Studies on generalizations of the classical orthogonal polynomials where gaps are allowed in their degree sequences

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Chapter 1

Introduction

In this thesis we study several generalizations of the classical orthogonal polynomials (COP). These generalizations include the exceptional orthogonal polynomials (XOP), the Dunkl-supersymmetric orthogonal functions and orthogonal polynomials whose degree sequence is $0,2,2,4,4,\ldots$. A common feature shared by these generalizations when they appear as polynomials is that the degree sequence of them are not a set where all the non-negative integers are included. Here we say a polynomial $p(x)$ is of degree n if the highest degree of the variable x is n. Specifically, let us consider a (finite or infinite) sequence of polynomials $\{P_n(x)\}$ that satisfy certain orthogonality, denote the degree sequence of $\{P_n(x)\}$ by $\mathbb{S}$, and let $\mathbb{N}_0 = \{0,1,2,\ldots\}$. For the orthogonal polynomials we shall consider in this thesis, one always has

$$\mathbb{S} = \mathbb{N}_0 \backslash \mathbb{C}, \tag{1.0.1}$$

where the set $\mathbb{C} \subset \mathbb{N}$ can be finite or infinite. The significance of studying these generalizations of COP is self-evident once the readers come to realize the great theoretical value and rich applications of COP. We would like to invite the readers to follow us into this short but pleasing journey playing with generalizations of COP.

1.1 Classical orthogonal polynomials

1.1.1 History and definitions

First, we shall quickly review the history of the orthogonal polynomials (OP) in general. The origin of OP goes back to the theory of continued fractions studied by Stieltjes in the late nineteenth century [72]. Over the past hundred years, voluminous achievements on the theory and applications of OP have been contributed by a great number of outstanding mathematicians, to name a few, Markov, Padé, Hamburger, Hausdorff, Carleman, Perron, Szegö [10, 34, 35, 53, 61, 62, 74]. Especially, after the publication of Szegö's famous treatise on the theory of OP, increasing interest has been attracted to this subject. The basic general theory of OP was further developed by Chihara in his well-known book [12], where many necessary background materials are also included.

Along with the development of the theories of OP, it has been widely applied to many different branches of mathematics and physics, such as special functions, integrable systems, approximation theory, numerical analysis, random matrix, quantum mechanics and combinatorial theory. In addition, the theories developed upon that of OP furnish comparatively general and instructive illustrations of certain situations in the theory of orthogonal systems. Recently, some of these polynomials have been shown to be of great significance in quantum informatics [7, 14, 43] and in machine learning [48, 71].

Now let us introduce the definition of OP. For a comprehensive review of the theory of OP, one can refer to the special issues dedicated to such topics [12, 47, 74]. Let $\mathscr{L}$ be a linear functional from $\mathbb{R}[x]$ to $\mathbb{R}$. The orthogonal polynomial sequence (OPS) related to the functional $\mathscr{L}$ are defined as a sequence of polynomials $\{p_n(x)\}_{n=0}^{\infty}$ satisfying the following conditions:

$$\mathscr{L}[p_n(x)p_m(x)] = h_n\delta_{m,n}, \quad h_n \neq 0, \tag{1.1.1a}$$
$$\deg(p_n(x)) = n. \tag{1.1.1b}$$

If in additional we also have $h_n = 1$, $n \geq 0$, then it will be called an orthonormal polynomial sequence.

For convenience, unless otherwise specified we will assume that the OPS mentioned in this thesis are always monic (which means their leading coefficients in the variable is 1). An equivalent definition of OPS was then provided by Favard [20] in 1935 as the existence of the three-term recurrence relations:

$$xp_n(x) = p_{n+1}(x) + a_n p_n(x) + b_n p_{n-1}(x), \quad p_{-1}(x) = 0, \quad (b_n \neq 0), \quad n = 0, 1, 2, \ldots \tag{1.1.2}$$

Moreover, the OPS $\{p_n(x)\}_{n=0}^{\infty}$ is called positive-definite if a_n is real and $b_n > 0$. This characterization of OPS is sometimes even more important since it relates OP to a tridiagonal matrix, which is usually called a Jacobi matrix. This key feature is the starting point of many applications of OP. The Jacobi matrix plays an important role in several areas including quantum theory, integrable systems, numerical analysis, random matrices and antisymmetric simple exclusion process (ASEP) which are nowadays extensively studied and investigated [4, 6, 11, 68, 78, 80].

Three well-known examples of OP, the Hermite, Laguerre and Jacobi (including the special cases Tchebichef, Legendre, Gagenbauer) polynomials, have long been at the center of the studies of OP. These three systems were called collectively the classical orthogonal polynomials (COP). In many literatures the term "classical" means that the OP satisfy certain second-order differential equations

$$(A(x)\partial_x^2 + B(x)\partial_x + C(x))p_n(x) = 0, \tag{1.1.3}$$

where $\partial_x = \frac{d}{dx}$, $A(x)$ and $B(x)$ are polynomials of degrees not exceeding 2 and 1, $C(x)$ is constant. These COP have many properties in common. One of them is that the derivative of $p_n(x)$ is a constant times $q_{n-1}(x)$ where $\{p_n(x)\}$ is in one of these COP and $\{q_n(x)\}$ is also. These are the only sets of OP with the property that their derivatives are also orthogonal.

Later, the concept of COP has also been extended to a discrete variable case and they are defined as polynomials satisfying a second-order difference equation

$$(A(x)\Delta_x^2 + B(x)\Delta_x + C(x))p_n(x) = 0 \tag{1.1.4}$$

or a second-order q-difference equation

$$(A(x)(\Delta_x^q)^2 + B(x)\Delta_x^q + C(x))p_n(x) = 0, \tag{1.1.5}$$

where Δ_x is a difference operator defined by $\Delta_x f(x) = f(x+1) - f(x)$ and Δ_x^q is the q-difference operator defined by $\Delta_x^q f(x) = (f(qx) - f(x))/(q-1)x$. The orthogonal polynomials which are solutions of (1.1.3), (1.1.4) or (1.1.5) are characterized as the Askey scheme or the q-Askey scheme [57] and these polynomials are explicitly written in terms of hypergeometric functions [22].

In the book of Koekoek and coworkers [44], the Hermite, Laguerre and Jacobi polynomials are called "very classical orthogonal polynomials", and (following Andrews & Askey [2]) the authors called all families in the (q-)Askey scheme classical. The families in the (q-)Askey scheme have found interpretations in various settings, for instance in the representation theory of specific Lie or finite or quantum groups, in combinatorics and in probability theory. Some of the limits in the scheme could also be brought over to limit relations of the structures where the polynomials were interpreted.

In this thesis we would like to follow the statement in Koekoek's book, which means in what follows, the term COP will always refer to all the members in the (q-)Askey scheme.

1.2 Duality and classical orthogonal polynomials

As we have seen, classical orthogonal polynomials are always equipped with three-term recurrence relations and a second-order equation simultaneously. This property is called duality. In the infinite-dimensional case there are several possibilities for duality property. The "classical" duality means that orthogonal polynomials $p_n(x)$ satisfy both the recurrence relation (1.1.2) and one of the second-order equations (1.1.3), (1.1.4) and (1.1.5). In the finite-dimensional case, the duality can be understood with the help of a Leonard pair. The relationship between a Leonard pair and orthogonal polynomials has been explained explicitly in [75, 76]. In what follows, we would like to briefly introduce it.

Let V denote a vector space over a field $\mathbb{K}$ with finite positive dimension $N+1$. By definition, a pair of linear operators $X : V \to V$ and $Y : V \to V$ form a Leonard pair if there exist two basis for V, say e_n and d_n, $n = 0, 1, 2, \ldots, N$, such that, on the one hand, with respect to the basis e_n, $n = 0, 1, 2, \ldots, N$, X is diagonal and Y is tridiagonal:

$$Xe_n = \lambda_n e_n, \quad Ye_n = \xi_{n+1} e_{n+1} + \eta_n e_n + \xi_n e_{n-1}, \quad n = 0, 1, 2, \ldots N;$$

on the other hand, with respect to the basis d_n, $n = 0, 1, 2, \ldots, N$, Y is diagonal and X is tridiagonal:

$$Yd_n = \mu_n d_n, \quad Xd_n = a_{n+1} d_{n+1} + b_n d_n + a_n d_{n-1}, \quad n = 0, 1, 2, \ldots N$$

where $a_n, \xi_n \neq 0$, $n = 0, 1, \ldots, N$, and $a_{N+1} = \xi_{N+1} = 0$. If there exist functions ω_n and polynomials $\psi_n(x)$, $n = 0, 1, \ldots, N$, such that the following expansions hold

$$e_s = \sum_{n=0}^{N} \sqrt{\omega_s} \psi_n(\lambda_s) d_n, \quad d_n = \sum_{s=0}^{N} \sqrt{\omega_s} \psi_n(\lambda_s) e_s,$$

then $\psi_n(x)$ are orthonormal polynomials defined by the three-term recurrence relation

$$x\psi_n(x) = a_{n+1} \psi_{n+1}(x) + b_n \psi_n(x) + a_n \psi_{n-1}(x), \tag{1.2.1}$$

where $\psi_{-1}(x) = 0$, $\psi_0(x) = 1$. These polynomials are orthonormal with respect to the weights ω_s

$$\sum_{s=0}^{N} \omega_s \psi_n(\lambda_s) \psi_m(\lambda_s) = \delta_{nm}. \tag{1.2.2}$$

For readers who are not familiar with the above discussions we would like to give some explanations on the calculations leading to (1.2.1) and (1.2.2). First, it follows from the expansion of e_s that

$$Xe_s = \sum_{n=0}^{N} \sqrt{\omega_s} \psi_n(\lambda_s) X d_n = \sum_{n=0}^{N} \sqrt{\omega_s} \psi_n(\lambda_s) (a_{n+1} d_{n+1} + b_n d_n + a_n d_{n-1}),$$

while it also holds that

$$Xe_s = \lambda_s e_n = \sum_{n=0}^{N} \sqrt{\omega_s} \psi_n(\lambda_s) \lambda_s d_n.$$

By comparing the right-hand sides of these two equation one arrives (1.2.1). The orthogonality relation (1.2.2) follows directly from the expansions:

$$d_n = \sum_{s=0}^{N} \sqrt{\omega_s} \psi_n(\lambda_s) \sum_{m=0}^{N} \sqrt{\omega_s} \psi_m(\lambda_s) d_m = \sum_{m=0}^{N} \left(\sum_{s=0}^{N} \omega_s \psi_n(\lambda_s) \psi_m(\lambda_s) \right) d_m.$$

Again, if there exist functions $\tilde{\omega}_n$ and polynomials $\chi_n(x)$, $n = 0, 1, \ldots, N$, such that the (dual) expansions hold

$$d_s = \sum_{n=0}^{N} \sqrt{\tilde{\omega}_s} \chi_n(\mu_s) e_n, \quad e_n = \sum_{s=0}^{N} \sqrt{\tilde{\omega}_s} \chi_n(\mu_s) d_s,$$

then the (dual) polynomials $\chi_n(x)$ are orthonormal defined by the three-term recurrence relation

$$x\chi_n(x) = \xi_{n+1}\chi_{n+1}(x) + \eta_n\chi_n(x) + \xi_n\chi_{n-1}(x), \tag{1.2.3}$$

where $\chi_{-1}(x) = 0, \chi_0(x) = 1$. They are orthogonal with respect to (dual) weights $\tilde{\omega}_s$

$$\sum_{s=0}^{N} \tilde{\omega}_s \chi_n(\mu_s) \chi_m(\mu_s) = \delta_{nm}. \tag{1.2.4}$$

Moreover, comparison between the two types of expansions of e_n, d_n leads to the Leonard duality:

$$\sqrt{\omega_s}\psi_n(\lambda_s) = \sqrt{\tilde{\omega}_n}\chi_s(\mu_n). \tag{1.2.5}$$

If we multiply $\sqrt{\tilde{\omega}_n/\omega_s}$ in both sides of the recurrence relations (1.2.3) with n replaced by s and $x = \mu_n$

$$\mu_n \sqrt{\tilde{\omega}_n/\omega_s}\chi_s(\mu_n) = \xi_{s+1}\sqrt{\tilde{\omega}_n/\omega_s}\chi_{s+1}(\mu_n) + \eta_s\sqrt{\tilde{\omega}_n/\omega_s}\chi_s(\mu_n) + \xi_s\sqrt{\tilde{\omega}_n/\omega_s}\chi_{s-1}(\mu_n)$$

and then substitute the relation (1.2.5) into the above, it turns out that polynomials $\psi_n(x)$ satisfy the second-order difference equation

$$A(s)\left(\psi_n(\lambda_{s+1}) - \psi_n(\lambda_s)\right) + B(s)\left(\psi_n(\lambda_{s-1}) - \psi_n(\lambda_s)\right) + C(s)\psi_n(\lambda_s) = \mu_n\psi_n(\lambda_s)$$

where

$$A(s) = \xi_{s+1}\sqrt{\omega_{s+1}/\omega_s}, \quad B(s) = \xi_s\sqrt{\omega_{s-1}/\omega_s}, \quad C(s) = \eta_s + A(s) + B(s).$$

1.3 Algebraic representations

Bispectral pair is a generalization of Leonard pair. With the help of this concept, the polynomials in the (q-)Askey scheme are related with very elegant algebras, among which the most general one is the Askey-Wilson algebra (or Zhedanov algebra) [32, 87]. All the polynomials in the (q-)Askey scheme can be realized by this algebra or its degenerations. The Askey-Wilson (AW(3)) algebra is defined as the algebra with three generators X, Y and Z subject to the relations

$$[X,Y]_q = Z, \tag{1.3.1a}$$
$$[Y,Z]_q = BX + A_1Y + C_1, \tag{1.3.1b}$$
$$[Z,X]_q = BX + A_2Y + C_2, \tag{1.3.1c}$$

where A_1, A_2, B, C_1, C_2 are complex constants, and $[X,Y]_q = XY - qYX$ is called q-mutator. Due to simple q-mutation relations its representations, spectra, overlaps and other properties can be obtained immediately [31]. Later, The Z_3 form of the AW(3) algebra was also found [85]:

$$[X,Y]_q = a_3Z + w_3, \quad [Y,Z]_q = a_1X + w_1, \quad [Z,X]_q = a_2Z + w_2.$$

In case if $a_1a_2a_3 \neq 0$ it is possible to put $a_1 = a_2 = a_3 = 1$, then there are four independent parameters: $\omega_1, \omega_2, \omega_3$ and the value Q of the Casimir operator of this algebra. They correspond to the 4 parameters of Askey-Wilson polynomials.

When some parameters are zero then the Aksey-Wilson polynomials degenerate to other polynomials from the (q-)Askey scheme. For example, put $q = -1$, the algebra

$$\{X,Y\} = a_3 Z + w_3, \quad \{Y,Z\} = a_1 X + w_1, \quad \{Z,X\} = a_2 Z + w_2,$$

describes the Bannai-Ito polynomials (which will appear in Chapter 3) [3, 79], where $\{X,Y\} = XY + YX$ is the anticommutator. In addition, if $a_1 = 0$ then the degeneration corresponds to big -1 Jacobi polynomials [84]. If $a_1 = \omega_1 = 0$ then the degeneration corresponds to little -1 Jacobi polynomials [82]. For more interesting results on the algebras related with COP one can refer to [5, 21, 30–32, 75, 76, 85, 87].

1.4 Outline of thesis

The main purpose of this thesis is to deepen the understanding of classical orthogonal polynomials by studying their generalizations when dropping some restrictions on the degree sequence. Specifically, we consider the generalizations where the degree sequence of such an orthogonal polynomial system does not consist of all the nonnegative integers, i.e. gaps are allowed in their degree sequence.

This thesis unfolds as follows.

In chapter 2, we discuss about the electrostatic properties of zeros of exceptional extensions of the very classical orthogonal polynomials. We first give a brief review on the exceptional extensions of the very classical orthogonal polynomials. A powerful method in the construction of these exceptional polynomials is called the Darboux transformation. After introducing these concepts, we investigate a classical electrostatic problem related with the very classical orthogonal polynomials. This problem can be solved by deriving the configuration where the maximum value of a special energy function is obtained. We show that this energy function attains its maximum value at the zeros of some exceptional orthogonal polynomials under certain conditions.

In chapter 3, we construct an exceptional extension of the Bannai-Ito polynomials. In this construction, we generalize the Darboux transformation to a first-order Dunkl-type difference operator. From the generalized Darboux transformation we derive the exceptional Bannai-Ito operators which have polynomial eigenfunctions of all but a finite number of degrees. We also give more general results on the intertwining relations regarding the multiple-step exceptional Bannai-Ito operator, and derived their eigenfunctions. A special class of eigenfunctions of the Bannai-Ito operator which are called the quasi-polynomial eigenfunctions are also important in the construction of the exceptional Bannai-Ito polynomials. A quasi-polynomial eigenfunction consists of a gauge factor and a polynomial part. We show that there are 8 classes of gauge factors by comparing the coefficients of the conjugated Bannai-Ito operator and those of the Bannai-Ito operator. Then we construct the 1-step exceptional Bannai-Ito polynomials and show that they are orthogonal with respect to a discrete measure on the exceptional Bannai-Ito grid. Interestingly enough, the degree sequences of the exceptional Bannai-Ito polynomials demonstrate different rules compared with all the known 1-step XOPs. The positivity of the weight functions related to these 1-step exceptional Bannai-Ito polynomials is also considered, and we provide several sufficient conditions with respect to certain parameters.

In chapter 4, we introduced and characterized orthogonal functions that we have called Dunkl-supersymmetric. These functions are eigenfunctions of a class of Dunkl-type differential operators that can be cast within Supersymmetric Quantum Mechanics. This investigation has built and expanded upon the analysis in [65] where two examples had been studied. A significant feature of these orthogonal function families is that they do not involve polynomials of all degrees but are rather organized in pairs of polynomials both of the same degree (where the examples in terms of the Jacobi polynomials may be viewed as polynomials in another variable) . The connection with Supersymmetric Quantum Mechanics has been exploited to obtain a number of Dunkl-SUSY orthogonal functions from exactly solvable problems. Informed by these results we could offer a general characterization of the Dunkl-

SUSY OPs and could exhibit as well their recurrence relations. It would be of interest to relate the families of OPs that have been obtained as $q = -1$ limits of q-orthogonal polynomials [51, 79, 82, 84]. A challenging project for the future would be to undertake the study of multivariate supersymmetric polynomials.

In chapter 5, we give summary and plans of future works.

Chapter 2

Exceptional extensions of the very classical orthogonal polynomials and their electrostatic properties

2.1 Darboux transformation

The last decade has witnessed exciting developments in a new class of generalization of COP, which were given a kindly confusing name, the "exceptional" orthogonal polynomials (XOP). It is necessary to remark that the XOP are a generalization of the COP, since they have the latter as a special case. Here we say a polynomial $P_n(x)$ is of degree n if the highest degree of its variable is n. In most cases the XOP have "gaps" in their degree sequences, i.e. there are a finite number of missing degrees in their polynomial sequences (while the degree sequences of very COP are $\{0,1,2,\dots\}$). Extensive interest have been devoted to many aspects of the theory of XOP. See, for instance, [25] for the introduction of the exceptional flag which gives birth to XOP, and [24,26,69,77] for a systematic way of constructing XOP satisfying 2nd-order differential equations (or 2nd-order difference equations in [16–18]), as well as [23] for a complete classification of the (continuous) XOP.

In the construction of XOPs, the Darboux transformation (DT) plays an important role. It was further clarified that multiple-step or higher order DTs lead to XOPs labelled by multi-indices [27,29,59]. The 1-step (rational) DT was conducted on a 2nd-order differential operator $T = p(x)D_{xx} + q(x)D_x + r(x)$ and acts as $T \mapsto T^{(1)}$:

$$T = \mathscr{B} \circ \mathscr{A} + \lambda, \quad T^{(1)} = \mathscr{A} \circ \mathscr{B} + \lambda, \tag{2.1.1}$$

where $\mathscr{A}$, $\mathscr{B}$ are 1st-order differential operators [26]. An immediate consequence of (2.1.1) can be derived as the following intertwining relations

$$\mathscr{A} \circ T = T^{(1)} \circ \mathscr{A}, \quad T \circ \mathscr{B} = \mathscr{B} \circ T^{(1)},$$

which imply that the eigenvalue problem $T[y] = \lambda y$ is equivalent to $T^{(1)}[y^{(1)}] = \lambda y^{(1)}$ where $y^{(1)} = \mathscr{A}[y]$. Thus with a well selected "seed solution" ϕ such that $T[\phi] = \mu\phi$ and $\mathscr{A}[\phi] = 0$, it simply deletes degrees in the eigenfunction sequence $\{y^{(1)}\}$ of the Darboux transformed operator $T^{(1)}$.

In the above we described a rough image of a 1-step (rational) DT. Let us introduce the basic knowledge about DT in more details adopting the notations of [23]. Given a second-order differential operator $T = p(x)\partial_x^2 + q(x)\partial_x + r(x)$, let $\phi(x)$ be an eigenfunctions of T such that

$$T[\phi](x) = \lambda\phi(x),$$

where $p(x), q(x), r(x)$ are rational functions, λ is the corresponding eigenvalue.

Definition 2.1.1. *A rational factorization of T is a relation of the form*

$$T = BA + \lambda,$$

where A, B are first-order differential operators. Given a rational factorization, we call the second-order differential operator $\hat{T}$ defined by

$$\hat{T} = AB + \lambda$$

the partner operator of T and say that $T \mapsto \hat{T}$ is a rational Darboux transformation.

It is easy to see that T, $\hat{T}$ are related by the following intertwining relations

$$AT = \hat{T}A, \quad TB = B\hat{T},$$

which imply that the eigenvalue equation $T[\phi] = \lambda\phi$ is equivalent to the eigenvalue equation $\hat{T}[\hat{\phi}] = \lambda\hat{\phi}$ where $\hat{\phi} = A[\phi]$. Specifically, we denote the first-order differential operators A, B by

$$A = b(\partial_x - u), \quad B = \hat{b}(\partial_x - \hat{u}),$$

where $b, \hat{b}, u, \hat{u}$ are non-zero rational functions satisfying

$$\hat{b}b = p, \quad \hat{u} + u = -\frac{q}{p} + \frac{b'}{b},$$

and a Ricatti equation

$$p(u' + u^2) + qu + r = \lambda.$$

From the definition of T, $\hat{T}$ and the way they are being factorized, it follows immediately that:

Proposition 2.1.1. *Given two second-order differential operators T, $\hat{T}$:*

$$T = p\partial_x^2 + q\partial_x + r, \quad \hat{T} = \hat{p}\partial_x^2 + \hat{q}\partial_x + \hat{r},$$

if T, $\hat{T}$ are related by a rational Darboux transformation, then their coefficients satisfy

$$\hat{p} = p,$$
$$\hat{q} = q + p' - \frac{2b'}{b}p,$$
$$\hat{r} = r + q' + up' - \frac{b'}{b}(q + p') + \left(2\left(\frac{b'}{b}\right)^2 - \frac{b''}{b} + 2u'\right)p.$$

If we let ϕ_0 be a solution of $A[y] = 0$, consequently, $u = \phi_0'/\phi_0$, then there exist a constant λ_0 such that

$$T = BA + \lambda_0, \quad T[\phi_0] = \lambda_0\phi_0$$

which means that ϕ_0 is an eigenfunction of T with respect to the eigenvalue λ_0. Let $\{\phi_\alpha\}_{\alpha\in\mathbb{I}}$ be the set of eigenfunctions of T such that

$$T[\phi_\alpha] = \lambda_\alpha\phi_\alpha, \quad \alpha \in \mathbb{I}.$$

For the partner operator of T defined by $\hat{T} = AB + \lambda_0$, its eigenfunctions can be given by

$$\hat{\phi}_\alpha = \begin{cases} \dfrac{b}{p\omega\phi_0}, & \text{if } A[\phi_\alpha] = 0 \quad (2.1.2) \\ A[\phi_\alpha], & \text{otherwise} \quad (2.1.3) \end{cases}$$

where ω is given by $\omega = e^{\int \frac{q-p'}{p}}$. In fact, if $A[\phi_\alpha] = 0$, then

$$\hat{T}[\hat{\phi}_\alpha] = AB[\hat{\phi}_\alpha] + \lambda_0\hat{\phi}_\alpha = \lambda_0\hat{\phi}_\alpha$$

since $B[\hat{\phi}_\alpha] = 0$, and, if $A[\phi_\alpha] \neq 0$, then

$$\hat{T}[A[\phi_\alpha]] = ABA[\phi_\alpha] + \lambda_0\hat{\phi}_\alpha = A[(\lambda_\alpha - \lambda_0)\phi_\alpha] + \lambda_0\hat{\phi}_\alpha = \lambda_\alpha\hat{\phi}_\alpha.$$

Hence the rational Darboux transformation

$$(T, \{\phi_\alpha\}) \mapsto (\hat{T}, \{\hat{\phi_\alpha}\})$$

is an isospectral transformation:

$$\hat{T}[\hat{\phi}_\alpha] = \lambda_\alpha\hat{\phi}_\alpha, \quad \forall \alpha \in \mathbb{I}.$$

Next we consider iterated rational Darboux transformations.

Definition 2.1.2. *Let T, $\hat{T}$ be second-order differential operators with rational coefficients. We say that T and $\hat{T}$ are gauge-equivalent if there exist a complex-valued rational function σ such that*

$$\sigma T = \hat{T}\sigma,$$

where σ is referred as the gauge-factor. And say that $\hat{T}$ is Darboux connected to T if there exists a differential operator L such that

$$LT = \hat{T}L.$$

In particular, gauge-equivalent operators are Darboux connected since they are related by a zeroth-order intertwining relation. The relations between coefficients of gauge-equivalent operators T, $\hat{T}$ can be obtained from straight-forward computations:

$$\begin{aligned}
&\hat{p} = p, \\
&\hat{q} = q - \frac{2\sigma'}{\sigma}p, \\
&\hat{r} = r - \frac{\sigma'}{\sigma}q + \left(2\left(\frac{\sigma'}{\sigma}\right)^2 - \frac{\sigma''}{\sigma}\right)p.
\end{aligned}$$

Proposition 2.1.2. *Two second-order differential operators with rational coefficients T, $\hat{T}$ are Darboux connected if and only if they are either gauge-equivalent, or they are connected by a factorization chain, i.e., there exist second-order differential operators T_i with $T_0 = T$ and $T_n = \hat{T}$ such that*

$$\begin{aligned}
&T_i = B_iA_i + \lambda_i, \quad i = 0, 1, \dots, n-1 \\
&T_{i+1} = A_iB_i + \lambda_i,
\end{aligned}$$

where A_i, B_i are first-order differential opeartors, λ_i are constants, $i = 0, 1, \dots, n-1$.

In fact, the existence of factorization chain between T and $\hat{T}$ can be demonstrated as the following sequence of eigenvalue equations which are indeed the iterated utilization of rational Darboux transformations

$$\begin{aligned}
T[\phi_0] = T_0[\phi_0] &= \lambda_0\phi_0, \\
&T_1[\phi_1] = \lambda_1\phi_1, \quad T_1[\hat{\phi}_0] = \lambda_0\hat{\phi}_0, \\
&T_2[\phi_2] = \lambda_2\phi_2, \quad T_2[\hat{\phi}_1] = \lambda_1\hat{\phi}_1, \\
&\vdots \\
\hat{T}[\phi_n] = T_n[\hat{\phi}_{n-1}] &= \lambda_{n-1}\hat{\phi}_{n-1}.
\end{aligned}$$

For simplicity of computation, here we assume that $\lambda_0, \lambda_1, \cdots, \lambda_{n-1}$ are distinct numbers. First, we find a seed solution of $T_0[\phi^{(0)}] = \lambda^{(0)}\phi^{(0)}$ $(\lambda^{(0)} \neq \lambda_0)$, let $A_0 = b_0(\partial_x - \phi'^{(0)}/\phi^{(0)})$. Notice that $A_0[\phi_0] \neq 0$, denote $\hat{\phi}_0 = A_0[\phi_0]$ then we get $T_1[\hat{\phi}_0] = \lambda_0\hat{\phi}_0$. Let $A_1 = b_1(\partial_x - \hat{\phi}_0'/\hat{\phi}_0)$, $A_1[\phi_1] \neq 0$ and $\hat{\phi}_1 = A_1[\phi_1] = b_1(\phi_1' - \phi_1\hat{\phi}_0'/\hat{\phi}_0) = b_1\mathrm{Wr}[\hat{\phi}_0, \phi_1]/\hat{\phi}_0$, here Wr represents the Wronskian type determinant. In the same way we will find that $A_2 = b_2(\partial_x - \hat{\phi}_1'/\hat{\phi}_1)$ and $\hat{\phi}_2 = A_2[\phi_2] = b_2(\phi_2' - \phi_2\hat{\phi}_1'/\hat{\phi}_1) = b_2\mathrm{Wr}[\hat{\phi}_1, \phi_2]/\hat{\phi}_1$. Continue this procedure, it turns out that

$$\hat{\phi}_{n-1} = \frac{b_{n-1}}{\hat{\phi}_{n-2}}\mathrm{Wr}[\hat{\phi}_{n-2}, \phi_{n-1}].$$

In the case where $b_0 = b_1 = \cdots = b_{n-1} = 1$, it follows inductively

$$\hat{\phi}_{n-1} = \frac{\mathrm{Wr}[\phi^{(0)}, \phi^{(1)}, \ldots, \phi^{(n-1)}, \phi^{(n)}]}{\mathrm{Wr}[\phi^{(0)}, \phi^{(1)}, \ldots, \phi^{(n-1)}]},$$

here $\phi^{(i)}$, $i = 0, 1, \ldots, n$ are different eigenfunctions of T_0.

Till now we have shown how exceptional polynomial sequence can be obtained by a rational Darboux transformation and iterated rational Darboux transformations. The operator related to exceptional polynomial sequences are called the exceptional operators.

Definition 2.1.3. *A second-order differential operator T is exceptional if T has polynomial eigenfunctions for all but finitely many degrees. Specifically, there exists a finite set of natural numbers $\{k_1, \ldots, k_m\} \subset \mathbb{N}$ such that for all $k \notin \{k_1, \ldots, k_m\}$, there exists a polynomial y_k of degree k satisfying the following eigenvalue equation:*

$$T[y_k] = \lambda_k y_k, \quad \lambda_k \in \mathbb{C},$$

while no such polynomials exists if $k \in \{k_1, \ldots, k_m\}$. Such a polynomial system is called the exceptional orthogonal polynomial system, where $k_1, \ldots, k_m$ are the exceptional degrees, and m is the codimension.

The following theorem implies that every exceptional operator is Darboux connected to a classical operator.

Theorem 2.1.1 (M. García-Ferrero, D. Gómez-Ullate and R. Milson [23])**.** *Every exceptional orthogonal polynomial system can be obtained by applying a finite sequence of Darboux transformations to a classical orthogonal polynomial system.*

Note that this theorem was only proved for the "very classical orthogonal polynomials" (the Hermite, Laguerre and Jacobi polynomials), it may not hold true for all the COP but still has great instructions for deriving exceptional extensions of COP.

2.2 Exceptional extensions of the very classical orthogonal polynomials

In this section we will introduce the definition and properties of exceptional extensions of the very classical orthogonal polynomials. First, we quickly review some properties of the very classical orthogonal polynomials. The eigenvalue equation of the very classical orthogonal polynomials can be rewritten as the well known Sturm-Liouville type equation

$$(P(x)y'(x))' + R(x)y(x) = \lambda\omega(x)y(x),$$

where $P(x) = \omega(x)p(x)$, $R(x) = \omega(x)r(x)$. The weight function $\omega(x)$ satisfies the Pearson equation

$$\big(p(x)w(x)\big)' = q(x)w(x) \tag{2.2.1}$$

and the conditions

$$p(x)w(x)x^k = 0, \quad k \in \mathbb{N} \tag{2.2.2}$$

on the boundary of the interval I.

Denote $\mathscr{P}$ the ring of polynomials. Let us introduce the definition of the exceptional extensions of the very classical orthogonal polynomials [23].

Definition 2.2.1. *(Exceptional orthogonal polynomials)*
A sequence of polynomials $\{y_k(x)\}_{k\in\mathbb{N}/\{k_1,\cdots,k_m\}}$ is called a sequence of exceptional orthogonal polynomials if

(1) the y_k's are the eigenfunctions of a second-order differential operator T, $T = p\partial_x^2 + q\partial_x + r$, where p, q, r are rational functions on x;

(2) there is an open interval $I \in \mathbb{R}$ such that

(1-a) the associated weight function $w(x)$, as given in (2.2.1), is single valued, and integrable on I, and moreover,

(1-b) all moments are finite, i.e.

$$\int_I x^j \omega(x)dx < \infty, \quad j \in \mathbb{N}/\{k_1,\cdots,k_m\};$$

(1-b) $y(x)p(x)\omega(x) \to 0$ at the endpoints of I for every polynomial $y \in \mathscr{P}$.

(3) the vector space span $\{y_k : k \notin \{k_1,\cdots,k_m\}\}$ is dense in the weighted Hilbert space $L^2(\omega(x)dx, I)$.

The weight functions associated with these exceptional polynomials turn out to the those of the classical ones over the square of a polynomial [23].

Theorem 2.2.1. *The weight function $\omega(x)$ of XOP has the form*

$$\hat{\omega}(x) = \frac{\omega(x)}{\eta^2(x)},$$

where $\eta(x)$ is a real-valued polynomial which is non-vanishing on I, $\omega(x)$ is the weight function of a classical orthogonal polynomial system.

Remark 2.2.1. *Note that all the zeros of $\eta(x)$ lie outside I by assumption (2) in the Definition 2.2.1. If an exceptional orthogonal polynomial system has polynomials for all degrees (i.e. $m = 0$), then it defines a classical orthogonal polynomial system, which up to an affine transformation must be Hermite, Laguerre or Jacobi polynomials.*

Specifically, the second-order differential equations satisfied by the three types exceptional orthogonal polynomials are given by [16–18]

$$H_n''(x) - 2\left(x + \frac{\eta_H'(x)}{\eta_H(x)}\right)H_n'(x) + \left(\frac{\eta_H''(x)}{\eta_H(x)} + 2x\frac{\eta_H'(x)}{\eta_H(x)} + 2n - 2k - 2u_{\mathscr{F}}^H\right)H_n(x) = 0, \tag{2.2.3}$$

$$\begin{aligned} &xL_n''(x) + \left(\alpha + k' + 1 - x - 2x\frac{\eta_L'(x)}{\eta_L(x)}\right)L_n'(x) \\ &+ \left(x\frac{\eta_L''(x)}{\eta_L(x)} + (x - \alpha - k')\frac{\eta_L'(x)}{\eta_L(x)} + n - k_1 - u_{\mathscr{F}}^L\right)L_n(x) = 0, \quad \alpha > -1, k' > 0, \end{aligned} \tag{2.2.4}$$

$$
\begin{aligned}
&(1-x^2)P_n''(x)+\left(\beta-\alpha-2k_2'-(\alpha+\beta+2k_1'+2)x-2(1-x^2)\frac{\eta_J'(x)}{\eta_J(x)}\right)P_n'(x)\\
&+\left((1-x^2)\frac{\eta_L''(x)}{\eta_L(x)}+\left[\alpha-\beta+2k_2'+(2k_1'+\alpha+\beta)x\right]\frac{\eta_J'(x)}{\eta_J(x)}+\lambda(n-u_{\mathscr{F}}^J)-\lambda(k_1')\right)P_n(x)=0,\\
&\alpha,\beta>-1,k_1'+k_2'>0,
\end{aligned}
\tag{2.2.5}
$$

where $H_n(x)$, $L_n(x)$, $P_n(x)$ denote exceptional Hermite, Laguerre, Jacobi polynomials of degree n, respectively. $\eta_H(x)$, $\eta_L(x)$, $\eta_J(x)$ are polynomials whose degrees coincide with the codimension of the related XOPS, α, β, k, k', k_1, k_1', k_2', $u_{\mathscr{F}}^H$, $u_{\mathscr{F}}^L$, $u_{\mathscr{F}}^J$ are certain constants and $\lambda(x)$ is a real-valued function, we shall omit the details about these functions and constants here for the convenience of discussion.

2.3 Stieltjes-Calogero type relations

There are many literatures considering the Stieltjes-Calogero type relations for zeros of orthogonal polynomials, the most famous result among which was obtained by T. J. Stieltjes [73] as follow

$$\sum_{k=1,k\neq j}^{n}\frac{1}{x_j-x_k}=x_j,$$

where $x_1,x_2,\cdots,x_n$ are zeros of Hermite polynomial of degree n. Stieltjes noted that this result implies an appealing interpretation of the location of zeros of Hermite polynomials as equilibrium positions of a simple one-dimensional n-particle problem. Moreover, He obtained similar relations for zeros of Laguerre and Jacobi polynomials thereafter. Interest in such kind of relations was revived by the work of Calogero and co-workers on integrable many-body systems [1, 8, 9]. Since then substantial efforts have been made on finding the Stieltjes-Calogero type relations for the purpose of revealing the relationship between zeros of polynomial systems and certain many-body systems.

To the best of the author's knowledge, the existing most generic method of obtaining this kind of relations was described in [67]. We apply this method to give some nontrivial results in the proceeding part. Let

$$S_{m,j}:=\sum_{k=1,k\neq j}^{n}\frac{1}{(x_j-x_k)^m},$$

if it satisfies that

$$\sum_{k=1,k\neq j}^{n}\frac{1}{(x_j-x_k)^m}=f(x_j),$$

where $f(x_j)$ is a rational function about x_j, then the above formula is called a Stieltjes-Calogero type relation.

Consider an n-th order differential equation,

$$\sum_{i=0}^{n}A_i(x)y^{(n-i)}(x)=f(x),\tag{2.3.1}$$

where $A_i(x)$ and $f(x)$ belong to $C^\infty(-\infty,\infty)$. Suppose that (2.6) has a monic polynomial solution $y(x)$ with simple roots:

$$y(x)=\prod_{i=1}^{n}(x-x_i),$$

then let $y_j(x)$ be defined as $y(x) = (x - x_j)y_j(x)$, i.e.

$$y_j(x) = \prod_{i=1, i \neq j}^{n} (x - x_i).$$

It follows that

$$y^{(r)}(x_j) = r y_j^{(r-1)}(x_j), \quad r \geq 1,$$

so that (2.3.1) becomes, after division by $y'(x)$ and evaluation at $x = x_j$,

$$\sum_{i=0}^{n-1} (n-i) A_i(x_j) \frac{y_j^{(n-i-1)}(x_j)}{y_j(x_j)} = \frac{f(x_j)}{y'(x_j)}. \tag{2.3.2}$$

$S_{1,j}$ can easily be obtained by observing the right hand side of the following formula

$$S_{1,j} = \frac{y_j'(x)}{y_j(x)}\Big|_{x=x_j}$$

thus the other terms immediately follow by differentiating at $x = x_j$

$$\left(\frac{y_j'(x)}{y_j(x)}\right)^{(s)}\Big|_{x=x_j} = (-1)^s s! S_{s+1,j}, \quad s = 0, 1, 2, \cdots.$$

In light of the above formula $S_{r,j} (r = 2, 3, \cdots)$ can be derived by analyzing a new function $Z_r(x)$

$$Z_r(x) := \frac{y_j^{(r)}(x)}{y_j(x)}$$

where $Z_r(x)$ satisfies a recurrence relation

$$Z_{r+1}(x) = Z_r'(x) + Z_1(x) Z_r(x),$$

and the initial condition

$$Z_1(x_j) = S_{1,j}.$$

Immediately we can rewrite (2.3.2) as

$$\sum_{i=0}^{n-1} (n-i) A_i(x_j) Z_{n-i-1}(x_j) = \frac{f(x_j)}{y'(x_j)}. \tag{2.3.3}$$

In the case of exceptional orthogonal polynomials, a second-order differential equation with rational coefficients was satisfied

$$p(x)y''(x) + q(x)y'(x) + r(x)y(x) = \lambda y(x), \tag{2.3.4}$$

one can easily obtain

$$S_{1,j} = -\frac{q(x_j)}{2p(x_j)}, \tag{2.3.5}$$

$$S_{2,j} = \frac{2[p'(x_j) + q(x_j)]S_{1,j} + [q'(x_j) + r(x_j)]}{3p(x_j)} + S_{1,j}^2, \tag{2.3.6}$$

$$S_{3,j} = -\frac{1}{8p(x_j)} \Big\{ 3[2p'(x_j) + q(x_j)][S_{1,j}^2 - S_{2,j}] + 2[p''(x_j) + 2q'(x_j) + r(x_j)]S_{1,j} \Big\} + \frac{3}{2} S_{1,j} S_{2,j} - \frac{1}{2} S_{1,j}^3, \tag{2.3.7}$$

and $S_{4,j}$, $S_{5,j}$, $\cdots$, by inductively calculating $Z_r(x)$, $r=2,3,\cdots$, and differentiating on both sides of (2.3.4).

Making use of the above method, we obtain the following properties on the zeros of exceptional orthogonal polynomials according to the second-order differential equations (2.2.3), (2.2.4) and (2.2.5).

Let x_1, $\cdots$, x_n denote the n zeros of the exceptional Hermite polynomial of degree n, then the Stieltjes-Calogero type relations of $x_1,\cdots,x_n$ follow

$$\begin{aligned}
S_{1,j} &= x_j + \frac{\eta_H'(x_j)}{\eta_H(x_j)},\\
S_{2,j} &= \frac{2}{3}(n-1-k-u_{\mathscr{F}}^H) - \frac{1}{3}\left[x_j^2 + \frac{\eta_H''(x_j)}{\eta_H(x_j)} - \left(\frac{\eta_H'(x_j)}{\eta_H(x_j)}\right)^2\right],\\
S_{3,j} &= \frac{1}{2}x_j.
\end{aligned}$$

Let x_1, $\cdots$, x_n denote the n zeros of the exceptional Laguerre polynomial of degree n, then the Stieltjes-Calogero type relations of $x_1,\cdots,x_n$ follow

$$\begin{aligned}
S_{1,j} &= -\frac{\alpha+1+k'-x_j}{2x_j} + \frac{\eta_L'(x_j)}{\eta_L(x_j)},\\
S_{2,j} &= -\frac{1}{12}\left\{\frac{(\alpha+1+k')(\alpha+5+k')}{x_j^2} - \frac{2(2n+\alpha+1+k'-2k_1'-2u_{\mathscr{F}}^L+2\frac{\eta_L'(x_j)}{\eta_L(x_j)})}{x_j}\right.\\
&\qquad\left. +1+4\frac{\eta_L''(x_j)}{\eta_L(x_j)} - 4\left(\frac{\eta_L'(x_j)}{\eta_L(x_j)}\right)^2\right\}.
\end{aligned}$$

Let $x_1,\cdots,x_n$ denote the n zeros of the exceptional Jacobi polynomial of degree n, then the Stieltjes-Calogero type relations of $x_1,\cdots,x_n$ follow

$$S_{1,j} = -\frac{\alpha-\beta+2k_2'+(\alpha+\beta+2+2k_1')x_j}{2(1-x_j^2)} + \frac{\eta_J'(x_j)}{\eta_J(x_j)}.$$

Remark 2.3.1. *Only the first several terms of these relations are listed here, the other terms, which tend to be more complicated (although some special terms may have elegant forms like $S_{3,j}$ for the zeros of exceptional Hermite polynomials), can be easily computed using this method. Notice that in the case of classical orthogonal polynomials all the terms containing k, k', k_1, k_1', k_2', $u_{\mathscr{F}}^a$, $\eta_a'(x_j)/\eta_a(x_j)$ and $\eta_a''(x_j)/\eta_a(x_j)$ $(a=H,L,J)$ disappear automatically.*

2.4 The electrostatic properties of zeros of the exceptional extensions of the very classical polynomials

The zeros of the exceptional extensions of the very classical polynomials can be divided into two groups: regular zeros which lie in the domain of orthogonality, and exceptional zeros (usually complex) which lie in the exterior of the domain. A conjecture considering the location of zeros of these exceptional orthogonal polynomials was drafted as follow:

Conjection 2.4.1 (A. B. Kuijlaars and R. Milson, [49])**.** *The regular zeros of exceptional orthogonal polynomials have the same asymptotic behavior as the zeros of their classical counterpart. The exceptional zeros converge to the zeros of the denominator polynomial $\eta(x)$.*

Moreover, properties like the location and asymptotic behavior of zeros of exceptional Hermite polynomials are described by A. B. Kuijlaars and R. Milson [49], of exceptional Laguerre and Jacobi polynomials by C. L. Ho, R. Sasaki [36] and D. Gómez-Ullate, M. García-Ferrero, R. Milson [28]. It concludes that the zeros of exceptional orthogonal polynomials usually share similar properties as their classical counterparts, especially for the regular zeros.

Below we revisit an energy problem by making use of properties of exceptional orthogonal polynomials. Considering the maximum of the following energy function

$$T_{\omega}(x_1,\cdots,x_n)=\prod_{j=1}^{n}\omega(x_j)\prod_{1\leq i<j\leq n}|x_i-x_j|^2, \tag{2.4.1}$$

where the n points x_1, $\cdots$, x_n lie on a compact set E. In the case of $\omega(x)=1$, I. Schur showed that the maximum of T_{ω} is obtained at the zeros of certain orthogonal polynomials [70]. If $\omega(x)$ takes a classical weight, namely with Hermite weight $\omega(x)=e^{-x^2}$, with Laguerre weights $\omega_{\alpha}(x)=x^{\alpha}e^{-x}$, with Jacobi weights $\omega_{\alpha,\beta}(x)=(1-x)^{\alpha}(1+x)^{\beta}$, then the maximum of T_{ω} is attained at the zeros of orthogonal polynomials corresponding to ω, $\omega_{\alpha-1}$, $\omega_{\alpha-1,\beta-1}$, respectively [37]. Results for the zeros of general orthogonal polynomials can be found in [40]. In addition, Á. P. Horv*á*th proved that the set of regular zeros of exceptional Hermite polynomials is the solution of the maximum problem with respect to the weight $\hat{\omega}(x)P_m^2(x)$, where $\hat{\omega}(x)$ is the weight of exceptional Hermite polynomials, $P_m(x)$ is a polynomial whose zeros are the exceptional zeros of an exceptional Hermite polynomial of codimension m [38]. Similar results have also been reported in the cases of the so-called X_m-Laguerre polynomials and X_m-Jacobi polynomials [39].

Remark 2.4.1. *As is pointed out in* [40]*, T_{ω} is called an energy function in light of its potential theoretic background. In fact, taking the logarithm in* (1.1)*, the maximization problem of* (1.1) *is equivalent to the minimization problem of the following function*

$$-\ln\left(T_{\omega}\right)=\sum_{j=1}^{n}\ln\frac{1}{\omega(x_i)}+\sum_{1\leq i<j\leq n}\ln\frac{1}{|x_i-x_j|^2}.$$

The second summation in the right-hand side can be interpreted as the energy of a system of n like-charged particles located at the points $\{x_i\}_{i=1}^{n}$, where the repelling force between two particles is proportional to the reciprocal of the square of the distance between them. The first summation refers to the total external potential of this system. Thus, $-\ln\left(T_{\omega}\right)$ is the total energy of this n-particle system.

In what follows, we investigate the maximum of the energy function (2.4.1) with respect to $\omega(x)=\hat{\omega}(x)p(x)$, where $p(x)$ is the coefficient of the following second-order differential equation satisfied by the exceptional orthogonal polynomials with respect to $\hat{\omega}(x)$

$$p(x)y''(x)+q(x)y'(x)+r(x)y(x)=\lambda y(x), \tag{2.4.2}$$

the prime denotes derivative with respect to x, $y'(x)=dy(x)/dx$.

Before proving the main result of this section we shall introduce some lemmas.

Lemma 2.4.1. *An Hermitian strictly diagonally dominant matrix with real positive diagonal entries is positive definite.*

Proof. Let A denote an Hermitian strictly diagonally dominant matrix with real positive diagonal entries, then it follows from the Gershgorin circle theorem that all the eigenvalues of A are positive, which implies that A is positive definite. □

Lemma 2.4.2 (Uniqueness of the maximum point of T_{ω})**.** *Let $\omega(x)$ be a non-nagative, continuous weight on $I\subset\mathbb{R}$ such that* $\ln\omega(x)$ *is concave, i.e.* $(\ln\omega(x))''\leq 0$, $\forall x\in I$*, then the maximum point of T_{ω} is unique.*

Proof. Assume that $\{a_i\}_{i=1}^n$ and $\{b_i\}_{i=1}^n$ are maximum points of T_ω enumerated in increasing order, let $c_i = (a_i + b_i)/2$. We consider the value of T_ω at the point $\{c_i\}_{i=1}^n$. Rewrite T_ω as

$$T_\omega(x_1,\cdots,x_n) = \prod_{j=1}^n \omega(x_j) \prod_{1\le i<j\le n} |x_i - x_j|^2 = \prod_{1\le i<j\le n} |x_i - x_j|^2 [\omega(x_i)\omega(x_j)]^{\frac{4}{n(n-1)}},$$

then because of the ordering of the points $\{a_i\}_{i=1}^n$, $\{b_i\}_{i=1}^n$ and the log-concavity of $\omega(x)$, we have

$$\begin{aligned}
\ln\left(|c_i - c_j|^2(\omega(c_i)\omega(c_j))^{\frac{4}{n(n-1)}}\right) &= \ln|c_i - c_j|^2 + \frac{4}{n(n-1)}(\ln\omega(c_i) + \ln\omega(c_j)) \\
&= \ln\big(|\frac{a_i - a_j}{2}| + |\frac{b_i - b_j}{2}|\big)^2 + \frac{4}{n(n-1)}\left[\ln\omega(\frac{a_i + b_i}{2}) + \ln\omega(\frac{a_j + b_j}{2})\right] \\
&\ge \ln|a_i - a_j||b_i - b_j| + \frac{2}{n(n-1)}(\ln\omega(a_i) + \ln\omega(b_i) + \ln\omega(a_j) + \ln\omega(b_j)) \\
&= \frac{1}{2}\ln\left(|a_i - a_j|^2(\omega(a_i)\omega(a_j))^{\frac{4}{n(n-1)}}\right) + \frac{1}{2}\ln\left(|b_i - b_j|^2(\omega(b_i)\omega(b_j))^{\frac{4}{n(n-1)}}\right)
\end{aligned}$$

where the arithmetic-geometric mean inequality was used, and the equality holds if and only if $a_i = b_i$, $i = 1,\cdots,n$, which establishes the uniqueness. □

As pointed out in [81], Stieltjes showed that (when $\omega(x)$ is a classical weight) $-\ln T_\omega(x_1,\cdots,x_n)$ attains a minimum when $x_1,\cdots,x_n$ are the zeros of the corresponding classical orthogonal polynomial. However, Stieljes did not explicitly show that this position is a minimum (even though he explicitly mentions that it is a minimum). Here we reformulate these results as the following theorem and give an explicit proof.

Theorem 2.4.1. *Let $\omega(x) = \hat{\omega}(x)p(x)$, where $\hat{\omega}(x)$ takes a classical weight, $p(x)$ is the coefficient in (2.4.2), namely, $\omega(x) = e^{-x^2}$ for Hermite polynomials, or $\omega(x) = x\cdot x^\alpha e^{-x}$ for Laguerre polynomials, or $\omega(x) = (1-x^2)\cdot(1-x)^\alpha(1+x)^\beta$ for Jacobi polynomials. Then in the domain I with respect to $\hat{\omega}(x)$, the energy function T_ω attains its maximum at the set of zeros of the corresponding orthogonal polynomials.*

Proof. Let $x_1,\cdots,x_n$ denote the zeros of a classical orthogonal polynomial of degree n with respect to the weight $\hat{\omega}(x)$ (with $\eta(x) = 1$). By differentiating $\ln T_\omega(y_1,\cdots,y_n)$ in y_i, $i = 1,2,\ldots,n$, we have

$$\begin{aligned}
\frac{\partial \ln T_\omega(y_1,\cdots,y_n)}{\partial y_i} &= \big(\frac{\omega'}{\omega}\big)(y_i) + \sum_{k=1,k\ne i}^n \frac{2}{y_i - y_k}, \\
&= \frac{\hat{\omega}'(y_i)}{\hat{\omega}(y_i)} + \frac{p'(y_i)}{p(y_i)} + \sum_{k=1,k\ne i}^n \frac{2}{y_i - y_k},
\end{aligned}$$

It follows from Pearson equation (2.2.1) and the Stieltjes-Calogero type relation (2.3.5) that

$$\frac{\hat{\omega}'(x)}{\hat{\omega}(x)} + \frac{p'(x)}{p(x)} = \frac{q(x)}{p(x)}, \quad S_{1,i} = \sum_{k=1,k\ne i}^n \frac{1}{x_i - x_k} = -\frac{q(x_i)}{2p(x_i)}.$$

which imply that

$$\frac{\partial \ln T_\omega(x_1,\cdots,x_n)}{\partial x_i} = 0.$$

Thus, $X = (x_1, \cdots, x_n)$ is a critical point of the energy function T_ω, which means T_ω has a local extremum at X. Next we consider the Hessian matrix H of $(-\ln T_\omega)$, if H is positive definite at X, then T_ω has a local maximum at X. The off-diagonal and diagonal elements of H are given by

$$
\begin{aligned}
H_{ij} &= \frac{\partial^2(-\ln(T_\omega(y_1, \cdots, y_n)))}{\partial y_i \partial y_j} = -\frac{2}{(y_i - y_j)^2}, \quad i \neq j \\
H_{ii} &= \frac{\partial^2(-\ln(T_\omega(y_1, \cdots, y_n)))}{\partial y_i^2} = (-\frac{\omega'}{\omega})'(y_i) + \sum_{j=1, j\neq i}^{n} \frac{2}{(y_i - y_j)^2} \\
&= \frac{q(y_i)p'(y_i) - p(y_i)q'(y_i)}{p(y_i)^2} + \sum_{j=1, j\neq i}^{n} \frac{2}{(y_i - y_j)^2}.
\end{aligned}
$$

Since $q(x)p'(x) - p(x)q'(x) > 0$, $\forall x \in \mathbb{R}$, it follows that H is Hermitian, strictly diagonally dominant, and has real positive diagonal entries, thus H is positive definite. This means that T_ω has a maximum value at the point $(x_1, \cdots, x_n)$. In fact, $q(x)p'(x) - p(x)q'(x) > 0$ is always true in the case of classical orthogonal polynomials. Denote the left hand side of the inequality by $F(x)$. For Hermite polynomials, $p(x) = 1, q(x) = -2x$, $F(x) = 2 > 0$; for Laguerre polynomials, $p(x) = x, q(x) = \alpha + 1 - x$, $F(x) = \alpha + 1 > 0$ (since $\alpha > -1$); for Jacobi polynomials, $p(x) = 1 - x^2, q(x) = \beta - \alpha - (\alpha + \beta + 2)x$, $F(x) = (\alpha + \beta + 2)(1 + x^2) - (\beta - \alpha)2x > 0$ (since $\alpha, \beta > -1$).

The uniqueness of the maximum point follows from the fact that each weight $\omega(x)$ is log-concave in the related domain I. Moreover, T_ω tends to zero at the boundary of the domain related to $\hat{\omega}(x)$, thus it attains a unique maximum at $(x_1, \cdots, x_n)$. □

Note that the zeros of classical orthogonal polynomials are all real, simple and distinct [74, chapter 6.2], which guarantees that T_ω dose not vanish at these zeros. However, the exceptional orthogonal polynomials have complex zeros and were conjectured to have simple zeros except possibly for the zeros at $z = 0$ [49]. Here we assume an exceptional orthogonal polynomial $P_{n+m}(z)$ of degree $n + m$ has $n + m$ simple zeros , and we denote the set consisting of these zeros by

$$Z = \{z_1, \cdots, z_n, z_{n+1}, \cdots, z_{n+m}\}$$

where $z_1 = x_1$, $\cdots$, $z_n = x_n$ are the n real zeros and $z_{n+1} = x_{n+1} + i\mu_1$, $\cdots$, $z_{n+m} = x_{n+m} + i\mu_m$ are the m complex zeros. Here we consider the function $T_\omega(Y) := T_\omega(y_1, \cdots, y_n, y_{n+1} + i\mu_1, \cdots, y_{n+m} + i\mu_m)$ with $n + m$ real variables. $T_\omega(Y)$ is a complex-valued function as long as $m \geq 1$, so we check the maximum value of $|T_\omega(Y)|^2 = T_\omega(Y)\overline{T_\omega(Y)}$ instead. First, rewrite $T_\omega(Y)$ as

$$
\begin{aligned}
T_\omega(Y) = \prod_{i=1}^{n} \omega(y_i) \cdot \prod_{j=1}^{m} \omega(y_{n+j} + i\mu_j) \cdot \prod_{1\leq i<j\leq n} |y_i - y_j|^2 \cdot \prod_{1\leq k<l\leq m} |y_{n+k} + i\mu_k - (y_{n+l} + i\mu_l)|^2 \\
\cdot \prod_{\substack{1\leq s\leq n \\ 1\leq t\leq m}} |y_s - (y_{n+t} + i\mu_t)|^2,
\end{aligned}
$$

then we have

$$
\begin{aligned}
|T_\omega(Y)|^2 = \prod_{i=1}^{n} \omega^2(y_i) \cdot \prod_{j=1}^{m} \omega(y_{n+j} + i\mu_j)\omega(y_{n+j} - i\mu_j) \cdot \prod_{1\leq i<j\leq n} |y_i - y_j|^4 \\
\cdot \prod_{1\leq k<l\leq m} |(y_{n+k} - y_{n+l})^2 + (\mu_k - \mu_l)^2|^2 \cdot \prod_{\substack{1\leq s\leq n \\ 1\leq t\leq m}} |(y_s - y_{n+t})^2 + \mu_t^2)|^2.
\end{aligned}
$$

For $1 \le i \le n$, we have

$$\frac{\partial \ln |T_\omega(Y)|^2}{\partial y_i} = 2\frac{\omega'(y_i)}{\omega(y_i)} + \sum_{j=1, j\neq i}^{n} \frac{4}{y_i - y_j} + \sum_{t=1}^{m} \frac{4(y_i - y_{n+t})}{(y_i - y_{n+t})^2 + \mu_t^2},$$

$$= 2\frac{\omega'(y_i)}{\omega(y_i)} + \sum_{j=1, j\neq i}^{n} \frac{4}{y_i - y_j} + \sum_{t=1}^{m} \frac{4}{y_i - (y_{n+t} + i\mu_t)} - \sum_{t=1}^{m} \frac{4i\mu_t}{(y_i - y_{n+t})^2 + \mu_t^2}.$$

Notice that the sum of the first three terms on the right-hand side of the last equation equals 0 at the point $(x_1, \cdots, x_{n+m})$ due to (2.2.1) and (2.3.4). This together with the fact that the left-hand side of the above equations is real implies that

$$\sum_{t=1}^{m} \frac{\mu_t}{(x_i - x_{n+t})^2 + \mu_t^2} = 0. \tag{2.4.3}$$

For $n+1 \le i \le n+m$, we have

$$\frac{\partial \ln |T_\omega(Y)|^2}{\partial y_i} = \frac{\omega'(y_i + i\mu_{i-n})}{\omega(y_i + i\mu_{i-n})} + \frac{\omega'(y_i - i\mu_{i-n})}{\omega(y_i - i\mu_{i-n})} + \sum_{l=1, l\neq i-n}^{m} \frac{4(y_i - y_{n+l})}{(y_i - y_{n+l})^2 + (\mu_{i-n} - \mu_l)^2} + \sum_{s=1}^{n} \frac{4(y_i - y_s)}{(y_i - y_s)^2 + \mu_{i-n}^2}$$

$$= 2\frac{\omega'(y_i + i\mu_{i-n})}{\omega(y_i + i\mu_{i-n})} + \sum_{l=1, l\neq i-n}^{m} \frac{4}{(y_i + i\mu_{i-n}) - (y_{n+l} + i\mu_l)} + \sum_{s=1}^{n} \frac{4}{(y_i + i\mu_{i-n}) - y_s}$$

$$+ \frac{\omega'(y_i - i\mu_{i-n})}{\omega(y_i - i\mu_{i-n})} - \frac{\omega'(y_i + i\mu_{i-n})}{\omega(y_i + i\mu_{i-n})} + \sum_{l=1, l\neq i-n}^{m} \frac{4i(\mu_{i-n} - \mu_l)}{(y_i - y_{n+l})^2 + (\mu_{i-n} - \mu_l)^2} + \sum_{s=1}^{n} \frac{4i\mu_{i-n}}{(y_i - y_s)^2 + \mu_{i-n}^2}.$$

Again, we find that the sum of the first three terms on the right-hand side of the last equation equals 0 at the point $(x_1, \cdots, x_{n+m})$, thus implies

$$\frac{\omega'(x_i - i\mu_{i-n})}{\omega(x_i - i\mu_{i-n})} - \frac{\omega'(x_i + i\mu_{i-n})}{\omega(x_i + i\mu_{i-n})} + \sum_{l=1, l\neq i-n}^{m} \frac{4i(\mu_{i-n} - \mu_l)}{(x_i - x_{n+l})^2 + (\mu_{i-n} - \mu_l)^2} + \sum_{s=1}^{n} \frac{4i\mu_{i-n}}{(x_i - x_s)^2 + \mu_{i-n}^2} = 0. \tag{2.4.4}$$

Therefore we have shown that $(x_1, \cdots, x_{n+m})$ is a critical point of $|T_\omega(Y)|^2$.

The Hessian matrix H of $(-\ln |T_\omega(Y)|^2)$ has four types off-diagonal elements and two types diagonal elements:

$$H_{ij} = -\frac{4}{(y_i - y_j)^2}, \quad 1 \le i \le n, 1 \le j \le n, i \neq j,$$

$$H_{ij} = -\frac{4[(y_i - y_j)^2 - \mu_{j-n}^2]}{[(y_i - y_j)^2 + \mu_{j-n}^2]^2}, \quad 1 \le i \le n, n+1 \le j \le n+m,$$

$$H_{ij} = -\frac{4[(y_i - y_j)^2 - \mu_{i-n}^2]}{[(y_i - y_j)^2 + \mu_{i-n}^2]^2}, \quad n+1 \le i \le n+m, 1 \le j \le n,$$

$$H_{ij} = -\frac{4[(y_i - y_j)^2 - (\mu_{i-n} - \mu_{j-n})^2]}{[(y_i - y_j)^2 + (\mu_{i-n} - \mu_{j-n})^2]^2}, \quad n+1 \le i \le n+m, n+1 \le j \le n+m, i \neq j,$$

and

$$H_{ii} = \left(-\frac{2\omega'(y_i)}{\omega(y_i)}\right)' + \sum_{j=1,j\neq i}^{n} \frac{4}{(y_i - y_j)^2} + \sum_{t=1}^{m} \frac{4[(y_i - y_{n+t})^2 - \mu_t^2]}{[(y_i - y_{n+t})^2 + \mu_t^2]^2}, \quad 1 \le i \le n,$$

$$H_{ii} = \left(-\frac{\omega'(y_i + i\mu_{i-n})}{\omega(y_i + i\mu_{i-n})}\right)' + \left(-\frac{\omega'(y_i - i\mu_{i-n})}{\omega(y_i - i\mu_{i-n})}\right)' + \sum_{l=1,l\neq i}^{m} \frac{4[(y_i - y_{n+l})^2 - (\mu_{i-n} - \mu_l)^2]}{[(y_i - y_{n+l})^2 + (\mu_{i-n} - \mu_l)^2]^2}$$
$$+ \sum_{s=1}^{n} \frac{4[(y_i - y_s)^2 - \mu_{i-n}^2]}{[(y_i - y_s)^2 + \mu_{i-n}^2]^2}, \quad n+1 \le i \le n+m.$$

In order to find the condition for H to be positive definite, the following should be satisfied

$$H_{ii} > 0 \quad \text{and} \quad H_{ii} > \sum_{j=1,j\neq i}^{n+m} |H_{ij}|, \quad 1 \le i \le n+m,$$

which is equivalent to

$$H_{ii} > \sum_{j=1,j\neq i}^{n+m} |H_{ij}|, \quad 1 \le i \le n+m.$$

For $1 \le i \le n$, we have

$$\begin{aligned}
H_{ii} - \sum_{j=1,j\neq i}^{n+m} |H_{ij}| &= \left(-\frac{2\omega'(y_i)}{\omega(y_i)}\right)' + \sum_{t=1}^{m} \frac{4[(y_i - y_{n+t})^2 - \mu_t^2]}{[(y_i - y_{n+t})^2 + \mu_t^2]^2} - \sum_{t=1}^{m} \left| \frac{4[(y_i - y_{n+t})^2 - \mu_t^2]}{[(y_i - y_{n+t})^2 + \mu_t^2]^2} \right| \\
&= \left(-\frac{2\omega'(y_i)}{\omega(y_i)}\right)' + \sum_{t=1}^{m} \left[\frac{4}{(y_i - y_{n+t})^2 + \mu_t^2} - \frac{8\mu_t^2}{[(y_i - y_{n+t})^2 + \mu_t^2]^2} \right] \\
&\quad - \sum_{t=1}^{m} \left| \frac{4}{(y_i - y_{n+t})^2 + \mu_t^2} - \frac{8\mu_t^2}{[(y_i - y_{n+t})^2 + \mu_t^2]^2} \right| \\
&\ge \left(-\frac{2\omega'(y_i)}{\omega(y_i)}\right)' - \sum_{t=1}^{m} \frac{16\mu_t^2}{[(y_i - y_{n+t})^2 + \mu_t^2]^2} \\
&\ge \left(-\frac{2\omega'(y_i)}{\omega(y_i)}\right)' - \sum_{t=1}^{m} \frac{4}{(y_i - y_{n+t})^2},
\end{aligned}$$

for $n+1 \le i \le n+m$, we have

$$\begin{aligned}
H_{ii} - \sum_{j=1,j\neq i}^{n+m} |H_{ij}| &= \left(-\frac{\omega'(y_i + i\mu_{i-n})}{\omega(y_i + i\mu_{i-n})}\right)' + \left(-\frac{\omega'(y_i - i\mu_{i-n})}{\omega(y_i - i\mu_{i-n})}\right)' + \sum_{l=1,l\neq i-n}^{m} \frac{4[(y_i - y_{n+l})^2 - (\mu_{i-n} - \mu_l)^2]}{[(y_i - y_{n+l})^2 + (\mu_{i-n} - \mu_l)^2]^2} \\
&\quad + \sum_{s=1}^{n} \frac{4[(y_i - y_s)^2 - \mu_{i-n}^2]}{[(y_i - y_s)^2 + \mu_{i-n}^2]^2} - \sum_{l=1,l\neq i-n}^{m} \left| \frac{4[(y_i - y_{n+l})^2 - (\mu_{i-n} - \mu_l)^2]}{[(y_i - y_{n+l})^2 + (\mu_{i-n} - \mu_l)^2]^2} \right| - \sum_{s=1}^{n} \left| \frac{4[(y_i - y_s)^2 - \mu_{i-n}^2]}{[(y_i - y_s)^2 + \mu_{i-n}^2]^2} \right| \\
&\ge \left(-\frac{\omega'(y_i + i\mu_{i-n})}{\omega(y_i + i\mu_{i-n})}\right)' + \left(-\frac{\omega'(y_i - i\mu_{i-n})}{\omega(y_i - i\mu_{i-n})}\right)' - \sum_{l=1,l\neq i-n}^{m} \frac{4}{(y_i - y_{n+l})^2} - \sum_{s=1}^{n} \frac{4}{(y_i - y_s)^2} \\
&= \left(-\frac{\omega'(y_i + i\mu_{i-n})}{\omega(y_i + i\mu_{i-n})}\right)' + \left(-\frac{\omega'(y_i - i\mu_{i-n})}{\omega(y_i - i\mu_{i-n})}\right)' - \sum_{j=1,j\neq i}^{n+m} \frac{4}{(y_i - y_j)^2}.
\end{aligned}$$

The above inequalities imply that if

$$\Big(-\frac{2\omega'(x_i)}{\omega(x_i)}\Big)' > \sum_{j=n+1,j\neq i}^{n+m} \frac{4}{(x_i-x_j)^2} \tag{2.4.5}$$

and

$$\Big(-\frac{\omega'(x_i+i\mu_{i-n})}{\omega(x_i+i\mu_{i-n})}\Big)' + \Big(-\frac{\omega'(x_i-i\mu_{i-n})}{\omega(x_i-i\mu_{i-n})}\Big)' > \sum_{j=1,j\neq i}^{n+m} \frac{4}{(x_i-x_j)^2} \tag{2.4.6}$$

hold, then $|T_\omega(Y)|^2$ has a (local) maximum value at $X=(x_1,\cdots,x_n,x_{n+1},\cdots,x_{n+m})$. According to these discussions below we provide a sufficient condition for $|T_\omega(Y)|^2$ to obtain its maximum value at the point X.

Theorem 2.4.2. *Let $\omega(x)=\hat{\omega}(x)p(x)$, where $\hat{\omega}(x)$ takes an exceptional weight, $p(x)$ is the coefficient in (2.4.2), namely, $\omega(x)=e^{-x^2}/\eta_H^2(x)$ for exceptional Hermite polynomials, or $\omega(x)=x\cdot x^\alpha e^{-x}/\eta_L^2(x)$ for exceptional Laguerre polynomials, or $\omega(x)=(1-x^2)\cdot(1-x)^\alpha(1+x)^\beta/\eta_J^2(x)$ for exceptional Jacobi polynomials. Let $P_{n+m}(x)$ be an exceptional polynomial of degree $n+m$ corresponding to the weight $\hat{\omega}(x)$. Assume that the zeros of $P_{n+m}(x)$ are all simple, and denote x_i, $i=1,2,\ldots,n+m$, the the real parts of the zeros of $P_{n+m}(x)$. If the denominators $\eta_H(x)$, $\eta_L(x)$, $\eta_J(x)$ satisfy the following conditions*

$$\big(\ln\eta_\alpha(x)\big)''+k_\alpha \geq 0, \quad x\in I, \tag{2.4.7}$$

$$\big(\ln\eta_\alpha(x)\big)''|_{x=z_i}+k_\alpha > \sum_{j=n+1,j\neq i}^{n+m}\frac{1}{(x_i-x_j)^2}, \quad 1\leq i\leq n+m, \tag{2.4.8}$$

then in the domain I with respect to $\hat{\omega}(x)$, the real-valued function $|T_\omega(Y)|^2$ attains its maximum value at X, where the subscript α can be replaced by H, L, J, respectively, $k_H=1$, $k_L=k_J=0$.

Proof. Till now it has been known that if (2.4.5) and (2.4.6) are satisfied then $|T_\omega(Y)|^2$ has a (local) maximum value at X. The uniqueness requires that $(\ln\omega(x))''=(q(x)/p(x))'\leq 0$, $\forall x\in I$, provided the information of $p(x)$, $q(x)$ are given in (2.2.3), (2.2.4), (2.2.5), respectively, we check case by case using the same notations as we did in the proof of Theorem 4.3. Assuming it satisfies that

$$\big(\ln\eta_H(x)\big)''+1\geq 0, \quad x\in(-\infty,\infty), \tag{2.4.9}$$

$$\big(\ln\eta_L(x)\big)''\geq 0, \quad x\in(0,\infty), \tag{2.4.10}$$

$$\big(\ln\eta_J(x)\big)''\geq 0, \quad x\in(-1,1), \tag{2.4.11}$$

then for exceptional Hermite polynomials, it holds that

$$F(x)=2+2\big(\ln\eta_H(x)\big)''\geq 0,$$

as well as for exceptional Laguerre polynomials ($\alpha>-1, k'>0$) we have

$$F(x)=\alpha+k'+1+2x^2\big(\ln\eta_L(x)\big)''\geq 0,$$

and for exceptional Jacobi polynomials ($\alpha,\beta>-1, k_1'+k_2'>0$) we have

$$F(x)=(\alpha+\beta+2k_1'+2)(1+x^2)-(\beta-\alpha-2k_2')2x+2(1-x^2)^2\big(\ln\eta_J(x)\big)''\geq 0.$$

Moreover, since it holds respectively for the weight functions of exceptional Hermite, Laguerre, Jacobi polynomial that

$$\left(-\frac{\omega'(x)}{\omega(x)}\right)' = \begin{cases} 2+2\big(\ln\eta_H(x)\big)'', \\ \frac{\alpha+k'+1}{x^2}+2\big(\ln\eta_L(x)\big)'' > 2\big(\ln\eta_L(x)\big)'', \\ \frac{(\alpha+\beta+2k_1'+2)(1+x^2)-(\beta-\alpha-2k_2')2x}{(1-x^2)^2}+2\big(\ln\eta_J(x)\big)'' > 2\big(\ln\eta_J(x)\big)'', \end{cases}$$

we then rewrite (2.4.5) and (2.4.6) into the following conditions which can be implied by (2.4.8):

$$\begin{cases} 1+\big(\ln\eta_H(x_i)\big)'' \\ \big(\ln\eta_L(x_i)\big)'' \\ \big(\ln\eta_J(x_i)\big)'' \end{cases} > \sum_{j=n+1, j\neq i}^{n+m} \frac{1}{(x_i-x_j)^2}, \quad 1\le i\le n \tag{2.4.12}$$

and

$$\begin{cases} 2+\big(\ln\eta_H(x_i+i\mu_{i-n})\big)''+\big(\ln\eta_H(x_i-i\mu_{i-n})\big)'' \\ \big(\ln\eta_L(x_i+i\mu_{i-n})\big)''+\big(\ln\eta_L(x_i-i\mu_{i-n})\big)'' \\ \big(\ln\eta_J(x_i+i\mu_{i-n})\big)''+\big(\ln\eta_J(x_i-i\mu_{i-n})\big)'' \end{cases} > \sum_{j=1, j\neq i}^{n+m} \frac{2}{(x_i-x_j)^2}, \quad n+1\le i\le n+m. \tag{2.4.13}$$

Recall that $\omega(x)$ decays quickly at the boundary, thus $|T_\omega(Y)|^2$ tends to zero at the boundary. Concludingly, $|T_\omega(Y)|^2$ has a unique maximum at X if (2.4.7), (2.4.8) are satisfied. □

Notice that in the equations (2.4.3) and (2.4.4) we have

$$\frac{\mu_t}{(x_i-x_{n+t})^2+\mu_t^2} = \frac{1}{2i}\left[\frac{1}{(x_i-x_{n+t})-i\mu_t} - \frac{1}{(x_i-x_{n+t})+i\mu_t}\right],$$

and

$$\frac{4i(\mu_{i-n}-\mu_l)}{(x_i-x_{n+l})^2+(\mu_{i-n}-\mu_l)^2} = 2\left[\frac{1}{(x_i-x_{n+l})-i(\mu_{i-n}-\mu_l)} - \frac{1}{(x_i-x_{n+l})+i(\mu_{i-n}-\mu_l)}\right],$$

$$\frac{4i\mu_{i-n}}{(x_i-x_s)^2+\mu_{i-n}^2} = 2\left[\frac{1}{(x_i-x_s)-i\mu_{i-n}} - \frac{1}{(x_i-x_s)+i\mu_{i-n}}\right],$$

which lead to the following result.

Corollary 2.4.1. *If an exceptional orthogonal polynomial $P_{n+m}(z)$ has $n+m$ simple zeros consisting of n real zeros and m complex zeros:*

$$z_1 = x_1, \dots, z_n = x_n, z_{n+1} = x_{n+1}+i\mu_1, \dots, z_{n+m} = x_{n+m}+i\mu_m,$$

where $x_i\in\mathbb{R}, i=1,\dots,n+m$, $\mu_j\in\mathbb{R}, j=1,\dots,m$, then it holds that

$$\sum_{t=1}^{m}\frac{1}{(x_i-x_{n+t})+i\mu_t} = \sum_{t=1}^{m}\frac{1}{(x_i-x_{n+t})-i\mu_t}, \quad 1\le i\le n, \tag{2.4.14}$$

and

$$\begin{aligned} &\frac{\omega'(x_i+i\mu_{i-n})}{\omega(x_i+i\mu_{i-n})} + \sum_{l=1, l\neq i-n}^{m}\frac{2}{(x_i-x_{n+l})+i(\mu_{i-n}-\mu_l)} + \sum_{s=1}^{n}\frac{2}{(x_i-x_s)+i\mu_{i-n}} \\ = &\frac{\omega'(x_i-i\mu_{i-n})}{\omega(x_i-i\mu_{i-n})} + \sum_{l=1, l\neq i-n}^{m}\frac{2}{(x_i-x_{n+l})-i(\mu_{i-n}-\mu_l)} + \sum_{s=1}^{n}\frac{2}{(x_i-x_s)-i\mu_{i-n}}, \quad n+1\le i\le n+m. \end{aligned} \tag{2.4.15}$$

In particular, notice that

$$\frac{\omega'(x_i+i\mu_{i-n})}{\omega(x_i+i\mu_{i-n})}=\frac{\hat{\omega}'(x_i+i\mu_{i-n})}{\hat{\omega}(x_i+i\mu_{i-n})}+\frac{p'(x_i+i\mu_{i-n})}{p(x_i+i\mu_{i-n})}=-2S_{1,i},$$

it follows that the left-hand side of (2.4.15) is 0, consequently implies

$$\frac{\omega'(x_i-i\mu_{i-n})}{\omega(x_i-i\mu_{i-n})}+\sum_{l=1,l\neq i-n}^{m}\frac{2}{(x_i-x_{n+l})-i(\mu_{i-n}-\mu_l)}+\sum_{s=1}^{n}\frac{2}{(x_i-x_s)-i\mu_{i-n}}=0,\quad n+1\leq i\leq n+m.$$

2.4.1 Examples

Here we provide some examples which give evidence for our main result considering the case of exceptional Hermite polynomials. The exceptional Hermite polynomials are defined upon Wronskian determinants whose entries are Hermite polynomials according to a double partition [24]. Let $\lambda=(\lambda_1,\cdots,\lambda_r)$ be a non-decreasing sequence of non-negative integers

$$0\leq\lambda_1\leq\lambda_2\leq\cdots\leq\lambda_r,$$

we call λ a double (or even) partition if r is even and $\lambda_{2i-1}=\lambda_{2i}$, $i=1,\cdots,r/2$. The exceptional Hermite polynomials with respect to λ are defined as

$$H_n^{(\lambda)}=\mathrm{Wr}[H_{\lambda_1},H_{\lambda_2+1},\cdots,H_{\lambda_r+r-1},H_{n-|\lambda|+r}],\quad n-|\lambda|+r\in\mathbb{N}\backslash\{\lambda_1,\lambda_2+1,\cdots,\lambda_r+r-1\},$$

where Wr denotes the Wronskian determinant, H_j is the jth Hermite polynomial and $|\lambda|=\sum_i^r\lambda_i$. From this definition it is clear that $\deg H_n^{(\lambda)}(z)=n$. Recall from table 1 the weight function of exceptional Hermite polynomials is $\hat{\omega}_H(z)=e^{-z^2}/\eta_H^2(z)$, where we can now give η_H as

$$\eta_H:=\eta_H^{(\lambda)}=\mathrm{Wr}[H_{\lambda_1},H_{\lambda_2+1},\cdots,H_{\lambda_r+r-1}].$$

It is known that η_H has no zeros on the real line when λ is a double partition [24], hence $\hat{\omega}_H$ is a well-defined weight function on the real line. Since $\deg\eta_H=|\lambda|$, η_H has $|\lambda|$ complex zeros. According to theorem 2.3 of [49], if all the zeors of $H_n^{(\lambda)}$ are simple then the exceptional (complex) zeros converge to the zeros of η_H.

The problem described in the introduction is to find the maximum value of

$$T_\omega(x_1,\cdots,x_n)=\prod_{j=1}^{n}\omega(x_j)\prod_{1\leq i<j\leq n}|x_i-x_j|^2,$$

where $\omega=\hat{\omega}p$, specifically $\omega(x)=e^{-x^2}/\eta_H^2(x)$ in the current case. Let $Z=\{z_1,\cdots,z_n\}$ be the set of zeros of $H_n^{(\lambda)}(z)$. In order to check whether $|T_\omega|$ has a maximum value at Z or not, let us define

$$f(z)=\left|\frac{T_\omega(z_1+z,\cdots,z_n+z)}{T_\omega(z_1,\cdots,z_n)}\right|,$$

for different partition λ we observe the value of $f(z)$ around $z=0$.

Example 2.4.1. *When $\lambda=(1,1,1,1)$, $\eta_H=Wr[H_1,H_2,H_3,H_4]$, the associated exceptional Hermite polynomials are*

$$H_n^{(\lambda)}=Wr[H_1,H_2,H_3,H_4,H_n],\quad n\notin\{1,2,3,4\}.$$

Let $n = 8$, then $H_n^{(\lambda)}(z)$ has 4 complex zeros and 4 real zeros, $Z = \{z_1, \cdots, z_8\}$. Numerical results show that $z = 0$ is a saddle point of $f(z)$ when $z \in \mathbb{C}$ (since $T_\omega(z_1 + z, \cdots, z_n + z)$ is a holomorphic function, according to the maximum modulus principle the modulus $|T_\omega(z_1 + z, \cdots, z_n + z)|$ cannot exhibit a true local maximum within the domain). Nevertheless, if $z \in \mathbb{R}$, $f(z)$ attains its maximum at $z = 0$.

Example 2.4.2. *For $\lambda = (1,1,3,3)$, $\eta_H = Wr[H_1, H_2, H_5, H_6]$, the associated exceptional Hermite polynomials are*

$$H_n^{(\lambda)} = Wr[H_1, H_2, H_5, H_6, H_{n-4}], \quad n - 4 \notin \{1,2,5,6\}.$$

Let $n = 8$, then $H_n^{(\lambda)}(z)$ has 6 complex zeros and 2 real zeros, $Z = \{z_1, \cdots, z_8\}$. Again, it follows numerically that $z = 0$ is a saddle point of $f(z)$ when $z \in \mathbb{C}$ and a maximum point of $f(z)$ if $z \in \mathbb{R}$.

Remark 2.4.2. *The above two examples show that in some cases Z is a saddle point of $|T_\omega|$ while at the same time a maximum point of $|T_\omega|$ if all the imaginary parts of z_i's are fixed. However, this phenomenon does not arise for all cases.*

Example 2.4.3. *For $\lambda = (2,2,3,3)$, $\eta_H = Wr[H_2, H_3, H_5, H_6]$, the associated exceptional Hermite polynomials are*

$$H_n^{(\lambda)} = Wr[H_2, H_3, H_5, H_6, H_{n-6}], \quad n \notin \{2,3,5,6\}.$$

Let $n = 10$, then $H_n^{(\lambda)}(z)$ has 8 complex zeros and 2 real zeros, $Z = \{z_1, \cdots, z_{10}\}$. In this case one can observe from the numerical simulation of $f(z)$ that $z = 0$ is neither a maximum point nor a saddle point of $f(z)$, hence $|T_\omega|$ has no maximum at Z.

Chapter 3

Exceptional Bannai-Ito polynomials

In this chapter, we derive the exceptional extensions of the Bannai-Ito polynomials.

3.1 Bannai-Ito polynomials

First, let us introduce the definition and some basic properties of the Bannai-Ito polynomials. The Bannai-Ito polynomials, originally introduced in [3], are recently classified as a new kind of "classical" orthogonal polynomials [79] since they are identified to be the eigenfunctions of the difference operator

$$H = \alpha(x)(R - I) + \beta(x)(TR - I). \tag{3.1.1}$$

H is a Dunkl shift operator, where R is the reflection operator, T is the forward shift operator, and I is the identity operator acting as

$$R[f(x)] = f(-x), \quad T[f(x)] = f(x+1), \quad I[f(x)] = f(x).$$

Throughout this paper the operators R, T and I only influence x, for example, $R[f(x+1)] = f(-x+1)$ not $f(-x-1)$, and $T[f(-x)] = f(-x-1)$ not $f(-x+1)$. It is known that the Dunkl shift operator has polynomial eigenfunctions of all degrees if and only if its coefficients are given by

$$\alpha(x) = \frac{(x-\rho_1)(x-\rho_2)}{-2x}, \quad \beta(x) = \frac{(x-r_1+1/2)(x-r_2+1/2)}{2x+1}, \tag{3.1.2}$$

where r_1, r_2, ρ_1, ρ_2 are real numbers. In this setting the Dunkl shift operator is called the Bannai-Ito operator. The eigenfunctions of the Bannai-Ito operator are the Bannai-Ito polynomials $B_n(x)$,

$$H[B_n(x)] = \alpha(x)(B_n(-x) - B_n(x)) + \beta(x)(B_n(-x-1) - B_n(x)) = \lambda_n B_n(x),$$

where $B_n(x)$ is of degree n, and the eigenvalues are given by

$$\lambda_n = \begin{cases} \dfrac{n}{2}, & \text{if } n \text{ is even}, \quad (3.1.3)\\ r_1 + r_2 - \rho_1 - \rho_2 - \dfrac{n+1}{2}, & \text{if } n \text{ is odd}. \quad (3.1.4) \end{cases}$$

One should notice that the Bannai-Ito polynomials are defined upon four parameters, i.e. $B_n(x) := B_n(x;\rho_1,\rho_2,r_1,r_2)$, we use the former for simplicity.

The Bannai-Ito polynomials are discrete orthogonal polynomials. They are orthogonal with respect to a discrete, positive measure of weight function $\omega(x)$ on the Bannai-Ito grid $\{x_s\}_{s=0}^{N-1}$:

$$\sum_{s=0}^{N-1} \omega(x_s) B_n(x_s) B_m(x_s) = h_n \delta_{nm} \quad (h_n > 0; \quad 0 \le n, m < N),$$

where x_s $(s = 0, 1, \ldots, N-1)$ are the simple roots of $B_N(x)$ [79].

3.2 Generalized Darboux transformation of Dunkl shift operator

It has been addressed before that the DT is one of the most powerful tools for constructing XOPs. The rational DTs (or the Darboux-Crum transformations) factorize a second-order differential or difference operator into two first-order differential or difference operators, hence the exceptional operator can be obtained by exchanging the two 1st-order operators. Unfortunately, in our case the Dunkl shift operator is a 1st-order difference operator, which makes it difficult to apply the rational DTs directly. In this section we present a generalized DT of the Dunkl shift operator, and then give exceptional Bannai-Ito operators explicitly.

Consider the eigenvalue problem of the Dunkl shift operator

$$H[\phi(x)] = \alpha(x)(R-I)[\phi(x)] + \beta(x)(TR-I)[\phi(x)] = \mu\phi(x),$$

where $\alpha(x)$, $\beta(x)$ are functions in x. Then we choose an eigenfunction $\phi(x)$ (not necessarily to be polynomial) of H as a seed solution and let

$$\chi(x) = (I-R)[\phi(x)] = \phi(x) - \phi(-x), \tag{3.2.1}$$

$$\tilde{\chi}(x) = (I+TR)[\beta(-x-1)\phi(x)] = \beta(-x-1)\phi(x) + \beta(x)\phi(-x-1). \tag{3.2.2}$$

The functions $\chi(x)$ and $\tilde{\chi}(x)$ satisfy the following properties

$$\chi(-x) = -\chi(x), \quad \tilde{\chi}(-x-1) = \tilde{\chi}(x),$$

and the eigenvalue problem $H[\phi(x)] = \mu\phi(x)$ can be written as

$$-\alpha(x)\chi(x) + \tilde{\chi}(x) = (\mu + \beta(x) + \beta(-x-1))\phi(x). \tag{3.2.3}$$

Substituting x by $-x-1$, the above equation becomes

$$-\alpha(-x-1)\chi(-x-1) + \tilde{\chi}(x) = (\mu + \beta(-x-1) + \beta(x))\phi(-x-1), \tag{3.2.4}$$

the operation $(3.2.3)\cdot\beta(-x-1) + (3.2.4)\cdot\beta(x)$ then implies

$$\alpha(x)\beta(-x-1)\chi(x) + \alpha(-x-1)\beta(x)\chi(-x-1) + \mu\tilde{\chi}(x) = 0. \tag{3.2.5}$$

After substituting x by $-x$ in (3.2.3) and then subtracting the result by (3.2.3) we have

$$\tilde{\chi}(-x) - \tilde{\chi}(x) = -\chi(x)(\mu + \alpha(x) + \alpha(-x) + \beta(x) + \beta(-x-1)), \tag{3.2.6}$$

which holds under the condition

$$\beta(-x) + \beta(x-1) = \beta(x) + \beta(-x-1). \tag{3.2.7}$$

The properties of $\chi(x)$ and $\tilde{\chi}(x)$ are very important, as well as the equations (3.2.3), (3.2.4), (3.2.5), (3.2.6) and the condition (3.2.7), which will be used frequently in the DT with respect to the Dunkl shift operator H.

Now we define the operator

$$\mathscr{F}_\phi = \frac{1}{\chi(x)}(R-I) + \frac{1}{\tilde{\chi}(x)}(TR+I)\beta(-x-1) \tag{3.2.8}$$

such that $\mathscr{F}_\phi[\phi(x)] = 0$. It is easily seen that if the intertwining relation

$$\mathscr{F}_\phi \circ H = H^{(1)} \circ \mathscr{F}_\phi \tag{3.2.9}$$

holds for a new Dunkl shift operator $H^{(1)}$, then for any eigenfunction $\psi(x)$ ($\neq \phi(x)$) of H with eigenvalue ν ($\neq \mu$)), one has

$$H^{(1)}\left[\mathscr{F}_\phi[\psi(x)]\right] = \mathscr{F}_\phi \circ H[\psi(x)] = \nu \cdot \mathscr{F}_\phi[\psi(x)].$$

The equation with respect to the most left and the most right terms means that $\mathscr{F}_\phi[\psi(x)]$ is the eigenfunction of $H^{(1)}$ with eigenvalue ν. Before deriving the explicit expression of the operator $H^{(1)}$ we first give the following lemma for the convenience of calculation.

Lemma 3.2.1. *The operators R, T and I satisfy*

$$RR = I, \quad TRTR = I, \quad RTRT = I.$$

Moreover, for any function $f(x)$, it holds that

$$\begin{aligned}
&(R-I)f(x)(R-I) = (f(x)+f(-x))(I-R),\\
&(TR+I)f(x)(TR+I) = (f(x)+f(-x-1))(TR+I),\\
&(TR+I)f(x)(TR-I) = (f(x)-f(-x-1))(TR-I),\\
&(TR-I)f(x)(TR+I) = (f(-x-1)-f(x))(TR+I),\\
&(R-I)f(x)(TR-I) = f(-x)RTR - f(x)TR - f(-x)R + f(x)I,\\
&(R-I)f(x)(TR+I) = f(-x)RTR - f(x)TR + f(-x)R - f(x)I,\\
&(TR-I)f(x)(R-I) = f(-x-1)T - f(-x-1)TR - f(x)R + f(x)I,\\
&(TR+I)f(x)(R-I) = f(-x-1)T - f(-x-1)TR + f(x)R - f(x)I.
\end{aligned}$$

The above formulas follow from the definitions of R, T, I and elementary calculations, thus we may omit the proof.

Using the formulas in Lemma 3.2.1 we are able to derive the explicit expression of the operator $H^{(1)}$ from (3.2.9). Denote the coefficients of $H^{(1)}$ by $\alpha^{(1)}(x)$, $\beta^{(1)}(x)$ and $\gamma^{(1)}(x)$:

$$H^{(1)} = \alpha^{(1)}(x)(R-I) + \beta^{(1)}(x)(TR-I) + \gamma^{(1)}(x).$$

Proposition 3.2.1. *The Dunkl shift operator $H^{(1)}$ which satisfies (3.2.9) with $\mathscr{F}_\phi$ given by (3.2.8) is*

$$H^{(1)} = \frac{\tilde{\chi}(-x)}{\chi(x)}(R-I) + \frac{\alpha(-x-1)\beta(x)\chi(-x-1)}{\tilde{\chi}(x)}(TR-I) + \frac{\tilde{\chi}(-x)-\tilde{\chi}(x)}{\chi(x)}. \tag{3.2.10}$$

Proof. We derive $H^{(1)}$ directly from (3.2.9). According Lemma 2.1, the left-hand side of (3.2.9) is

$$\begin{aligned}
\mathscr{F}_\phi \circ H = &\frac{\beta(-x)}{\chi(x)}RTR + \frac{\beta(x)\alpha(-x-1)}{\tilde{\chi}(x)}T - \left(\frac{\beta(x)\alpha(-x-1)}{\tilde{\chi}(x)} + \frac{\beta(x)}{\chi(x)}\right)TR\\
&+\left(\frac{\beta(-x-1)\alpha(x)}{\tilde{\chi}(x)} - \frac{\alpha(x)+\alpha(-x)+\beta(-x)}{\chi(x)}\right)R\\
&-\left(\frac{\beta(-x-1)\alpha(x)}{\tilde{\chi}(x)} - \frac{\alpha(x)+\alpha(-x)+\beta(x)}{\chi(x)}\right)I,
\end{aligned}$$

and the right-hand side of (3.2.9) is

$$H^{(1)} \circ \mathscr{F}_\phi = \frac{\alpha^{(1)}(x)\beta(-x)}{\tilde{\chi}(-x)}RTR + \frac{\beta^{(1)}(x)}{\chi(-x-1)}T - \left(\frac{(\alpha^{(1)}(x)-\gamma^{(1)}(x))\beta(x)}{\tilde{\chi}(x)} + \frac{\beta^{(1)}(x)}{\chi(-x-1)}\right)TR$$

$$+\Big(\frac{\alpha^{(1)}(x)\beta(x-1)}{\tilde{\chi}(-x)}+\frac{\gamma^{(1)}(x)-\beta^{(1)}(x)}{\chi(x)}\Big)R$$
$$+\Big(\frac{(\gamma^{(1)}(x)-\alpha^{(1)}(x))\beta(-x-1)}{\tilde{\chi}(x)}+\frac{\beta^{(1)}(x)-\gamma^{(1)}(x)}{\chi(x)}\Big)I.$$

Then by comparing the coefficients of the operators RTR, T, TR, R and I one has

$$\alpha^{(1)}(x)=\frac{\tilde{\chi}(-x)}{\chi(x)},\ \ \beta^{(1)}(x)=\frac{\alpha(-x-1)\beta(x)\chi(-x-1)}{\tilde{\chi}(x)}, \tag{3.2.11}$$

$$\gamma^{(1)}(x)=\frac{\tilde{\chi}(-x)-\tilde{\chi}(x)}{\chi(x)}=-(\mu+\alpha(x)+\alpha(-x)+\beta(x)+\beta(-x-1)), \tag{3.2.12}$$

where the second equation in (3.2.12) follows from (3.2.6). □

If we add the intertwining relation $H\circ\mathscr{B}_\phi=\mathscr{B}_\phi\circ H^{(1)}$ where $\mathscr{B}_\phi$ is also a Dunkl shift operator, then it will be given by (we rearranged it for the convenience of checking (3.2.14) and (3.2.15))

$$\mathscr{B}_\phi=\alpha(x)(R-I)\tilde{\chi}(x)+(TR+I)\alpha(x)\beta(-x-1)\chi(x). \tag{3.2.13}$$

Further calculations imply that if the condition (3.2.7) holds then the products of $\mathscr{F}_\phi$ and $\mathscr{B}_\phi$ can be expressed in terms of H and $H^{(1)}$, respectively:

$$\mathscr{B}_\phi\circ\mathscr{F}_\phi=(H-\mu)\circ(H+\beta(x)+\beta(-x-1)), \tag{3.2.14}$$
$$\mathscr{F}_\phi\circ\mathscr{B}_\phi=(H^{(1)}-\mu)\circ(H^{(1)}+\beta(x)+\beta(-x-1)). \tag{3.2.15}$$

The above equations can be considered as a generalized DT of the Dunkl shift operator H, and $H^{(1)}$ is the 1-step Darboux transformed Dunkl shift operator.

Remark 3.2.1. *In order to make sure that this generalized DT can be applied on $H^{(1)}$ in the same manner as before, the coefficients $\alpha^{(1)}(x)$, $\beta^{(1)}(x)$ and $\gamma^{(1)}(x)$ should satisfy the same properties as those of H. Again, we denote the 2-step Darboux transformed Dunkl shift operator by $H^{(2)}$ with the form*

$$H^{(2)}=\alpha^{(2)}(x)(R-I)+\beta^{(2)}(x)(TR-I)+\gamma^{(2)}(x),$$

and similarly with (3.2.8) we define the operator

$$\mathscr{F}^{(2)}=\frac{1}{\chi^{(2)}(x)}(R-I)+\frac{1}{\tilde{\chi}^{(2)}(x)}(TR+I)\beta^{(1)}(-x-1),$$

where $\chi^{(2)}(x)=(I-R)[\phi_2^{(2)}(x)]$, $\tilde{\chi}^{(2)}(x)=(I+TR)[\beta^{(1)}(-x-1)\phi_2^{(2)}(x)]$, $\phi_2^{(2)}(x)$ is the second-step seed solution which is an eigenfunction of $H^{(1)}$ with eigenvalue μ_2: $\phi_2^{(2)}(x)=\mathscr{F}_\phi[\phi_2^{(1)}(x)]$ (we may denote $\mathscr{F}_\phi$ by $\mathscr{F}^{(1)}$ and the first-step seed solution $\phi(x)$ by $\phi_1^{(1)}(x)$ such that $\phi_2^{(2)}(x)=\mathscr{F}^{(1)}[\phi_2^{(1)}(x)]$, $\phi_2^{(1)}(x)\neq\phi_1^{(1)}(x)$). Then it again follows from the following intertwining relation

$$\mathscr{F}^{(2)}\circ H^{(1)}=H^{(2)}\circ\mathscr{F}^{(2)}$$

that

$$\alpha^{(2)}(x)=\frac{\tilde{\chi}^{(2)}(-x)}{\chi^{(2)}(x)},\ \ \beta^{(2)}(x)=\frac{\alpha^{(1)}(-x-1)\beta^{(1)}(x)\chi^{(2)}(-x-1)}{\tilde{\chi}^{(2)}(x)},$$

and

$$\gamma^{(2)}(x) = \frac{\tilde{\chi}^{(2)}(-x) - \tilde{\chi}^{(2)}(x)}{\chi^{(2)}(x)} + \gamma^{(1)}(-x-1) = \frac{\tilde{\chi}^{(2)}(-x) - \tilde{\chi}^{(2)}(x)}{\chi^{(2)}(x)} + \gamma^{(1)}(-x)$$

$$= \frac{\tilde{\chi}^{(2)}(-x) - \tilde{\chi}^{(2)}(x)}{\chi^{(2)}(x)} + \gamma^{(1)}(x).$$

The three expressions of $\gamma^{(2)}(x)$ imply $\gamma^{(1)}(-x-1) = \gamma^{(1)}(-x) = \gamma^{(1)}(x)$, which further requires $\alpha(x) + \alpha(-x) = \alpha(-x-1) + \alpha(x+1)$ and (3.2.7) according to (3.2.12). In the second and the third equation with respect to $\gamma^{(2)}(x)$ we have assumed that $\beta^{(1)}(x)$ satisfies the condition (3.2.7). Note that these three expressions did not appear in the calculation of $\gamma^{(1)}(x)$ since $\gamma^{(0)}(x) = 0$ in H. Therefore, by repeating this procedure we can conclude as follow.

Lemma 3.2.2. *Denote the n-step Darboux transformed Dunkl shift operator by $H^{(n)}$ ($n = 1, 2, \ldots$) with the form*

$$H^{(n)} = \alpha^{(n)}(x)(R - I) + \beta^{(n)}(x)(TR - I) + \gamma^{(n)}(x). \tag{3.2.16}$$

If the condition

$$\alpha(x) + \alpha(-x) = \alpha(-x-1) + \alpha(x+1) \tag{3.2.17}$$

and (3.2.7) *are satisfied, then the generalized DT can be applied on each $H^{(n)}$ ($n = 1, 2, \ldots$) in the same manner as we did on H.*

Proof. By repeating the procedure in Remark 3.2.1 one finds that the conditions

$$\alpha^{(n)}(x) + \alpha^{(n)}(-x) = \alpha^{(n)}(-x-1) + \alpha^{(n)}(x+1), \tag{3.2.18}$$

$$\beta^{(n)}(-x) + \beta^{(n)}(x-1) = \beta^{(n)}(x) + \beta^{(n)}(-x-1), \tag{3.2.19}$$

$$\gamma^{(n)}(-x-1) = \gamma^{(n)}(-x) = \gamma^{(n)}(x). \tag{3.2.20}$$

are sufficient for deriving the coefficients $\alpha^{(n+1)}(x)$, $\beta^{(n+1)}(x)$, $\gamma^{(n+1)}(x)$. On the other hand, from the calculations of $H^{(1)}$ and $H^{(2)}$ it is easy to conclude that for $n = 1, 2, \ldots$,

$$\alpha^{(n)}(x) = \frac{\tilde{\chi}^{(n)}(-x)}{\chi^{(n)}(x)}, \quad \beta^{(n)}(x) = \frac{\alpha^{(n-1)}(-x-1)\beta^{(n-1)}(x)\chi^{(n)}(-x-1)}{\tilde{\chi}^{(n)}(x)}, \tag{3.2.21}$$

$$\gamma^{(n)}(x) = -(\mu^{(n)} + \alpha^{(n-1)}(x) + \alpha^{(n-1)}(-x) + \beta^{(n-1)}(x) + \beta^{(n-1)}(-x-1)) \tag{3.2.22}$$

where the properties $\chi^{(n)}(-x) = -\chi^{(n)}(x)$, $\tilde{\chi}^{(n)}(-x-1) = \tilde{\chi}^{(n)}(x)$ always hold. Then inductively one can see that the conditions (3.2.18), (3.2.19), (3.2.20) hold for $n = 1, 2, \ldots$ if (3.2.17) and (3.2.7) are satisfied. □

Let us notice that the conditions (3.2.17) and (3.2.7) are already satisfied by the coefficients of the Bannai-Ito operator, thus a multiple-step DT can be performed on the Bannai-Ito operator smoothly. In the next subsection, we will derive the 1-step exceptional Bannai-Ito operator and the corresponding eigenfunctions. Some important expressions about the eigenfunctions of the n-step exceptional Bannai-Ito operator will also be given thereafter.

3.2.1 Generalized Darboux transformation of the Bannai-Ito operator

If H is a Bannai-Ito operator where $\alpha(x)$, $\beta(x)$ are defined by (3.1.2), then $H^{(1)}$ can be called the 1-step exceptional Bannai-Ito operator. In this case, it holds that

$$\alpha(x)+\alpha(-x)=\rho_1+\rho_2:=\alpha, \quad \beta(x)+\beta(-x-1)=-(r_1+r_2):=-\beta, \tag{3.2.23}$$

hence

$$\gamma^{(1)}(x)=-(\mu+\alpha(x)+\alpha(-x)+\beta(x)+\beta(-x-1))=-(\mu+\alpha-\beta). \tag{3.2.24}$$

Therefore, the 1-step exceptional Bannai-Ito operator becomes

$$H^{(1)}=\frac{\tilde{\chi}(-x)}{\chi(x)}(R-I)+\frac{\alpha(-x-1)\beta(x)\chi(-x-1)}{\tilde{\chi}(x)}(TR-I)-(\mu+\alpha-\beta). \tag{3.2.25}$$

For normalization purpose we may rewrite the operators $\mathscr{F}_\phi$, $\mathscr{B}_\phi$ and $H^{(1)}$ into

$$\hat{\mathscr{F}}_\phi=r(x)\mathscr{F}_\phi, \quad \hat{\mathscr{B}}_\phi=\mathscr{B}_\phi r^{-1}(x), \quad \hat{H}^{(1)}=r(x)H^{(1)}r^{-1}(x), \tag{3.2.26}$$

where $r(x)$ is a decoupling coefficient whose explicit expression will be given in Lemma 3.4.1.

Adopting the notations of [77] here we may call $\hat{\mathscr{F}}_\phi$ a "dressing" operator and $\hat{\mathscr{B}}_\phi$ an "undressing" operator in view of their acting as dressing and undressing of a superscript $^{(1)}$:

$$\psi^{(1)}(x):=\begin{cases}\hat{\mathscr{F}}_\phi[\psi(x)], & \text{if } \hat{\mathscr{F}}_\phi[\psi(x)]\neq 0 \quad (3.2.27)\\ \dfrac{\sigma(x)r(x)}{\tilde{\chi}(x)\chi(x)\alpha(x)\omega(x)}, & \text{otherwise} \quad (3.2.28)\end{cases}$$

$$\hat{\mathscr{B}}_\phi[\psi^{(1)}(x)]=(\nu-\mu)(\nu-\beta)\psi(x),$$

where $\sigma(x)$ satisfies $\sigma(x+1)=\sigma(x)$ and $\sigma(-x)=-\sigma(x)$, for example, $\sigma(x)=\sin(2\pi x)$, and $\omega(x)$ is the weight function associated with the Bannai-Ito operator H. It can be easily checked by using the results in Section 3.4 (Lemma 3.4.3) that

$$\hat{H}^{(1)}\left[\frac{\sigma(x)r(x)}{\tilde{\chi}(x)\chi(x)\alpha(x)\omega(x)}\right]=\mu\frac{\sigma(x)r(x)}{\tilde{\chi}(x)\chi(x)\alpha(x)\omega(x)}, \tag{3.2.29}$$

thus $\psi^{(1)}(x)$ is the eigenfunction of the normalized 1-step exceptional Bannai-Ito operator $\hat{H}^{(1)}$. Therefore, the DT

$$(H,\{\psi(x)\})\mapsto(\hat{H}^{(1)},\{\psi^{(1)}(x)\})$$

is an isospectral transformation:

$$H[\psi(x)]=\nu\psi(x), \quad \hat{H}^{(1)}[\psi^{(1)}(x)]=\nu\psi^{(1)}(x).$$

In fact, the equation (3.2.29) is equivalent with

$$H^{(1)}\left[\frac{\sigma(x)}{\tilde{\chi}(x)\chi(x)\alpha(x)\omega(x)}\right]=\mu\frac{\sigma(x)}{\tilde{\chi}(x)\chi(x)\alpha(x)\omega(x)} \tag{3.2.30}$$

in view of (3.2.26). Here we briefly check (3.2.30) using the expression (3.2.10).

$$H^{(1)}\left[\frac{\sigma(x)}{\tilde{\chi}(x)\chi(x)\alpha(x)\omega(x)}\right]=\frac{\tilde{\chi}(-x)}{\chi(x)}\left(\frac{1}{\tilde{\chi}(-x)}-\frac{1}{\tilde{\chi}(x)}\right)\frac{\sigma(x)}{\chi(x)\alpha(x)\omega(x)}+\frac{\tilde{\chi}(-x)-\tilde{\chi}(x)}{\chi(x)}\frac{\sigma(x)}{\tilde{\chi}(x)\chi(x)\alpha(x)\omega(x)}$$
$$+\frac{\alpha(-x-1)\beta(x)\chi(-x-1)}{\tilde{\chi}(x)}\left(\frac{-\beta(-x-1)}{\chi(-x-1)\alpha(-x-1)}-\frac{\beta(x)}{\chi(x)\alpha(x)}\right)\frac{\sigma(x)}{\tilde{\chi}(x)\beta(x)\omega(x)}$$
$$=\frac{\sigma(x)}{\tilde{\chi}(x)\omega(x)}\left(\frac{-\beta(-x-1)}{\tilde{\chi}(x)}-\frac{\beta(x)\alpha(-x-1)\chi(-x-1)}{\tilde{\chi}(x)\chi(x)\alpha(x)}\right)$$
$$=\frac{\sigma(x)}{\tilde{\chi}(x)\omega(x)}\left(-\frac{\beta(-x-1)\alpha(x)\chi(x)+\beta(x)\alpha(-x-1)\chi(-x-1)}{\tilde{\chi}(x)\chi(x)\alpha(x)}\right).$$

In the first equation, the properties $\chi(-x)=-\chi(x)$, $\tilde{\chi}(-x-1)=\tilde{\chi}(x)$, $\sigma(-x)=-\sigma(x)$, $\sigma(-x-1)=\sigma(-x)=-\sigma(x)$ and (3.4.18), (3.4.19) in Lemma 4.7 have been used. Then the first 2 terms in the right-hand side of the first equation annihilate immediately, the third term can be simplified as the right-hand side of the second equation. Finally, with the help of (3.2.5) we arrive at (3.2.30).

In the same way it turns out that (see (3.2.13))

$$\mathscr{B}_\phi\left[\frac{\sigma(x)}{\tilde{\chi}(x)\chi(x)\alpha(x)\omega(x)}\right]=0, \tag{3.2.31}$$

since

$$(R-I)\left[\frac{\sigma(x)}{\chi(x)\alpha(x)\omega(x)}\right]=0,\quad (TR+I)\left[\frac{\beta(-x-1)\sigma(x)}{\tilde{\chi}(x)\omega(x)}\right]=0$$

hold for the same properties as we listed in the previous paragraph.

To summarize the above results we give the following theorem which serves as the formulation of the generalized Darboux transformation for the Bannai-Ito operator.

Theorem 3.2.1. *The 1-step exceptional Bannai-Ito operator $H^{(1)}$ and the Bannai-Ito operator H satisfy the following intertwining relations:*

$$\mathscr{F}_\phi\circ H=H^{(1)}\circ\mathscr{F}_\phi,\quad H\circ\mathscr{B}_\phi=\mathscr{B}_\phi\circ H^{(1)} \tag{3.2.32}$$

where $\mathscr{F}_\phi$, $\mathscr{B}_\phi$ are both Dunkl shift operators (see (3.2.8), (3.2.13)). The operator $\mathscr{F}_\phi$ satisfies the condition $\mathscr{F}_\phi[\phi(x)]=0$, where $\phi(x)$ is an eigenfunction of H called a seed solution. Moreover, the products of $\mathscr{F}_\phi$ and $\mathscr{B}_\phi$ can be expressed in terms of H and $H^{(1)}$:

$$\mathscr{B}_\phi\circ\mathscr{F}_\phi=(H-\mu)\circ(H-\beta), \tag{3.2.33}$$
$$\mathscr{F}_\phi\circ\mathscr{B}_\phi=(H^{(1)}-\mu)\circ(H^{(1)}-\beta). \tag{3.2.34}$$

The relations (3.2.33), (3.2.34) follow from (3.2.14), (3.2.15) and (3.2.23).

Later in Section 3.4 we will show that with a well selected seed solution $\phi(x)$ and the related decoupling coefficient $r(x)$, the 1-step Darboux transformed eigenfunctions $\{\hat{\mathscr{F}}_\phi[B_n(x)]\}$ ($B_n(x)$ are the Bannai-Ito polynomials) possess the "exceptional" feature (gaps in their degree sequences) and are orthogonal with respect to a discrete measure on the exceptional Bannai-Ito grid.

As an immediate result of the intertwining relations (3.2.32), we have

$$H\circ(\mathscr{B}_\phi\circ\mathscr{F}_\phi)=(\mathscr{B}_\phi\circ\mathscr{F}_\phi)\circ H,$$
$$(\mathscr{F}_\phi\circ\mathscr{B}_\phi)\circ H^{(1)}=H^{(1)}\circ(\mathscr{F}_\phi\circ\mathscr{B}_\phi),$$

which indicate that H and $H^{(1)}$ are commutable with $(\mathscr{B}_\phi \circ \mathscr{F}_\phi)$ and $(\mathscr{F}_\phi \circ \mathscr{B}_\phi)$, respectively. In a more generic setting, if we denote H by $H^{(0)}$, and the exceptional operator obtained after n steps of DT by $H^{(n)}$ as we did before, while the same notations adopting to the operators $\mathscr{F}^{(n)}$ and $\mathscr{B}^{(n)}$ with $\mathscr{F}^{(1)} = \mathscr{F}_\phi$, $\mathscr{B}^{(1)} = \mathscr{B}_\phi$, then we can give the intertwining relations with respect to the multiple-step Darboux transformed Bannai-Ito operators.

Corollary 3.2.1. *The exceptional Bannai-Ito operator $H^{(n+1)}$ and the Bannai-Ito operator $H^{(0)}$ satisfy the following intertwining relations for $n = 1, 2, \ldots$,*

$$(\mathscr{F}^{(n)} \circ \cdots \circ \mathscr{F}^{(1)}) \circ H^{(0)} = H^{(n+1)} \circ (\mathscr{F}^{(n)} \circ \cdots \circ \mathscr{F}^{(1)}), \tag{3.2.35}$$

$$H^{(0)} \circ (\mathscr{B}^{(1)} \circ \cdots \circ \mathscr{B}^{(n)}) = (\mathscr{B}^{(1)} \circ \cdots \circ \mathscr{B}^{(n)}) \circ H^{(n+1)}. \tag{3.2.36}$$

Proof. This corollary follows inductively from the construction of the multiple-step exceptional Bannai-Ito operators $H^{(n)}$ $(n = 1, 2, \ldots)$. According to Theorem 3.2.1 we know that the exceptional Bannai-Ito operators $H^{(1)}, H^{(2)}, H^{(3)}, \ldots$ can be obtained through the following intertwining relations

$$\begin{aligned}
&\mathscr{F}^{(1)} \circ H^{(0)} = H^{(1)} \circ \mathscr{F}^{(1)}, \qquad && H^{(0)} \circ \mathscr{B}^{(1)} = \mathscr{B}^{(1)} \circ H^{(1)},\\
&\mathscr{F}^{(2)} \circ H^{(1)} = H^{(2)} \circ \mathscr{F}^{(2)}, && H^{(1)} \circ \mathscr{B}^{(2)} = \mathscr{B}^{(2)} \circ H^{(2)},\\
&\mathscr{F}^{(3)} \circ H^{(2)} = H^{(3)} \circ \mathscr{F}^{(3)}, && H^{(2)} \circ \mathscr{B}^{(3)} = \mathscr{B}^{(3)} \circ H^{(3)},\\
&\qquad\qquad\qquad\vdots
\end{aligned}$$

By applying $\mathscr{F}^{(2)}$ on the left-hand side of the first equation and then rewriting the result using the third equation we have

$$\mathscr{F}^{(2)} \circ \mathscr{F}^{(1)} \circ H^{(0)} = \mathscr{F}^{(2)} \circ H^{(1)} \circ \mathscr{F}^{(1)} = H^{(2)} \circ \mathscr{F}^{(2)} \circ \mathscr{F}^{(1)}.$$

Similarly, by applying $\mathscr{B}^{(2)}$ on the right-hand side of the second equation and then rewriting the result using the fourth equation we have

$$H^{(0)} \circ \mathscr{B}^{(1)} \circ \mathscr{B}^{(2)} = \mathscr{B}^{(1)} \circ H^{(1)} \circ \mathscr{B}^{(2)} = \mathscr{B}^{(1)} \circ \mathscr{B}^{(2)} \circ H^{(2)}.$$

Repeating this procedure finally one will arrive at (3.2.35) and (3.2.36). □

Again, we can deduce

$$H^{(0)} \circ (\mathscr{B}^{(1)} \circ \cdots \circ \mathscr{B}^{(n)}) \circ (\mathscr{F}^{(n)} \circ \cdots \circ \mathscr{F}^{(1)}) = (\mathscr{B}^{(1)} \circ \cdots \circ \mathscr{B}^{(n)}) \circ (\mathscr{F}^{(n)} \circ \cdots \circ \mathscr{F}^{(1)}) \circ H^{(0)},$$

$$(\mathscr{F}^{(n)} \circ \cdots \circ \mathscr{F}^{(1)}) \circ (\mathscr{B}^{(1)} \circ \cdots \circ \mathscr{B}^{(n)}) \circ H^{(n+1)} = H^{(n+1)} \circ (\mathscr{F}^{(n)} \circ \cdots \circ \mathscr{F}^{(1)}) \circ (\mathscr{B}^{(1)} \circ \cdots \circ \mathscr{B}^{(n)}),$$

which indicate that H and $H^{(n+1)}$ are commutable with $(\mathscr{B}^{(1)} \circ \cdots \circ \mathscr{B}^{(n)}) \circ (\mathscr{F}^{(n)} \circ \cdots \circ \mathscr{F}^{(1)})$ and $(\mathscr{F}^{(n)} \circ \cdots \circ \mathscr{F}^{(1)}) \circ (\mathscr{B}^{(1)} \circ \cdots \circ \mathscr{B}^{(n)})$, respectively.

3.2.2 Determinant expression of multiple-step exceptional eigenfunctions

From the intertwining relations in Corollary 3.2.1 one knows that the eigenfunctions of the n-step exceptional Bannai-Ito operator $H^{(n)}$ can be given by

$$\phi_m^{(n)}(x) = \mathscr{F}^{(n-1)} \circ \cdots \circ \mathscr{F}^{(1)}[\phi_m^{(1)}(x)] \quad (n \geq 1), \tag{3.2.37}$$

where $\phi_m^{(1)}(x)$ is an eigenfunction of $H^{(0)}$ (or H, the original Bannai-Ito operator) with eigenvalue μ_m. Please do not mistake $\phi_m^{(k)}(x)$ and $\phi_n^{(k)}(x)$ by the eigenfunctions of order m and order n, here we use the subscripts m, n only to indicate they are different. Recall that

$$\mathscr{F}^{(n)} = \frac{1}{\chi^{(n)}(x)}(R-I) + \frac{1}{\tilde{\chi}^{(n)}(x)}(TR+I)\beta^{(n-1)}(-x-1), \tag{3.2.38}$$

where $\beta^{(n)}(x)$ is given by (3.2.21), and

$$\chi^{(n)}(x) := \chi_n^{(n)}(x) = (I-R)[\phi_n^{(n)}(x)], \tag{3.2.39}$$

$$\tilde{\chi}^{(n)}(x) := \tilde{\chi}_n^{(n)}(x) = (I+TR)[\beta^{(n-1)}(-x-1)\phi_n^{(n)}(x)]. \tag{3.2.40}$$

Namely, the left-hand sides of (3.2.1) and (3.2.2) are represented by $\chi^{(1)}(x)$ and $\tilde{\chi}^{(1)}(x)$, $\phi_n^{(n)}(x)$ is the nth-step seed solution:

$$H^{(n-1)}[\phi_n^{(n)}(x)] = \mu_n\phi_n^{(n)}(x), \quad \phi_n^{(n)}(x) = \mathscr{F}^{(n-1)}[\phi_n^{(n-1)}(x)]. \tag{3.2.41}$$

For the simplicity of calculation we introduce the following notations (whose special cases are (3.2.39) and (3.2.40))

$$\chi_m^{(n)}(x) = (I-R)[\phi_m^{(n)}(x)], \quad \tilde{\chi}_m^{(n)}(x) = (I+TR)[\beta^{(n-1)}(-x-1)\phi_m^{(n)}(x)]. \tag{3.2.42}$$

It then follows from the definition that, for $n \geq 2$ we have

$$\chi_m^{(n)}(x) = \frac{\tilde{\chi}_m^{(n-1)}(x)}{\tilde{\chi}^{(n-1)}(x)} - \frac{\tilde{\chi}_m^{(n-1)}(-x)}{\tilde{\chi}^{(n-1)}(-x)}, \tag{3.2.43}$$

and

$$\tilde{\chi}_m^{(n)}(x) = (\mu_m - \mu_{n-1})\frac{\tilde{\chi}_m^{(n-1)}(x)}{\tilde{\chi}^{(n-1)}(x)}, \tag{3.2.44}$$

where the expression

$$\phi_m^{(n)}(x) = \mathscr{F}^{(n-1)}[\phi_m^{(n-1)}(x)] = \frac{\tilde{\chi}_m^{(n-1)}(x)}{\tilde{\chi}^{(n-1)}(x)} - \frac{\chi_m^{(n-1)}(x)}{\chi^{(n-1)}(x)} \tag{3.2.45}$$

and the eigenvalue equation of $\phi_m^{(n-1)}(x)$ (specifically, the $(n-1)$-step version of (3.2.5)) have been used for deriving (3.2.43) and (3.2.44).

As it has been shown in [16–18, 24, 29, 59], multiple-step exceptional orthogonal polynomials can be expressed in Wronskian determinants whose entries are the classical orthogonal polynomials and their derivatives. Similarly, in the exceptional Bannai-Ito case, for example, the eigenfunctions of the 1-step exceptional Bannai-Ito operator $H^{(1)}$ are the following determinant.

$$\phi_m^{(2)}(x) = \frac{1}{\tilde{\chi}^{(1)}(x)\chi^{(1)}(x)}\begin{vmatrix} \tilde{\chi}_m^{(1)}(x) & \chi_m^{(1)}(x) \\ \tilde{\chi}^{(1)}(x) & \chi^{(1)}(x) \end{vmatrix}$$

For the eigenfunctions of the n-step exceptional Bannai-Ito operator $H^{(n)}$ ($n \geq 2$), we show in the next theorem that they can always be expressed in a 3×3 determinant.

Theorem 3.2.2. *The eigenfunctions of the n-th step exceptional Bannai-Ito operator $H^{(n)}$ ($n \geq 2$) can be expressed as the* 3×3 *determinant*

$$\phi_m^{(n+1)}(x) = \prod_{j=1}^{n-2} \frac{(\mu_m - \mu_j)}{(\mu_n - \mu_j)} \begin{vmatrix} \mu_m \tilde{\chi}_m^{(1)}(x) & \tilde{\chi}_m^{(1)}(x) & \tilde{\chi}_m^{(1)}(-x) \\ \mu_n \tilde{\chi}_n^{(1)}(x) & \tilde{\chi}_n^{(1)}(x) & \tilde{\chi}_n^{(1)}(-x) \\ \mu_{n-1} \tilde{\chi}_{n-1}^{(1)}(x) & \tilde{\chi}_{n-1}^{(1)}(x) & \tilde{\chi}_{n-1}^{(1)}(-x) \end{vmatrix} \cdot \left[(\mu_n - \mu_{n-1}) \tilde{\chi}_n^{(1)}(x) \begin{vmatrix} \tilde{\chi}_n^{(1)}(x) & \tilde{\chi}_n^{(1)}(-x) \\ \tilde{\chi}_{n-1}^{(1)}(x) & \tilde{\chi}_{n-1}^{(1)}(-x) \end{vmatrix} \right]^{-1} \tag{3.2.46}$$

where μ_n is the eigenvalue of $\phi_n^{(1)}(x) : H[\phi_n^{(1)}(x)] = \mu_n \phi_n^{(1)}(x)$, and

$$\tilde{\chi}_n^{(1)}(x) = \beta(-x-1)\phi_n^{(1)}(x) + \beta(x)\phi_n^{(1)}(-x-1).$$

Proof. First, it is easily seen from (3.2.43) and (3.2.44) that, for $n \geq 2$ we have

$$\tilde{\chi}_m^{(n)}(x) = \frac{\prod_{j=1}^{n-1}(\mu_m - \mu_j)}{\prod_{k=1}^{n-2}(\mu_{n-1} - \mu_k)} \frac{\tilde{\chi}_m^{(1)}(x)}{\tilde{\chi}_{n-1}^{(1)}(x)}, \quad \chi_m^{(n)}(x) = \frac{\prod_{j=1}^{n-2}(\mu_m - \mu_j)}{\prod_{k=1}^{n-2}(\mu_{n-1} - \mu_k)} \left(\frac{\tilde{\chi}_m^{(1)}(x)}{\tilde{\chi}_{n-1}^{(1)}(x)} - \frac{\tilde{\chi}_m^{(1)}(-x)}{\tilde{\chi}_{n-1}^{(1)}(-x)} \right).$$

Then from (3.2.45) it follows that

$$\begin{aligned} \phi_m^{(n+1)}(x) &= \frac{\tilde{\chi}_m^{(n)}(x)}{\tilde{\chi}^{(n)}(x)} - \frac{\chi_m^{(n)}(x)}{\chi^{(n)}(x)} \\ &= \prod_{j=1}^{n-1} \frac{(\mu_m - \mu_j)}{(\mu_n - \mu_j)} \frac{\tilde{\chi}_m^{(1)}(x)}{\tilde{\chi}_n^{(1)}(x)} - \prod_{j=1}^{n-2} \frac{(\mu_m - \mu_j)}{(\mu_n - \mu_j)} \frac{\tilde{\chi}_m^{(1)}(x)\tilde{\chi}_{n-1}^{(1)}(-x) - \tilde{\chi}_m^{(1)}(-x)\tilde{\chi}_{n-1}^{(1)}(x)}{\tilde{\chi}_n^{(1)}(x)\tilde{\chi}_{n-1}^{(1)}(-x) - \tilde{\chi}_n^{(1)}(-x)\tilde{\chi}_{n-1}^{(1)}(x)} \\ &= \prod_{j=1}^{n-2} \frac{(\mu_m - \mu_j)}{(\mu_n - \mu_j)} \left[\frac{(\mu_m - \mu_{n-1})\tilde{\chi}_m^{(1)}(x)}{(\mu_n - \mu_{n-1})\tilde{\chi}_n^{(1)}(x)} - \frac{\tilde{\chi}_m^{(1)}(x)\tilde{\chi}_{n-1}^{(1)}(-x) - \tilde{\chi}_m^{(1)}(-x)\tilde{\chi}_{n-1}^{(1)}(x)}{\tilde{\chi}_n^{(1)}(x)\tilde{\chi}_{n-1}^{(1)}(-x) - \tilde{\chi}_n^{(1)}(-x)\tilde{\chi}_{n-1}^{(1)}(x)} \right]. \end{aligned}$$

Finally, the formula in the square brackets can be rewritten into

$$\begin{vmatrix} \mu_m \tilde{\chi}_m^{(1)}(x) & \tilde{\chi}_m^{(1)}(x) & \tilde{\chi}_m^{(1)}(-x) \\ \mu_n \tilde{\chi}_n^{(1)}(x) & \tilde{\chi}_n^{(1)}(x) & \tilde{\chi}_n^{(1)}(-x) \\ \mu_{n-1} \tilde{\chi}_{n-1}^{(1)}(x) & \tilde{\chi}_{n-1}^{(1)}(x) & \tilde{\chi}_{n-1}^{(1)}(-x) \end{vmatrix} \cdot \left[(\mu_n - \mu_{n-1}) \tilde{\chi}_n^{(1)}(x) \begin{vmatrix} \tilde{\chi}_n^{(1)}(x) & \tilde{\chi}_n^{(1)}(-x) \\ \tilde{\chi}_{n-1}^{(1)}(x) & \tilde{\chi}_{n-1}^{(1)}(-x) \end{vmatrix} \right]^{-1}.$$

□

Let us observe the right-hand side of (3.2.46), $\phi_m^{(n+1)}(x)$ vanishes if $m = i$ for $i = 1, 2, \ldots, n$. The cases $m = n$ and $m = n-1$ are due to the 3×3 determinant part, while the cases $m \in \{1, 2, \ldots, n-2\}$ are due to the prefactor $\prod_{j=1}^{n-2}(\mu_m - \mu_j)$. In this way, there are in total n eigenfunctions been deleted from the eigenfunction sequence of the n-step exceptional Bannai-Ito operator $H^{(n)}$.

3.3 Quasi-polynomial eigenfunctions of Bannai-Ito operator

In this section we consider a special class of eigenfunctions of the Bannai-Ito operator, which are called quasi-polynomial eigenfunctions. A quasi-polynomial eigenfunction is the product of a gauge factor and a polynomial part:

$$H[\xi(x)p(x)] = \lambda\xi(x)p(x),$$

where $\xi(x)$ is a function in x and $p(x)$ is a polynomial in x, λ is the corresponding eigenvalue. The Bannai-Ito operator may have several sequences of quasi-polynomial eigenfunctions. From these quasi-polynomial eigenfunctions, in the next section, we will choose the seed solutions of the DT. This plays an important role in the construction of exceptional Bannai-Ito polynomials.

From the definition of the quasi-polynomial eigenfunction, we will derive all possible gauge factors $\xi(x)$. First, let us consider the conjugated operator $\tilde{H} = \xi^{-1}H\xi$:

$$\begin{aligned}\tilde{H} &= \frac{1}{\xi(x)}\Big[\alpha(x)(R-I)\xi(x) + \beta(x)(TR-I)\xi(x)\Big] \\ &= \alpha(x)\frac{\xi(-x)}{\xi(x)}(R-I) + \beta(x)\frac{\xi(-x-1)}{\xi(x)}(TR-I) + \alpha(x)\left[\frac{\xi(-x)}{\xi(x)} - 1\right] + \beta(x)\left[\frac{\xi(-x-1)}{\xi(x)} - 1\right].\end{aligned}$$

The operator $\tilde{H}$ has polynomial eigenfunctions if and only if $\tilde{H}$ is also a Bannai-Ito operator, i.e. there exist real numbers ρ_1', ρ_2', r_1', r_2' and ρ_1'', ρ_2'', r_1'', r_2'' such that both (3.3.1) and one of (3.3.2), (3.3.3) are satisfied

$$\alpha(x)\left[\frac{\xi(-x)}{\xi(x)} - 1\right] + \beta(x)\left[\frac{\xi(-x-1)}{\xi(x)} - 1\right] = const. \tag{3.3.1}$$

$$\alpha(x)\frac{\xi(-x)}{\xi(x)} = \frac{(x-\rho_1')(x-\rho_2')}{-2x}, \quad \beta(x)\frac{\xi(-x-1)}{\xi(x)} = \frac{(x-r_1'+\frac{1}{2})(x-r_2'+\frac{1}{2})}{2x+1}, \tag{3.3.2}$$

$$\alpha(x)\frac{\xi(-x)}{\xi(x)} = \frac{(x-\rho_1'')(x-\rho_2'')}{2x}, \quad \beta(x)\frac{\xi(-x-1)}{\xi(x)} = -\frac{(x-r_1''+\frac{1}{2})(x-r_2''+\frac{1}{2})}{2x+1}. \tag{3.3.3}$$

Further calculations lead to the following lemma.

Lemma 3.3.1. *Let $H = \alpha(x)(R-I) + \beta(x)(TR-I)$ be a Bannai-Ito operator, then the conjugated operator $\tilde{H} = \xi^{-1}H\xi$ has polynomial eigenfunctions if and only if $\xi(x)$ satisfies*

$$\frac{\xi(-x)}{\xi(x)} = \frac{(x-\rho_1')(x-\rho_2')}{(x-\rho_1)(x-\rho_2)}, \quad \frac{\xi(-x-1)}{\xi(x)} = \frac{(x-r_1'+\frac{1}{2})(x-r_2'+\frac{1}{2})}{(x-r_1+\frac{1}{2})(x-r_2+\frac{1}{2})}, \tag{3.3.4}$$

where $\rho_1'\rho_2' = \rho_1\rho_2$ and $r_1'r_2' = r_1r_2$; or $\xi(x)$ satisfies

$$\frac{\xi(-x)}{\xi(x)} = -\frac{(x-\rho_1'')(x-\rho_2'')}{(x-\rho_1)(x-\rho_2)}, \quad \frac{\xi(-x-1)}{\xi(x)} = -\frac{(x-r_1''+\frac{1}{2})(x-r_2''+\frac{1}{2})}{(x-r_1+\frac{1}{2})(x-r_2+\frac{1}{2})}, \tag{3.3.5}$$

where $\rho_1''\rho_2'' = -\rho_1\rho_2$ and $r_1''r_2'' = -r_1r_2$.

Proof. It is easily seen that (3.3.4) and (3.3.5) follow from (3.3.2) and (3.3.3), respectively. Thus, (3.3.1) can be rewritten into

$$\begin{aligned}const. &= \frac{(x-\rho_1')(x-\rho_2') - (x-\rho_1)(x-\rho_2)}{-2x} + \frac{(x-r_1'+\frac{1}{2})(x-r_2'+\frac{1}{2}) - (x-r_1+\frac{1}{2})(x-r_2+\frac{1}{2})}{2x+1} \\ &= -\frac{\rho_1+\rho_2-\rho_1'-\rho_2'}{2} + \frac{r_1+r_2-r_1'-r_2'}{2} - \frac{\rho_1'\rho_2'-\rho_1\rho_2}{2x} + \frac{r_1'r_2'-r_1r_2}{2x+1}\end{aligned}$$

which implies $\rho_1'\rho_2' - \rho_1\rho_2 = 0$ and $r_1'r_2' - r_1r_2 = 0$; or

$$const. = \frac{(x-\rho_1'')(x-\rho_2'')+(x-\rho_1)(x-\rho_2)}{2x} - \frac{(x-r_1''+\frac{1}{2})(x-r_2''+\frac{1}{2})+(x-r_1+\frac{1}{2})(x-r_2+\frac{1}{2})}{2x+1}$$
$$= -\frac{\rho_1+\rho_2+\rho_1''+\rho_2''}{2} + \frac{r_1+r_2+r_1''+r_2''}{2} - \frac{1}{2} + \frac{\rho_1''\rho_2''+\rho_1\rho_2}{2x} - \frac{r_1''r_2''+r_1r_2}{2x+1}$$

which implies $\rho_1''\rho_2'' + \rho_1\rho_2 = 0$ and $r_1''r_2'' + r_1r_2 = 0$. □

It then follows that there are both 4 sets of parameterizations (σ_1, σ_2, σ_3, σ_4) for ρ_1', ρ_2', r_1', r_2' and ρ_1'', ρ_2'', r_1'', r_2'' (σ_5, σ_6, σ_7, σ_8):

$$\sigma_1 = \{\rho_1,\rho_2,r_1,r_2\}, \quad \sigma_2 = \{-\rho_1,-\rho_2,-r_1,-r_2\},$$
$$\sigma_3 = \{-\rho_1,-\rho_2,r_1,r_2\}, \quad \sigma_4 = \{\rho_1,\rho_2,-r_1,-r_2\},$$
$$\sigma_5 = \{-\rho_1,\rho_2,-r_1,r_2\}, \quad \sigma_6 = \{\rho_1,-\rho_2,r_1,-r_2\},$$
$$\sigma_7 = \{\rho_1,-\rho_2,-r_1,r_2\}, \quad \sigma_8 = \{-\rho_1,\rho_2,r_1,-r_2\}.$$

Remark 3.3.1. *One may ask why there are only 8 sets of parameterizations, for example, the condition $\rho_1'\rho_2' = \rho_1\rho_2$ leads to $\rho_1' = k\rho_1$ and $\rho_2' = \rho_2/k$ where k can be any real number. We will show that the conditions (3.3.4) and (3.3.5) imply that only the choices $k = \pm 1$ are allowed. In fact, if we let $\rho_1' = k\rho_1$ and $\rho_2' = \rho_2/k$, then the first equation of (3.3.4) can be rewritten into*

$$\frac{\xi(-x)}{\xi(x)} = \frac{(x-k\rho_1)(x-\rho_2/k)}{(x-\rho_1)(x-\rho_2)}, \tag{3.3.6}$$

which becomes the next equation with x replaced by $-x$

$$\frac{\xi(x)}{\xi(-x)} = \frac{(x+k\rho_1)(x+\rho_2/k)}{(x+\rho_1)(x+\rho_2)}. \tag{3.3.7}$$

Then we have

$$1 = \frac{\xi(-x)}{\xi(x)} \cdot \frac{\xi(x)}{\xi(-x)} = \frac{(x-k\rho_1)(x-\rho_2/k)}{(x-\rho_1)(x-\rho_2)} \cdot \frac{(x+k\rho_1)(x+\rho_2/k)}{(x+\rho_1)(x+\rho_2)} = \frac{(x^2-k^2\rho_1^2)(x^2-\rho_2^2/k^2)}{(x^2-\rho_1^2)(x^2-\rho_2^2)}.$$

The above equation have 4 solutions: $k^2 = 1$ and $k^2 = \rho_2^2/\rho_1^2$. However, the former two solutions lead to $(\rho_1',\rho_2') = (\rho_1,\rho_2)$ or $(-\rho_1,-\rho_2)$ while the latter two solutions lead to $(\rho_1',\rho_2') = (\rho_2,\rho_1)$ or $(-\rho_2,-\rho_1)$. One should notice that nothing changes if we exchange ρ_1' with ρ_2' (ρ_1'' with ρ_2'') or r_1' with r_2' (r_1'' with r_2'') due to the symmetry of the right-hand sides of (3.3.2) *(*(3.3.3)*). In fact, the solutions $k^2 = \rho_2^2/\rho_1^2$ lead to the same gauge factors as the solutions $k^2 = 1$. Therefore, we drop the solutions $k^2 = \rho_2^2/\rho_1^2$ and keep $k^2 = 1$. This reasoning can also be applied to the remaining cases. In this way we conclude that there are in total 8 cases of parameterizations. These parameterizations correspond to the following 8 classes of quasi-polynomial eigenfunctions.*

Theorem 3.3.1. *The Bannai-Ito operator has 8 sequences of quasi-polynomial eigenfunctions:* $\{\xi_d(x)p_m^{(d)}(x)\}_{m=0}^{\infty}$, $d \in \{1,2,\ldots,8\}$. *The 8 gauge factors are*

$$
\begin{aligned}
\xi_1(x) &= 1,\\
\xi_2(x) &= \frac{\Gamma(1/2+r_1+x)\Gamma(1/2+r_1-x)\Gamma(1/2+r_2+x)\Gamma(1/2+r_2-x)}{\Gamma(\rho_1-x)\Gamma(1+\rho_1+x)\Gamma(\rho_2-x)\Gamma(1+\rho_2+x)},\\
\xi_3(x) &= \frac{1}{\Gamma(\rho_1-x)\Gamma(1+\rho_1+x)\Gamma(\rho_2-x)\Gamma(1+\rho_2+x)},\\
\xi_4(x) &= \Gamma(1/2+r_1+x)\Gamma(1/2+r_1-x)\Gamma(1/2+r_2+x)\Gamma(1/2+r_2-x),\\
\xi_5(x) &= \frac{\Gamma(1/2+r_1+x)\Gamma(1/2+r_1-x)}{[\Gamma(\rho_1-x)\Gamma(1+\rho_1+x)},\\
\xi_6(x) &= \frac{\Gamma(1/2+r_2+x)\Gamma(1/2+r_2-x)}{\Gamma(\rho_2-x)\Gamma(1+\rho_2+x)},\\
\xi_7(x) &= \frac{\Gamma(1/2+r_1+x)\Gamma(1/2+r_1-x)}{\Gamma(\rho_2-x)\Gamma(1+\rho_2+x)},\\
\xi_8(x) &= \frac{\Gamma(1/2+r_2+x)\Gamma(1/2+r_2-x)}{\Gamma(\rho_1-x)\Gamma(1+\rho_1+x)}.
\end{aligned}
$$

And the polynomials $p_m^{(d)}(x) = B_n(x;\sigma_d)$ *for* $m \in \{0,1,2,\ldots\}$, $d \in \{1,2,\ldots,8\}$. *Moreover, the eigenvalues of the quasi-polynomial eigenfunctions* $\{\xi_d(x)p_m^{(d)}(x)\}$ *are*

$$
\mu_{\boldsymbol{d}} = \mu_{d,m} = \begin{cases} \lambda_m(\sigma_d)+C_d, & \text{if } d \in \{1,2,3,4\},\\ -\lambda_m(\sigma_d)+C_d, & \text{if } d \in \{5,6,7,8\}, \end{cases} \tag{3.3.8}
$$

where $\lambda_m(\sigma_d)$ *is the eigenvalue of the Bannai-Ito polynomial* $B_m(x)$ *(refers to (3.1.3), (3.1.4)) with parameters given by* σ_d*, and the definition of the constant* C_d *is*

$$
C_d = \begin{cases} -\dfrac{\rho_1+\rho_2-\rho_1'-\rho_2'}{2}+\dfrac{r_1+r_2-r_1'-r_2'}{2}, & \text{if } \{\rho_1',\rho_2',r_1',r_2'\} = \sigma_d \text{ and } d \in \{1,2,3,4\},\\ -\dfrac{\rho_1+\rho_2+\rho_1''+\rho_2''}{2}+\dfrac{r_1+r_2+r_1''+r_2''-1}{2}, & \text{if } \{\rho_1'',\rho_2'',r_1'',r_2''\} = \sigma_d \text{ and } d \in \{5,6,7,8\}. \end{cases}
$$

Proof. Here we derive the above quasi-polynomial eigenfunctions using Lemma 3.3.1. Notice that $\xi(-x)/\xi(-x-1) = F(x)$ leads to $\xi(x+1)/\xi(x) = F(-x-1)$ if one substitute x by $-x-1$, hence it is convenient to construct the gauge factors with the help of the Gamma function.

In the first case we have $\xi_1(x+1)/\xi_1(x) = 1$, which implies $\xi_1(x)$ is a constant.

In the second case we have

$$
\frac{\xi_2(x+1)}{\xi_2(x)} = \frac{(x-\rho_1+1)(x-\rho_2+1)(x+r_1+1/2)(x+r_2+1/2)}{(x+\rho_1+1)(x+\rho_2+1)(x-r_1+1/2)(x-r_2+1/2)}.
$$

Recall that $\Gamma(x+1)/\Gamma(x) = x$, we can express $\xi_2(x)$ in terms of the Gamma functions

$$
\xi_2(x) = c_2(x)\frac{\Gamma(x-\rho_1+1)\Gamma(x-\rho_2+1)\Gamma(x+r_1+1/2)\Gamma(x+r_2+1/2)}{\Gamma(x+\rho_1+1)\Gamma(x+\rho_2+1)\Gamma(x-r_1+1/2)\Gamma(x-r_2+1/2)},
$$

where $c_2(x)$ is periodic function of period 1, $c_2(x+1) = c_2(x)$. The fact that $\xi_2(x)$ must be an eigenfunction of H implies that $c_2(x)$ cannot be a constant. If we let

$$
c_2(x) = \frac{\sin[\pi(x-\rho_1+1)]\sin[\pi(x-\rho_2+1)]}{\sin[\pi(x-r_1+1/2)]\sin[\pi(x-r_2+1/2)]},
$$

then the following expression of $\xi_2(x)$ satisfies $H[\xi_2(x)] = (r_1 + r_2 - \rho_1 - \rho_2)\xi_2(x)$.

$$\xi_2(x) = \frac{\Gamma(x+r_1+1/2)\Gamma(-x+r_1+1/2)\Gamma(x+r_2+1/2)\Gamma(-x+r_2+1/2)}{\Gamma(x+\rho_1+1)\Gamma(-x+\rho_1)\Gamma(x+\rho_2+1)\Gamma(-x+\rho_2)}$$

In the derivation of the above expression of $\xi_2(x)$, Euler's reflection formula

$$\Gamma(x)\Gamma(1-x) = \pi/\sin(\pi x), \quad x \notin \mathbb{Z}$$

has been used (assuming $x-\rho_1+1, x-\rho_2+1, x-r_1+1/2, x-r_2+1/2 \notin \mathbb{Z}$).

The remaining $\xi_k(x)$'s can be obtained in the same way by choosing suitable periodic function $c(x)$'s and applying Euler's reflection formula. We shall assume that the restriction $x \notin \mathbb{Z}$ is always satisfied wherever Euler's reflection formula was applied. This is not difficult since ρ_1, ρ_2, r_1, r_2 can be any real numbers.

According to (3.3.1), (3.3.2), (3.3.3) and Lemma 3.3.1, it is easily seen that the conjugated operator

$$\tilde{H} = \begin{cases} H(\sigma_d) + C_d, & \text{if } d \in \{1,2,3,4\}, \\ -H(\sigma_d) + C_d, & \text{if } d \in \{5,6,7,8\}, \end{cases}$$

thus $p_n^{(d)}(x) = B_n(x;\sigma_d)$ and (3.3.8) follow immediately. □

3.4 Exceptional Bannai-Ito polynomials

Using the results of Section 3.2 and Section 3.3, we are now able to construct the exceptional Bannai-Ito polynomials. We first show that there are missing degrees in the constructed exceptional Bannai-Ito polynomial sequences. Notably their missing degrees demonstrate different rules compared with the known 1-step XOPs. And then we prove that the exceptional Bannai-Ito polynomials are orthogonal with respect to a discrete measure on the exceptional Bannai-Ito grid.

Define an index set $\mathbf{D} = \{1,2,\ldots,8\} \times \mathbb{Z}_{\geq 0}$. For the sake of simplicity, we assume that for any index $\mathbf{d} = (d,m) \in \mathbf{D}$, a quasi-polynomial eigenfunction $\phi_{\mathbf{d}}(x) = \xi_d(x) p_m^{(d)}(x)$ is uniquely determined upon the constant multiplier. Last but not least, we assume that the Bannai-Ito polynomials mentioned in this paper are always monic (i.e. the coefficient of the highest order term is 1), hence $p_n^{(d)}(x)$ are always monic too. One could refer to Theorem 3.3.1.

Now we take a quasi-polynomial eigenfunction $\phi_{\mathbf{d}}(x)$ with $\mathbf{d} = (d,m)$ as a seed solution and show that the Darboux transformed eigenfunction $\hat{\mathscr{F}}_{\phi_{\mathbf{d}}}[B_n(x)]$ is just the exceptional Bannai-Ito polynomial we want. Firstly, a well selected decoupling coefficient $r(x)$ is essential.

Lemma 3.4.1. *Assume that the decoupling coefficient $r(x)$ is given by*

$$r(x) = \tilde{\chi}(x)\chi(x)\frac{\eta_d(x)}{x\xi_d(x)}, \tag{3.4.1}$$

where $\eta_d(x)$ is the polynomial of lowest degree such that

$$\frac{\xi_d(-x)}{\xi_d(x)} = \frac{\eta_d(-x)}{\eta_d(x)}.$$

Then the Darboux transformed eigenfunction

$$\hat{\mathscr{F}}_{\phi_{\mathbf{d}}}[B_n(x)] = \frac{r(x)}{\chi(x)\tilde{\chi}(x)} \begin{vmatrix} (I-R)[\phi_{\mathbf{d}}(x)] & (I-R)[B_n(x)] \\ (I+TR)[\beta(-x-1)\phi_{\mathbf{d}}(x)] & (I+TR)[\beta(-x-1)B_n(x)] \end{vmatrix}$$

is a polynomial.

Proof. Given the seed solution $\phi_{\mathbf{d}}(x) = \xi_d(x)p_m^{(d)}(x)$ whose eigenvalue is $\mu_{\mathbf{d}}$, we have

$$\begin{aligned}
\frac{\chi(x)\tilde{\chi}(x)}{r(x)}\hat{\mathscr{F}}_{\phi_{\mathbf{d}}}[B_n(x)] &= (\phi_{\mathbf{d}}(x)-\phi_{\mathbf{d}}(-x))(\beta(-x-1)B_n(x)+\beta(x)B_n(-x-1)) \\
&\quad -(B_n(x)-B_n(-x))(\beta(-x-1)\phi_{\mathbf{d}}(x)+\beta(x)\phi_{\mathbf{d}}(-x-1)) \\
&= (\phi_{\mathbf{d}}(x)-\phi_{\mathbf{d}}(-x))[(\lambda_n+\beta(x)+\beta(-x-1))B_n(x)+\alpha(x)(B_n(x)-B_n(-x))] \\
&\quad -(B_n(x)-B_n(-x))[(\mu_{\mathbf{d}}+\beta(x)+\beta(-x-1))\phi_{\mathbf{d}}(x)+\alpha(x)(\phi_{\mathbf{d}}(x)-\phi_{\mathbf{d}}(-x))] \\
&= (\lambda_n+\beta(x)+\beta(-x-1))B_n(x)(\phi_{\mathbf{d}}(x)-\phi_{\mathbf{d}}(-x)) \\
&\quad -(\mu_{\mathbf{d}}+\beta(x)+\beta(-x-1))\phi_{\mathbf{d}}(x)(B_n(x)-B_n(-x)) \\
&= \frac{x\xi_d(x)}{\eta_d(x)}\Bigg[(\lambda_n+\beta(x)+\beta(-x-1))B_n(x)\Big(\frac{\eta_d(x)p_m^{(d)}(x)-\eta_d(-x)p_m^{(d)}(-x)}{x}\Big) \\
&\quad -(\mu_{\mathbf{d}}+\beta(x)+\beta(-x-1))\eta_d(x)p_m^{(d)}(x)\Big(\frac{B_n(x)-B_n(-x)}{x}\Big)\Bigg],
\end{aligned}$$

where the second equation follows from equation (3.2.3) which can be used as

$$\begin{aligned}
\beta(-x-1)\phi_{\mathbf{d}}(x)+\beta(x)\phi_{\mathbf{d}}(-x-1) &= (\mu_{\mathbf{d}}+\beta(x)+\beta(-x-1))\phi_{\mathbf{d}}(x)+\alpha(x)(\phi_{\mathbf{d}}(x)-\phi_{\mathbf{d}}(-x)), \\
\beta(-x-1)B_n(x)+\beta(x)B_n(-x-1) &= (\lambda_n+\beta(x)+\beta(-x-1))B_n(x)+\alpha(x)(B_n(x)-B_n(-x)).
\end{aligned}$$

The third equation is obtained after the elimination of

$$\alpha(x)(B_n(x)-B_n(-x))(\phi_{\mathbf{d}}(x)-\phi_{\mathbf{d}}(-x)).$$

Finally, by introducing the polynomial $\eta_d(x)$ we arrive at the fourth equation. Notice that the function in the square brackets is just the desired polynomial. Therefore, the decoupling coefficient should be

$$r(x) = \tilde{\chi}(x)\chi(x)\frac{\eta_d(x)}{x\xi_d(x)}.$$

□

Here we give all the functions $\eta_d(x)$ explicitly for later convenience. This list is obtained via Lemma 3.3.1,

$$\begin{aligned}
&\eta_1(x) = 1, && \eta_2(x) = (x-\rho_1)(x-\rho_2), \\
&\eta_3(x) = (x-\rho_1)(x-\rho_2), && \eta_4(x) = 1, \\
&\eta_5(x) = (x-\rho_1), && \eta_6(x) = (x-\rho_2), \\
&\eta_7(x) = (x-\rho_2), && \eta_8(x) = (x-\rho_1).
\end{aligned}$$

With $r(x)$ given by Lemma 3.4.1, let $B_{\mathbf{d},n}^{(1)}(x) = \hat{\mathscr{F}}_{\phi_{\mathbf{d}}}[B_n(x)]$, then $\{B_{\mathbf{d},n}^{(1)}(x)\}$ are the polynomial eigenfunctions of $\hat{H}^{(1)}$: $\hat{H}^{(1)}[B_{\mathbf{d},n}^{(1)}(x)] = \lambda_n B_{\mathbf{d},n}^{(1)}(x)$ $(\lambda_n \neq \mu_{\mathbf{d}})$. In what follows, we give an analysis of the degree of $B_{\mathbf{d},n}^{(1)}(x)$ and show that there are missing degrees in their polynomial sequences. From the proof of Lemma 3.4.1, we have

$$\begin{aligned}
B_{\mathbf{d},n}^{(1)}(x) = (\lambda_n-\beta)\left(\frac{\eta_d(x)p_m^{(d)}(x)-\eta_d(-x)p_m^{(d)}(-x)}{x}\right)B_n(x) \\
-(\mu_{\mathbf{d}}-\beta)\left(\frac{B_n(x)-B_n(-x)}{x}\right)\eta_d(x)p_m^{(d)}(x),
\end{aligned} \tag{3.4.2}$$

where the constant $\beta = -(\beta(x)+\beta(-x-1)) = r_1+r_2$ (refers to (3.2.22)).

Remark 3.4.1. *Note that $\mu_{4,0} = r_1 + r_2 = \beta$ (refers to (3.3.8)), in this case the polynomials $B^{(1)}_{4,0,n}(x) = 0$ for $n = 0, 1, 2, \ldots$, which implies that $\boldsymbol{d} = (4, 0)$ cannot be chosen as the index of a seed solution.*

In order to see the degree of $B^{(1)}_{\mathbf{d},n}(x)$, let

$$B_n(x) = x^n + a_{n-1}x^{n-1} + \cdots \tag{3.4.3}$$

then from Theorem 3.3.1 we have

$$p^{(d)}_n(x) = B_n(x; \sigma_d) = x^n + a_{n-1}(\sigma_d)x^{n-1} + \cdots$$

where $a_i(\sigma_d)$ $(i = 0, 1, \ldots, n-1)$ are the coefficients with respect to the parameterization σ_d. For $d = 1, \ldots, 8$, denote the degree of $\eta_d(x)$ by κ_d such that $\eta_d(x) = x^{\kappa_d} + b^{(d)}_{\kappa_d - 1}x^{\kappa_d - 1} + \cdots$. Then

$$\eta_d(x)p^{(d)}_m(x) = x^{m+\kappa_d} + (a_{m-1}(\sigma_d) + b^{(d)}_{\kappa_d-1})x^{m+\kappa_d-1} + \cdots, \tag{3.4.4}$$

where $\kappa_d = 0$ for $d \in \{1, 4\}$; $\kappa_d = 2$ for $d \in \{2, 3\}$; and $\kappa_d = 1$ for $d \in \{5, 6, 7, 8\}$.

Proposition 3.4.1. *Let S be the set of degrees of $\{B^{(1)}_{\boldsymbol{d},n}(x)\}$, where the index $\boldsymbol{d} \in \boldsymbol{D} \backslash \{(1, n), (4, 0)\}$. If the conditions (4.14) and (4.15) are satisfied, then we have*

- *for m is odd,*
  - $d = 1 : S = \{m-1, m, m+1, \cdots, 2m-2, 2m, \cdots\}$;
  - $d = 4 : S = \{m-1, m, m+1, m+2, m+3, \cdots\}$;
  - $d = 2, 3 : S = \{m+1, m+2, m+3, m+4, m+5, \cdots\}$;
  - $d = 5, 6, 7, 8 : S = \{m-1, m+1, m+1, m+3, m+3, \cdots\}$;
- *for m is even,*
  - $d = 1 : S = \{m-2, m, m, \cdots, 2m-4, 2m-4, 2m-2, 2m, 2m, \cdots\}$;
  - $d = 4 : S = \{m-2, m, m, m+2, m+2, \cdots\}$;
  - $d = 2, 3 : S = \{m, m+2, m+2, m+4, m+4, \cdots\}$;
  - $d = 5, 6, 7, 8 : S = \{m, m+1, m+2, m+3, m+4, \cdots\}$.

Proof. According to (3.4.3) and (3.4.4), the right-hand side of (3.4.2) can be expanded as

$$\begin{aligned}
B^{(1)}_{\mathbf{d},n}(x) &= (\lambda_n - \beta)[x^{m+\kappa_d-1} + (-x)^{m+\kappa_d-1} + (a_{m-1}(\sigma_d) + b_{\kappa_d-1})(x^{m+\kappa_d-2} + (-x)^{m+\kappa_d-2}) + \cdots](x^n + a_{n-1}x^{n-1} + \cdots) \\
&\quad - (\mu_{\mathbf{d}} - \beta)[x^{n-1} + (-x)^{n-1} + a_{n-1}(x^{n-2} + (-x)^{n-2}) + \cdots][x^{m+\kappa_d} + (a_{m-1}(\sigma_d) + b_{\kappa_d-1})x^{m+\kappa_d-1} + \cdots] \\
&= (\lambda_n - \beta)[x^{m+\kappa_d-1} + (-x)^{m+\kappa_d-1} + (a_{m-1}(\sigma_d) + b_{\kappa_d-1})(x^{m+\kappa_d-2} + (-x)^{m+\kappa_d-2})]x^n \\
&\quad - (\mu_{\mathbf{d}} - \beta)[x^{n-1} + (-x)^{n-1} + a_{n-1}(x^{n-2} + (-x)^{n-2})]x^{m+\kappa_d} + \cdots.
\end{aligned}$$

Note that $x^k + (-x)^k = 2x^k$ if k is even, otherwise $x^k + (-x)^k = 0$. The degree of $B^{(1)}_{\mathbf{d},n}(x)$ depends on the parities of $m + \kappa_d$ and n. Specifically, the leading term of $B^{(1)}_{\mathbf{d},n}(x)$ is given by:

$$B^{(1)}_{\mathbf{d},n}(x) = \begin{cases} 2(\lambda_n - \beta)x^{n+m+\kappa_d-1} + \cdots, & \text{if } m + \kappa_d \text{ is odd and } n \text{ is even,} \\ 2(\lambda_n - \mu_{\mathbf{d}})x^{n+m+\kappa_d-1} + \cdots, & \text{if } m + \kappa_d \text{ is odd and } n \text{ is odd,} \\ 2C_{d,m,n}x^{n+m+\kappa_d-2} + \cdots, & \text{if } m + \kappa_d \text{ is even and } n \text{ is even,} \\ -2(\mu_{\mathbf{d}} - \beta)x^{n+m+\kappa_d-1} + \cdots, & \text{if } m + \kappa_d \text{ is even and } n \text{ is odd,} \end{cases}$$

where $C_{n,m,d} = (\lambda_n - \beta)(a_{m-1}(\sigma_d) + b^{(d)}_{\kappa_d - 1}) - (\mu_{\mathbf{d}} - \beta)a_{n-1}$. Recall that in the case $d = 1$, the seed solution is $\phi_{(1,m)} = B_m(x)$, thus $B^{(1)}_{\mathbf{d},n}(x) = 0$ for $d = 1$, $n = m$ since $\hat{\mathscr{F}}_{\phi_{(1,m)}}[B_m(x)] = 0$. In the other cases if we assume that the coefficient of the leading term of $B^{(1)}_{\mathbf{d},n}(x)$ is always non-zero, i.e.

$$\lambda_n - \beta \neq 0, \quad \text{if } n \text{ is even}, \tag{3.4.5}$$

$$\mu_{\mathbf{d}} - \beta \neq 0, \quad \text{if } d \in \{1,2,3,4\} \text{ and } m \text{ is even; or } d \in \{5,6,7,8\} \text{ and } m \text{ is odd}, \tag{3.4.6}$$

$$\lambda_n - \mu_{\mathbf{d}} \neq 0, \quad \text{if } d \in \{1,2,3,4\}, m \text{ is odd and } n \text{ is odd; or } d \in \{5,6,7,8\}, m \text{ is even and } n \text{ is odd}, \tag{3.4.7}$$

$$C_{d,m,n} \neq 0, \quad \text{if } d \in \{1,2,3,4\}, m \text{ is even and } n \text{ is even; or } d \in \{5,6,7,8\}, m \text{ is odd and } n \text{ is even}, \tag{3.4.8}$$

are satisfied, then for the degree of $B^{(1)}_{\mathbf{d},n}(x)$ we have

$$\deg(B^{(1)}_{\mathbf{d},n}(x)) = \begin{cases} n + m + \kappa_d - 1, & \text{if } m + \kappa_d \text{ is odd; or } m + \kappa_d \text{ is even and } n \text{ is odd}, & (3.4.9) \\ n + m + \kappa_d - 2, & \text{if } m + \kappa_d \text{ is even and } n \text{ is even}. & (3.4.10) \end{cases}$$

By analyzing the parity of m and n, it turns out that (3.4.9) leads to the first three cases for m is odd and the last case for m is even, while (3.4.10) leads to the other cases in Proposition 3.4.1.

Finally, let us consider under which conditions will (3.4.5)-(3.4.8) be satisfied. It follows from (3.1.3), (3.1.4) and (3.2.23) that

$$\lambda_n - \beta = \begin{cases} n/2 - (r_1 + r_2), & \text{if } n \text{ is even}, & (3.4.11) \\ -(\rho_1 + \rho_2) - (n+1)/2, & \text{if } n \text{ is odd}, & (3.4.12) \end{cases}$$

thus (3.4.5) holds under the condition

$$r_1 + r_2 \notin \mathbb{Z}. \tag{3.4.13}$$

In Section 3.6 we list the explicit expressions for $\mu_{\mathbf{d}} - \beta$, $\lambda_n - \mu_{\mathbf{d}}$ and $C_{d,m,n}$ in the corresponding cases. From (3.6.1)-(3.6.24) we can see that (3.4.6)-(3.4.8) are satisfied under the conditions

$$r_1 + r_2, \ \ \rho_1 + \rho_2, \ \ r_1 + r_2 + \rho_1 + \rho_2, \ \ r_1 + r_2 - \rho_1 - \rho_2 \notin \mathbb{Z}, \tag{3.4.14}$$

$$\frac{r_1 - r_2 - \rho_1 + \rho_2 + 1}{2}, \ \ \frac{r_1 - r_2 + \rho_1 - \rho_2 + 1}{2}, \ \ r_i - \rho_j + \frac{1}{2}, \ \ r_i + \rho_j + \frac{1}{2} \notin \mathbb{Z}, \ \ i, j \in \{1,2\}, \tag{3.4.15}$$

and the index $\mathbf{d} = (d,m) \notin \{(1,n), (4,0)\}$.

□

Remark 3.4.2. *As we addressed in the proof of Proposition 3.4.1, in both cases $d = 1$ there are missing degrees ($2m-1$ and $2m-2$, respectively) in the degree sequence of $\{B^{(1)}_{\mathbf{d},n}(x)\}$ when $n = m$, since the seed solutions $\phi_{(1,m)} = B_m(x)$ and the trivial eigenfunctions $\hat{\mathscr{F}}_{\phi_{(1,m)}}[B_m(x)] = 0$. On the other hand, the nontrivial eigenfunction given by* (3.2.28) *becomes*

$$\phi^{(1)}_{\mathbf{d}}(x) = \frac{\sigma(x) r(x)}{\tilde{\chi}(x)\chi(x)\alpha(x)\omega(x)} = \frac{\sigma(x)\eta_d(x)}{x\alpha(x)\omega(x)\xi_d(x)}.$$

Here we may choose $\sigma(x) = x\alpha(x)\omega(x)\xi_1(x)/\eta_1(x)$. With this choice it holds that $\sigma(x+1) = \sigma(x)$ and $\sigma(-x) = -\sigma(x)$, then $\phi^{(1)}_{\mathbf{d}}(x) = \eta_d(x)\xi_1(x)/\eta_1(x)\xi_d(x)$, such that only when $d = 1$ the nontrivial eigenfunction $\phi^{(1)}_{\mathbf{d}}(x)$ is a polynomial and $\phi^{(1)}_{(1,m)}(x) = 1$. This eigenfunction should be added to *the sequence* $\{B^{(1)}_{(1,m),n}(x)\}$*, hence the polynomial sequence starts from degree* 0*. However, for the convenience of later discussion, we will not include this term into the XBI polynomial sequence.*

Notice that in each case there are missing degrees in the degree sequence S, and the degrees of $\{B^{(1)}_{\mathbf{d},n}(x)\}$ demonstrate exactly opposite features regarding the parity of m. Specifically, in the first three cases when m is odd and the in the last case when m is even, S behaves similarly as the known 1-step XOPs, where S is cofinite (the complement of S is finite). However, in the other cases S is not cofinite and only contains even degrees. This fact implies that in these cases, the normalized 1-step exceptional Bannai-Ito operator $\hat{H}^{(1)}$ only has even-order eigenpolynomials, and there are two different series of these eigenpolynomials. It would be better to say that the eigenpolynomials of odd degrees are not been deleted but are just replaced by the ones of even degrees. For example, in the case $m = 2$ and $d \in \{2,3\}$, the degree set of $\{B^{(1)}_{\mathbf{d},n}(x)\}$ is $S = \{2,4,4,6,6,\ldots\}$. The polynomials $B^{(1)}_{\mathbf{d},n}(x)$ are different from each other even when they have the same degree, and by no exception they are orthogonal according to Theorem 4.11.

The feature that S is not cofinite naturally conflicts with the definition of XOPs which satisfy a second-order differential (difference) equation. This is not surprising, the constraint that S should be cofinite is just the consequence of the way XOPs in [16–18, 23–27, 69] are presented, the reflection operator R has not appeared in their eigenvalue equations. Taking this opportunity, we would like to modify the definition of XOPs as the generalization of COPs where the only condition to be removed is that it contains polynomials of all degrees. By this means, the XOPs are characterized by orthogonality and forming the polynomial eigenfunctions of certain differential (difference) operators. From now on, we call $\{B^{(1)}_{\mathbf{d},n}(x)\}$ the 1-step exceptional Bannai-Ito (XBI) polynomials.

Proposition 3.4.2. *The exceptional Bannai-Ito polynomials* $B^{(1)}_{\boldsymbol{d},n}(x)$ *can be expressed as the linear combination of the Bannai-Ito polynomials* $B_n(x)$ *and* $B_n(-x) - B_n(x)$*,*

$$B^{(1)}_{\boldsymbol{d},n}(x) = C^{(1)}_{\boldsymbol{d},n}(x)B_n(x) + C^{(2)}_{\boldsymbol{d}}(x)(B_n(x) - B_n(-x)),$$

where

$$C^{(1)}_{\boldsymbol{d},n}(x) = (\lambda_n - \beta)\left(\frac{\hat{\phi}^{(0)}_{\boldsymbol{d}}(x) - \hat{\phi}^{(0)}_{\boldsymbol{d}}(-x)}{x}\right), \quad C^{(2)}_{\boldsymbol{d}}(x) = -(\mu_{\boldsymbol{d}} - \beta)\frac{\hat{\phi}^{(0)}_{\boldsymbol{d}}(x)}{x},$$

and $\hat{\phi}^{(0)}_{\boldsymbol{d}}(x)$ *is the normalized seed solution which is a polynomial:*

$$\hat{\phi}^{(0)}_{\boldsymbol{d}}(x) = \eta_d(x)p^{(d)}_m(x) = \phi_{\boldsymbol{d}}(x)\frac{\eta_d(x)}{\xi_d(x)}. \tag{3.4.16}$$

Proof. The above result follows directly from (3.4.2). □

Corollary 3.4.1. *The exceptional Bannai-Ito polynomials* $B^{(1)}_{\boldsymbol{d},n}(x)$ *satisfy*

$$B^{(1)}_{\boldsymbol{d},n}(x) - B^{(1)}_{\boldsymbol{d},n}(-x) = \frac{1}{x}(\lambda_n - \mu_{\boldsymbol{d}})(\hat{\phi}^{(0)}_{\boldsymbol{d}}(x) - \hat{\phi}^{(0)}_{\boldsymbol{d}}(-x))(B_n(x) - B_n(-x)). \tag{3.4.17}$$

Proof. From Proposition 4.5, we have

$$\begin{aligned} B^{(1)}_{\mathbf{d},n}(x) - B^{(1)}_{\mathbf{d},n}(-x) &= C^{(1)}_{\mathbf{d},n}(x)B_n(x) - C^{(1)}_{\mathbf{d},n}(-x)B_n(-x) \\ &\quad + (C^{(2)}_{\mathbf{d}}(x) + C^{(2)}_{\mathbf{d}}(-x))(B_n(-x) - B_n(x)). \end{aligned}$$

Since $C^{(1)}_{\mathbf{d},n}(x) = C^{(1)}_{\mathbf{d},n}(-x)$, it turns out that

$$\begin{aligned} B^{(1)}_{\mathbf{d},n}(x) - B^{(1)}_{\mathbf{d},n}(-x) &= (C^{(1)}_{\mathbf{d},n}(x) + C^{(2)}_{\mathbf{d}}(x) + C^{(2)}_{\mathbf{d}}(-x))(B_n(-x) - B_n(x)) \\ &= \frac{1}{x}(\lambda_n - \mu_{\mathbf{d}})(\hat{\phi}^{(0)}_{\mathbf{d}}(x) - \hat{\phi}^{(0)}_{\mathbf{d}}(-x))(B_n(-x) - B_n(x)). \end{aligned}$$

□

3.4.1 Orthogonality

A finite difference operator L is said to be symmetric with respect to an inner product $\langle , \rangle_{\omega(x)}$ if it satisfies $\langle L[p(x)], q(x)\rangle_{\omega(x)} = \langle p(x), L[q(x)]\rangle_{\omega(x)}$ for any functions $p(x)$ and $q(x)$, where the inner product is defined by $\langle p(x), q(x)\rangle_{\omega(x)} = \sum_{x\in\chi} \omega(x)p(x)q(x)$. It is known from the Lemma 2.4 of [16] that if a difference operator is symmetric with respect to an inner product $\langle , \rangle_{\omega(x)}$, then its eigenfunctions are orthogonal with respect to $\omega(x)$.

Assume that the operator $\mathscr{L}$ has polynomial eigenfunctions $\{p_n(x)\}$

$$\mathscr{L}[p_n(x)] = \lambda_n p_n(x) \quad (\lambda_n \neq \lambda_m, n \neq m),$$

the linearity of the inner product $\langle , \rangle_{\omega(x)}$ implies

$$\begin{aligned} &\langle \mathscr{L}[p_n(x)], p_m(x)\rangle_{\omega(x)} = \lambda_n \langle p_n(x), p_m(x)\rangle_{\omega(x)}, \\ &\langle p_n(x), \mathscr{L}[p_m(x)]\rangle_{\omega(x)} = \lambda_m \langle p_n(x), p_m(x)\rangle_{\omega(x)}. \end{aligned}$$

Then if $\mathscr{L}$ is symmetric with respect to $\langle , \rangle_{\omega(x)}$, it holds that

$$\langle p_n(x), p_m(x)\rangle_{\omega(x)} = 0 \quad (n \neq m),$$

which demonstrate the orthogonality of $\{p_n(x)\}$ with respect to $\omega(x)$. In light of this conclusion we need first to derive the conditions for $\mathscr{L}$ to be symmetric.

Lemma 3.4.2. *Let $\omega(x)$ be a weight function supported on a countable set $\chi \subset \mathbb{R}$. $\mathscr{L}$ is a Dunkl shift operator of the form $\mathscr{L} = F(x)R + G(x)TR + C(x)$. Assume that the functions $F(x)$, $G(x)$ and $\omega(x)$ satisfy the following relations*

$$\omega(x)F(x) = \omega(-x)F(-x), \tag{3.4.18}$$

$$\omega(x)G(x) = \omega(-x-1)G(-x-1), \tag{3.4.19}$$

for $x \in \mathbb{R}$, and the boundary conditions

$$F(x) = 0 \quad \text{for } x \in \chi \backslash (-\chi), \tag{3.4.20}$$

$$G(x) = 0 \quad \text{for } x \in \chi \backslash (-\chi - 1), \tag{3.4.21}$$

then $\mathscr{L}$ is symmetric with respect to $\omega(x)$. Here we denote by $-\chi$ and $-\chi - 1$ the sets $-\chi = \{-x : x \in \chi\}$ and $-\chi - 1 = \{-x-1 : x \in \chi\}$, respectively.

Proof. According to the conditions, it holds for any functions $p(x)$ and $q(x)$ that

$$\begin{aligned} \sum_{x\in\chi} \omega(x)F(x)p(-x)q(x) &= \sum_{x\in-\chi} \omega(-x)F(-x)p(x)q(-x) \\ &= \sum_{x\in(-\chi)\cap\chi} \omega(x)F(x)p(x)q(-x) = \sum_{x\in\chi} \omega(x)F(x)p(x)q(-x), \end{aligned}$$

and

$$\sum_{x\in\chi}\omega(x)G(x)p(-x-1)q(x)=\sum_{x\in(-\chi-1)}\omega(-x-1)G(-x-1)p(x)q(-x-1)$$

$$=\sum_{x\in(-\chi-1)\cap\chi}\omega(x)G(x)p(x)q(-x-1)=\sum_{x\in\chi}\omega(x)G(x)p(x)q(-x-1).$$

These equations imply that

$$\sum_{x\in\chi}\omega(x)\big[F(x)p(-x)+G(x)p(-x-1)\big]q(x)=\sum_{x\in\chi}\omega(x)p(x)\big[F(x)q(-x)+G(x)q(-x-1)\big].$$

The above equation is equivalent to $\langle\mathscr{L}[p(x)],q(x)\rangle_{\omega(x)}=\langle p(x),\mathscr{L}[q(x)]\rangle_{\omega(x)}$, thus $\mathscr{L}$ is symmetric with respect to $\omega(x)$. □

Lemma 3.4.3. *Assume that $\omega(x)$ is the weight function associated with a Dunkl-shift operator $\mathscr{L}=F(x)R+G(x)TR+C(x)$ such that (3.4.18), (3.4.19), (3.4.20) and (3.4.21) hold, then it satisfies*

$$\frac{\omega(x+1)}{\omega(x)}=\frac{F(-x-1)G(x)}{F(x+1)G(-x-1)}.$$

Proof. The equations

$$\omega(x)F(x)=\omega(-x)F(-x),\quad \omega(x)G(x)=\omega(-x-1)G(-x-1)$$

imply that

$$\frac{\omega(-x)}{\omega(-x-1)}=\frac{F(x)G(-x-1)}{F(-x)G(x)},$$

after substituting x by $-x-1$ then we get the desired result. □

Now we are able to give the weight functions of the exceptional Bannai-Ito operator by using the properties of the Gamma function as we did in Section 3.3. However, it takes less steps if the relationship between the weight functions of the exceptional Bannai-Ito operator and the Bannai-Ito operator is available, since the weight functions of the Bannai-Ito polynomials are already known in [79]. Below we give the weight function of the exceptional Bannai-Ito polynomials $\{B^{(1)}_{\mathbf{d},n}(x)\}$ and show their orthogonality explicitly. These results can be extended to the multiple-step exceptional Bannai-Ito polynomials.

Theorem 3.4.1. *Let $\hat{\omega}^{(1)}(x)$ be the weight function associated with the exceptional Bannai-Ito operator $\hat{H}^{(1)}$, and $\omega(x)$ be the weight function of the Bannai-Ito operator H, then it holds that*

$$\hat{\omega}^{(1)}(x)=c(x)\frac{\tilde{\chi}(x)\chi(x)\alpha(x)}{r^2(x)}\omega(x), \tag{3.4.22}$$

where $c(x)$ is a 1-periodic function $c(x+1)=c(x)$, and it satisfies $c(-x)=c(x)$.

Proof. According to (3.2.25), (3.2.26), the normalized 1-step exceptional Bannai-Ito operator is

$$\hat{H}^{(1)}=\frac{r(x)\tilde{\chi}(-x)}{r(-x)\chi(x)}(R-I)+\frac{r(x)\alpha(-x-1)\beta(x)\chi(-x-1)}{r(-x-1)\tilde{\chi}(x)}(TR-I)$$
$$+\frac{\alpha(-x-1)\beta(x)\chi(-x-1)}{\tilde{\chi}(x)}\left(\frac{r(x)}{r(-x-1)}-1\right).$$

Then from Lemma 3.4.3, we have

$$\frac{\hat{\omega}^{(1)}(x+1)}{\hat{\omega}^{(1)}(x)}=\frac{\tilde{\chi}(x+1)\chi(x+1)r^2(x)\alpha(-x-1)\beta(x)}{\tilde{\chi}(x)\chi(x)r^2(x+1)\alpha(x)\beta(-x-1)}=\frac{\tilde{\chi}(x+1)\chi(x+1)r^2(x)\alpha(x+1)\omega(x+1)}{\tilde{\chi}(x)\chi(x)r^2(x+1)\alpha(x)\omega(x)},$$

hence

$$\hat{\omega}^{(1)}(x)=c(x)\frac{\tilde{\chi}(x)\chi(x)\alpha(x)\omega(x)}{r^2(x)},$$

where $c(x)$ is a periodic function of period 1, $c(x+1)=c(x)$. Moreover, if we check the relations (3.4.18) and (3.4.19) with respect to the coefficients of $\hat{H}^{(1)}$, it turns out that

$$c(-x)=c(x),\quad c(-x-1)=c(x).$$

Notice that $c(-x-1)=c(x)$ follows from the conditions $c(x+1)=c(x)$ and $c(-x)=c(x)$, thus only the latter two conditions are essential. In view of these properties, it may sometimes be convenient to choose $c(x)$ as a constant. □

It remains to derive the exceptional Bannai-Ito grid (from the simple roots of exceptional Bannai-Ito polynomials), which varies in the choice of the seed solution. It is known that the Bannai-Ito polynomials have simple and distinct real roots [79] as the other COPs do [74]. Specifically, when n is odd, if we assume that $r_2=\rho_2+n/2$, then the Bannai-Ito polynomial $B_n(x)$ has n simple roots given by

$$\rho_2,\ \ -\rho_2-1,\ \ \rho_2+1,\ \ \cdots,\ \ -\rho_2-\frac{n-1}{2},\ \ \rho_2+\frac{n-1}{2};$$

when n is even, assume that $\rho_1=-\rho_2-n/2$, then the n simple roots of $B_n(x)$ are

$$\rho_2,\ \ -\rho_2-1,\ \ \rho_2+1,\ \ -\rho_2-2,\ \ \cdots,\ \ \rho_2+\frac{n-2}{2},\ \ -\rho_2-\frac{n}{2}.$$

These roots can be rewritten into a more elegant form which was called the Bannai-Ito grid: $x_s=-1/4+(-1)^s(x_0+s/2+1/4)$ $(s=0,1,\ldots,n-1)$ with $x_0=\rho_2$.

Remark 3.4.3. *Note that in the case when n is odd there are 4 possible conditions:* $r_i-\rho_j=n/2$, $i,j=1,2$, *where we just restrict with the condition* $r_2=\rho_2+n/2$ *for the sake of simplicity. And in the case when n is even there are also 2 possible conditions:* $\rho_1+\rho_2=-n/2$ *and* $r_1+r_2=n/2$, *for the same reason we restrict with the condition* $\rho_1+\rho_2=-n/2$. *More details about Bannai-Ito grid can be found in [79].*

It then follows from Proposition 3.4.2 and the above results that $B^{(1)}_{\mathbf{d},n}(x)=Q_{\mathbf{d},n}(x)B_n(x)$, where

$$Q_{\mathbf{d},n}(x)=\begin{cases} C^{(1)}_{\mathbf{d},n}(x)+2xC^{(2)}_{\mathbf{d}}(x)/(x-\rho_2), & \text{if } n \text{ odd and } r_2=\rho_2+\frac{n}{2},\\ C^{(1)}_{\mathbf{d},n}(x)+nxC^{(2)}_{\mathbf{d}}(x)/((x-\rho_2)(x+\rho_2+\frac{n}{2})), & \text{if } n \text{ even and } \rho_1=-\rho_2-\frac{n}{2}.\end{cases}$$

Note that $C^{(1)}_{\mathbf{d},n}(x)$ is a polynomial in x, $2xC^{(2)}_{\mathbf{d}}(x)/(x-\rho_2)$ is a polynomial for $d=1,2,5,6$, and $nxC^{(2)}_{\mathbf{d}}(x)/(x-\rho_2)(x+\rho_2+\frac{n}{2})$ is a polynomial for $d=1,2$. In these cases, the roots of $B_n(x)$ belong to the simple roots of $B^{(1)}_{\mathbf{d},n}(x)$. In other cases only a part of the former belong to the latter.

Let $\chi^{(1)}_{\mathbf{d}}$ be the set whose elements come from the exceptional Bannai-Ito grid, thus these elements are the simple roots of $B^{(1)}_{\mathbf{d},N}(x)$. For simplicity's sake, we rewrite the normalized exceptional Bannai-Ito operator into

$$\hat{H}^{(1)}=\hat{\alpha}^{(1)}(x)(R-I)+\hat{\beta}^{(1)}(x)(TR-I)+\hat{\gamma}^{(1)}(x),$$

and consider the eigenvalue equation $\hat{H}^{(1)}[B^{(1)}_{\mathbf{d},N}(x)] = \lambda_N B^{(1)}_{\mathbf{d},N}(x)$. Assume that $x^{(1)}_s \in \chi^{(1)}_{\mathbf{d}}$, then this eigenvalue equation becomes

$$\hat{\alpha}^{(1)}(x^{(1)}_s)B^{(1)}_{\mathbf{d},N}(-x^{(1)}_s) + \hat{\beta}^{(1)}(x^{(1)}_s)B^{(1)}_{\mathbf{d},N}(-x^{(1)}_s - 1) = 0.$$

If $x^{(1)}_s \in \chi^{(1)}_{\mathbf{d}} \backslash (-\chi^{(1)}_{\mathbf{d}})$ and $x^{(1)}_s \in \chi^{(1)}_{\mathbf{d}} \cap (-\chi^{(1)}_{\mathbf{d}} - 1)$, which means $B^{(1)}_{\mathbf{d},N}(-x^{(1)}_s) \neq 0$ and $B^{(1)}_{\mathbf{d},N}(-x^{(1)}_s - 1) = 0$, then $\hat{\alpha}^{(1)}(x^{(1)}_s) = 0$. On the other hand, if $x^{(1)}_s \in \chi^{(1)}_{\mathbf{d}} \backslash (-\chi^{(1)}_{\mathbf{d}} - 1)$ and $x^{(1)}_s \in \chi^{(1)}_{\mathbf{d}} \cap (-\chi^{(1)}_{\mathbf{d}})$, which means $B^{(1)}_{\mathbf{d},N}(-x^{(1)}_s - 1) \neq 0$ and $B^{(1)}_{\mathbf{d},N}(-x^{(1)}_s) = 0$, then $\hat{\beta}^{(1)}(x^{(1)}_s) = 0$. Using these results together with the boundary conditions in Lemma 3.4.2, we can conclude that

$$\chi^{(1)}_{\mathbf{d}} \backslash (-\chi^{(1)}_{\mathbf{d}}) \subseteq \chi^{(1)}_{\mathbf{d}} \cap (-\chi^{(1)}_{\mathbf{d}} - 1), \quad \chi^{(1)}_{\mathbf{d}} \backslash (-\chi^{(1)}_{\mathbf{d}} - 1) \subseteq \chi^{(1)}_{\mathbf{d}} \cap (-\chi^{(1)}_{\mathbf{d}}),$$

hence $\chi^{(1)}_{\mathbf{d}} = \chi^{(1)}_{\mathbf{d}} \cap (-\chi^{(1)}_{\mathbf{d}}) \cap (-\chi^{(1)}_{\mathbf{d}} - 1) + \chi^{(1)}_{\mathbf{d}} \backslash (-\chi^{(1)}_{\mathbf{d}}) + \chi^{(1)}_{\mathbf{d}} \backslash (-\chi^{(1)}_{\mathbf{d}} - 1)$. The first set in the right-hand side consists of part of the roots of $B_N(x)$, while the remaining 2 sets can be obtained from the simple roots of $\hat{\alpha}^{(1)}(x)$ and $\hat{\beta}^{(1)}(x)$.

Theorem 3.4.2. *The exceptional Bannai-Ito polynomials $\{B^{(1)}_{\boldsymbol{d},n}(x)\}$ satisfy the discrete orthogonality relation*

$$\sum_{x \in \chi^{(1)}_{\boldsymbol{d}}} \hat{\omega}^{(1)}(x) B^{(1)}_{\boldsymbol{d},n}(x) B^{(1)}_{\boldsymbol{d},m}(x) = h^{(1)}_{\boldsymbol{d},n} \delta_{nm} \quad (0 \leq n,m < N), \tag{3.4.23}$$

where $h^{(1)}_{\boldsymbol{d},n}$ is constant. If N is odd and $r_2 = \rho_2 + N/2$,

$$d = 1,5 : \chi^{(1)}_{\boldsymbol{d}} = \{x_1, \ldots, x_{N-1}\}, \quad d = 2,6 : \chi^{(1)}_{\boldsymbol{d}} = \{x_0, \ldots, x_N\},$$

$$d = 3,7 : \chi^{(1)}_{\boldsymbol{d}} = \{x_0, \ldots, x_{N-1}\}, \quad d = 4,8 : \chi^{(1)}_{\boldsymbol{d}} = \{x_1, \ldots, x_N\};$$

if N is even and $\rho_1 = -\rho_2 - N/2$,

$$d = 1,4 : \chi^{(1)}_{\boldsymbol{d}} = \{x_1, \ldots, x_{N-2}\}, \quad d = 2,3 : \chi^{(1)}_{\boldsymbol{d}} = \{x_0, \ldots, x_{N-1}\},$$

$$d = 5,8 : \chi^{(1)}_{\boldsymbol{d}} = \{x_1, \ldots, x_{N-1}\}, \quad d = 6,7 : \chi^{(1)}_{\boldsymbol{d}} = \{x_0, \ldots, x_{N-2}\},$$

where $x_s = -1/4 + (-1)^s(\rho_2 + s/2 + 1/4)$.

Remark 3.4.4. *It should be noted that the weight $\hat{\omega}^{(1)}(x_s)$ is not always positive. From the formula (3.4.22) we know that the positivity of $\hat{\omega}^{(1)}(x_s)$ depends on that of $\tilde{\chi}(x_s)\chi(x_s)\alpha(x_s)/r^2(x_s)$. In fact, we can choose a positive 1-periodic function $c(x)$, besides, the Bannai-Ito weight $\omega(x_s)$ is positive by construction [79]. Let us rewrite this expression into*

$$\frac{\tilde{\chi}(x)\chi(x)\alpha(x)}{r^2(x)} = \frac{x^2\xi_d^2(x)\alpha(x)}{\eta_d^2(x)\tilde{\chi}(x)\chi(x)}$$

$$= \frac{x}{\eta_d(x)p^{(d)}_m(x) - \eta_d(-x)p^{(d)}_m(-x)} \cdot \frac{x\alpha(x)}{\eta_d(x)\left(\beta(-x-1)p^{(d)}_m(x) + \beta(x)\frac{\xi_d(-x-1)}{\xi_d(x)}p^{(d)}_m(-x-1)\right)}.$$

It is convenient to discuss the positivity of $E_{\boldsymbol{d}}(x) := E^{(1)}_d(x)E^{(2)}_{\boldsymbol{d}}(x)E^{(3)}_{\boldsymbol{d}}(x)$ instead:

$$E^{(1)}_d(x) := \frac{x\alpha(x)}{\eta_d(x)}, \quad E^{(2)}_{\boldsymbol{d}}(x) := \frac{\eta_d(x)p^{(d)}_m(x) - \eta_d(-x)p^{(d)}_m(-x)}{x},$$

$$E_{\boldsymbol{d}}^{(3)}(x) := \beta(-x-1)p_m^{(d)}(x) + \beta(x)\frac{\xi_d(-x-1)}{\xi_d(x)}p_m^{(d)}(-x-1).$$

That is, the positivity of the weight $\hat{\omega}^{(1)}(x_s)$ is equivalent with that of $E_{\boldsymbol{d}}(x_s)$. Consider the case $m = 1$, N is odd and $r_2 = \rho_2 + N/2$, the expressions of $E_{\boldsymbol{d}}(x)$ follow as:

$$E_{1,1}(x) = (x-\rho_1)(x-\rho_2)\Big[(x+\frac{1}{2})^2 + \frac{(\rho_1+\frac{1}{2})(\rho_2+\frac{1}{2}) - (\rho_1+\rho_2+1)r_1}{2r_1-2\rho_1+N-2}N + \frac{\rho_2(2\rho_2+1)(2\rho_1+1) - r_1(2\rho_2(2\rho_2+1)-(2\rho_1+1))}{2(2r_1-2\rho_1+N-2)}\Big], \tag{3.4.24}$$

$$E_{2,1}(x) = (x+r_1+\frac{1}{2})(x+\rho_2+\frac{N+1}{2})\Big[x^2 + \frac{\rho_1\rho_2 - (r_1+\frac{1}{2})(\rho_1+\rho_2)}{2r_1-2\rho_1+N+2}N + \frac{\rho_1(2\rho_2(2\rho_2+1)-(2r_1+1)) - \rho_2(2\rho_2+1)(2r_1+1)}{2(2r_1-2\rho_1+N+2)}, \tag{3.4.25}$$

$$E_{3,1}(x) = \Big[x^2 + \frac{\rho_1\rho_2 + (r_1-\frac{1}{2})(\rho_1+\rho_2)}{2r_1+2\rho_1+4\rho_2+N-2}N + \frac{\rho_1((4\rho_2-1)(\rho_2+2r_1-1)-\rho_2) + \rho_2(2\rho_2-1)(2r_1-1)}{2(2r_1+2\rho_1+4\rho_2+N-2)}\Big] \cdot\Big[(x+\frac{1}{2})^2 + \frac{(\rho_1-\frac{1}{2})(\rho_2-\frac{1}{2}) + r_1(\rho_1+\rho_2-1)}{2r_1+2\rho_1+4\rho_2+N-2}N + \frac{r_1((4\rho_2-1)(\rho_2+2\rho_1-1)-\rho_2) + \rho_2(2\rho_2-1)(2\rho_1-1)}{2(2r_1+2\rho_1+4\rho_2+N-2)}\Big], \tag{3.4.26}$$

$$E_{4,1}(x) = (x-\rho_1)(x-\rho_2)(x+r_1+\frac{1}{2})(x+\rho_2+\frac{N+1}{2}), \tag{3.4.27}$$

$$E_{5,1}(x) = \frac{(N-1)(2\rho_1+2\rho_2+N-1)^2(2r_1-2\rho_1+1)}{4(2\rho_1-2r_1+N-2)^2}(x-\rho_2)(x+r_1+\frac{1}{2}), \tag{3.4.28}$$

$$E_{6,1}(x) = \frac{(N+1)(2r_1+2\rho_2-1)^2(2r_1-2\rho_1-1)}{4(2\rho_1-2r_1+N+2)^2}(x-\rho_1)(x+\rho_2+\frac{N+1}{2}), \tag{3.4.29}$$

$$E_{7,1}(x) = \frac{(4\rho_2+N-1)^2(2r_1-2\rho_2+1)(2\rho_2-2\rho_1+N-1)}{4(4\rho_2-2\rho_1-2r_1+N-2)^2}(x-\rho_1)(x+r_1+\frac{1}{2}), \tag{3.4.30}$$

$$E_{8,1}(x) = \frac{(2r_1+2\rho_1-1)^2(2r_1-2\rho_2-1)(2\rho_2-2\rho_1+N+1)}{4(4\rho_2-2\rho_1-2r_1+N+2)^2}(x-\rho_2)(x+\rho_2+\frac{N+1}{2}). \tag{3.4.31}$$

It is not difficult to derive some sufficient conditions for $E_{d,1}(x) > 0$, where $x \in \chi_{d,1}^{(1)}$. Let us take the case $d = 3$ for an example, from (3.4.26) we know that $E_{3,1}(x) > 0$ if

$$\frac{\rho_1\rho_2 + (r_1-\frac{1}{2})(\rho_1+\rho_2)}{2r_1+2\rho_1+4\rho_2+N-2}N + \frac{\rho_1((4\rho_2-1)(\rho_2+2r_1-1)-\rho_2) + \rho_2(2\rho_2-1)(2r_1-1)}{2(2r_1+2\rho_1+4\rho_2+N-2)}$$

and

$$\frac{(\rho_1-\frac{1}{2})(\rho_2-\frac{1}{2}) + r_1(\rho_1+\rho_2-1)}{2r_1+2\rho_1+4\rho_2+N-2}N + \frac{r_1((4\rho_2-1)(\rho_2+2\rho_1-1)-\rho_2) + \rho_2(2\rho_2-1)(2\rho_1-1)}{2(2r_1+2\rho_1+4\rho_2+N-2)}$$

are both positive. These conditions are immediately satisfied if we assume that

$$r_1, \rho_1, \rho_2 > \frac{1}{2}. \tag{3.4.32}$$

For the other cases, we list some sufficient conditions below. These conditions are obtained similarly by observing the right-hand sides of (3.4.24), (3.4.25), and (3.4.27)-(3.4.31).

$$
\begin{aligned}
&d=1: 0<r_1<\frac{(\rho_1+\frac{1}{2})(\rho_2+\frac{1}{2})}{\rho_1+\rho_2+1}, -\frac{1}{2}<\rho_1<\rho_2+1 \text{ and } \rho_2>-\frac{1}{2};\\
&d=2: \frac{N-3}{2}<r_1<\frac{N-2}{2}, \rho_1<0 \text{ and } -\frac{1}{2}<\rho_2<r_1-\frac{N-2}{2};\\
&d=4: r_1>\frac{N-3}{2}, \rho_1<\frac{1}{2} \text{ and } \rho_2>-\frac{1}{2};\\
&d=5: -1<r_1<0, \rho_1<r_1+\frac{1}{2} \text{ and } \rho_2>-\frac{1}{2};\\
&d=6: r_1>-\frac{N-3}{4}, \rho_1<\rho_2 \text{ and } -\frac{N+1}{4}<\rho_2<-\frac{N-1}{4};\\
&d=7: r_1>0, -\frac{1}{2}<\rho_1<\rho_2 \text{ and } r_1-\frac{1}{2}<\rho_2<r_1+\frac{1}{2};\\
&d=8: r_1>\rho_2+\frac{1}{2}, \rho_1<\rho_2+\frac{N+1}{2} \text{ and } -\frac{N+3}{4}<\rho_2<-\frac{N-1}{4}.
\end{aligned}
$$

Example 3.4.1. *In this example we demonstrate the orthogonality of the exceptional Bannai-Ito polynomials explicitly. Consider the case $\boldsymbol{d}=(3,1)$, where the seed solution is given by $\phi_{(3,1)}=\xi_3(x)p_1^{(3)}(x)=\xi_3(x)B_1(x;-\rho_1,-\rho_2,r_1,r_2)$, and its eigenvalue is $\mu_{(3,1)}=r_1+r_2-1$. According to Proposition 3.4.2, we can give the related exceptional Bannai-Ito polynomials:*

$$
B^{(1)}_{(3,1),n}(x)=(\lambda_n-\beta)\frac{\hat{\phi}^{(0)}_{(3,1)}(x)-\hat{\phi}^{(0)}_{(3,1)}(-x)}{x}B_n(x)-(\mu_{(3,1)}-\beta)\frac{\hat{\phi}^{(0)}_{(3,1)}(x)}{x}(B_n(x)-B_n(-x)),
$$

where $\hat{\phi}^{(0)}_{(3,1)}(x)=\eta_3(x)p_1^{(3,1)}(x)=(x-\rho_1)(x-\rho_2)B_1(x;-\rho_1,-\rho_2,r_1,r_2)$. Assume that N is odd and $r_2=\rho_2+\frac{N}{2}$, then $\chi^{(1)}_{(3,1)}=\{\rho_2,-\rho_2-1,\rho_2+1,\cdots,-\rho_2-\frac{N-1}{2},\rho_2+\frac{N-1}{2}\}$ is the corresponding exceptional Bannai-Ito grid. The discrete orthogonality (3.4.23) holds for the weight function

$$
\hat{\omega}^{(1)}(x)=\frac{\sin(2\pi x)\Gamma(x-r_1+\frac{1}{2})\Gamma(-x-r_1+\frac{1}{2})\Gamma(x+\rho_1+1)\Gamma(-x+\rho_1)}{\Gamma(x+r_2+\frac{1}{2})\Gamma(-x+r_2+\frac{1}{2})\Gamma(x-\rho_2+1)\Gamma(-x-\rho_2)y_1(x)y_2(x)},
$$

where $y_1(x)$, $y_2(x)$ are the polynomials

$$
\begin{aligned}
y_1(x)=&(r_1+r_2+\rho_1+\rho_2-1)x^2+r_1\rho_1\rho_2+r_2\rho_1\rho_2+r_1r_2\rho_1+r_1r_2\rho_2-\rho_1\rho_2\\
&-\frac{r_1\rho_1+r_1\rho_2+r_2\rho_1+r_2\rho_2}{2}+\frac{\rho_1+\rho_2}{4},\\
y_2(x)=&(r_1+r_2+\rho_1+\rho_2-1)x^2+(r_1+r_2+\rho_1+\rho_2-1)x+r_1\rho_1\rho_2+r_2\rho_1\rho_2+r_1r_2\rho_1+r_1r_2\rho_2\\
&-r_1r_2-\frac{r_1\rho_1+r_1\rho_2+r_2\rho_1+r_2\rho_2-r_1-r_2}{2}+\frac{\rho_1+\rho_2-1}{4}.
\end{aligned}
$$

The orthogonality constant in the right-hand side of (3.4.23) is given by $h^{(1)}_{(3,1),n}=h^{(1)}_{(3,1),0}u_1^{(1)}\cdots u_n^{(1)}$, where $h^{(1)}_{(3,1),0}=\sum_{x\in\chi^{(1)}_{(3,1)}}\hat{\omega}^{(1)}(x)B^{(1)}_{(3,1),0}(x)^2$, and

$$
u_n^{(1)}=\begin{cases}
-\dfrac{n(2r_1+2\rho_2+N-n)^2(2r_1-2\rho_1+N-n)(2r_1+2\rho_2+N-n-2)}{8(2r_1-2\rho_1+N-2n)^2(\rho_1+\rho_2+\frac{n}{2}-1)}, & \text{if } n \text{ is even,}\\
\dfrac{2(N-n)(2r_1-2\rho_1-n)(2r_1-2\rho_2-n)(\rho_1+\rho_2+\frac{n-1}{2})(\rho_1+\rho_2+\frac{n+1}{2})(\rho_1-\rho_2-\frac{N-n}{2})}{(2r_1-2\rho_1+N-2n)^2(2r_1+2\rho_2+N-n+1)(2r_1+2\rho_2+N-n-1)}, & \text{if } n \text{ is odd.}
\end{cases}
$$

3.5 Some notes on the generalized Darboux transformation

This paper starts from the original idea that exceptional Dunkl shift operators can be obtained from the intertwining relations which always appear in the Darboux transformations. We call this method a generalized Darboux transformation (on first-order difference operators). After the 1-step and the multiple-step exceptional Dunkl shift operators being successfully obtained through this method, we are able to give the exceptional Bannai-Ito operators with the restriction on certain coefficients. Especially, in this paper we mainly focus on the 1-step exceptional Bannai-Ito polynomials, which form the eigenpolynomials of the normalized 1-step exceptional Bannai-Ito operator.

In this generalized Darboux transformation the crucial role is played by the operator $\mathscr{F}_\phi$ which annihilates the seed solution $\phi(x)$. In fact, we should realize that the choice of the operator $\mathscr{F}_\phi$ in Section 3.2 is not unique. The only restriction we have used is that $\mathscr{F}_\phi$ is also a Dunkl shift operator. Without loss of generality, we may define $\mathscr{F}$ as

$$\mathscr{F} = -\frac{R-I+f_1(x)}{\phi(-x)-\phi(x)+f_1(x)\phi(x)} + \frac{TR-I+f_2(x)}{\phi(-x-1)-\phi(x)+f_2(x)\phi(x)} \tag{3.5.1}$$

such that $\mathscr{F}[\phi(x)] = 0$, and correspondingly,

$$\chi(x) = \phi(x)-\phi(-x)-f_1(x)\phi(x), \quad \tilde{\chi}(x) = \phi(-x-1)-\phi(x)+f_2(x)\phi(x).$$

In the case regarding $\mathscr{F}_\phi$, we have let

$$f_1(x) = 0, \quad f_2(x) = (\beta(-x-1)+\beta(x))/\beta(x). \tag{3.5.2}$$

Recall that the 1-step exceptional Dunkl shift operator has the form

$$H^{(1)} = \alpha^{(1)}(x)(R-I)+\beta^{(1)}(x)(TR-I)+\gamma^{(1)}(x),$$

then from the intertwining relation $\mathscr{F}\circ H = H^{(1)}\circ\mathscr{F}$ one can obtain the coefficients of $H^{(1)}$ by comparing the coefficients of the operators RTR, T, TR, R, I appeared in each side. Specifically, from the coefficients of RTR and T we have

$$\alpha^{(1)}(x) = \frac{\beta(-x)[\phi(x-1)-\phi(-x)+f_2(-x)\phi(-x)]}{\phi(x)-\phi(-x)-f_1(x)\phi(x)}, \tag{3.5.3}$$

$$\beta^{(1)}(x) = \frac{\alpha(-x-1)[\phi(-x-1)-\phi(x+1)-f_1(-x-1)\phi(-x-1)]}{\phi(-x-1)-\phi(x)+f_2(x)\phi(x)}. \tag{3.5.4}$$

After substituting (3.5.3), (3.5.4) into the remaining three equations with respect to the coefficients of TR, R, I we can derive three different expressions of $\gamma^{(1)}(x)$ (which are omitted in view of their length). Of course, these three expressions of $\gamma^{(1)}(x)$ must be equal to each other, hence one can derive the restrictions regarding $f_1(x)$ and $f_2(x)$ from this fact. However, this is not an easy task as it seems to be, since the equations with respect to $\gamma^{(1)}(x)$ are complicated and difficult to solve. Three other feasible cases we have found are:

$$f_1(x) = 0, f_2(x) = 0; \tag{3.5.5}$$

$$f_1(x) = (\alpha(-x)+\alpha(x))/\alpha(x), f_2(x) = 0; \tag{3.5.6}$$

$$f_1(x) = (\alpha(-x)+\alpha(x))/\alpha(x), f_2(x) = (\beta(-x-1)+\beta(x))/\beta(x). \tag{3.5.7}$$

As for the general cases of $f_1(x)$ and $f_2(x)$, we shall leave it as an open problem for the readers of interest.

If one look at the 1-step exceptional eigenfunction $\mathscr{F}[B_n(x)]$, the following two expressions can be obtained similarly as we did in the proof of Lemma 3.4.1:

$$
\begin{aligned}
\beta(x)\chi(x)\tilde{\chi}(x)\mathscr{F}[B_n(x)] &= (\lambda_n + \alpha(x)f_1(x) + \beta(x)f_2(x))\,B_n(x)(\phi(-x) - \phi(x)) \\
&\quad - (\mu + \alpha(x)f_1(x) + \beta(x)f_2(x))\,\phi(x)(B_n(-x) - B_n(x)) \\
&\quad + (\lambda_n - \mu)f_1(x)B_n(x)\phi(x), \\
\alpha(x)\chi(x)\tilde{\chi}(x)\mathscr{F}[B_n(x)] &= (\mu + \alpha(x)f_1(x) + \beta(x)f_2(x))\,\phi(x)(B_n(-x-1) - B_n(x)) \\
&\quad - (\lambda_n + \alpha(x)f_1(x) + \beta(x)f_2(x))\,B_n(x)(\phi(-x-1) - \phi(x)) \\
&\quad + (\mu - \lambda_n)f_2(x)B_n(x)\phi(x).
\end{aligned}
$$

Recall that for the coefficients $\alpha(x)$, $\beta(x)$ of the Bannai-Ito operator, $\alpha(-x) + \alpha(x)$ and $\beta(-x-1) + \beta(x)$ are both constants (see (3.2.23)), hence $\alpha(x)f_1(x) + \beta(x)f_2(x)$ is always constant in the four cases with respect to (3.5.2), (3.5.5)-(3.5.7). Thus, one can derive 1-step exceptional Bannai-Ito polynomials from the normalizations of these expressions. It turns out (3.5.2), (3.5.5)-(3.5.7) actually lead to different exceptional polynomials. Discussions on the orthogonality with respect to (3.5.5)-(3.5.7) can be made in the same manner as that of (3.5.2). In view of this fact, there are more than one type of exceptional Bannai-Ito polynomials. This is the nontrivial aspect of our "generalized" Darboux transformation, due to the non-uniqueness of $\mathscr{F}$.

3.6 Supplymentary data

For readers' convenience, we list some data for the coefficients $\mu_{d,m} - \beta$, $\lambda_n - \mu_{d,m}$ and $C_{d,m,n}$, which have been used in the proof of Proposition 3.4.1.

For m is even, we have

$$\mu_{1,m} - \beta = \frac{m}{2} - r_1 - r_2, \tag{3.6.1}$$

$$\mu_{2,m} - \beta = \frac{m}{2} - \rho_1 - \rho_2, \tag{3.6.2}$$

$$\mu_{3,m} - \beta = \frac{m}{2} - r_1 - r_2 - \rho_1 - \rho_2, \tag{3.6.3}$$

$$\mu_{4,m} - \beta = \frac{m}{2}, \tag{3.6.4}$$

for m is odd, we have

$$\mu_{5,m} - \beta = \frac{m}{2} - r_2 - \rho_1, \tag{3.6.5}$$

$$\mu_{6,m} - \beta = \frac{m}{2} - r_1 - \rho_2, \tag{3.6.6}$$

$$\mu_{7,m} - \beta = \frac{m}{2} - r_2 - \rho_2, \tag{3.6.7}$$

$$\mu_{8,m} - \beta = \frac{m}{2} - r_1 - \rho_1. \tag{3.6.8}$$

For m is odd and n is odd, we have

$$\lambda_n - \mu_{1,m} = \frac{m-n}{2}, \tag{3.6.9}$$

$$\lambda_n - \mu_{2,m} = r_1 + r_2 - \rho_1 - \rho_2 + \frac{m-n}{2}, \tag{3.6.10}$$

$$\lambda_n - \mu_{3,m} = -\rho_1 - \rho_2 + \frac{m-n}{2}, \tag{3.6.11}$$

$$\lambda_n - \mu_{4,m} = r_1 + r_2 + \frac{m-n}{2}, \tag{3.6.12}$$

for m is even and n is odd, we have

$$\lambda_n - \mu_{5,m} = r_1 - \rho_1 + \frac{m-n}{2}, \tag{3.6.13}$$

$$\lambda_n - \mu_{6,m} = r_2 - \rho_2 + \frac{m-n}{2}, \tag{3.6.14}$$

$$\lambda_n - \mu_{7,m} = r_1 - \rho_2 + \frac{m-n}{2}, \tag{3.6.15}$$

$$\lambda_n - \mu_{8,m} = r_2 - \rho_1 + \frac{m-n}{2}. \tag{3.6.16}$$

For m is even and n is even, we have

$$C_{1,m,n} = -\frac{(r_1+r_2-\frac{m}{2})(r_1+r_2-\frac{n}{2})(\frac{m-n}{2})(r_1+r_2-\rho_1-\rho_2)}{(r_1+r_2-\rho_1-\rho_2-m)(r_1+r_2-\rho_1-\rho_2-n)}, \tag{3.6.17}$$

$$C_{2,m,n} = \frac{(\rho_1+\rho_2-\frac{m}{2})(r_1+r_2-\frac{n}{2})(r_1+r_2-\rho_1-\rho_2+\frac{m-n}{2})(r_1+r_2-\rho_1-\rho_2)}{(r_1+r_2-\rho_1-\rho_2+m)(r_1+r_2-\rho_1-\rho_2-n)}, \tag{3.6.18}$$

$$C_{3,m,n} = \frac{(r_1+r_2+\rho_1+\rho_2-\frac{m}{2})(r_1+r_2-\frac{n}{2})(\rho_1+\rho_2-\frac{m-n}{2})(r_1+r_2-\rho_1-\rho_2)}{(r_1+r_2+\rho_1+\rho_2-m)(r_1+r_2-\rho_1-\rho_2-n)}, \tag{3.6.19}$$

$$C_{4,m,n} = \frac{(-\frac{m}{2})(r_1+r_2-\frac{n}{2})(r_1+r_2+\frac{m-n}{2})(r_1+r_2-\rho_1-\rho_2)}{(r_1+r_2+\rho_1+\rho_2+m)(r_1+r_2-\rho_1-\rho_2-n)}, \tag{3.6.20}$$

for m is odd and n is even, we have

$$C_{5,m,n} = \frac{(r_2+\rho_1-\frac{m}{2})(r_1+r_2-\frac{n}{2})(r_1-\rho_1+\frac{m-n}{2})(r_1+r_2-\rho_1-\rho_2)}{(r_1-r_2-\rho_1+\rho_2+m)(r_1+r_2-\rho_1-\rho_2-n)}, \tag{3.6.21}$$

$$C_{6,m,n} = -\frac{(r_1+\rho_2-\frac{m}{2})(r_1+r_2-\frac{n}{2})(r_2-\rho_2+\frac{m-n}{2})(r_1+r_2-\rho_1-\rho_2)}{(r_1-r_2-\rho_1+\rho_2-m)(r_1+r_2-\rho_1-\rho_2-n)}, \tag{3.6.22}$$

$$C_{7,m,n} = \frac{(r_2+\rho_2-\frac{m}{2})(r_1+r_2-\frac{n}{2})(r_1-\rho_2+\frac{m-n}{2})(r_1+r_2-\rho_1-\rho_2)}{(r_1-r_2+\rho_1-\rho_2+m)(r_1+r_2-\rho_1-\rho_2-n)}, \tag{3.6.23}$$

$$C_{8,m,n} = -\frac{(r_1+\rho_1-\frac{m}{2})(r_1+r_2-\frac{n}{2})(r_2-\rho_1+\frac{m-n}{2})(r_1+r_2-\rho_1-\rho_2)}{(r_1-r_2+\rho_1-\rho_2-m)(r_1+r_2-\rho_1-\rho_2-n)}. \tag{3.6.24}$$

Chapter 4

Dunkl-Supersymmetric orthogonal functions

In this chapter, we introduce a new type of orthogonal functions related with the theory of supersymmetry.

4.1 A supersymmetric quantum mechanics model with Dunkl-type supercharges

Supersymmetric quantum mechanics (SUSY QM) has been useful in the study of exactly solvable quantum mechanical models [13, 86]. In [65], the authors presented supersymmetric quantum mechanical models in one dimension involving differential operators of Dunkl-type (see also [63, 64]). In this realization, the reflection operator appears in both the supersymmetric Hamiltonian and the supercharge. The wave functions for two such systems have been obtained in [65] and seen to define orthogonal polynomials that are themselves expressed in terms of Hermite and little -1 Jacobi polynomials respectively. We here propose to pursue the exploration of the orthogonal functions that occur as eigenfunctions of such Dunkl-type supercharges,specifically of the operator

$$\mathscr{L} = \partial_x R + v(x), \tag{4.1.1}$$

where $v(-x) = -v(x)$, R is the reflection operator acts on the variable x, $Rf(x) = f(-x)$.

A Hamiltonian H is said to be supersymmetric if there are supercharges Q, $Q^\dagger$ such that the following superalgebra relations are satisfied

$$[Q,H] = 0, \quad [Q^\dagger,H] = 0, \quad H = \{Q,Q^\dagger\}. \tag{4.1.2}$$

The brackets $[,]$ and $\{,\}$ are called the commutator and the anticommutator, respectively:

$$[A,B] = AB - BA, \quad \{A,B\} = AB + BA.$$

If the supercharge Q is self-adjoint, i.e., $Q^\dagger = Q$, it follows from (4.1.2) that the $H = 2Q^2$, and the model is said to be $N = 1/2$ supersymmetric. Realizations of $N = 1/2$ supersymmetric systems have been obtained in [65] by taking the supercharge as the following Dunkl-type differential operator:

$$Q = 2^{-\frac{1}{2}}(\partial_x R + u(x)R + v(x)), \tag{4.1.3}$$

where $u(x)$ is even, $v(x)$ is odd (i.e., $u(-x) = u(x)$, $v(-x) = -v(x)$), and the operator R is the reflection operator which acts on x as $Rf(x) = f(-x)$. It is clear that Q is self-adjoint, $Q^\dagger = Q$, and the

Hamiltonian H is then

$$H = -\partial_x^2 + (u^2(x) + v^2(x) + u'(x)) - v'(x)R. \tag{4.1.4}$$

Notice that if $u(x) = 0$, then the supercharge Q and the Hamiltonian H become

$$Q = 2^{-\frac{1}{2}}(\partial_x R + v(x)), \quad H = -\partial_x^2 + v^2(x) - v'(x)R, \tag{4.1.5}$$

and they satisfy

$$\{Q, R\} = 0, \quad [H, R] = 0. \tag{4.1.6}$$

The assumption that $v(x)$ is odd is essential for the relations (4.1.6) to be achieved. Consequently, these relations together with (4.1.2) imply that, for Q and H given in (4.1.5):

(a) the operators Q and H share the same eigenfunctions: $Q\psi(x) = \nu\psi(x)$, $H\psi(x) = E\psi(x)$, where $E = 2\nu^2$;
(b) their eigenfunctions appear in pairs $\psi(x), \psi(-x)$:

$$\begin{aligned} Q\psi(x) &= \nu\psi(x), \quad Q\psi(-x) = -\nu\psi(-x); \\ H\psi(x) &= E\psi(x), \quad H\psi(-x) = E\psi(-x). \end{aligned} \tag{4.1.7}$$

We shall focus on models described by (4.1.5) in this chapter and will assume that the operator $\mathscr{L}$ is non-degenerate, i.e., all that eigenvalues of $\mathscr{L}$ are distinct. For results on the eigenvalue problem related with the most general first-order Dunkl-type differential operator

$$L = F_0(x) + F_1(x)R + G_0(x)\partial_x + G_1(x)\partial_x R$$

with arbitrary functions $F_0(x)$, $F_1(x)$, $G_0(x)$, $G_1(x)$ one can refer to [83].

4.2 The eigenvalue problem of a Hamiltonian with reflection

In this section, we give an analysis on the eigenvalue problem related to the Hamiltonian

$$H = -\partial_x^2 + v^2(x) - v'(x)R \tag{4.2.1}$$

where $v(x)$ is odd, $v(-x) = -v(x)$. First, let us notice that H can be rewritten into the following two Hamiltonians

$$\begin{aligned} H_1 &= -\partial_x^2 + v^2(x) - v'(x) := -\partial_x^2 + V_1(x), \\ H_2 &= -\partial_x^2 + v^2(x) + v'(x) := -\partial_x^2 + V_2(x), \end{aligned} \tag{4.2.2}$$

by restricting H on even or odd functions, respectively. In this way, we can avoid coping with the reflection R directly. The potentials $V_1(x)$ and $V_2(x)$ are **even** under the assumption that $v(x)$ is odd, and the relation $V_2(x) = V_1(x) + 2v'(x)$ holds. In this case the function $v(x)$ plays the role of the superpotential, the potentials $V_1(x)$ and $V_2(x)$ are known as a pair of supersymmetric partner potentials [13].

In view of the property (4.1.7), let us assume that H has a discrete sequence of eigenfunctions:

$$H\psi_n(x) = E_n\psi_n(x), \quad n = 0, \pm 1, \pm 2, \ldots$$

where $E_0 = 0$, $E_{-n} = E_n$, $\psi_{-n}(x) = \psi_n(-x)$, $n = 1,2,\dots$. If we apply the decompositions

$$\psi_{\pm n}(x) = e_n(x) \pm o_n(x), \tag{4.2.3}$$

where $e_n(x)$ and $o_n(x)$ are the even and odd components of $\psi_{\pm n}(x)$, respectively, then the eigenvalue equation of H can be rewritten into

$$H\psi_{\pm n}(x) = H_1 e_n(x) \pm H_2 o_n(x) = E_n(e_n(x) \pm o_n(x))$$

which lead to the following eigenvalue equations

$$H_1 e_n(x) = E_n e_n(x), \quad H_2 o_n(x) = E_n o_n(x). \tag{4.2.4}$$

Lemma 4.2.1. *If there exist a sequence of eigenfunctions of H_1 which are all even and a sequence of eigenfunctions of H_2 which are all odd, and their eigenvalues satisfy the condition (4.2.5), then the eigenfunctions of H can be expressed as linear combinations of those of H_1 and H_2.*

Proof. Denote the eigenfunctions and eigenvalues of H_1 and H_2 by $\psi_n^{(1)}(x)$, $E_n^{(1)}$ and $\psi_n^{(2)}(x)$, $E_n^{(2)}$, respectively. Let $\psi_{N(n)}^{(1)}(x)$ be the even eigenfunctions of H_1 and $\psi_{M(n)}^{(2)}(x)$ be the odd eigenfunctions of H_2, where the indices $N(n)$ and $M(n)$ are both increasing, namely,

$$0 \le N(0) < N(1) < \cdots; \quad 0 \le M(0) < M(1) < \cdots.$$

Then, by defining

$$e_n(x) = C^{(e)}\psi_{N(n)}^{(1)}(x), \quad o_n(x) = C^{(o)}\psi_{M(n)}^{(2)}(x)$$

with arbitrary constants $C^{(e)}$, $C^{(o)}$ which are not identically zero, and imposing the condition

$$E_{N(n)}^{(1)} = E_{M(n)}^{(2)} \tag{4.2.5}$$

one can solve the eigenvalue problem of H as follow:

$$\psi_n(x) = C^{(e)}\psi_{N(n)}^{(1)}(x) + C^{(o)}\psi_{M(n)}^{(2)}(x), \quad E_n = E_{N(n)}^{(1)} = E_{M(n)}^{(2)}. \tag{4.2.6}$$

□

Remark 4.2.1. *Recall that the eigenvalue problem of the operator H_1 (H_2) on some interval (a,b) with boundary conditions is a Sturm-Liouville problem. For example, the eigenvalue problem*

$$\begin{aligned}\mathscr{H}\phi(x) = (-\partial_x^2 + V(x))\phi(x) = \lambda\phi(x), \quad x \in (a,b)\\ c_a\phi(a) + d_a\phi'(a) = 0,\\ c_b\phi(b) + d_b\phi'(b) = 0\end{aligned}$$

is a regular Sturm-Liouville problem. According to the Sturm-Liouville theory, if $V(x)$ is continuous and regular in (a,b), then

(1) Eigenvalues of the operator $\mathscr{H}$ are real, simple and non-degenerate (eigenvalues of different eigenfunctions are distinct, $\lambda_m \neq \lambda_n$, $\forall m \neq n$). Further, the eigenvalues form an infinite sequence, and can be ordered according to increasing magnitude so that $\lambda_0 < \lambda_1 < \cdots$ and $\lim_{n\to\infty}\lambda_n = \infty$.

(2) The eigenfunctions of $\mathscr{H}$ are orthogonal:

$$\int_a^b \phi_m(x)\phi_n(x)dx = 0, \quad m \neq n.$$

Remark 4.2.2. *Since the reflection R is involved in H, the range of the coordinate x must be invariant under R, namely, it should be $(-a,a)$ (a can be finite or infinite). Thus, the range of the coordinate x in H_1 and H_2 should both be $(-a,a)$. From the construction of H_1 and H_2 it is easily seen that once H_1 satisfies this condition, then the same holds for H_2. We shall distinguish the following two cases: (A) a "genuine" $(-a,a)$ model and (B) two copies of $(0,a)$ model. Note that the potential $V_1(x)$ ($V_2(x)$) is even here.*

In case (A), let us consider the operator H_1 on $(-a,a)$. Assume that H_1 has an infinite sequence of eigenfunctions, $H_1\psi_n^{(1)}(x) = E_n^{(1)}\psi_n^{(1)}(x)$ ($n = 0,1,\ldots$) with $0 = E_0 < E_1 < \cdots$, then the eigenfunctions and eigenvalues of H_2 follow from the relations (4.3.1) and (4.3.2) automatically. Thus those of H can be derived using Lemma 4.2.1.

In case (B), let us consider the operator H_1 on $(0,a)$. In this case, we assume that the potentials $V_1(x)$, $v(x)$ are singular at $x = 0$, and H_1 has an infinite sequence of eigenfunctions, $H_1\psi_n^{(1)}(x) = E_n^{(1)}\psi_n^{(1)}(x)$ ($n = 0,1,2,\ldots$) with $0 = E_0 < E_1 < \cdots$. In particular, we assume that $\psi_n^{(1)}(x)$ satisfies $\psi_n^{(1)}(0) = (\psi_n^{(1)})'(0) = 0$. Define the Hamiltonian $\tilde{H}_1$ of a new model on $(-a,a)$ by $\tilde{H}_1 = H_1$, which is singular at $x = 0$. We will see in Section 4.3 that H_1 can be factorized as $H_1 = A^\dagger A$, where A and its conjugation $A^\dagger$ are first order differential operators, thus by defining the operators $\tilde{A}$ and $\tilde{A}^\dagger$ of new model on $(-a,a)$ as $\tilde{A} = A$ and $\tilde{A}^\dagger = A^\dagger$, we have $\tilde{H} = \tilde{A}^\dagger\tilde{A}$. Let us define $\tilde{\psi}_n^{(1)}(x)$ on $(-a,a)$ as follows:

$$\tilde{\psi}_{2n}^{(1)}(x) = \begin{cases} \psi_n^{(1)}(x) & (0 \le x < a) \\ \psi_n^{(1)}(-x) & (-a < x < 0) \end{cases}, \quad \tilde{\psi}_{2n+1}^{(1)}(x) = \begin{cases} \psi_n^{(1)}(x) & (0 \le x < a) \\ -\psi_n^{(1)}(-x) & (-a < x < 0) \end{cases} \tag{4.2.7}$$

which satisfy

$$\tilde{\psi}_n^{(1)}(-x) = (-1)^n\tilde{\psi}_n^{(1)}(x). \tag{4.2.8}$$

Then we have

$$\tilde{H}_1\tilde{\psi}_n^{(1)}(x) = \tilde{E}_n\tilde{\psi}_n^{(1)}(x), \quad \tilde{E}_{2n} = \tilde{E}_{2n+1} = E_n \quad (n \ge 0).$$

The energy eigenvalues are doubly degenerate, which is allowed by the singularity of $x = 0$. The eigenfunctions $\tilde{\psi}_{2n}^{(1)}(x)$ and $\tilde{\psi}_{2m+1}^{(1)}(x)$ are orthogonal: $\int_{-a}^{a}\tilde{\psi}_{2n}^{(1)}(x)\tilde{\psi}_{2m+1}^{(1)}(x)dx = 0$. Again, using the relations (4.3.1), (4.3.2) and Lemma 4.2.1 one can obtain the eigenfunctions and eigenvaules of H.

4.3 Supersymmetric quantum mechanics and shape invariant even potentials

In the theory of SUSY QM [13], the Hamiltonians H_1 and H_2 can be factorized as follow:

$$H_1 = A^\dagger A + E_0^{(1)}, \quad H_2 = AA^\dagger + E_0^{(1)},$$

where $A^\dagger$ is the conjugation of A,

$$A = \partial_x + v(x), \quad A^\dagger = -\partial_x + v(x).$$

If we consider the unbroken SUSY where the ground state energy is zero, namely, $E_0^{(1)} = 0$, then we can choose $v(x) = -(\ln \psi_0^{(1)}(x))'$ such that $H\psi_0^{(1)}(x) = A^\dagger A\psi_0^{(1)}(x) = 0$. This follows from the fact that A annihilates the ground state wave function $\psi_0^{(1)}(x)$.

Again, let us denote the eigenfunctions and eigenvalues of H_1 and H_2 by $\psi_n^{(1)}(x)$, $E_n^{(1)}$ and $\psi_n^{(2)}(x)$, $E_n^{(2)}$, respectively. They satisfy the equations

$$H_1\psi_n^{(1)}(x) = A^\dagger A\psi_n^{(1)}(x) = E_n^{(1)}\psi_n^{(1)}(x), \quad H_2 A\psi_n^{(1)}(x) = AA^\dagger A\psi_n^{(1)}(x) = E_n^{(1)} A\psi_n^{(1)}(x),$$
$$H_2\psi_n^{(2)}(x) = AA^\dagger\psi_n^{(2)}(x) = E_n^{(2)}\psi_n^{(2)}(x), \quad H_1 A^\dagger\psi_n^{(2)}(x) = A^\dagger AA^\dagger\psi_n^{(2)}(x) = E_n^{(2)} A^\dagger\psi_n^{(2)}(x),$$

from which it follows that

$$E_n^{(2)} = E_{n+1}^{(1)}, \quad E_0^{(1)} = 0, \tag{4.3.1}$$

$$\psi_n^{(2)}(x) = (C_n^{(1)})^{-1} A\psi_{n+1}^{(1)}(x), \tag{4.3.2}$$

$$\psi_{n+1}^{(1)}(x) = (C_{n+1}^{(2)})^{-1} A^\dagger\psi_n^{(2)}(x), \tag{4.3.3}$$

where the coefficients $C_n^{(1)}$ and $C_n^{(2)}$ satisfy the condition $C_n^{(1)} C_{n+1}^{(2)} = E_{n+1}^{(1)}$. Note that the relations (4.3.2), (4.3.3) and the definitions of $A, A^\dagger$ imply that $\psi_{n+1}^{(1)}(x)$ and $\psi_n^{(2)}(x)$ have different parity, namely, if $\psi_{n+1}^{(1)}(x)$ is even, then $\psi_n^{(2)}(x)$ is odd; if $\psi_{n+1}^{(1)}(x)$ is odd, then $\psi_n^{(2)}(x)$ is even.

In what follows we adopt the assumption in the proof of Lemma 4.2.1 that $\psi_{N(n)}^{(1)}(x)$ are even and $\psi_{M(n)}^{(2)}(x)$ are odd for $n = 0, 1, \ldots$. This can be achieved through some minor trick. (In fact, if $\psi_n^{(1)}(x)$ and $\psi_n^{(2)}(x)$ do not have definite parity, we can redefine them by

$$\tilde{\psi}_n^{(1)}(x) := \frac{1}{2}(\psi_n^{(1)}(x) + \psi_n^{(1)}(-x)), \quad \tilde{\psi}_n^{(2)}(x) := \frac{1}{2}(\psi_n^{(2)}(x) - \psi_n^{(2)}(-x))$$

which are still eigenfunctions of H_1 and H_2 with eigenvalues $E_n^{(1)}$ and $E_n^{(2)}$, respectively. This is because $\psi_n^{(1)}(-x)$ and $\psi_n^{(2)}(-x)$ are also eigenfunctions of H_1 and H_2 with eigenvalues $E_n^{(1)}$ and $E_n^{(2)}$, respectively. Obviously, the new defined eigenfunctions are even and odd, respectively.)

If we let $v(x)$ in the operator $\mathscr{L}$ be defined by $v(x) = -(\ln \psi_0^{(1)}(x))'$, then the operators A and $A^\dagger$ turn out to be the restrictions of $\mathscr{L}$ on even and odd functions, respectively. It follows that

$$\mathscr{L}\psi_{N(n)}^{(1)}(x) = A\psi_{N(n)}^{(1)}(x) = C_{N(n)-1}^{(1)}\psi_{N(n)-1}^{(2)}(x), \tag{4.3.4}$$

$$\mathscr{L}\psi_{M(n)}^{(2)}(x) = A^\dagger\psi_{M(n)}^{(2)}(x) = C_{M(n)+1}^{(2)}\psi_{M(n)+1}^{(1)}(x). \tag{4.3.5}$$

From these relations we can derive the eigenfunctions of $\mathscr{L}$.

Lemma 4.3.1. *Let* $C_{N(n)-1}^{(1)} = C_{N(n)}^{(2)} = \sqrt{E_{N(n)}^{(1)}}$, $n = 0, 1, \ldots$, *and*

$$\psi_{N(n)-1}^{(2)}(x) = \left(\sqrt{E_{N(n)}^{(1)}}\right)^{-1} A\psi_{N(n)}^{(1)}(x). \tag{4.3.6}$$

If we further assume that $M(n) = N(n) - 1$, $n = 0, 1, \ldots$, *then the eigenvalue problem* $\mathscr{L}\psi_{\pm n}(x) = \lambda_{\pm n}\psi_{\pm n}(x)$ *can be solved as follow:*

$$\psi_{\pm n}(x) = \psi_{N(n)}^{(1)}(x) \pm \psi_{N(n)-1}^{(2)}(x), \quad \lambda_{\pm n} = \pm\sqrt{E_{N(n)}^{(1)}}. \tag{4.3.7}$$

Proof. The condition $M(n) = N(n) - 1$ is equivalent with (4.2.5) in view of the relation (4.3.1), then it follows from Lemma 4.2.1 that the eigenfunctions of H as well as those of $\mathscr{L}$ can be expressed in terms of the linear combination of $\psi_n^{(1)}(x)$ and $\psi_n^{(2)}(x)$. Using this condition and the relations (4.3.4), (4.3.5) one can easily check the following eigenvalue equations

$$\mathscr{L}\left(\psi_{N(n)}^{(1)}(x) \pm \sqrt{C_{N(n)-1}^{(1)}/C_{N(n)}^{(2)}}\,\psi_{N(n)-1}^{(2)}(x)\right) = \pm\sqrt{E_{N(n)}^{(1)}}\left(\psi_{N(n)}^{(1)}(x) \pm \sqrt{C_{N(n)-1}^{(1)}/C_{N(n)}^{(2)}}\,\psi_{N(n)-1}^{(2)}(x)\right).$$

Then (4.3.7) follows immediately from the assumption $C_{N(n)-1}^{(1)} = C_{N(n)}^{(2)} = \sqrt{E_{N(n)}^{(1)}}$. □

4.3.1 Shape invariant even potentials

It is now clear that once the even potentials $V_1(x), V_2(x)$ and their corresponding eigenfunctions and eigenvalues are known, then the eigenfunctions and eigenvalues of $\mathscr{L}$ with $v(x)$ given by the superpotential related to $V_1(x), V_2(x)$ follow automatically from Lemma 4.3.1.

A good class of potentials are the shape invariant potentials which satisfy the condition

$$V_2(x;a_1) = V_1(x;a_2) + R(a_1), \tag{4.3.8}$$

where a_1 is a set of parameters, a_2 is a translation of a_1, and it follows that

$$R(a_1) = V_2(x;a_1) - V_1(x;a_2) = V_1(x;a_1) - V_1(x;a_2) + 2v'(x;a_1).$$

Unless otherwise stated, for any function $f(x)$ appear later we default $f(x)$ stands for $f(x;a_1)$, in other words, a_1 and a_2 must appear simultaneously. The condition (4.3.8) implies that

$$H_2\psi_m^{(1)}(x;a_2) = [E_m^{(1)}(a_2) + R(a_1)]\psi_m^{(1)}(x;a_2).$$

By comparing this with the eigenvalue equation $H_2\psi_n^{(2)}(x;a_1) = E_n^{(2)}(a_1)\psi_n^{(2)}(x;a_1)$ we can conclude that if $E_n^{(2)}(a_1) = E_m^{(1)}(a_2) + R(a_1)$ holds for some indices m and n, then

$$\psi_n^{(2)}(x;a_1) \propto \psi_m^{(1)}(x;a_2). \tag{4.3.9}$$

In particular, if $m = n$, then (4.3.9) becomes (4.3.12) and it means that the eigenfunctions of H_1 and H_2 coincide through a translation on certain parameters. Fortunately, it turns out that this is true for all the examples we shall consider in this paper (see Remark 4.3.1). Combining the relations (4.3.6) and (4.3.12), then we have

$$\psi_{N(n)-1}^{(2)}(x;a_1) = \left(\sqrt{E_{N(n)}^{(1)}(a_1)}\right)^{-1} A\psi_{N(n)}^{(1)}(x;a_1) \propto \psi_{N(n)-1}^{(1)}(x;a_2). \tag{4.3.10}$$

Recall that $\psi_{N(n)-1}^{(2)}(x;a_1)$ is odd and $\psi_{N(n)}^{(1)}(x;a_1)$ is even, thus $\psi_{N(n)-1}^{(1)}(x;a_1)$ is odd too since the translation on the parameter(s) a_1 does not change the parity in x. So $\psi_n^{(1)}(x)$ is symmetric:

$$\psi_n^{(1)}(-x) = (-1)^n\psi_n^{(1)}(x). \tag{4.3.11}$$

And $\psi_n^{(2)}(x)$ should also be symmetric due to the relation (4.3.2).

A list of shape invariant potentials and of the corresponding wavefunctions related with supersymmetric quantum mechanics is presented in [13] (Table 4.1). We can readily obtain from this table the even potentials by putting restrictions on certain parameters. The results are given in Table 1 (which is split in two parts). Specifically, the examples of **shifted oscillator**, **Scarf II or Rosen-Morse II (hyperbolic)** and **Scarf I** potentials belong to case (A) in Remark 4.2.2 while the examples of **3d oscillator**, **generalized Pöschl-Teller** and **Pöschl-Teller** potentials belong to case (B). For convenience we shall call them the type (A) examples and the type (B) examples, respectively.

Remark 4.3.1. *From Table 1 one can see that in all the examples the relation*

$$E_n^{(1)}(a_2)+R(a_1)=E_n^{(2)}(a_1),$$

holds, which leads to

$$\psi_n^{(2)}(x;a_1)\propto\psi_n^{(1)}(x;a_2). \tag{4.3.12}$$

The above relation together with Lemma 4.3.1 implies that the eigenfunctions of $\mathscr{L}$ with $v(x)$ given by the superpotential in Table 4.1 can be written as:

$$\psi_{\pm n}(x;a_1)=\psi_{N(n)}^{(1)}(x;a_1)\pm\psi_{N(n)-1}^{(2)}(x;a_1)=\psi_{N(n)}^{(1)}(x;a_1)\pm\tilde{C}_n\psi_{N(n)-1}^{(1)}(x;a_2), \tag{4.3.13}$$

where it follows from (4.3.10) that

$$\tilde{C}_n=\left(\sqrt{E_{N(n)}^{(1)}(a_1)}\right)^{-1}\frac{A\psi_{N(n)}^{(1)}(x;a_1)}{\psi_{N(n)-1}^{(1)}(x;a_2)}. \tag{4.3.14}$$

Recall that the indices $N(n)$, $n=0,1,\ldots$, are chosen in such a way that $\psi_{N(n)}^{(1)}(x)$ are even and $\psi_{N(n)-1}^{(1)}(x)$ are odd. Since the Hermite polynomials $H_n(x)$ are symmetric, and the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ are symmetric when $\alpha=\beta$, we observe in Table 1 that all the eigenfunctions of the type (A) examples (the first three examples) are symmetric, and those of the type (B) examples can be constructed as symmetric functions using the method (4.2.7) introduced in Remark 4.2.2. Then it turns out that $N(n)=2n$, $n=0,1,\ldots$, and (4.3.13) reads

$$\psi_{\pm n}(x;a_1)=\psi_{2n}^{(1)}(x;a_1)\pm\tilde{C}_n\psi_{2n-1}^{(1)}(x;a_2). \tag{4.3.15}$$

To summarize, we provide a list of these eigenfunctions in Table 4.2. For the explicit definitions and properties of these classical orthogonal polynomials (Hermite, Laguerre and Jacobi polynomials) one can refer to Section 4.6.

4.4 Dunkl-SUSY orthogonal functions in terms of classical orthogonal polynomials

In this section we shall give some examples of Dunkl-SUSY orthogonal functions explicitly. Before that we may apply a gauge transformation on the operator $\mathscr{L}$ as follow:

$$Y:=(\psi_0^{(1)}(x))^{-1}\mathscr{L}\psi_0^{(1)}(x)=\partial_xR+v(x)(I-R). \tag{4.4.1}$$

The eigenfunctions of the new operator Y are $Q_n(x)=(\psi_0^{(1)}(x))^{-1}\psi_n^{(1)}(x)$ $(n=0,1,\ldots)$. We will show that these eigenfunctions also satisfy certain orthogonality relations, that will deem giving them the name of Dunkl-Supersymmetric (Dunkl-SUSY) orthogonal functions.

Table 4.1 Shape invariant even potentials derived from [13] (Table 4.1), where the parameters a_1 and a_2 are related by a translation $a_2 = a_1 + \alpha$. Here we replaced the parameter ω in [13] with $\omega = 2s^2$ for our convenience. Unless specified explicitly otherwise, the parameters A, B, α, s, l are all taken ≥ 0, and the range of potentials is $-\infty \leq x \leq \infty$, $0 \leq r \leq \infty$.

Name of potential	$v(x)$	$V_1(x;a_1)$	y	$\psi_n^{(1)}(y)$
shifted oscillator	s^2x	$s^2(s^2x^2-1)$	sx	$e^{-\frac{1}{2}y^2}H_n(y)$
Scarf II or Rosen-Morse II (hyperbolic)	$A\tanh(\alpha x)$	$A^2 - A(A+\alpha)\mathrm{sech}^2(\alpha x)$	$\sinh(\alpha x)$	$i^n(y^2+1)^{-\frac{A}{2\alpha}}$ $\cdot P_n^{(-\frac{A}{\alpha}-\frac{1}{2},-\frac{A}{\alpha}-\frac{1}{2})}(iy)$
Scarf I (trigonometric)	$A\tan(\alpha x)$ $(-\frac{\pi}{2\alpha} \leq x \leq \frac{\pi}{2\alpha})$	$-A^2 + A(A-\alpha)\sec^2(\alpha x)$	$\sin(\alpha x)$	$(1-y^2)^{\frac{A}{2\alpha}}$ $\cdot P_n^{(\frac{A}{\alpha}-\frac{1}{2},\frac{A}{\alpha}-\frac{1}{2})}(y)$
3d oscillator	$s^2r - \frac{l+1}{r}$	$s^4r^2 + \frac{l(l+1)}{r^2} - (2l+3)s^2$	s^2r^2	$y^{\frac{l+1}{2}}e^{-\frac{y}{2}}L_n^{l+\frac{1}{2}}(y)$
generalized Pöschl-Teller	$A\coth(\alpha r) - B\mathrm{cosech}(\alpha r)$ $(A<B)$	$A^2 + (B^2+A^2+A\alpha)\mathrm{cosech}^2(\alpha r)$ $-B(2A+\alpha)\coth(\alpha r)\mathrm{cosech}(\alpha r)$	$\cosh(\alpha r)$	$(y-1)^{\frac{B-A}{2\alpha}}(y+1)^{-\frac{A+B}{2\alpha}}$ $\cdot P_n^{(\frac{B-A}{\alpha}-\frac{1}{2},-\frac{A+B}{\alpha}-\frac{1}{2})}(y)$
Pöschl-Teller	$A\tan(\alpha r) - B\cot(\alpha r)$ $(A,B>0,\ 0<r<\frac{\pi}{2\alpha})$	$-(A+B)^2 + A(A-\alpha)\sec^2(\alpha r)$ $+B(B-\alpha)\mathrm{cosec}^2(\alpha r)$	$\cos(2\alpha r)$	$(1-y)^{\frac{B}{2\alpha}}(1+y)^{\frac{A}{2\alpha}}$ $\cdot P^{(\frac{B}{\alpha}-\frac{1}{2},\frac{A}{\alpha}-\frac{1}{2})}(y)$

Name of potential	a_1	a_2	$E_n^{(1)}(a_1)$	$E_n^{(2)}(a_1)$	$E_m^{(1)}(a_2)+R(a_1)$
shifted oscillator	s	s	$2ns^2$	$2(n+1)s^2$	$2(m+1)s^2$
Scarf II or Rosen-Morse II (hyperbolic)	A	$A-\alpha$	$2nA\alpha - n^2\alpha^2$	$2(n+1)A\alpha - (n+1)^2\alpha^2$	$2(m+1)A\alpha - (m+1)^2\alpha^2$
Scarf I (trigonometric)	A	$A+\alpha$	$2nA\alpha + n^2\alpha^2$	$2(n+1)A\alpha + (n+1)^2\alpha^2$	$2(m+1)A\alpha + (m+1)^2\alpha^2$
3d oscillator	l	$l+1$	$4ns^2$	$4(n+1)s^2$	$4(m+1)s^2$
generalized Pöschl-Teller	A	$A-\alpha$	$2nA\alpha - n^2\alpha^2$	$2(n+1)A\alpha - (n+1)^2\alpha^2$	$2(m+1)A\alpha - (m+1)^2\alpha^2$
Pöschl-Teller	A,B	$A+\alpha, B+\alpha$	$4n\alpha(A+B+n\alpha)$	$4(n+1)\alpha(A+B+(n+1)\alpha)$	$4(m+1)\alpha(A+B+(m+1)\alpha)$

The weight function $\omega(x)$ associated with the operator Y satisfies to [13,51]

$$\frac{\omega'(x)}{\omega(x)} = -2v(x) = 2\frac{\psi_0'(x)}{\psi_0(x)}$$

and hence $\omega(x) = (\psi_0^{(1)}(x))^2$. Therefore the orthogonality relation of $\{Q_n(x)\}_{n=0,\pm1,\pm2,\ldots}$ are

$$\int_I (\psi_0^{(1)}(x))^2 Q_n(x) Q_m(x) dx = 0, \quad n \neq m, \tag{4.4.2}$$

where the interval I will be determined from the weight function $(\psi_0^{(1)}(x))^2$.

With an eye to presenting a model-independent description of Dunkl-SUSY orthogonal functions, we now extract from Table 4.2 the following families of such orthogonal functions that are defined in terms of classical orthogonal polynomials. We assume that all the Hermite, Laguerre, Jacobi polyno-

Table 4.2 Eigenfunctions of the operator $\mathscr{L} = \partial_x R + v(x)$ with $v(x)$ given by the superpotentials in table 1.

$v(x)$	$\tilde{C}_n$	$\psi_{\pm n}(x)$
$s^2 x$	$2\sqrt{n}$	$e^{-\frac{1}{2}s^2x^2}[H_{2n}(sx) \pm \tilde{C}_n H_{2n-1}(sx)]$
$A\tanh(\alpha x)$	$\frac{1}{2}\sqrt{\frac{A-n\alpha}{n\alpha}}$	$(-1)^n \cosh(\alpha x)^{-\frac{A}{\alpha}}[P_{2n}^{(-\frac{A}{\alpha}-\frac{1}{2}),-\frac{A}{\alpha}-\frac{1}{2})}(i\sinh(\alpha x))$ $\mp \tilde{C}_n i\cosh(\alpha x) P_{2n-1}^{(-\frac{A}{\alpha}+\frac{1}{2}),-\frac{A}{\alpha}+\frac{1}{2})}(i\sinh(\alpha x))]$
$A\tan(\alpha x)$	$\frac{1}{2}\sqrt{\frac{A+n\alpha}{n\alpha}}$	$\lvert\cos(\alpha x)\rvert^{\frac{A}{\alpha}}[P_{2n}^{(\frac{A}{\alpha}-\frac{1}{2},\frac{A}{\alpha}-\frac{1}{2})}(\sin(\alpha x)) \pm \tilde{C}_n \lvert\cos(\alpha x)\rvert P_{2n-1}^{(\frac{A}{\alpha}+\frac{1}{2},\frac{A}{\alpha}+\frac{1}{2})}(\sin(\alpha x)]$
$s^2 r - \frac{l+1}{r}$	$-\frac{1}{\sqrt{n}}$	$\lvert sr\rvert^{l+1} e^{-\frac{1}{2}s^2r^2}[L_n^{(l+\frac{1}{2})}(s^2r^2) \pm \tilde{C}_n sr L_{n-1}^{(l+\frac{3}{2})}(s^2r^2)]$
$A\coth(\alpha r)$ $-B\text{cosech}(\alpha r)$	$\frac{1}{2}\sqrt{\frac{2A-n\alpha}{n\alpha}}$	$(\cosh(\alpha r)-1)^{\frac{B-A}{2\alpha}}(\cosh(\alpha r)+1)^{-\frac{B+A}{2\alpha}}[P_n^{(\frac{B-A}{\alpha}-\frac{1}{2},-\frac{B+A}{\alpha}-\frac{1}{2})}(\cosh(\alpha r)$ $\pm \tilde{C}_n \sinh(\alpha r) P_{n-1}^{(\frac{B-A}{\alpha}+\frac{1}{2},-\frac{B+A}{\alpha}+\frac{1}{2})}(\cosh(\alpha r)]$
$A\tan(\alpha r)$ $-B\cot(\alpha r)$	$\frac{1}{2}\sqrt{\frac{A+B+n\alpha}{n\alpha}}$	$(1-\cos(2\alpha r))^{\frac{B}{2\alpha}}(1+\cos(2\alpha r))^{\frac{A}{2\alpha}}[P_n^{(\frac{B}{\alpha}-\frac{1}{2},\frac{A}{\alpha}-\frac{1}{2})}(\cos(2\alpha r))$ $\pm \tilde{C}_n \sin(2\alpha r) P_n^{(\frac{B}{\alpha}+\frac{1}{2},\frac{A}{\alpha}+\frac{1}{2})}(\cos(2\alpha r))]$

mials ($\hat{H}_n(x)$, $\hat{L}_n^{(\alpha)}(x)$, $\hat{P}_n^{(\alpha,\beta)}(x)$) involved are orthonormal:

$$\int_{-\infty}^{\infty} \hat{H}_m(x)\hat{H}_n(x)dx = \delta_{m,n}, \quad \int_0^{\infty} \hat{L}_m^{(\alpha)}(x)\hat{L}_n^{(\alpha)}(x)dx = \delta_{m,n}, \quad \int_{-1}^{1} \hat{P}_m^{(\alpha,\beta)}(x)\hat{P}_n^{(\alpha,\beta)}(x)dx = \delta_{m,n}.$$

Specifically, let $H_n(x)$, $L_n^{(\alpha)}(x)$, $P_n^{(\alpha,\beta)}(x)$ be defined as in Section 4.6, then

$$\hat{H}_n(x) = (2^n n!\sqrt{\pi})^{-\frac{1}{2}} H_n(x), \quad \hat{L}_n^{(\alpha)}(x) = \left(\frac{\Gamma(n+\alpha+1)}{n!}\right)^{-\frac{1}{2}} L_n^{(\alpha)}(x),$$

$$\hat{P}_n^{(\alpha,\beta)}(x) = \left(\frac{2^{\alpha+\beta+1}\Gamma(\alpha+n+1)\Gamma(\beta+n+1)}{n!\Gamma(\alpha+\beta+n+1)(\alpha+\beta+2n+1)}\right)^{-\frac{1}{2}} P_n^{(\alpha,\beta)}(x).$$

Now we are ready to provide the following examples of Dunkl-SUSY orthogonal functions.

- Dunkl-SUSY orthogonal functions in terms of the orthonormal Hermite polynomials $\hat{H}_n(x)$, which is related with the **shifted oscillator** potential:

$$Q_{\pm n}^{(H)}(x) = \frac{1}{\sqrt{2}}\left(\hat{H}_{2n}(sx) \pm \hat{H}_{2n-1}(sx)\right), \quad n \geq 1, \quad Q_0^{(H)}(x) = 1, \tag{4.4.3}$$

$$Y = \partial_x R + s^2 x, \quad YQ_{\pm n}^{(H)}(x) = \pm\sqrt{E_{2n}}Q_{\pm n}^{(H)}(x), \quad E_n = 2ns^2, \tag{4.4.4}$$

$$\int_{-\infty}^{\infty} e^{-s^2x^2} Q_n^{(H)}(x) Q_m^{(H)}(x)dx = \delta_{nm}, \quad m,n \in \mathbb{Z}. \tag{4.4.5}$$

- Dunkl-SUSY orthogonal functions in terms of the orthonormal Laguerre polynomials $\hat{L}_n^{(\alpha)}(x)$, which is related with the **3d oscillator** potential ($l + \frac{1}{2} \to \alpha$):

$$Q_{\pm n}^{(L)}(x) = \frac{1}{\sqrt{2}}\left(\hat{L}_n^{(\alpha)}(s^2x^2) \mp x\hat{L}_{n-1}^{(\alpha+1)}(s^2x^2)\right), \quad n \geq 1, \quad Q_0^{(L)}(x) = 1, \tag{4.4.6}$$

$$Y = \partial_x R + s^2 x - \frac{\alpha + 1/2}{x}, \quad YQ_{\pm n}^{(L)}(x) = \pm\sqrt{E_n}Q_{\pm n}^{(L)}(x), \quad E_n = 4ns^2, \tag{4.4.7}$$

$$\int_{-\infty}^{\infty} e^{-s^2x^2}\lvert sx\rvert^{2\alpha+1} Q_n^{(L)}(x) Q_m^{(L)}(x)dx = \delta_{nm}, \quad m,n \in \mathbb{Z}. \tag{4.4.8}$$

(In fact, the above example returns to the example of the Hermite case when $\alpha = -\frac{1}{2}$, this is due to the relations 4.6.1 and 4.6.2. It is also obvious from the eigenvalue equation of Y.)

- Dunkl-SUSY orthogonal functions in terms of the orthonormal Jacobi polynomials $\hat{P}_n^{(\alpha,\beta)}(x)$: the example related with the **Scarf II or Rosen-Morse II (hyperbolic)** potential,

$$Q_{\pm n}^{(J,1)}(x) = \frac{(-1)^n}{\sqrt{2}}\left(\hat{P}_{2n}^{(-\frac{A}{\alpha}-\frac{1}{2},-\frac{A}{\alpha}-\frac{1}{2})}(i\sinh(\alpha x)) \pm \cosh(x)\hat{P}_{2n-1}^{(-\frac{A}{\alpha}+\frac{1}{2},-\frac{A}{\alpha}+\frac{1}{2})}(i\sinh(\alpha x))\right),\ n \geq 1, \tag{4.4.9}$$

$$Y = \partial_x R + A\tanh(\alpha x), \quad YQ_{\pm n}^{(J,1)}(x) = \pm\sqrt{E_{2n}}Q_{\pm n}^{(J,.1)}(x), \quad E_n = 2nA\alpha - n^2\alpha^2, \tag{4.4.10}$$

$$\int_{-\frac{i\pi}{2\alpha}}^{\frac{i\pi}{2\alpha}} |\cosh(\alpha x)|^{-\frac{A}{\alpha}} Q_n^{(J,1)}(x)Q_m^{(J,1)}(x)dx = \delta_{nm}, \quad m,n \in \mathbb{Z}; \tag{4.4.11}$$

the example related with the **Scarf I (trigonometric)** potential,

$$Q_{\pm n}^{(J,2)}(x) = \frac{1}{\sqrt{2}}\left(\hat{P}_{2n}^{(\frac{A}{\alpha}-\frac{1}{2},\frac{A}{\alpha}-\frac{1}{2})}(\sin(\alpha x)) \pm \cos(\alpha x)\hat{P}_{2n-1}^{(\frac{A}{\alpha}+\frac{1}{2},\frac{A}{\alpha}+\frac{1}{2})}(\sin(\alpha x))\right), \quad n \geq 1, \tag{4.4.12}$$

$$Y = \partial_x R + A\tan(\alpha x), \quad YQ_{\pm n}^{(J,2)}(x) = \pm\sqrt{E_{2n}}Q_{\pm n}^{(J,2)}(x), \quad E_n = 2nA\alpha + n^2\alpha^2, \tag{4.4.13}$$

$$\int_{-\frac{\pi}{2\alpha}}^{\frac{\pi}{2\alpha}} |\cos(\alpha x)|^{-\frac{A}{\alpha}} Q_n^{(J,2)}(x)Q_m^{(J,2)}(x)dx = \delta_{nm}, \quad m,n \in \mathbb{Z}; \tag{4.4.14}$$

the example related with the **generalized Pöschl-Teller** potential ($A < B$),

$$Q_{\pm n}^{(J,3)}(x) = \frac{1}{\sqrt{2}}\left(\hat{P}_n^{(\frac{B-A}{\alpha}-\frac{1}{2},-\frac{B+A}{\alpha}-\frac{1}{2})}(\cosh(\alpha x)) \mp i\sinh(\alpha x)\hat{P}_{n-1}^{(\frac{B-A}{\alpha}+\frac{1}{2},-\frac{B+A}{\alpha}+\frac{1}{2})}(\cosh(\alpha x))\right),\ n \geq 1, \tag{4.4.15}$$

$$Y = \partial_x R + A\coth(\alpha x) - B\mathrm{cosech}(\alpha x),$$

$$YQ_{\pm n}^{(J,3)}(x) = \pm\sqrt{E_n}Q_{\pm n}^{(J,3)}(x), \quad E_n = 2nA\alpha - n^2\alpha^2, \tag{4.4.16}$$

$$\int_{-\frac{i\pi}{\alpha}}^{\frac{i\pi}{\alpha}} (\cosh(\alpha r) - 1)^{\frac{B-A}{2\alpha}} (\cosh(\alpha r) + 1)^{-\frac{B+A}{2\alpha}} Q_n^{(J,3)}(x)Q_m^{(J,3)}(x)dx = \delta_{nm}, \quad m,n \in \mathbb{Z}; \tag{4.4.17}$$

the example related with the **Pöschl-Teller** potential ($A, B > 0$),

$$Q_{\pm n}^{(J,4)}(x) = \frac{1}{\sqrt{2}}\left(\hat{P}_n^{(\frac{B}{\alpha}-\frac{1}{2},\frac{A}{\alpha}-\frac{1}{2})}(\cos(2\alpha x)) \pm \sin(2\alpha x)\hat{P}_{n-1}^{(\frac{B}{\alpha}+\frac{1}{2},\frac{A}{\alpha}+\frac{1}{2})}(\cos(2\alpha x))\right), \quad n \geq 1, \tag{4.4.18}$$

$$Y = \partial_x R + A\tan(\alpha x) - B\cot(\alpha x),$$

$$YQ_{\pm n}^{(J,4)}(x) = \pm\sqrt{E_n}Q_{\pm n}^{(J,4)}(x), \quad E_n = 4n\alpha(A + B + n\alpha), \tag{4.4.19}$$

$$\int_{-\frac{\pi}{2\alpha}}^{\frac{\pi}{2\alpha}} (1 - \cos(2\alpha x))^{\frac{B}{\alpha}} (1 + \cos(2\alpha x))^{\frac{A}{\alpha}} Q_n^{(J,4)}(x)Q_m^{(J,2)}(x)dx = \delta_{nm}, \quad m,n \in \mathbb{Z}, \tag{4.4.20}$$

and $Q_{\pm 0}^{(J,i)}(x) = 1$, $i = 1,2,3,4$.

4.5 The recurrence relation of the Dunkl-supersymmetric orthogonal polynomials

Notice that in the previous section the examples of Dunkl-SUSY orthogonal functions in terms of the Hermite polynomials and the Laguerre polynomials are also polynomials, we call them Dunkl-supersymmetric orthogonal polynomials (Dunkl-SUSY OPs). Using these examples we shall identify the main properties of these polynomials so as to offer in this section a characterization which is more intrinsic. The most fundamental features of the Dunkl-SUSY OPs can be identified as:

(A) For all positive and negative integers n, the polynomial system $\{Q_n(x)\}_{n=0,\pm1,\pm2,\dots}$ satisfy an orthogonality relation,

$$\int_I Q_n(x)Q_m(x)\omega(x)dx = h_n\delta_{n,m}, \quad (n,m=\dots,-1,0,1,\dots);$$

(B) The polynomial $Q_{-n}(x)$ with negative index has the same degree as the polynomial $Q_n(x)$ with positive index,

$$Q_{-n}(x) := R[Q_n(x)] = Q_n(-x). \quad (n=1,2,\dots);$$

(C) $\{Q_n(x)\}$ are the polynomial parts of the eigenfunctions of a Dunkl-type differential operator of the form

$$\mathscr{L} = \partial_x R + v(x), \quad (v(-x) = -v(x)).$$

Let us now address the question of what can be said about the polynomial system $\{Q_n(x)\}_{n=0,\pm1,\pm2,\dots}$ satisfying the conditions (A) and (B) if it is not assumed that they satisfy an eigenvalue equation. The answer to this question is given by the following theorem. Without loss of generality, from now on we take $Q_n(x)$ monic, i.e., with the coefficient of the highest degree term in x equal to 1.

Theorem 4.5.1. *A necessary and sufficient condition for the existence of a polynomial system $\{Q_n(x)\}_{n=0,\pm1,\pm2,\dots}$ which satisfies the conditions (A) and (B) is that $Q_n(x)$ are expressed as*

$$\begin{aligned} Q_n(x) &= S_{2n}(x) + a_n S_{2n-1}(x), \\ Q_{-n}(x) &= S_{2n}(x) - a_n S_{2n-1}(x), \end{aligned} \quad n=1,2,\dots \tag{4.5.1}$$

with $Q_0(x)=1$, where the coefficients a_n depend on the polynomials $S_n(x)$ (see (4.5.9)), and with $\{S_n(x)\}_{n=0,1,2\dots}$ a monic symmetric orthogonal polynomial system:

$$S_n(-x) = (-1)^n S_n(x), \quad \int_I S_n(x)S_m(x)\omega(x)dx = k_n\delta_{n,m}.$$

Proof. The sufficiency is straightforward. If (4.5.1) holds, then it immediately follows that $Q_{-n}(x) = Q_n(-x)$, thus (B) is satisfied. For all nonnegative integers n,m, we have

$$\begin{aligned} \int_I Q_n(x)Q_m(x)\omega(x)dx &= \int_I (S_{2n}(x)+a_nS_{2n-1}(x))(S_{2m}(x)+a_mS_{2m-1}(x))\omega(x)dx \\ &= (k_{2n}+a_na_mk_{2n-1})\delta_{n,m} + a_mk_{2n}\delta_{2n,2m-1} + a_nk_{2n-1}\delta_{2n-1,2m} \\ &= (k_{2n}+a_na_mk_{2n-1})\delta_{n,m}, \end{aligned}$$

$$\begin{aligned} \int_I Q_n(x)Q_{-m}(x)\omega(x)dx &= \int_I (S_{2n}(x)+a_nS_{2n-1}(x))(S_{2m}(x)-a_mS_{2m-1}(x))\omega(x)dx \\ &= (k_{2n}-a_na_mk_{2n-1})\delta_{n,m} - a_mk_{2n}\delta_{2n,2m-1} + a_nk_{2n-1}\delta_{2n-1,2m} \\ &= (k_{2n}-a_na_mk_{2n-1})\delta_{n,m}, \end{aligned}$$

$$\int_I Q_{-n}(x)Q_{-m}(x)\omega(x)dx = \int_I (S_{2n}(x) - a_n S_{2n-1}(x))(S_{2m}(x) - a_m S_{2m-1}(x))\omega(x)dx$$
$$= (k_{2n} + a_n a_m k_{2n-1})\delta_{n,m} - a_m k_{2n}\delta_{2n,2m-1} - a_n k_{2n-1}\delta_{2n-1,2m}$$
$$= (k_{2n} + a_n a_m k_{2n-1})\delta_{n,m}.$$

Therefore, condition (A) is also satisfied. Besides, from the first and the third equation we also have

$$h_n = h_{-n} = k_{2n} + a_n^2 k_{2n-1}. \tag{4.5.2}$$

As for the necessity, suppose that $\{Q_n(x)\}_{n=0,\pm1,\pm2,\ldots}$ satisfies the conditions (A) and (B). For $n = 1,2,\ldots$, $Q_n(x)$ can be expressed as $Q_n(x) = e_n(x) + o_n(x)$, where $e_n(x)$ and $o_n(x)$ are even and odd polynomials, respectively. Then from condition (B) we have $Q_{-n}(x) = e_n(x) - o_n(x)$, while condition (A) implies that for any positive integers $n \neq m$, one has the relations

$$0 = \langle Q_n, Q_m\rangle = \langle e_n, e_m\rangle + \langle e_n, o_m\rangle + \langle o_n, e_m\rangle + \langle o_n, o_m\rangle, \tag{4.5.3}$$

$$0 = \langle Q_n, Q_{-m}\rangle = \langle e_n, e_m\rangle - \langle e_n, o_m\rangle + \langle o_n, e_m\rangle - \langle o_n, o_m\rangle, \tag{4.5.4}$$

$$0 = \langle Q_{-n}, Q_m\rangle = \langle e_n, e_m\rangle + \langle e_n, o_m\rangle - \langle o_n, e_m\rangle - \langle o_n, o_m\rangle, \tag{4.5.5}$$

$$0 = \langle Q_{-n}, Q_{-m}\rangle = \langle e_n, e_m\rangle - \langle e_n, o_m\rangle - \langle o_n, e_m\rangle + \langle o_n, o_m\rangle, \tag{4.5.6}$$

which together lead to

$$\langle e_n, e_m\rangle = \langle e_n, o_m\rangle = \langle o_n, e_m\rangle = \langle o_n, o_m\rangle = 0, \tag{4.5.7}$$

where the inner product $\langle f, g\rangle = \int_I f(x)g(x)\omega(x)dx$. Note that (4.5.4) and (4.5.5) also hold for $n = m$, which implies that

$$\langle e_n, e_n\rangle = \langle o_n, o_n\rangle. \tag{4.5.8}$$

The relations (4.5.7) and (4.5.8) mean that the polynomials $\{e_n(x), o_n(x)\}_{n=0,1,2,\ldots}$ form an orthogonal polynomial system, more exactly, in view of the parities of $e_n(x)$ and $o_n(x)$, they form a symmetric orthogonal polynomial system:

$$e_n(x) = S_{2n}(x), \quad o_n(x) = a_n S_{2n-1}(x),$$

where the coefficients a_n can be obtained from (4.5.8) and are:

$$a_n = \sqrt{\frac{\langle S_{2n}(x), S_{2n}(x)\rangle}{\langle S_{2n-1}(x), S_{2n-1}(x)\rangle}} = \sqrt{\frac{k_{2n}}{k_{2n-1}}}, \quad (n = 1,2,\ldots). \tag{4.5.9}$$

Note that the subscripts in $S_{2n}(x)$ and $S_{2n-1}(x)$ do not necessarily represent the corresponding degrees. We have hence shown that the conditions (A) and (B) lead to expression (4.5.1), thus proving necessity. □

Theorem 4.5.1 provides a general presentation of the Dunkl-SUSY OPs. Conversely, if we are given a set of OPs satisfying the conditions (A) and (B), we can always recover the corresponding set of symmetric OPs $S_n(x)$.

Moreover, according to the relations (4.5.2) and (4.5.9), the orthogonality constant of the polynomials defined by (4.5.1) turn out to be

$$h_n = h_{-n} = 2k_{2n}, \quad (n = 1,2,\ldots) \tag{4.5.10}$$

and $h_0 = k_0$, where k_n are the orthogonality constant of $\{S_n(x)\}_{n=0,1,2,\ldots}$.

The recurrence relations can be given as follow.

Theorem 4.5.2. *Let the monic symmetric OPs* $\{S_n(x)\}_{n=0,1,2,\ldots}$ *defined by the three-term recurrence relation:*

$$S_n(x) = xS_{n-1}(x) - \gamma_n S_{n-2}(x), \quad (n = 1,2,\ldots)$$

with $S_{-1}(x) = 0$*,* $S_0(x) = 1$*, then the monic polynomial system* $\{Q_n(x)\}_{n=0,\pm1,\pm2,\ldots}$ *defined by* (4.5.1) *satisfies the recurrence relations:*

$$\begin{aligned} Q_{n+1}(x) = &\frac{1}{2}\left[x^2 + (a_{n+1} - \frac{\gamma_{2n+1}}{a_n})x - \gamma_{2n+2} - \frac{\gamma_{2n+1}a_{n+1}}{a_n}\right]Q_n(x) \\ &+\frac{1}{2}\left[x^2 + (a_{n+1} + \frac{\gamma_{2n+1}}{a_n})x - \gamma_{2n+2} + \frac{\gamma_{2n+1}a_{n+1}}{a_n}\right]Q_{-n}(x), \end{aligned} \quad n = 1,2,\ldots \tag{4.5.11}$$

$$\begin{aligned} Q_{-(n+1)}(x) = &\frac{1}{2}\left[x^2 - (a_{n+1} + \frac{\gamma_{2n+1}}{a_n})x - \gamma_{2n+2} + \frac{\gamma_{2n+1}a_{n+1}}{a_n}\right]Q_n(x) \\ &+\frac{1}{2}\left[x^2 - (a_{n+1} - \frac{\gamma_{2n+1}}{a_n})x - \gamma_{2n+2} - \frac{\gamma_{2n+1}a_{n+1}}{a_n}\right]Q_{-n}(x). \end{aligned} \quad n = 1,2,\ldots \tag{4.5.12}$$

with $Q_0(x) = 1$.

Proof. First, it follows from (4.5.1) that

$$S_{2n}(x) = \frac{Q_n(x) + Q_{-n}(x)}{2}, \quad S_{2n-1}(x) = \frac{Q_n(x) - Q_{-n}(x)}{2a_n}. \tag{4.5.13}$$

By definition, we have

$$\begin{aligned} Q_{n+1}(x) &= S_{2n+2}(x) + a_{n+1}S_{2n+1}(x) = (x + a_{n+1})S_{2n+1}(x) - \gamma_{2n+2}S_{2n}(x) \\ &= (x + a_{n+1})(xS_{2n}(x) - \gamma_{2n+1}S_{2n-1}) - \gamma_{2n+2}S_{2n}(x) \\ &= (x^2 + a_{n+1}x - \gamma_{2n+2})S_{2n}(x) - \gamma_{2n+1}(x + a_{n+1})S_{2n-1}, \end{aligned}$$

where the three-term recurrence relation of $\{S_n(x)\}$ has been used twice. Substituting (4.5.13) into the above then leads to

$$\begin{aligned} 2Q_{n+1}(x) &= (x^2 + a_{n+1}x - \gamma_{2n+2})(Q_n(x) + Q_{-n}(x)) - \frac{\gamma_{2n+1}}{a_n}(x + a_{n+1})(Q_n(x) - Q_{-n}(x)) \\ &= \left[x^2 + (a_{n+1} - \frac{\gamma_{2n+1}}{a_n})x - \gamma_{2n+2} - \frac{\gamma_{2n+1}a_{n+1}}{a_n}\right]Q_n(x) \\ &\quad + \left[x^2 + (a_{n+1} + \frac{\gamma_{2n+1}}{a_n})x - \gamma_{2n+2} + \frac{\gamma_{2n+1}a_{n+1}}{a_n}\right]Q_{-n}(x), \end{aligned}$$

from which we obtain (4.5.11). The relation (4.5.12) is obtained in the same manner. □

Note that the polynomials in the set $\{Q_n(x)\}_{n=0,\pm1,\pm2,\ldots}$ can be ordered as follows

$$Q_0(x),\ Q_1(x),\ Q_{-1}(x),\ \cdots,\ Q_n(x),\ Q_{-n}(x), \cdots$$

since $Q_n(x)$ and $Q_{-n}(x)$ have the same degree. This means that the relations (4.5.11) and (4.5.12) can be viewed as the three-term recurrence relations of $\{Q_n(x)\}_{n=0,\pm1,\pm2,\ldots}$.

4.6 Supplymentary data

Hermite polynomials

- The Hermite polynomials are orthogonal on the interval $(-\infty,\infty)$ with respect to the weight function e^{-x^2}. They satisfy the orthogonality relations:

$$\int_{-\infty}^{\infty} H_m(x)H_n(x)e^{-x^2}dx = 2^n n!\sqrt{\pi}\delta_{mn}$$

where $H_n(x)$ is the Hermite polynomial of degree n, δ_{mn} is Kronecher's delta.
- Three term recurrence relations:

$$H_n(x) = 2xH_{n-1}(x) - 2(n-1)H_{n-2}(x), \quad n \geq 1, \quad H_0(x) = 1.$$

Laguerre polynomials

- The Laguerre polynomials are orthogonal over $[0,\infty)$ with respect to the weight function $x^{\alpha}e^{-x}$. They satisfy the orthogonality relations:

$$\int_{0}^{\infty} L_m^{(\alpha)}(x)L_n^{(\alpha)}(x)x^{\alpha}e^{-x}dx = \frac{\Gamma(n+\alpha+1)}{n!}\delta_{mn}$$

where $L_n^{(\alpha)}(x)$ is the Laguerre polynomial of degree n.
- Three term recurrence relations:

$$L_n^{(\alpha)}(x) = \frac{2n-1+\alpha-x}{n}L_{n-1}^{(\alpha)}(x) - \frac{n-1+\alpha}{n}L_{n-2}^{(\alpha)}(x), \quad n \geq 1, \quad L_0^{(\alpha)}(x) = 1.$$

- Relation to Hermite polynomials:

$$H_{2n}(x) = (-1)^n 2^{2n} n! L_n^{(-1/2)}(x^2), \tag{4.6.1}$$

$$H_{2n+1}(x) = (-1)^n 2^{2n+1} n! x L_n^{(1/2)}(x^2). \tag{4.6.2}$$

Jacobi polynomials

- The Jacobi polynomials are orthogonal on the interval $(-1,1)$ with respect to the weight function $(1-x)^{\alpha}(1+x)^{\beta}$. They satisfy the orthogonality relations:

$$\int_{-\infty}^{\infty} P_m^{(\alpha,\beta)}(x)P_n^{(\alpha,\beta)}(x)(1-x)^{\alpha}(1+x)^{\beta}dx = \frac{2^{\alpha+\beta+1}\Gamma(\alpha+n+1)\Gamma(\beta+n+1)}{n!\Gamma(\alpha+\beta+n+1)(\alpha+\beta+2n+1)}\delta_{mn}$$

where $P_n^{(\alpha,\beta)}(x)$ is the Jacobi polynomial of degree n, and $\alpha,\beta > -1$.
- Three term recurrence relations:

$$P_n^{(\alpha,\beta)}(x) = \left[\frac{(2n+\alpha+\beta-1)(2n+\alpha+\beta)}{2n(n+\alpha+\beta)}x - \frac{(\beta^2-\alpha^2)(2n+\alpha+\beta-1)}{2n(n+\alpha+\beta)(2n+\alpha+\beta-2)}\right]P_{n-1}^{(\alpha,\beta)}(x)$$

$$-\frac{2(n+\alpha-1)(n+\beta-1)(2n+\alpha+\beta)}{2n(n+\alpha+\beta)(2n+\alpha+\beta-2)}P_{n-2}^{(\alpha,\beta)}(x), \quad n \geq 1 \quad P_0^{(\alpha,\beta)}(x) = 1.$$

Chapter 5

Summary and future works

We discussed several generalizations of the classical orthogonal polynomials and their properties. Let us briefly summarize the main results we have presented in this thesis and then discuss some ideas on the future works of this research.

5.1 Summary

In chapter 1, the history background and the definitions as well as the rich applications of the classical orthogonal polynomials are introduced. An important property called duality which reads as the equivalence of a three-term recurrence relation and an eigenvalue equation satisfied by the classical orthogonal polynomials is illustrated. Generalizing the eigenvalue equation is a key in deriving the generalizations of the classical orthogonal polynomials. In chapter 2, we studied the electrostatic properties of the zeros of exceptional extensions of the very classical orthogonal polynomials. We have shown that the maximum value of the modulus of a special energy function is attained on the zeros of exceptional extensions of the very classical orthogonal polynomials under certain conditions. In chapter 3, we established an exceptional extension of the Bannai-Ito polynomials. Interestingly enough, the degree sequences of these exceptional Bannai-Ito polynomials demonstrate different rules compared with those of the exceptional extensions of the very classical orthogonal polynomials, that is, there are cases where the degree sequence is consist of even integers only. In chapter 4, we introduced and characterized orthogonal functions that we have called Dunkl-supersymmetric. These functions are eigenfunctions of a class of Dunkl-type differential operators that can be cast within supersymmetric quantum mechanics. A significant feature of these orthogonal function families is that they do not involve polynomials of all degrees but are rather organized in pairs of polynomials both of the same degree (where the examples in terms of the Jacobi polynomials may be viewed as polynomials in certain special variables). The connection with supersymmetric quantum mechanics has been exploited to obtain a number of Dunkl-supersymmetric orthogonal functions from exactly solvable problems. Informed by these results we could offer a general characterization of the Dunkl-supersymmetric orthogonal polynomials and could exhibit as well their recurrence relations.

5.2 Future works

As we have already mentioned, there are examples in the exceptional Bannai-Ito polynomials and the Dunkl-supersymmetric orthogonal polynomials that their degree sequences are consist of even integers only, for instance, $\{0,2,2,4,4,6,6,\ldots\}$. These examples have seldom been mentioned in the literature as far as we know. Therefore, it is of great interest to study this type of orthogonal polynomials in general. In what follows, we would like to provide some results on this proceeding research which also gives a rough image of our future works.

Consider a general eigenvalue problem

$$LP_n(x) = \lambda_n P_n(x), \quad n = 0,1,2,\ldots$$

where the eigenfunctions $P_n(x)$ are polynomials. If a bounded operator L is self-adjoint and nondegenerate (i.e. $\lambda_n \neq \lambda_m, \forall n \neq m$), then its eigenfunctions $P_n(x)$, $n = 0,1,2,\ldots$, are orthogonal with respect to certain weight function. To the end we assume that L is self-adjoint and nondegenerate.

Definition 5.2.1. *A sequence of polynomials $\{P_n(x)\}_{n=0,1,2,\ldots}$ is called orthogonal polynomials sequence of single-parity degrees (OPSPD) if they are orthogonal with respect to certain linear functional $\mathscr{L}$*

$$\mathscr{L}[P_m(x)P_n(x)] = h_n\delta_{m,n}, \quad h_n \neq 0$$

and the degree sequence of $\{P_n(x)\}_{n=0,1,2,\ldots}$ is consist of even or odd integers only.

If $\{P_n(x)\}_{n=0,1,2,\ldots}$ is a finite polynomial sequence which satisfies the conditions in Definition 5.2.1, then it is called a finite OPSPD. If $h_n > 0$ for $i = 0,1,2,\ldots$, then the OPSPD is called positive definite.

A simple approach towards the construction of OPSPD is based on observations of how the operator L acts on the monomials, $1, x, x^2, \ldots$. Denote the degree sequence of the polynomial eigenfunctions of L by S_L. For convenience, here we call the polynomial eigenfunctions of a self-adjoint operator L **type I** OPSPD if $S_L = \{0,2,2,4,4,\ldots\}$. The other cases of OPSPD and their classifications will be leave as open problems. The following lemma concludes a sufficient condition for the existence of the **type I** OPSPD.

Lemma 5.2.1. *Let L be a linear operator on a Hilbert space. Suppose that L maps every monomial x^i, $i = 0,1,2,\ldots$, to a polynomial of degree $2\lceil \frac{i}{2} \rceil$ (the nearest even number $\geq i$), namely, $Lx^0 = k_{0,0}$ and*

$$Lx^{2i-1} = \sum_{j=0}^{2i} k_{2i-1,j}x^j, \quad Lx^{2i} = \sum_{j=0}^{2i} k_{2i,j}x^j, \quad i = 1,2,\ldots \tag{5.2.1}$$

where $k_{i,j}$'s are constants and $k_{2i-1,2i}, k_{2i,2i} \neq 0$, $\forall i = 1,2,\ldots$. Let

$$\Delta_m = (k_{2m,2m} - k_{2m-1,2m-1})^2 + 4k_{2m,2m-1}k_{2m-1,2m}, \tag{5.2.2}$$

if $\Delta_m > 0$ for $m = 1,2,\ldots$, then L has polynomial eigenfunctions whose degree sequence is $S_L = \{0,2,2,4,4,\ldots\}$.

Proof. Assume that $P_n(x) = \sum_{i=0}^{n} a_{n,i}x^i$ is a polynomial eigenfunction of L, then we have

$$\lambda_n P_n(x) = LP_n(x) = \sum_{i=0}^{n} a_{n,i} \sum_{j=0}^{2\lceil \frac{i}{2} \rceil} k_{i,j}x^j = \sum_{j=0}^{2\lceil \frac{n}{2} \rceil} \sum_{i=\max(0,2\lceil \frac{j}{2} \rceil - 1)}^{n} a_{n,i}k_{i,j}x^j,$$

which can be written as

$$\sum_{j=0}^{2\lceil \frac{n}{2} \rceil} \left(\sum_{i=\max(0,2\lceil \frac{j}{2} \rceil - 1)}^{n} a_{n,i}k_{i,j} \right) x^j = \sum_{j=0}^{n} \lambda_n a_{n,j}x^j. \tag{5.2.3}$$

Here n must be even such that $2\lceil \frac{n}{2} \rceil = n$. Let $n = 2m$, then (5.2.3) is equivalent with

$$\sum_{i=\max(0,2\lceil \frac{j}{2} \rceil - 1)}^{2m} a_{2m,i}k_{i,j} = \lambda_{2m}a_{2m,j}, \quad j = 0,1,\ldots,2m. \tag{5.2.4}$$

For convenience, we assume that $P_{2m}(x)$ is monic ($a_{2m,2m} = 1$) and $a_{2m,2m-1} \neq 0$. It follows from the last two equations in (5.2.4) which read as

$$(\lambda_{2m} - k_{2m-1,2m-1})a_{2m,2m-1} = k_{2m,2m-1}a_{2m,2m},$$
$$(\lambda_{2m} - k_{2m,2m})a_{2m,2m} = k_{2m-1,2m}a_{2m,2m-1},$$

that λ_{2m} is the solution of the following equation

$$\lambda_{2m}^2 - (k_{2m,2m} + k_{2m-1,2m-1})\lambda_{2m} + k_{2m,2m}k_{2m-1,2m-1} - k_{2m,2m-1}k_{2m-1,2m} = 0. \tag{5.2.5}$$

The discriminant of this equation is (5.2.2). If $\Delta_m > 0$, then there exists two solutions for the equation (5.2.5), say λ_{2m} and λ_{-2m}, which satisfy

$$\lambda_{2m} + \lambda_{-2m} = k_{2m,2m} + k_{2m-1,2m-1}, \tag{5.2.6}$$

and

$$\lambda_{2m}\lambda_{-2m} = k_{2m,2m}k_{2m-1,2m-1} - k_{2m,2m-1}k_{2m-1,2m}. \tag{5.2.7}$$

The other coefficients of $P_{2m}(x)$ then can be derived inductively from (5.2.4) under the assumption that the denominators involved are not zero:

$$a_{2m,2m-2l-1} = \left[(\lambda_{2m} - k_{2m-2l,2m-2l})(\lambda_{2m} - k_{2m-2l-1,2m-2l-1}) - k_{2m-2l-1,2m-2l}k_{2m-2l,2m-2l-1}\right]^{-1}$$
$$\cdot \sum_{i=2m-2l+1}^{2m} a_{2m,i}\left[(\lambda_{2m} - k_{2m-2l,2m-2l})k_{i,2m-2l-1} + k_{2m-2l,2m-2l-1}k_{i,2m-2l}\right], \quad l = 0,\ldots,m-1,$$
$$a_{2m,2m-2l} = \left[(\lambda_{2m} - k_{2m-2l,2m-2l})(\lambda_{2m} - k_{2m-2l-1,2m-2l-1}) - k_{2m-2l-1,2m-2l}k_{2m-2l,2m-2l-1}\right]^{-1}$$
$$\cdot \sum_{i=2m-2l+1}^{2m} a_{2m,i}\left[(\lambda_{2m} - k_{2m-2l-1,2m-2l-1})k_{i,2m-2l} + k_{2m-2l-1,2m-2l}k_{i,2m-2l-1}\right], \; l = 1,\ldots,m-1,$$

and

$$a_{2m,0} = \frac{1}{\lambda_{2m} - k_{0,0}} \sum_{i=1}^{2m} a_{2m,i}k_{i,0}.$$

□

5.2.1 Algebraic Heun operators and the construction of type I OPSPD

The algebraic Heun (AH) operators come from the duality of COP. They can be constructed using the bispectral pair of operators related with COP. It is known that the AH operators are the most general operators that map any polynomial of degree n into a polynomial of degree $n+1$ [33]. Let us consider the case where L maps the monomials $1, x, x^2, x^3, x^4, \ldots$ into polynomials of degrees $0, 2, 2, 4, 4, \ldots$, respectively. Since L raises the degree of every odd monomial by 1 and preserves the degrees of every even monomial, we can make use of the AH operators by defining

$$L[x^n] := \frac{(1+(-1)^n)}{2}H[x^n] + \frac{(1-(-1)^n)}{2}W[x^n], \tag{5.2.8}$$

where H is a linear operator that maps x^n to a polynomial of degree n and W is an AH operator. In fact, (5.2.8) can be realized with the help of the reflection operator R ($R(f(x)) = f(-x)$). Let

$$L = \frac{1}{2}(H+W) + \frac{1}{2}(H-W)R, \tag{5.2.9}$$

then (5.2.8) holds immediately.

By choosing H as the spectral operator related to certain COP $\{Q_n(x)\}_{n=0,1,2,\ldots}$ and W as the corresponding AH operator, one can make use of the theories of COP and their generalizations. Let us take the Bannai-Ito case for an example. Recall that the Bannai-Ito polynomials are eigenfunctions of the operator

$$L_{BI} = \frac{(x-\rho_1)(x-\rho_2)}{-2x}(R-I) + \frac{(x-r_1+1/2)(x-r_2+1/2)}{2x+1}(TR-I), \tag{5.2.10}$$

where T is the shift operator, I is the identity, $Tf(x) = f(x+1)$, $If(x) = f(x)$.

The algebraic Heun Bannai-Ito (AHBI) operator can be given by

$$W = \tau_1 XY + \tau_2 YX + \tau_3 X + \tau_4 Y + \tau_0, \tag{5.2.11}$$

where $\tau_i, i = 0,\ldots,4$, are real coefficients. The operators X,Y are generators of the Bannai-Ito algebra:

$$\{X,Y\} = Z+\omega_3, \quad \{Y,Z\} = X+\omega_1, \quad \{X,Z\} = Y+\omega_2, \tag{5.2.12}$$

where $\omega_i, i = 1,2,3$ are constants [79]. Specifically,

$$X = 2L_{BI} + (\rho_1+\rho_2-r_1-r_2+\frac{1}{2}), \quad Y = x,$$

$$\omega_1 = 4r_2r_1 + 4\rho_2\rho_1, \quad \omega_2 = -2{r_1}^2 - 2{r_2}^2 + 2{\rho_1}^2 + 2{\rho_2}^2, \quad \omega_3 = -4r_2r_1 + 4\rho_2\rho_1.$$

Let $H = X$, then it follows from (5.2.9) that

$$2L = W|_{\tau_3=\tau_3+1} - W|_{\tau_3=\tau_3-1}R.$$

For generic parameters $\tau_i, i = 0,\ldots,4$, the operator L involves TR, I, R and T. However, the shift operator T is not self-adjoint, here we set some conditions to annihilate T in L. Let $\tau_1 = \tau_2, \tau_3 = \tau_2+1$, then we write L as L_0:

$$L_0 = CL_1(x)TR + CL_2(x)R + CL_3(x)I, \tag{5.2.13}$$

where

$$CL_1(x) = \frac{(2x-2r_2+1)(2x-2r_1+1)}{2x+1},$$

$$CL_2(x) = \frac{-4(\tau_2+\tau_4+1)x^2 + 4((2r_1r_2-2\rho_1\rho_2+\rho_1+\rho_2)\tau_2 - 2\tau_0 - \tau_4 + 4\rho_1 + 4\rho_2)x - 8(\tau_2+\frac{1}{2})\rho_1\rho_2)}{2x},$$

$$CL_3(x) = 2(\tau_2+\tau_4)x - 4r_1r_2\tau_2 + 4\rho_1\rho_2\tau_2 - 2\rho_1\tau_2 - 2\tau_2\rho_2 + \tau_0 + \frac{\tau_4}{2} + \frac{2(1+2\tau_2)\rho_1\rho_2}{x} - \frac{4r_2r_1}{2x+1}.$$

The operator L_0 acts on the monomials as:

$$L_0[x^{2m}] = (2\rho_1+2\rho_2-2r_1-2r_2+4m+1)x^{2m} + \cdots,$$

$$L_0[x^{2m-1}] = 4(\tau_2+\tau_4)x^{2m}+$$

$$((8\rho_1\rho_2 - 8r_1r_2 - 4\rho_1 - 4\rho_2)\tau_2 + 2r_1 + 2r_2 - 2\rho_1 - 2\rho_2 + 2\tau_0 + \tau_4 - (4m-1))x^{2m-1} + \cdots,$$

thus the following condition must be satisfied so that L_0 maps the monomials to polynomials of degree $0,2,2,4,4,\ldots$,

$$2\rho_1 + 2\rho_2 - 2r_1 - 2r_2 \neq -(4m+1), \quad m = 0,1,2,\ldots,$$
$$\tau_2 + \tau_4 \neq 0. \tag{5.2.14}$$

Suppose that L_0 possesses polynomial eigenfunctions with distinct eigenvalues,

$$L_0 P_{\pm 2m} = \lambda_{\pm 2m} P_{\pm 2m}, \quad m = 0,1,2,\ldots,$$

then it follows from the relation (5.2.6) that

$$\lambda_{2m} + \lambda_{-2m} = (8\rho_1\rho_2 - 8r_1r_2 - 4\rho_1 - 4\rho_2)\tau_2 + 2\tau_0 + \tau_4 + 2, \quad m = 0,1,2,\ldots. \tag{5.2.15}$$

5.2.2 A generalization of the Bannai-Ito algebra

Let $Y_L := ax + b$ and $X_L := cL_0 + d$ with

$$a = 4b, \quad d = \left(\left(2\rho_1 + 2\rho_2 - 4\rho_1\rho_2 + 4r_1r_2 + \frac{1}{2}\right)\tau_2 - \tau_0\right)c.$$

It turns out that X_L, Y_L satisfy the following anticommutation relations:

$$\{X_L, Y_L\} = C_1 Y_L^2 + Z_L + K_3, \tag{5.2.16}$$
$$\{Y_L, Z_L\} = C_2 X_L + K_1, \tag{5.2.17}$$
$$\{Z_L, X_L\} = C_3 X_L + C_4 Y_L^2 + C_5 Y_L + K_2, \tag{5.2.18}$$

where

$$C_1 = \frac{c}{b}(\tau_2+\tau_4),\ C_2 = 4b^2,\ C_3 = 4bc(\tau_2+\tau_4),\ C_4 = -\frac{c^2}{b}(\tau_2+\tau_4)(\tau_2+\tau_4+2),\ C_5 = c^2(\tau_2+\tau_4+2)^2,$$

$$K_3 = -bc(\tau_2 + \tau_4 - 32\rho_1\rho_2\tau_2 - 16\rho_1\rho_2 + 16r_1r_2),$$

$$K_1 = 32b^2c(2\rho_1\rho_2\tau_2 + \rho_1\rho_2 + r_1r_2),$$

$$K_2 = bc^2(64\,{r_1}^2{r_2}^2{\tau_2}^2 - 128\,{\tau_2}^2 r_1 r_2 \rho_1\rho_2 + 64\,{\rho_1}^2{\rho_2}^2{\tau_2}^2 + 64\,r_1r_2\rho_1{\tau_2}^2 + 64\,r_1r_2\rho_2{\tau_2}^2 - 64\,{\rho_1}^2\rho_2{\tau_2}^2 -$$
$$64\,\rho_1{\rho_2}^2{\tau_2}^2 + 64\,r_1r_2\rho_1\tau_2 + 64\,r_1r_2\rho_2\tau_2 - 32\,r_1r_2\tau_0\tau_2 - 16\,\tau_2r_1r_2\tau_4 - 64\,{\rho_1}^2\rho_2\tau_2 + 16\,{\rho_1}^2{\tau_2}^2 -$$
$$64\,\rho_1{\rho_2}^2\tau_2 + 32\,\rho_1\rho_2\tau_0\tau_2 - 16\,\rho_1\rho_2\tau_2\tau_4 + 16\,{\rho_2}^2{\tau_2}^2 + 16\,r_2r_1\tau_2 + 16\,r_1r_2\tau_4 + 32\,\tau_2{\rho_1}^2 - 16\,\rho_1\rho_2\tau_2 -$$
$$16\,\rho_1\rho_2\tau_4 - 16\,\rho_1\tau_0\tau_2 - 8\,\tau_2\rho_1\tau_4 + 32\,{\rho_2}^2\tau_2 - 16\,\rho_2\tau_0\tau_2 - 8\,\tau_2\rho_2\tau_4 - 16\,{r_1}^2 - 16\,{r_2}^2 + 16\,{\rho_1}^2 -$$
$$16\,\rho_1\tau_0 - 8\,\rho_1\tau_4 + 16\,{\rho_2}^2 - 16\,\tau_0\rho_2 - 8\,\rho_2\tau_4 + 4\,{\tau_0}^2 + 4\,\tau_4\tau_0 - {\tau_2}^2 - 2\,\tau_2\tau_4 - 2\,\tau_2 - 2\,\tau_4).$$

The algebra generated by X_L, Y_L and Z_L subject to the relations (5.2.16)-(5.2.18) can be considered a generalization of the Bannai-Ito algebra. In fact, if one choose the parameters $\tau_2 = \tau_4 = 0, \tau_0 = 0$ and

$b = c = 1/2$, then this algebra is exactly the Bannai-Ito algebra (5.2.12). This fact also addresses the necessity of the condition (5.2.14) in this scheme.

The Casimir operator Q_L commuting with all the generator X_L, Y_L, Z_L of this algebra has the form:

$$Q_L = C_2X_L^2 + C_5Y_L^2 + Z_L^2 + C_2C_4Y_L - C_3Z_L, \tag{5.2.19}$$

which acts as a constant in this realization:

$$Q_L = 16b^2c^2(2\rho_1^2 + 2\rho_2^2 + 2r_1^2 + 2r_2^2 - \frac{1}{4}) + 2b(K_2 + 16bc^2(r_1^2 + r_2^2 - \rho_1^2 - \rho_2^2)) -$$

$$b^2c^2(\tau_2 + \tau_4)(64r_1r_2 + 3(\tau_2 + \tau_4)).$$

From the anticommutation relations (5.2.16)-(5.2.18) one can also rewrite Q_L as follow:

$$Q_L = (\sqrt{C_5}Y_L + Z_L - \frac{C_3}{2})^2 + C_2X_L^2 - C_2\sqrt{C_5}X_L - \sqrt{C_5}K_1 - \frac{C_3^2}{4}. \tag{5.2.20}$$

Let us introduce the operator by the following formula,

$$J_1 = (Y_L + N_1Z_L + M_1)(X_L + k_1) + t, \tag{5.2.21}$$

where N_1, M_1, k_1, t are constants.

Lemma 5.2.2. *If these constants are defined by*

$$N_1 = -\frac{C_1}{C_4}, \quad M_1 = \frac{C_1C_3}{2C_4}, \quad k_1 = \frac{C_4}{2C_1}, \quad t = -\frac{C_3}{4} - \frac{K_3}{2} + \frac{C_1}{2C_4}K_2,$$

then we have

$$\{J_1, X_L\} = \frac{1}{N_1}J_1 = c(\tau_2 + \tau_4 + 2)J_1. \tag{5.2.22}$$

The relation (5.2.22) follows from (5.2.16)-(5.2.18) through straightforward calculations. In later discussions we will see that J_1 is a ladder operator associated with L_0. Note that it is the existence of the Y_L^2-terms in (5.2.16) and (5.2.18) that causes the uniqueness of the constant N_1 (while there are two choices of N_1 in the case of the ordinary Bannai-Ito algebra), hence there is only one ladder operator of L_0 in the form (5.2.21).

The operator J_1 here shares similar properties with the ladder operator J_+ in the ordinary Bannai-Ito algebra [79]. The operator J_1 annihilates any constant $J_1[1] = 0$ and maps the monomials $x, x^2, x^3, x^4, \ldots$, into polynomials of degrees $2, 2, 4, 4, \ldots$, respectively.

Suppose that the operator L_0 has an infinite sequence of polynomial eigenfunctions in the means:

$$L_0P_{\pm 2m}(x) = \lambda_{\pm 2m}P_{\pm 2m}(x), \quad m = 0, 1, 2, \ldots$$

where $\lambda_{\pm 2m}$ are distinct eigenvalues, and $\deg P_{\pm 2m}(x) = 2m$. Obviously, $P_{\pm 2m}(x)$ are also eigenfunctions of the operator X_L:

$$X_LP_{\pm 2m}(x) = \mu_{\pm 2m}P_{\pm 2m}(x), \quad m = 0, 1, 2, \ldots$$

where

$$\mu_{\pm 2m} = c\left(\lambda_{\pm 2m} + \left(2\rho_1 + 2\rho_2 - 4\rho_1\rho_2 + 4r_1r_2 + \frac{1}{2}\right)\tau_2 - \tau_0\right). \tag{5.2.23}$$

It then follows from the relation (5.2.22) that $\hat{P}_{\pm 2m}(x) = J_1 P_{\pm 2m}(x)$ are again eigenfunctions of the operator X_L with the eigenvalues

$$\hat{\mu}_{\pm 2m} = c\left(-\lambda_{\pm 2m} - \left(2\rho_1 + 2\rho_2 - 4\rho_1\rho_2 + 4r_1r_2 - \frac{1}{2}\right)\tau_2 + \tau_4 + \tau_0 + 2\right).$$

Substitute the relation (5.2.15) into the right-hand side then it turns out

$$\hat{\mu}_{\pm 2m} = c\left(\lambda_{\mp 2m} + \left(2\rho_1 + 2\rho_2 - 4\rho_1\rho_2 + 4r_1r_2 + \frac{1}{2}\right)\tau_2 - \tau_0\right) = \mu_{\mp 2m}, \tag{5.2.24}$$

which means that J_1 acts on the eigenfunctions of L_0 in the way that it exchanges $P_{2m}(x)$ with $P_{-2m}(x)$:

$$J_1 P_{2m}(x) \propto P_{-2m}(x), \quad J_1 P_{-2m}(x) \propto P_{2m}(x).$$

As an immediate consequence of the relation (5.2.22), J_1^2 commutes with the operator X_L:

$$[X_L, J_1^2] = 0.$$

It follows from the anticommutation relations (5.2.16)-(5.2.18) that

$$(X_L + k_1)(Y_L + N_1 Z_L + M_1) = -(Y_L + N_1 Z_L + M_1)(X_L + k_1) - 2t,$$

thus we can express J_1^2 as

$$J_1^2 = -(Y_L + N_1 Z_L + M_1)^2 (X_L + k_1)^2 + t^2.$$

Notice that $N_1 = (\sqrt{C_5})^{-1}$ and $M_1\sqrt{C_5} = -C_3/2$, it then follows from (5.2.20) that J_1^2 is a fourth-order polynomial in X_L:

$$J_1^2 = -\frac{1}{C_5}\left(Q_L - C_2 X_L^2 + C_2\sqrt{C_5}X_L + \sqrt{C_5}K_1 + \frac{C_3^2}{4}\right)^2 (X_L + k_1)^2 + t^2.$$

We still want to find the ladder operators that transform $P_{2m}(x)$ ($P_{-2m}(x)$) to their neighbors $P_{2(m-1)}(x)$, $P_{2(m+1)}(x)$ ($P_{-2(m-1)}(x)$, $P_{-2(m+1)}(x)$). However, we are not able to obtain these ladder operators at the present stage. We will leave this to our future works.

According to numerical analysis we have the following conjectures.

Conjection 5.2.1. *Assume that the condition in Lemma 5.2.1. is satisfied by the operator L_0, and the polynomial eigenfunctions $\{P_{\pm 2m}\}_{m=0,1,2...}$ of L_0 are monic, then they satisfy the following recurrence relations:*

$$P_{2(m+1)}(x) = (x^2 + a_{2m}x + b_{2m})\frac{P_{2m}(x) + P_{-2m}(x)}{2} + c_{2m}(P_{2m}(x) - P_{-2m}(x)) +$$
$$d_{2m}\frac{P_{2(m-1)}(x) + P_{-(2m-1)}(x)}{2} + e_{2m}(P_{2m-1}(x) - P_{-(2m-1)}(x)),$$

$$P_{-(2m+1)}(x) = (x^2 + a_{-2m}x + b_{-2m})\frac{P_{2m}(x) + P_{-2m}(x)}{2} + c_{-2m}(P_{2m}(x) - P_{-2m}(x)) +$$
$$d_{-2m}\frac{P_{2m-1}(x) + P_{-(2m-1)}(x)}{2} + e_{-2m}(P_{2m-1}(x) - P_{-(2m-1)}(x)),$$

where the (a_{2m}, a_{-2m})'s are a pair of solutions of a quadratic equation.

Conjection 5.2.2. *The above conjecture holds for all the* **type I** *OPSPD.*

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List of Authors Papers and Works Related to the Thesis

Original Papers

[1] Yu Luo and Satoshi Tsujimoto, Exceptional Bannai-Ito polynomials, *J. Approx. Theor.* **239** (2019) 144-173.

[2] Y. Luo, S. Tsujimoto, L. Vinet and A. Zhedanov, Dunkl-Supersymmetric orthogonal functions associated with classical orthogonal polynomials, *J. Phys. A: Math. Theor.* https://doi.org/10.1088/1751-8121/ab63a9, 16pages.

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