\alpha)}(x)t^n = \sum_{n=2}^{\infty} (n-1)L_{n-1}^{(\alpha)}(x)t^n + \sum_{n=1}^{\infty} L_{n-1}^{(\alpha)}(x)t^n = t^2\dot{G} + tG.$$

Using all of this, we can put our relation into standard form:

$$\dot{G} + \left[\frac{x + (\alpha + 1)(t - 1)}{1 - 2t + t^2} \right] G = 0; \quad G(0; x) = 1.$$

The integrating factor in this equation turns out to be $\mu = \exp \left[\int \frac{x + (\alpha + 1)(t - 1)}{1 - 2t + t^2} dt \right]$ and through partial fraction decomposition, we obtain the general solution

$$G(t; x) = c(x, \alpha)(t - 1)^{-(\alpha + 1)} \exp \left(\frac{x}{t - 1} \right).$$

Therefore, from using our initial condition to determine $c(x, \alpha)$, we establish the solution

$$G(t; x) = \sum_{n=0}^{\infty} L_n^{(\alpha)}(x)t^n = (t - 1)^{-(\alpha + 1)} \exp \left(\frac{xt}{t - 1} \right),$$

which is the Sheffer A-Type 0 generating function for the Laguerre polynomials.

Example 2.4. For a more detailed example, we now consider the Meixner–Pollaczek polynomials. These polynomials have the unrestricted three-term recurrence relation

$$(n+1)P_{n+1}^{(\lambda)}(x; \phi) - 2[x \sin \phi + (n + \lambda) \cos \phi]P_n^{(\lambda)}(x; \phi) + (n + 2\lambda - 1)P_{n-1}^{(\lambda)}(x; \phi) = 0.$$

We then multiply this relation by t^n , take $c_n \equiv 1$ and sum for $n = 0, 1, 2, \dots$. From letting $H := H(t; x, \lambda, \phi) := \sum_{n=0}^{\infty} P_n^{(\lambda)}(x; \phi)t^n$ we achieve the differential equation

$$\dot{H} + 2 \left(\frac{\lambda(t - \cos \phi) - x \sin \phi}{1 - 2 \cos \phi t + t^2} \right) H = 0; \quad H(0; x, \lambda, \phi) = 1.$$

The solution to this equation can be obtained by partial fraction decomposition, and several manipulations, to be

$$H(t; x, \lambda, \phi) = \sum_{n=0}^{\infty} P_n^{(\lambda)}(x; \phi)t^n = (1 - e^{i\phi}t)^{-\lambda + ix} (1 - e^{-i\phi}t)^{-\lambda - ix}.$$

2.3 Differential Equations Part II

We now discuss some additional characterizations of classical orthogonal sets via differential equations. These results lead to a way to solve the time-independent Schrödinger equation. Through our development of each characterization, additional results, definitions and concepts are addressed, which are important unto themselves. We also supplement our characterizations by covering specific details for the Laguerre polynomials and discuss how similar results can be achieved for other *A-Type 0* sets. This section is based on much of the analysis conducted in [3–5, 7, 9, 16, 21, 23]. We begin with an important fundamental condition.

Lemma 2.1. An Equivalent Orthogonality Condition: *The set $\{P_n(x)\}_{n=0}^{\infty}$ is orthogonal with respect to the weight function $w(x) > 0$ on Ω_1 if and only if*

$$\int_{\Omega_1} x^j P_n(x) w(x) dx = 0, \quad \forall j = 0, 1, 2, \dots, n-1. \quad (2.7)$$

Proof. (\Rightarrow) Assume (2.7) holds. It is clear that there exist constants $\{\eta_{m,j}\}$ such that

$$P_m(x) = \sum_{j=0}^m \eta_{m,j} x^j.$$

We first assume that $m < n$, in which case we have

$$\int_{\Omega_1} P_m(x) P_n(x) w(x) dx = \sum_{j=0}^m \eta_{m,j} \int_{\Omega_1} x^j P_n(x) w(x) dx = 0,$$

because $j \leq m < n$. If $m > n$, we can simply interchange m with n in the logic used above. Hence, we have shown that given (2.7) it necessarily follows that

$$\int_{\Omega_1} P_m(x)P_n(x)w(x)dx = 0, \text{ for } m \neq n,$$

and therefore $\{P_n(x)\}_{n=0}^{\infty}$ is an orthogonal set with respect to the weight function $w(x) > 0$ on Ω_1 .

(\Leftarrow) Assume the orthogonality relation directly above is true. Then, there exist constants $\{\tilde{\eta}_{m,j}\}$ such that

$$x^j = \sum_{m=0}^j \tilde{\eta}_{m,j} P_m(x).$$

Therefore, for every $j \in \{0, 1, \dots, n-1\}$, we know that

$$\int_{\Omega_1} x^j P_n(x)w(x)dx = \sum_{m=0}^j \tilde{\eta}_{m,j} \int_{\Omega_1} P_m(x)P_n(x)w(x)dx = 0,$$

because $m \leq j < n$, i.e., since $m \neq n$. □

We will also need the following result.

Lemma 2.2. *With α_n as in (2.1) and c_n as in (2.4), we have*

$$\alpha_n = \prod_{k=1}^n c_k.$$

Proof. We first multiply both sides of (2.4) by $P_{n-1}(x)w(x)$ and integrate over Ω_1 , leading to

$$\begin{aligned} \int_{\Omega_1} P_{n+1}(x)P_{n-1}(x)w(x)dx &= \int_{\Omega_1} xP_n(x)P_{n-1}(x)w(x)dx \\ &\quad - b_n \int_{\Omega_1} P_n(x)P_{n-1}(x)w(x)dx \\ &\quad - c_n \int_{\Omega_1} P_{n-1}(x)P_{n-1}(x)w(x)dx. \end{aligned}$$

From the orthogonality relation (2.1), we observe that our relation directly above becomes

$$c_n \alpha_{n-1} = \int_{\Omega_1} xP_n(x)P_{n-1}(x)w(x)dx.$$

Since our polynomial sequence $\{P_n(x)\}_{n=0}^{\infty}$ is monic, we have

$$\begin{aligned}
c_n \alpha_{n-1} &= \int_{\Omega_1} P_n(x) (P_n(x) + \mathcal{O}(x^{n-1})) w(x) dx \\
&= \int_{\Omega_1} P_n^2(x) w(x) dx \\
&= \alpha_n,
\end{aligned}$$

which follows from Lemma 2.1 and (2.1). Thus, by iterating $c_n \alpha_{n-1} = \alpha_n$, with $\alpha_0 = 1$ via the normalization in Definition 2.3, we obtain our result. \square

Theorem 2.1 (The Christoffel–Darboux Identity). *For $N > 0$ we have*

$$\sum_{k=0}^{N-1} \frac{1}{\alpha_k} P_k(x) P_k(y) = \frac{P_N(x) P_{N-1}(y) - P_N(y) P_{N-1}(x)}{\alpha_{N-1}(x-y)}. \quad (2.8)$$

Proof. After replacing $Q_n(x)$ with $P_n(x)$ in (2.4), we multiply both sides of the resulting relation by $P_n(y)$, leading to

$$P_{n+1}(x) P_n(y) = x P_n(x) P_n(y) - b_n P_n(x) P_n(y) - c_n P_{n-1}(x) P_n(y). \quad (2.9)$$

We then exchange x with y in (2.9) and subtract this result from (2.9), which gives

$$\begin{aligned}
&P_{n+1}(x) P_n(y) - P_{n+1}(y) P_n(x) \\
&= (x-y) P_n(x) P_n(y) + c_n (P_n(x) P_{n-1}(y) - P_n(y) P_{n-1}(x)). \quad (2.10)
\end{aligned}$$

We then define the following operator:

$$\Delta_k^{x,y} := P_k(x) P_{k-1}(y) - P_k(y) P_{k-1}(x)$$

and we see that (2.10) becomes

$$(x-y) P_n(x) P_n(y) = \Delta_{n+1}^{x,y} - c_n \Delta_n^{x,y}.$$

Lastly, we divide both sides of the equation above by α_n and utilize Lemma 2.2, which yields

$$\frac{1}{\alpha_n} P_n(x) P_n(y) = \frac{1}{x-y} \left[\frac{1}{\alpha_n} \Delta_{n+1}^{x,y} - \frac{1}{\alpha_{n-1}} \Delta_n^{x,y} \right].$$

Summing both sides of this identity from 0 to $N-1$, we see that the right-hand side becomes a telescoping series that converges to the right-hand side of (2.8). \square

The limiting case $y \rightarrow x$ of (2.8) is readily achieved via L'Hôpital's Rule to be

$$\sum_{k=0}^{N-1} \frac{1}{\alpha_k} P_k^2(x) = \frac{P'_N(x) P_{N-1}(x) - P_N(x) P'_{N-1}(x)}{\alpha_{N-1}}. \quad (2.11)$$

The Christoffel–Darboux Identity has many general usages and will be needed throughout this chapter.

We next write $w(x)$ as in (2.1) as

$$w(x) = \exp(-v(x)), \quad (2.12)$$

where $v = v(x)$ is a twice continuously differentiable function on Ω_1 . For this section, we also use the *orthonormal* form $\{p_n(x)\}_{n=0}^\infty$ of $\{P_n(x)\}_{n=0}^\infty$. This definition is as follows.

Definition 2.8 (Orthonormality). It is a necessary and sufficient condition that an orthogonal polynomial sequence $\{p_n(x)\}_{n=0}^\infty$ satisfies an *orthonormal three-term recurrence relation* of the form

$$\begin{aligned} xp_n(x) &= a_{n+1}p_{n+1}(x) + b_np_n(x) + a_np_{n-1}(x), \\ \text{where } p_{-1}(x) &= 0 \text{ and } p_0(x) = 1. \end{aligned} \quad (2.13)$$

For c_n as in (2.4) we have (see [9]):

$$a_n = \sqrt{c_n}. \quad (2.14)$$

Therefore, we can of course equivalently write (2.13) as

$$xp_n(x) = \sqrt{c_{n+1}}p_{n+1}(x) + b_np_n(x) + \sqrt{c_n}p_{n-1}(x).$$

The orthonormal form $p_n(x)$ can be expressed in terms of $P_n(x)$ by

$$p_n(x) = \frac{1}{\sqrt{\alpha_n}}P_n(x). \quad (2.15)$$

This leads to the (continuous) *orthonormal relation*

$$\langle p_m(x), p_n(x) \rangle = \int_{\Omega_1} p_m(x)p_n(x)w(x)dx = \delta_{m,n}.$$

Remark 2.1. We do not call upon a discrete orthonormal relation in this section.

We now have the following.

Theorem 2.2. *If $v(x)$ is as defined in (2.12) and $\{p_n(x)\}_{n=0}^\infty$ is an orthonormal set as defined by Definition 2.8, then $p_n(x)$ satisfies the differential equation*

$$p'_n(x) = -B_n(x)p_n(x) + A_n(x)p_{n-1}(x), \quad (2.16)$$

with $A_n(x)$ and $B_n(x)$ as defined as

$$A_n(x) = a_n \left(\frac{p_n^2(y)w(y)}{y-x} \Big|_{\Omega_1} + \int_{\Omega_1} \frac{v'(x) - v'(y)}{x-y} p_n^2(y)w(y)dy \right), \quad (2.17)$$

$$B_n(x) = a_n \left(\frac{p_n(y)p_{n-1}(y)w(y)}{y-x} \Big|_{\Omega_1} + \int_{\Omega_1} \frac{v'(x) - v'(y)}{x-y} p_n(y)p_{n-1}(y)w(y)dy \right), \quad (2.18)$$

when the above integrals and boundary terms exist.

Proof. Since $\deg(p'_n(x)) = n - 1$, there exist constants $\{c_{n,k}\}$ such that

$$p'_n(x) = \sum_{k=0}^{n-1} c_{n,k} p_k(x). \quad (2.19)$$

We then multiply both sides of (2.19) by $p_m(x)w(x)$ and integrate over Ω_1 :

$$\int_{\Omega_1} p'_n(x)p_m(x)w(x)dx = \sum_{k=0}^{n-1} c_{n,k} \int_{\Omega_1} p_k(x)p_m(x)w(x)dx.$$

We then observe that the right-hand side is nonzero if and only if $m = k$, in which case we have

$$c_{n,k} = \int_{\Omega_1} p'_n(y)p_k(y)w(y)dy$$

after changing our integration variable to y . Then, using integration by parts (with the substitution $u = p_k(y)w(y)$), we obtain

$$\begin{aligned} c_{n,k} &= \int_{\Omega_1} p'_n(y)p_k(y)w(y)dy = p_n(y)p_k(y)w(y)|_{\Omega_1} \\ &\quad - \int_{\Omega_1} p_n(y) (p_k(y)w'(y) + p'_k(y)w(y)) dy. \end{aligned}$$

Via (2.12) we have $w'(y) = -v'(y)w(y)$ and therefore

$$c_{n,k} = p_n(y)p_k(y)w(y)|_{\Omega_1} - \int_{\Omega_1} p_n(y) (p'_k(y) - p_k(y)v'(y)) w(y)dy.$$

From Lemma 2.1, the integral with the $p'_k(y)$ -term is zero. This finally gives us

$$c_{n,k} = p_n(y)p_k(y)w(y)|_{\Omega_1} + \int_{\Omega_1} p_n(y)p_k(y)v'(y)w(y)dy.$$

From substituting this into (2.19) we have

$$p'_n(x) = w(y)p_n(y) \sum_{k=0}^{n-1} p_k(x)p_k(y) \Big|_{\Omega_1} + \int_{\Omega_1} p_n(y) \left(\sum_{k=0}^{n-1} p_k(x)p_k(y) \right) v'(y)w(y)dy.$$

Now notice, via Lemma 2.1, that the integral directly above is zero if $v'(y)$ is replaced by $v'(x)$. Thus, we can replace $v'(y)$ with $v'(y) - v'(x)$, in which case we see that

$$p'_n(x) = w(y)p_n(y) \sum_{k=0}^{n-1} p_k(x)p_k(y) \Big|_{\Omega_1} + \int_{\Omega_1} p_n(y) \left(\sum_{k=0}^{n-1} p_k(x)p_k(y) \right) (v'(y) - v'(x)) w(y)dy.$$

Next, via (2.15), we take $P_n(x) = \sqrt{\alpha_n}p_n(x)$ and use the Christoffel–Darboux Identity (Theorem 2.1) to evaluate each of the sums in the above equation. With some manipulations, we obtain (2.16). \square

Our next result relates $A(x)$ and $B(x)$ as in Theorem 2.2 and also plays a key role in our application to quantum mechanics.

Lemma 2.3. *The coefficients $A_n(x)$ and $B_n(x)$, as respectively defined in (2.17) and (2.18), satisfy the relation*

$$B_n(x) + B_{n+1}(x) = \frac{x - b_n}{a_n} A_n(x) - v'(x),$$

with $w(x)$ as defined in (2.12) and $w(x)$ vanishing at the boundary points of Ω_1 .

Proof. Assuming that $w(x)$ vanishes at the boundary points of Ω_1 , from (2.18) we have

$$B_n(x) + B_{n+1}(x) = a_n \int_{\Omega_1} \frac{v'(x) - v'(y)}{x - y} p_n(y)p_{n-1}(y)w(y)dy + a_{n+1} \int_{\Omega_1} \frac{v'(x) - v'(y)}{x - y} p_{n+1}(y)p_n(y)w(y)dy, \quad (2.20)$$

which can be written as

$$B_n(x) + B_{n+1}(x) = \int_{\Omega_1} p_n(y) \frac{v'(x) - v'(y)}{x - y} (a_{n+1}p_{n+1}(y) + a_n p_{n-1}(y)) w(y)dy. \quad (2.21)$$

From (2.13), it follows that $a_{n+1}p_{n+1}(y) + a_n p_{n-1}(y) = (y - b_n)p_n(y)$ and we therefore obtain

$$B_n(x) + B_{n+1}(x) = \int_{\Omega_1} \frac{v'(x) - v'(y)}{x - y} (y - b_n) p_n^2(y) w(y) dy. \quad (2.22)$$

We then take $y - b_n = (y - x) + (x - b_n)$ and see that the above integral becomes

$$\begin{aligned} & (x - b_n) \int_{\Omega_1} \frac{v'(x) - v'(y)}{x - y} p_n^2(y) w(y) dy - \int_{\Omega_1} (v'(x) - v'(y)) p_n^2(y) w(y) dy \\ &= (x - b_n) \frac{A_n(x)}{a_n} + \int_{\Omega_1} v'(y) p_n^2(y) w(y) dy - v'(x) \int_{\Omega_1} p_n^2(y) w(y) dy \\ &= \frac{x - b_n}{a_n} A_n(x) + \int_{\Omega_1} v'(y) p_n^2(y) w(y) dy - v'(x), \end{aligned}$$

where we have used (2.17) and the orthonormality of $\{p_n(x)\}_{n=0}^{\infty}$. From using integration by parts (with the substitution $u = v'(x)$) and orthonormality, we see that

$$\int_{\Omega_1} v'(y) p_n^2(y) w(y) dy = v'(x) \Big|_{\Omega_1} - \int_{\Omega_1} v''(y) dy = 0.$$

Hence, we have

$$B_n(x) + B_{n+1}(x) = \frac{x - b_n}{a_n} A_n(x) - v'(x). \quad \square$$

Theorem 2.3. *If $w(x)$ is as defined in (2.12) and $\{p_n(x)\}_{n=0}^{\infty}$ is an orthonormal set as defined by Definition 2.8, then $\{p_n(x)\}_{n=0}^{\infty}$ satisfies the (factored) second-order differential equation*

$$L_x^{2,n} \left(\frac{L_x^{1,n} p_n(x)}{A_n(x)} \right) = \frac{a_n}{a_{n-1}} A_{n-1}(x) p_n(x), \quad (2.23)$$

with the differential operators $L_x^{1,n}$ and $L_x^{2,n}$ defined as

$$L_x^{1,n} := \frac{d}{dx} + B_n(x) \quad (2.24)$$

$$L_x^{2,n} := -\frac{d}{dx} + B_n(x) + v'(x). \quad (2.25)$$

Proof. In light of (2.24), we can write (2.16) as

$$L_x^{1,n} p_n(x) = A_n(x) p_{n-1}(x). \quad (2.26)$$

Next, we define the weighted inner product

$$\langle p_m(x), p_n(x) \rangle_w := \int_{\Omega_1} p_m(x) p_n(x) w(x) dx$$

and utilize the *Hilbert Space* where the $\langle p_n, p_n \rangle_w$ is finite and $p_n(x)\sqrt{w(x)}$ is zero at the end points of Ω_1 (finite or infinite). Thus, $L_x^{2,n} = (L_x^{1,n})^*$.

Using (2.16) and (2.13) leads to the *adjoint* equation

$$\left(-\frac{d}{dx} + B_n(x) + v'(x)\right) p_{n-1}(x) = \frac{a_n}{a_{n-1}} A_{n-1}(x) p_n(x). \quad (2.27)$$

Thus, we can use (2.26) to readily obtain

$$\frac{L_x^{1,n} p_n(x)}{A_n(x)} = p_{n-1}(x)$$

and with (2.25) we can rewrite (2.27) as

$$L_x^{2,n} \left(\frac{L_x^{1,n} p_n(x)}{A_n(x)} \right) = \frac{a_n}{a_{n-1}} A_{n-1}(x) p_n(x)$$

and the theorem is established. \square

We additionally have an equivalent form for (2.23), which also emphasizes the fact that it is a second-order equation.

Corollary 2.1. *The differential equation (2.23) can equivalently be expressed as*

$$p_n''(x) + C_n(x)p_n'(x) + D_n(x)p_n(x) = 0, \quad (2.28)$$

where

$$C_n(x) := -v'(x) - \frac{A_n'(x)}{A_n(x)}, \quad (2.29)$$

$$D_n(x) := A_n(x) \frac{d}{dx} \left(\frac{B_n(x)}{A_n(x)} \right) - B_n(x) (v'(x) + B_n(x)) + \frac{a_n}{a_{n-1}} A_n(x) A_{n-1}(x). \quad (2.30)$$

Proof. By expanding the left-hand side of (2.23) and using some manipulations, we achieve (2.28). \square

Remark 2.2. We see that (2.24) is in fact a degree-lowering operator analogous to the ones used in Sheffer's analysis [22]. In contrast, we also note that (2.25) is a *degree-raising operator* or equivalently, a *ladder operator*. What has been shown through Corollary 2.1 is that every classical orthogonal polynomial sequence (written in orthonormal form) is a solution to a second-order linear differential equation or equivalently possesses a degree-raising operator.

In addition, classical orthogonal polynomials have an important connection to quantum mechanics via Theorem 2.3 (and Corollary 2.1). Namely, we can now show

that the solution to the time-independent Schrödinger equation can be expressed in terms of $\{p_n(x)\}_{n=0}^{\infty}$ if (2.23), or equivalently (2.28), is satisfied.

Theorem 2.4. *The second-order linear differential equation (2.23), or equivalently (2.28), can be written in the **Schrödinger form**:*

$$\Psi_n''(x) + V(x;n)\Psi_n(x) = 0, \quad (2.31)$$

where

$$\Psi_n(x) := \frac{\exp(-v(x)/2)}{\sqrt{A_n(x)}} p_n(x) \quad (2.32)$$

and

$$\begin{aligned} V(x;n) = & A_n(x) \frac{d}{dx} \left(\frac{B_n(x)}{A_n(x)} \right) - B_n(x) (v'(x) + B_n(x)) + \frac{a_n}{a_{n-1}} A_n(x) A_{n-1}(x) \\ & + \frac{1}{2} v''(x) + \frac{1}{2} \frac{d}{dx} \left(\frac{A_n'(x)}{A_n(x)} \right) - \frac{1}{4} \left(v'(x) + \frac{A_n'(x)}{A_n(x)} \right)^2. \end{aligned} \quad (2.33)$$

Proof. Substituting $\Psi_n(x)$ and $V(x;n)$ into the left-hand side of (2.31) and using manipulations, we see that the resulting expression vanishes. \square

In light of Theorem 2.4, we have the following discussion. For a particle confined to one dimension, the time-independent Schrödinger equation is written in the form

$$\psi''(x) + \frac{2m}{\hbar^2} (E - U(x))\psi(x) = 0, \quad (2.34)$$

where $\psi(x)$ represents the **wave function**, m the mass of a particle, $\hbar := h/(2\pi)$, where h is Planck's constant, E the total energy (constant), and $U(x)$ the potential energy. This equation is attributed to Erwin Schrödinger, who formulated it in late 1925 and published it in 1926, e.g., [18, 19]. We discuss this equation further.

To begin, the wave function $\psi(x)$ itself is not directly related to any actual physical phenomena. In addition, $\psi(x)$ may be a real- or complex-valued function. However, the square of its modulus (absolute magnitude) $|\psi(x)|^2$ when evaluated at a certain location in space is directly proportional to the **probability** of locating a particle in the same location. The quantity $|\psi(x)|^2$ is referred to as the **probability density**. In fact, from knowing $\psi(x)$ explicitly, the linear momentum, the energy, and other physical quantities of a particle can be inferred. We also mention that the entire field of quantum mechanics can basically be summarized as determining $\psi(x)$ for a given particle when its range of motion is restricted by potential fields.

The wave function $\psi(x)$ must adhere to certain physical restraints. One, since $|\psi(x)|^2$ is directly proportional to the probability, say \mathcal{P} , of locating a particle modeled by $\psi(x)$, it follows that the following must hold:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-\infty}^{\infty} \mathcal{P} dx = 1.$$

Intuitively, this means that if the particle exists, it must be somewhere in space. The above relation is a normalization. The probability that the particle will be discovered in a certain region of space, say $[a, b] \subseteq \mathbb{R}$, is then given by

$$\mathcal{P}_{[a,b]} := \int_a^b |\psi(x)|^2 dx \in [0, 1].$$

Now that the wave function $\psi(x)$ is better understood, we can discuss our equation at hand. By letting $V(x) := E - U(x)$ we can of course equivalently write (2.34) as

$$\psi''(x) + \frac{2m}{\hbar} V(x)\psi(x) = 0.$$

From this relation, it is clear why (2.31) is named as such. Moreover, in essence, the time-independent Schrödinger equation describes how the wave function evolves over space. Our relation (2.34), and therefore (2.31), is useful in many physical situations when the potential energy of a particle does not depend upon time.

To complete our discussion, it is noteworthy to mention that the time-dependent Schrödinger equation can be written as

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + U(x)\psi(x, t).$$

Furthermore, Schrödinger basically established his equation(s) based on thought experiments. In regard to his development, Richard Feynman said:

Where did we get that equation from? Nowhere. It is not possible to derive it from anything you know. It came out of the mind of Schrödinger.

For more details related to the Schrödinger equations and quantum mechanics, refer to [6, 20].

Next, we have another relationship between $A_n(x)$ and $B_n(x)$, which we use specifically in Example 2.1.

Theorem 2.5. *The coefficients $A_n(x)$ and $B_n(x)$ as respectively in (2.17) and (2.18) satisfy*

$$B_{n+1}(x) - B_n(x) = \frac{a_{n+1}A_{n+1}(x)}{x - b_n} - \frac{a_n^2 A_{n-1}(x)}{a_{n-1}(x - b_n)} - \frac{1}{x - b_n}. \quad (2.35)$$

Proof. Refer to [14]. □

We note that (2.35) is referred to as the *string equation*.

We use the following fundamental *special function* in what follows.

Definition 2.9. The *gamma function*, $\Gamma(z)$, is defined as

$$\Gamma(z) := \int_0^\infty \tau^{z-1} e^{-\tau} d\tau, \quad \operatorname{Re}(z) > 0.$$

Also, $\Gamma(z)$ satisfies the functional equation

$$\Gamma(z+1) = z\Gamma(z), \quad (2.36)$$

which in fact extends $\Gamma(z)$ to a meromorphic function with poles at all of the non-positive integers. See Chap. 2 of [17] for an extensive development of the gamma function.

From (2.36) and (2.6), we see that

$$(c)_n = \frac{\Gamma(c+n)}{\Gamma(c)}. \quad (2.37)$$

Example 2.5. We now discuss the details of how a particular Sheffer *A-Type 0* orthogonal set solves the Schrödinger Form (2.31). We first note that each classical orthogonal set yields a unique set of functions $\{A_n(x), B_n(x)\}$, which are of course dependent on the polynomials themselves, the corresponding interval of orthogonality Ω_1 , the weight function $w(x)$ [and therefore $v(x)$ as in (2.12)] as well as the recursion coefficient a_n . Therefore, each of the three Sheffer *A-Type 0* sets with continuous orthogonality relations (Hermite, Laguerre and Meixner–Pollaczek) has a unique wave function $\Psi_n(x)$ and consequently a unique kinetic energy function $V(x; n)$.

In general, we must first write our orthogonal set in orthonormal form. Then we must find $a_n, v(x), A_n(x)$, and $B_n(x)$. For our particular example, we use the Laguerre polynomials, which are defined as

$$L_n^{(\alpha)}(x) := \frac{(\alpha+1)_n}{n!} \sum_{k=0}^n \frac{(-n)_k}{(\alpha+1)_k} \frac{x^k}{k!}, \quad \alpha > -1 \quad (2.38)$$

and have the following (continuous) orthogonality relation

$$\int_0^\infty L_m^{(\alpha)}(x)L_n^{(\alpha)}(x)x^\alpha e^{-x}dx = \frac{\Gamma(\alpha+1+n)}{n!} \delta_{m,n}.$$

The restriction on α is essential, as $\{L_n^{(\alpha)}(x)\}_{n=0}^\infty$ is undefined for all $\alpha \leq -1$. It is worth noting that taking into account that $(\alpha+1)_n/(\alpha+1)_k = (\alpha+k+1)_{n-k}$ leads to the equivalent form

$$L_n^{(\alpha)}(x) = \frac{1}{n!} \sum_{k=0}^n \frac{(-n)_k}{k!} (\alpha+k+1)_{n-k} x^k.$$

Moreover, using this relationship, we can define the Laguerre polynomials for all $\alpha \in \mathbb{R}$.

For this application, we first assume $\alpha > 0$. We begin by putting our orthogonality relation in orthonormal form using (2.37) on $\Gamma(\alpha+1+n)$:

$$\int_0^{\infty} L_m^{(\alpha)}(x)L_n^{(\alpha)}(x)\frac{n!}{(\alpha+1)_n}\frac{x^\alpha e^{-x}}{\Gamma(\alpha+1)}dx = \delta_{m,n}. \quad (2.39)$$

This enables us to define

$$p_n(x) = (-1)^n \sqrt{\frac{n!}{(\alpha+1)_n}} L_n^{(\alpha)}(x) \quad (2.40)$$

and

$$w(x) = \frac{x^\alpha e^{-x}}{\Gamma(\alpha+1)}. \quad (2.41)$$

We first determine $A_n(x)$ as in (2.17) and begin by evaluating the boundary conditions, noting that the interval of orthogonality for the Laguerre polynomials is $\Omega_1 = [0, \infty)$. We readily obtain

$$\lim_{b \rightarrow \infty} \frac{p_n^2(y)w(y)}{y-x} \Big|_{y=0}^{y=b} = \frac{n!}{\Gamma(\alpha+1)(\alpha+1)_n} \lim_{b \rightarrow \infty} \frac{b^\alpha [L_n^{(\alpha)}(b)]^2}{e^b(b-x)} - 0 = 0.$$

Next, we see from (2.41) that

$$w(x) = \exp\left(-\ln\left(\frac{e^x \Gamma(\alpha+1)}{x^\alpha}\right)\right)$$

and therefore

$$\begin{aligned} v(x) &= \ln\left(\frac{e^x \Gamma(\alpha+1)}{x^\alpha}\right) \\ \Rightarrow v'(x) &= \frac{x-\alpha}{x}. \end{aligned} \quad (2.42)$$

Moreover,

$$\frac{v'(x) - v'(y)}{x-y} = \frac{\alpha}{xy}.$$

Putting all of this together, we thus far have

$$A_n(x) = \alpha \frac{a_n}{x} \int_0^{\infty} p_n^2(y) \frac{y^{\alpha-1} e^{-y}}{\Gamma(\alpha+1)} dy.$$

We evaluate the above integral using integration by parts (with the substitution $u = p_n^2(y)e^{-y}$), which leads to

$$A_n(x) = \frac{a_n}{x} \left(\lim_{b \rightarrow \infty} \frac{p_n^2(y)y^\alpha}{e^y} \Big|_0^b + \int_0^\infty p_n^2(y) \frac{y^\alpha e^{-y}}{\Gamma(\alpha + 1)} dy - 2 \int_0^\infty p_n(y)p_n'(y) \frac{y^\alpha e^{-y}}{\Gamma(\alpha + 1)} dy \right).$$

In the result directly above, it is clear that the boundary conditions equal zero. The middle integral is equal to 1 via the orthonormality relation in Definition 2.8. Using the fact that $\deg(p_n'(y)) = n - 1$ and Lemma 2.1, it follows that the last integral is equal to zero. This results in

$$A_n(x) = \frac{a_n}{x}. \tag{2.43}$$

We derive $B_n(x)$ in a similar fashion. In this case, it is also immediate that the boundary conditions for (2.18) are zero as well. Therefore, we have the following

$$B_n(x) = \alpha \frac{a_n}{x} \int_0^\infty p_n(y)p_{n-1}(y) \frac{y^{\alpha-1}e^{-y}}{\Gamma(\alpha + 1)} dy.$$

We use integration by parts on the above integral (with the substitution $u = p_n(y)p_{n-1}(y)e^{-y}$) and again call upon Lemma 2.1 to achieve

$$B_n(x) = -\frac{a_n}{x} \int_0^\infty p_{n-1}(y)p_n'(y) \frac{y^\alpha e^{-y}}{\Gamma(\alpha + 1)} dy. \tag{2.44}$$

In order to fully evaluate (2.44), we momentarily digress. We assume that $\{\mathcal{Q}_n(x)\}_{n=0}^\infty$ defines a generic orthogonal set, with $\mathcal{Q}_n(x) = q_{n,n}x^n + \mathcal{O}(x^{n-1})$. Then, using Lemma 2.1, we know that

$$\int_\Omega \mathcal{Q}_n^2(y)w(y)dy = \int_\Omega \mathcal{Q}_n(y)[q_{n,n}y^n + \mathcal{O}(y^{n-1})]w(y)dx = q_{n,n} \int_\Omega \mathcal{Q}_n(y)y^n w(y)dy.$$

Also, from directly evaluating (2.13), it is clear that the coefficient of y^n in $p_n(y)$ is $(a_1 \cdots a_n)^{-1}$. Thus, using this fact, our simple relation directly above and orthonormality, we have

$$\begin{aligned} a_n \int_0^\infty p_{n-1}(y)p_n'(y) \frac{y^\alpha e^{-y}}{\Gamma(\alpha + 1)} dy &= a_n \int_0^\infty p_{n-1}(y) \left[\frac{ny^{n-1}}{a_1 \cdots a_n} \right] \frac{y^\alpha e^{-y}}{\Gamma(\alpha + 1)} dy \\ &= n \int_0^\infty p_{n-1}(y) \left[\frac{y^{n-1}}{a_1 \cdots a_{n-1}} \right] \frac{y^\alpha e^{-y}}{\Gamma(\alpha + 1)} dy \\ &= n \int_0^\infty p_{n-1}^2(y) \frac{y^\alpha e^{-y}}{\Gamma(\alpha + 1)} dy \\ &= n \end{aligned}$$

and we conclude that

$$B_n(x) = \frac{-n}{x}. \quad (2.45)$$

To get a complete expression for $A_n(x)$, we must determine the recursion coefficient a_n , which of course can be done by using (2.14) and taking into account that the monic three-term recurrence relation for the Laguerre polynomials is

$$\begin{aligned} xQ_n(x) &= Q_{n+1}(x) + (2n + \alpha + 1)Q_n(x) + n(n + \alpha)Q_{n-1}(x), \\ Q_n(x) &:= (-1)^n n! L_n^{(\alpha)}(x). \end{aligned}$$

As it turns out, from our analysis above, we can also obtain a_n . We first substitute our relations (2.43) and (2.45) into the string equation (2.35), which yields

$$a_{n+1}^2 - a_n^2 = b_n. \quad (2.46)$$

Using Lemma 2.3 in the same way, we get

$$b_n = \alpha + 2n + 1. \quad (2.47)$$

Hence, (2.46) and (2.47) imply that

$$a_n = \sqrt{n(n + \alpha)}, \quad (2.48)$$

which follows since $n(n + \alpha)$ is nonnegative. Therefore, we have

$$A_n(x) = \frac{\sqrt{n(n + \alpha)}}{x}. \quad (2.49)$$

Furthermore, we can disregard the restriction $\alpha > 0$, as the above relation is clearly valid for $\alpha > -1$.

To evaluate the wave function $\Psi_n(x)$ in (2.32), we first note that

$$\exp(-v(x)/2) = \frac{x^{\alpha/2}}{e^{x/2}(\Gamma(\alpha + 1))^{1/2}}.$$

Using this relation and (2.49) we have

$$\Psi_n(x) = \frac{x^{\frac{\alpha+1}{2}} e^{-x/2} p_n(x)}{n^{1/4} (n + \alpha)^{1/4} (\Gamma(\alpha + 1))^{1/2}}. \quad (2.50)$$

Now, we substitute (2.49), (2.45), (2.48) and (2.42) into (2.33) and use manipulations to obtain the kinetic energy function

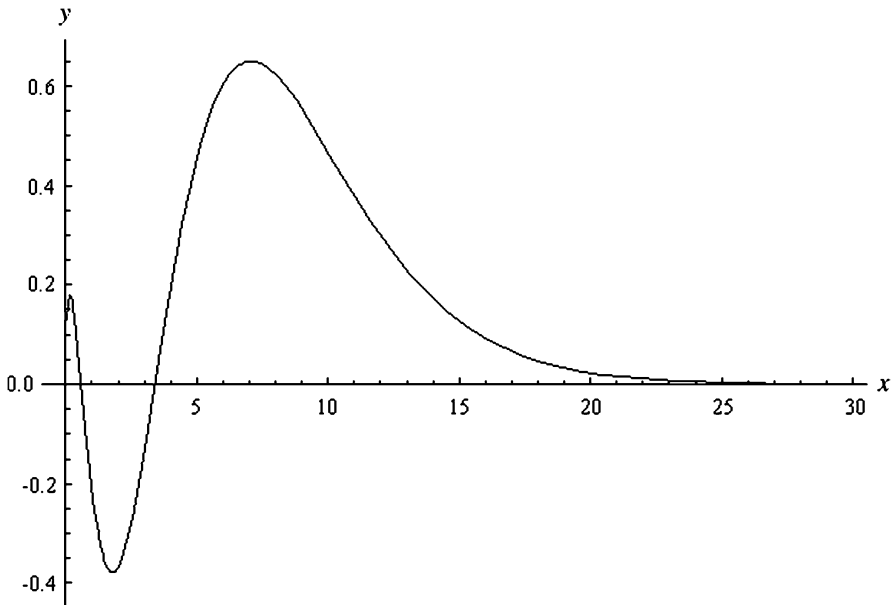


Fig. 2.1 $\Psi_2(x)$ for $\alpha = 0$

$$V(x;n) = \frac{-x^2 + 2(\alpha + 2n + 1)x + 1 - \alpha^2}{4x^2}. \tag{2.51}$$

Lastly, as a concrete example we take $\alpha = 0$ and $n = 2$, which gives the following wave and kinetic energy functions:

$$\Psi_2(x) = \frac{1}{2} \sqrt{\frac{xe^{-x}}{2}} p_2(x) \quad \text{and} \quad V(x;2) = \frac{-x^2 + 10x + 1}{4x^2}.$$

The graph of $\Psi_2(x)$ is displayed in Fig. 2.1.

We also display the graph of the kinetic energy function $V(x;2)$ in Fig. 2.2.

For both of these plots we used Mathematica[®].

Example 2.6. The motivated reader can show that for the Hermite polynomials, $v(x) = x^2$, $A_n(x) = \sqrt{2n}$ and $B_n(x) = 0$ and determine $\Psi_n(x)$ and $V(x;n)$ accordingly.

Next, we show how (2.16) of Theorem 2.2 and (2.28) of Corollary 2.1 can be applied to a specific Sheffer A -Type 0 set.

Example 2.7. Now that we have $A_n(x)$ and $B_n(x)$ for the Laguerre polynomials via Example 2.5, we can utilize these results in determining the specific differential equations (2.16) and (2.23) [and therefore (2.28)] that are satisfied by this particular A -Type 0 orthogonal set. Using $p_n(x)$ in (2.40), as well as (2.17) and (2.18) for $A_n(x)$ and $B_n(x)$, respectively, we see that (2.16) becomes

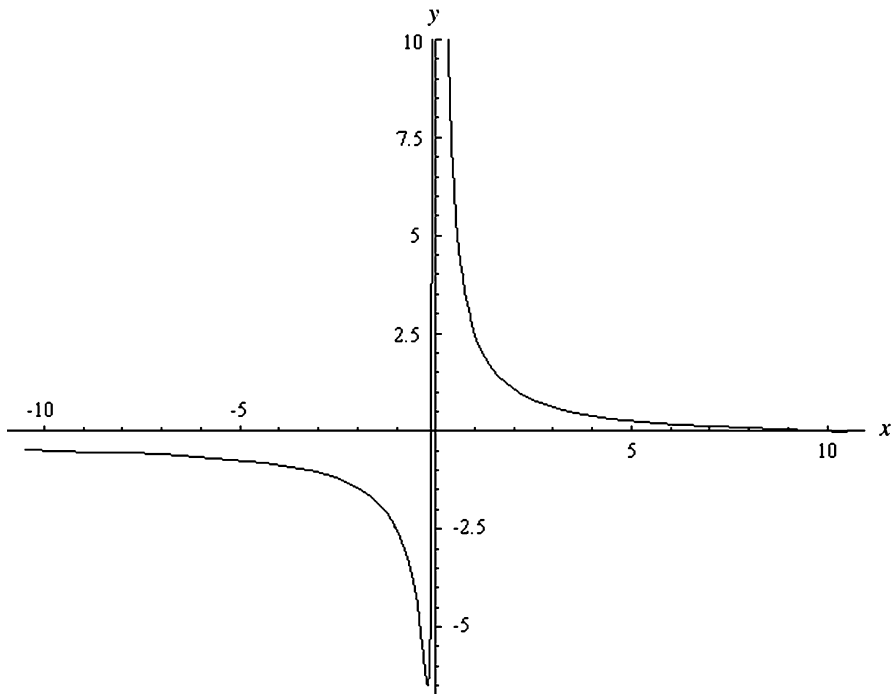


Fig. 2.2 $V(x;2)$ for $\alpha = 0$

$$\frac{d}{dx}L_n^{(\alpha)}(x) = \frac{n}{x}L_n^{(\alpha)}(x) - \frac{\alpha+n}{x}L_{n-1}^{(\alpha)}(x),$$

since $(\alpha+1)_n/(\alpha+1)_{n-1} = \alpha+n$. Similarly, (2.23) and (2.28) take on the form

$$x \frac{d^2}{dx^2}L_n^{(\alpha)}(x) + (1+\alpha+x) \frac{d}{dx}L_n^{(\alpha)}(x) + nL_n^{(\alpha)}(x) = 0.$$

2.4 Difference Equations

In Sects. 2.2 and 2.3, we gave examples of how continuous orthogonal polynomials are important in differential equations. Here, we show how discrete orthogonal polynomials play an important role in *difference equations*. In particular, what follows is a discrete analogue of the characterizations of Sect. 2.3 and is essentially based on [13].

To begin, we assume that $\{p_n(x)\}_{n=0}^{\infty}$ satisfies a discrete orthogonality relation as in (2.2). We expand on this assumption for this section by assuming the discrete weight function $w(x)$ is supported on the set $\{s, s+1, \dots, t\} \subset \mathbb{R}$, where s is a finite

number, but t may be either finite or infinite. We then write the orthogonality relation (2.2) as

$$\sum_{j=s}^t p_m(j)p_n(j)w(j) = \beta_n \delta_{m,n}, \quad w(s-1) = w(t+1) = 0. \quad (2.52)$$

In order to develop our analogues, we must find a discrete version of $v(x)$ as in (2.12). We call this analogue $u(x)$, which is defined as

$$u(x) := \frac{w(x-1) - w(x)}{w(x)}. \quad (2.53)$$

The discrete analogue of the Christoffel–Darboux Identity (Theorem 2.1) is

$$\sum_{k=0}^{n-1} \frac{p_k(x)p_k(y)}{\beta_n} = \frac{\gamma_{n-1}}{\gamma_n \beta_n} \left(\frac{p_n(x)p_{n-1}(y) - p_n(y)p_{n-1}(x)}{x-y} \right), \quad (2.54)$$

where γ_n denotes the leading coefficient of $p_n(x)$ —we use this notation throughout this entire section.

We now state the analogue of Theorem 2.2.

Theorem 2.6. *Let $\{p_n(x)\}_{n=0}^{\infty}$ satisfy (2.52). Then, we have*

$$\Delta p_n(x) = -B_n(x)p_n(x) + A_n(x)p_{n-1}(x), \quad (2.55)$$

where the linear difference operator Δ is defined as

$$\Delta f(x) := f(x+1) - f(x),$$

with

$$A_n(x) = \frac{\gamma_{n-1}}{\gamma_n \beta_{n-1}} \left(\frac{p_n(t+1)p_n(t)}{t-x} w(t) + \sum_{j=s}^t p_n(j)p_n(j-1) \frac{u(x+1) - u(j)}{x+1-j} w(j) \right) \quad (2.56)$$

and

$$B_n(x) = \frac{\gamma_{n-1}}{\gamma_n \beta_{n-1}} \left(\frac{p_n(t+1)p_{n-1}(t)}{t-x} w(t) + \sum_{j=s}^t p_n(j)p_{n-1}(j-1) \frac{u(x+1) - u(j)}{x+1-j} w(j) \right). \quad (2.57)$$

The s and t -values are as in (2.52).

Proof. The proof is similar to that of Theorem 2.2 and is left to the reader as an exercise. \square

Notice that in Theorem 2.6, $\{p_n(x)\}_{n=0}^{\infty}$ was only assumed to be an orthogonal set with respect to the discrete weight function $w(x)$. If it is further assumed that $\{p_n(x)\}_{n=0}^{\infty}$ is an orthonormal set, i.e., $\beta_n \equiv 1$, then it satisfies (2.13). Consequently, $\gamma_{n-1}/\gamma_n = a_n$, and $A_n(x)$ and $B_n(x)$ as respectively in (2.56) and (2.57) take on the form

$$A_n(x) = a_n \left(\frac{p_n(t+1)p_n(t)}{t-x} w(t) + \sum_{j=s}^t p_n(j)p_n(j-1) \frac{u(x+1)-u(j)}{x+1-j} w(j) \right) \quad (2.58)$$

and

$$B_n(x) = a_n \left(\frac{p_n(t+1)p_{n-1}(t)}{t-x} w(t) + \sum_{j=s}^t p_n(j)p_{n-1}(j-1) \frac{u(x+1)-u(j)}{x+1-j} w(j) \right). \quad (2.59)$$

To demonstrate the applicability of (2.55) to the discrete Sheffer A-Type 0 orthogonal sets, we consider the Meixner polynomials in our next example. To complete this example, we need the very useful **Chu-Vandermonde Sum**, which is

$${}_2F_1 \left(\begin{matrix} -n, b \\ c \end{matrix} \middle| 1 \right) = \frac{(c-b)_n}{(c)_n}.$$

It is worthwhile to note that the Chu-Vandermonde Sum can be obtained as the terminating version of the **Gauss Sum**:

$${}_2F_1 \left(\begin{matrix} a, b \\ c \end{matrix} \middle| 1 \right) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}, \quad \operatorname{Re}(c-a-b) > 0.$$

Namely, if in the Gauss Sum we replace a with $-n$, we are left with the Chu-Vandermonde Sum. Refer to Chap. 4 of [17] and Chap. 1 of [25] for more information on these and other similar sums.

Example 2.8. Here, we sketch the details of deriving the coefficients $A_n(x)$ and $B_n(x)$ in (2.55) for the Meixner polynomials. These polynomials can be defined as

$$M_n(x; \beta, c) := {}_2F_1 \left(\begin{matrix} -n, -x \\ \beta \end{matrix} \middle| 1 - \frac{1}{c} \right), \quad (2.60)$$

where $x = 0, 1, 2, \dots$. The weight function for the Meixner polynomials is

$$w(x) = \frac{(\beta)_x c^x}{x!}, \quad x = 0, 1, 2, \dots \quad (2.61)$$

via the discrete orthogonality relation

$$\sum_{x=0}^{\infty} M_m(x; \beta; c) M_n(x; \beta; c) \frac{(\beta)_x c^x}{x!} = \frac{n!(1-c)^{-\beta}}{c^n (\beta)_n} \delta_{m,n}. \quad (2.62)$$

Then, it follows from (2.53) that

$$u(x) = \frac{x}{(\beta + x - 1)c} - 1.$$

Next, we consider $q(x)$ such that $\deg(q(x)) \leq n$ and take c to be an arbitrary constant. Then, from our discrete analogue of the Christoffel–Darboux Identity (2.54), we observe that

$$\sum_{j=s}^t \frac{p_n(j)q(j)}{j-c} w(j) = q(c) \sum_{j=s}^t \frac{p_n(j)}{j-c} w(j), \quad (2.63)$$

which follows from (2.52). Using (2.63), as well as $A_n(x)$ in (2.56) and the Meixner weight function (2.61), it can be shown after several manipulations that

$$A_n(x) = \frac{\gamma_{n-1}}{\gamma_n \beta_{n-1}} \frac{p_n(-\beta)}{(\beta+x)c} \sum_{k=0}^{\infty} \frac{(\beta-1)_k c^k}{k!} p_n(k).$$

Using the definition of the Meixner polynomials (2.60), it can also be shown further that

$$A_n(x) = \frac{\gamma_{n-1}}{\gamma_n \beta_{n-1}} \frac{p_n(-\beta)}{(\beta+x)c} \sum_{j=0}^n \frac{(-n)_j}{j! (\beta)_j} \left(1 - \frac{1}{c}\right)^j (-1)^j \sum_{k=j}^{\infty} \frac{(\beta-1)_k c^k}{(k-j)!}.$$

For the next step, we call upon the **binomial theorem**, which we write using the Pochhammer symbol:

$$\sum_{n=0}^{\infty} \frac{(a)_n}{n!} z^n = (1-z)^{-a},$$

where, in general, we must require $|z| < 1$ if a is not a negative integer. We apply the binomial theorem to the right most sum in our last manipulation for $A_n(x)$ and also utilize the Chu-Vandermonde Sum to obtain

$$A_n(x) = \frac{\gamma_{n-1}}{\gamma_n \beta_{n-1}} \frac{p_n(-\beta)(1-c)^{1-\beta n!}}{c(\beta+x)(\beta)_n}.$$

The binomial theorem and (2.60) lead to

$$p_n(-\beta) = {}_1F_0 \left(\begin{matrix} -n \\ - \end{matrix} \middle| 1 - \frac{1}{c} \right) = \frac{1}{c^n}. \quad (2.64)$$

Then, from (2.60) and (2.62), we obtain

$$\gamma_n = \frac{1}{(\beta)_n} \left(1 - \frac{1}{c}\right)^n \quad \text{and} \quad \beta_n = \frac{n!}{c^n(1-c)^\beta(\beta)_n}.$$

By using (2.64) and the expressions for γ_n and β_n above to find γ_{n-1}/γ_n and β_{n-1} , we eventually have

$$A_n(x) = \frac{-n}{c(\beta+x)}.$$

To derive the expression for $B_n(x)$, we use (2.61), (2.56), (2.57), (2.63) and (2.64) to arrive at

$$B_n(x) = \frac{p_{n-1}(-\beta)}{p_n(-\beta)} A_n(x) = \frac{-n}{\beta+x}.$$

Collecting all of this analysis, we establish the following theorem.

Theorem 2.7. *With respect to the operator Δ as defined in Theorem 2.6, the Meixner polynomials satisfy the first-order difference equation*

$$\Delta M_n(x; \beta, c) = \left(\frac{n}{\beta+x}\right) M_n(x; \beta, c) - \left(\frac{n}{c(\beta+x)}\right) M_{n-1}(x; \beta, c).$$

Proof. See all of the above analysis. □

2.5 Gaussian Quadrature

Informally, the idea behind *Gaussian Quadrature* is to approximate the integral of a given function, say $f(x)$, multiplied by a weight function, with a linear combination of $f(x)$ at known x -values. That is given $f(x)$, we want to obtain

$$\int_{\mathbb{R}} f(x)w(x)dx \approx c_1f(x_1) + c_2f(x_2) + \cdots + c_Nf(x_N).$$

Of course, one would need to develop a method to accomplish this, i.e., how to specifically determine the c_i -terms, the N -value, and the set $\{x_k\}_{k=1}^N$. The essence of such a method was essentially devised by Carl F. Gauss.

As we have mentioned, this introduction is of course very informal, but should give a clear idea of our motivation. In this section, we show how Gaussian Quadrature is connected to classical orthogonal polynomial sequences and give a specific example using the Hermite *A-Type 0* polynomials. To begin, we must first discuss two important ideas that are necessary in the construction and proof of the main theorem of this section: the Lagrange Interpolation Polynomial and the nature of the zeros of classical monic orthogonal polynomials.

Definition 2.10. For a set of distinct points $\{x_1, \dots, x_n\}$, called *nodes*, the *Lagrange Fundamental Polynomial*, which we denote $l_k(x)$, is

$$l_k(x) := \prod_{j=1, j \neq k}^n \frac{(x - x_j)}{(x_k - x_j)} = \frac{S_n(x)}{S'_n(x_k)(x - x_k)}, \quad k \in \{1, \dots, n\},$$

with

$$S_n(x) = \prod_{j=1}^n (x - x_j).$$

As an immediate consequence, the *Lagrange Interpolation Polynomial* of a function $f(x)$ at the nodes $\{x_1, \dots, x_n\}$ is the unique polynomial $L(x)$ such that $\deg(L(x)) = n - 1$ and $f(x_j) = L(x_j)$ is satisfied. In addition, it is also immediate that $L(x)$ can be written as

$$L(x) = \sum_{k=1}^n l_k(x) f(x_k) = \sum_{k=1}^n f(x_k) \frac{S_n(x)}{S'_n(x_k)(x - x_k)}. \quad (2.65)$$

We emphasize that Lagrange Interpolation Polynomials do *not* form an orthogonal set and are not of any Sheffer *Type*. Nonetheless, as we discussed, they are necessary in the construction of the main result of this section. The interested reader can however refer to [24] for a more in-depth coverage of Lagrange Interpolation, including convergence properties.

We next state an important result about the zeros of classical monic orthogonal polynomials that will be needed in our main theorem. Moreover, for establishing this theorem, we call upon the Christoffel–Darboux Identity and its limiting case, which makes for a quite simple proof. For the remainder of this section we assume that $\{P_n(x)\}_{n=0}^{\infty}$ is a monic sequence of orthogonal polynomials that satisfy (2.4).

Theorem 2.8. *If $\mathcal{S} := \{P_n(x)\}_{n=0}^{\infty}$ satisfies the monic three-term recurrence relation (2.4), then the zeros of each $P_k(x) \in \mathcal{S}$ are both real and simple (distinct).*

Proof. Assume that $P_k(x)$ has a complex zero, say z . Then, since complex zeros of polynomials with real coefficients come in conjugate pairs, we know that \bar{z} is also a zero of $P_k(x)$. Now let $x = z$ and $y = \bar{z}$ and substitute these into (2.8). By the properties of the complex conjugate, we know that $P_k(\bar{z}) = \overline{P_k(z)}$ and therefore the right-hand side of (2.8) is zero. However, the left-hand side is nonzero. This contradiction implies that the zeros of each $P_k(x) \in \mathcal{S}$ are all real.

Next, assume that $P_k(x)$ has a zero of multiplicity 2, say x_0 . Then, the right-hand side of (2.11) is clearly zero since $P_k(x_0) = P'_k(x_0) = 0$, while the left-hand side is nonzero (positive). Therefore, we know that the zeros of each $P_k(x) \in \mathcal{S}$ are simple. \square

We now can prove the following.

Theorem 2.9 (Gauss–Jacobi Mechanical Quadrature). *Let $\{P_n(x)\}_{n=0}^{\infty}$ satisfy the monic three-term recurrence relation (2.4), with real and simple zeros ordered as*

$$x_{N,1} > x_{N,2} > \cdots > x_{N,N}.$$

Then, given a positive integer N , there exist a unique sequence of positive numbers $\{\lambda_k\}_{k=1}^N$ such that

$$\int_{\mathbb{R}} p(x)w(x)dx = \sum_{k=1}^N \lambda_k p(x_{N,k}), \quad (2.66)$$

which is valid for all polynomials $p(x)$ such that $\deg(p(x)) \leq 2N - 1$. Moreover, the λ_k -values, called the **Christoffel Numbers**, are not dependent on the polynomial $p(x)$ and can be computed via

$$\lambda_k = \int_{\mathbb{R}} \frac{P_N(x)w(x)dx}{P'_N(x_{N,k})(x - x_{N,k})}. \quad (2.67)$$

Proof. Let $L(x)$ be the Lagrange Interpolation Polynomial in (2.65) of $p(x)$ at the nodes $\{x_{N,k}\}_{k=1}^N$, which we assign to be the zeros of $\{P_n(x)\}_{n=0}^{\infty}$. These choices are permissible, as each of the zeros $\{P_n(x)\}_{n=0}^{\infty}$ is real and simple via Theorem 2.8 and can be ordered as in the statement of this theorem. Therefore,

$$L(x) = p(x) \text{ at } x = x_{N,k}, \quad \forall k \in \{1, 2, \dots, N\}.$$

Thus, there exists a polynomial $q(x)$ with $\deg(q(x)) \leq N - 1$ such that

$$p(x) - L(x) = P_N(x)q(x).$$

Multiplying the result directly above by $w(x)$ and integrating gives

$$\int_{\mathbb{R}} p(x)w(x)dx = \int_{\mathbb{R}} L(x)w(x)dx + \int_{\mathbb{R}} P_N(x)q(x)w(x)dx.$$

From Lemma 2.1, the rightmost integral is zero. By (2.65) with $S(x)$ replaced by $P_N(x)$ we see that our relation above becomes

$$\int_{\mathbb{R}} p(x)w(x)dx = \sum_{k=1}^N \left(\int_{\mathbb{R}} \frac{P_N(x)w(x)dx}{P'_N(x_{N,k})(x - x_{N,k})} \right) p(x_{N,k})$$

and (2.66) and (2.67) are both satisfied. Since we have proven (2.66), we can now apply it to $p(x) = P_N^2(x)/(x - x_{N,k})^2$, from which it follows that

$$\lambda_k = \int_{\mathbb{R}} \left(\frac{P_N(x)}{P'_N(x_{N,k})(x - x_{N,k})} \right)^2 w(x)dx.$$

This implies that $\{\lambda_k\}_{k=1}^N$ is a unique sequence of positive numbers. \square

We now demonstrate Theorem 2.9 concretely.

Example 2.9. We apply Theorem 2.9 to the polynomial $p(x) := 3x^3 - 2x^2$ using the Hermite polynomials, in which case $\Omega_1 = \mathbb{R}$. Since the weight function for the Hermite polynomials is $w(x) = e^{-x^2}$, we wish to evaluate

$$\int_{\mathbb{R}} (3x^3 - 2x^2) e^{-x^2} dx$$

via the right-hand side of (2.66). The Hermite polynomials are defined as

$$H_n(x) := n! 2^n \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(-1)^k x^{n-2k}}{2^{2k} k! (n-2k)!},$$

where $\lfloor n/2 \rfloor$ is the **floor function**. Through some manipulation, we can write these polynomials in the following hypergeometric form as in (2.5):

$$H_n(x) := (2x)^n {}_2F_0 \left(\begin{matrix} -n/2, (1-n)/2 \\ - \end{matrix} \middle| -\frac{1}{x^2} \right)$$

from which it is clear that the leading coefficient of $H_n(x)$ is 2^n . So, the monic form of the Hermite polynomials is $P_n(x) = 2^{-n} H_n(x)$. We next take $N = 3$ and thus

$$P_3(x) = \frac{1}{8} H_3(x) = x^3 - \frac{3}{2}x \Rightarrow P'_3(x) = 3x^2 - \frac{3}{2}.$$

The zeros of $P_3(x)$ give us the nodes

$$x_{3,1} = \sqrt{3/2},$$

$$x_{3,2} = 0,$$

$$x_{3,3} = -\sqrt{3/2}.$$

Also, we evaluate P and P' at each of these nodes to respectively obtain

$$P(x_{3,1}) = \frac{3}{4} (3\sqrt{6} - 4)$$

$$P(x_{3,2}) = 0$$

$$P(x_{3,3}) = -\frac{3}{4} (3\sqrt{6} - 4)$$

and

$$P'(x_{3,1}) = 3,$$

$$P'(x_{3,2}) = -3/2,$$

$$P'(x_{3,3}) = 3.$$

We next compute the λ_k -values using

$$\lambda_k = \int_{\mathbb{R}} \frac{P_3(x)e^{-x^2} dx}{P_3'(x_{3,k})(x - x_{3,k})}, \quad k = 1, 2, 3.$$

Specifically, this gives

$$\lambda_1 = \sqrt{\pi}/6,$$

$$\lambda_2 = 2\sqrt{\pi}/3,$$

$$\lambda_3 = \sqrt{\pi}/6.$$

Putting all of this together, after some calculations we obtain

$$\sum_{k=1}^3 \left(\int_{\mathbb{R}} \frac{P_3(x)e^{-x^2} dx}{P_3'(x_{3,k})(x - x_{3,k})} \right) p(x_{3,k}) = -\sqrt{\pi}$$

and of course

$$\int_{\mathbb{R}} (3x^3 - 2x^2) e^{-x^2} dx = -2 \int_{\mathbb{R}} x^2 e^{-x^2} dx = -2 \left(\frac{\sqrt{\pi}}{2} \right) = -\sqrt{\pi}$$

via the gamma function in Definition 2.9.

Also, the interested reader can consider instead using the Meixner–Pollaczek or the Laguerre polynomials for this example.

To summarize, we have established a numerical estimate of an integral by picking *optimal* abscissas (the x -values) at which to evaluate the function. The Gauss–Jacobi Mechanical Quadrature Theorem (Theorem 2.9) states that these values are exactly the roots of the orthogonal polynomial for the same interval and weight function as the integral being approximated. Gaussian Quadrature is optimal since it fits all polynomials up to degree $2N - 1$.

The natural question is of course how Gaussian Quadrature applies when $f(x)$ is a function more general than a polynomial of degree at most $2N - 1$. A detailed analysis of such a development and related results is quite detailed and a discussion of this nature is not germane to the work at hand. Nonetheless, it is certainly worthwhile to cover one such fundamental result and we refer the interested reader to [24] for a thorough treatment.

The result below essentially states that for large N , the quadrature of Theorem 2.9 becomes very close to the actual value of the integral $\int_a^b f(x) dx$, for which the integral exists.

Theorem 2.10. Let $w(x) > 0$ be a weight function defined on an arbitrary interval $[a, b]$ and $Q_N(f(x)) := \sum_{k=1}^N \lambda_k p(x_{N,k})$ the corresponding Gauss–Jacobi Mechanical Quadrature as in Theorem 2.9, where the λ_k -values are the Christoffel Numbers (2.67). Then the **quadrature convergence**

$$\lim_{N \rightarrow \infty} Q_N(f(x)) - \int_a^b f(x) dx = 0$$

holds for an arbitrary function $f(x)$ for which the above integral exists.

Proof. Refer to Chap. 15 of [24]. □

We conclude this section by briefly addressing two additional types of similar quadrature formulas. The first is **Radau Quadrature** [10], which is also a Gaussian Quadrature-like formula. In essence, Radau Quadrature requires $N + 1$ points and fits all polynomials up to degree $2N$ and hence yields exact results for all polynomials of degree $2N - 1$. This procedure requires the use of a weight function $W(x)$ in which the endpoint -1 in the interval $[-1, 1]$ is included in a total of N abscissas, leading to $N - 1$ free variables.

Also, **Laguerre-Gauss Quadrature** (often also called Gauss-Laguerre Quadrature) [2, 8] is additionally a Gaussian-like quadrature over the interval $[0, \infty)$ with the Laguerre $(L_n^{(0)}(x))$ weight function $W(x) = e^{-x^2}$. This procedure also fits all polynomials up to degree $2N - 1$.

2.6 Problems

We finalize this section by stating some interesting problems that naturally arise from the analysis we have covered.

Problem 1. Supply the rigorous details of Meixner–Pollaczek case of Example 2.4 and also consider applying the inverse method to the remaining three *A-Type 0* sets. For the Hermite polynomials $c_n := 1/n!$, for the Meixner polynomials $c_n := (\beta)_n/n!$, and for the Krawtchouk polynomials $c_n := C(N, n)$.

Problem 2. Develop an analogue of Example 2.5 for the Meixner–Pollaczek polynomials.

Problem 3. Construct an analogue of Example 2.8 for the other Sheffer Sequences that satisfy a discrete orthogonality, i.e., the Charlier and Krawtchouk polynomials.

Problem 4. Establish a discrete analogue of Theorem 2.4 and apply it to the Meixner, Charlier and Krawtchouk polynomials.

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